Dietrich O. Hummel

Atlas of Plastics Additives

Analysis by Spectrometric Methods

With 62 tables and 772 FTIR spectra

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Prof. Dr. Dietrich O. Hummel
Im Lindenhof 15
D-53773 Hennef

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Preface

Twenty years ago the 2nd edition of the text and spectra volume of Friedrich Scholl on the analysis of plastics additives was published, it can be found in most laboratories. He deceased shortly after his retirement, and my coworkers and I took over his heritage. Collecting samples of additives of all kind as well as the measurement of their *FTIR* spectra was done by Sigrun Wittmann, Liu Min, Mark Amberg, Vera Brunne, Astrid Baum and myself; my wife Doris digitised the structures. 752 spectra of the more important additives were selected from a total of 1630. To facilitate access for the analyst, the "triplets" (spectrum with peak table, structure, legend) were arranged according to a decimal system (technological class, chemical composition). Registers (chemical and trade name, empirical formula) help one to find the desired spectrum.

Literature on (predominantly) spectroscopic methods in the analysis of plastics additives was evaluated until 2001. Methods and experiments were critically reported; wherever possible the results were compressed in tables. In order to keep the volume of the book within limits only elementary methods for the separation of additives and matrices were described (2nd chapter). The chromatographic separation of mixtures had to be omitted; it is amply described in the book of Scholl and in later monographs. The reason why chapters 3 and 7 are so large is very simple: *(FT)IR* and mass spectrometries are by far the most important methods for identification and quantitative determination of additives. They are also suitable for combination with chromatographic and other analytical methods.

I owe gratitude to my coworkers for their zeal as well as to *Stiftung Industrieforschung* for generous support of our research, to many chemical companies for providing samples and to numerous colleagues sending reprints. Many thanks go to my colleagues B. Schrader (Uni. Essen), K.-W. Brzezinka (BAM, Berlin-Adlershof), K.-J. Eichhorn and D. Fischer (IPF Dresden) for measuring the Raman spectra of problematic samples. Finally, many thanks go to the editorial staff of *Springer Verlag* and to *medio Technologies* (producer) for skill and carefulness and for their patience with the author.

Dietrich O. Hummel
Summer 2002

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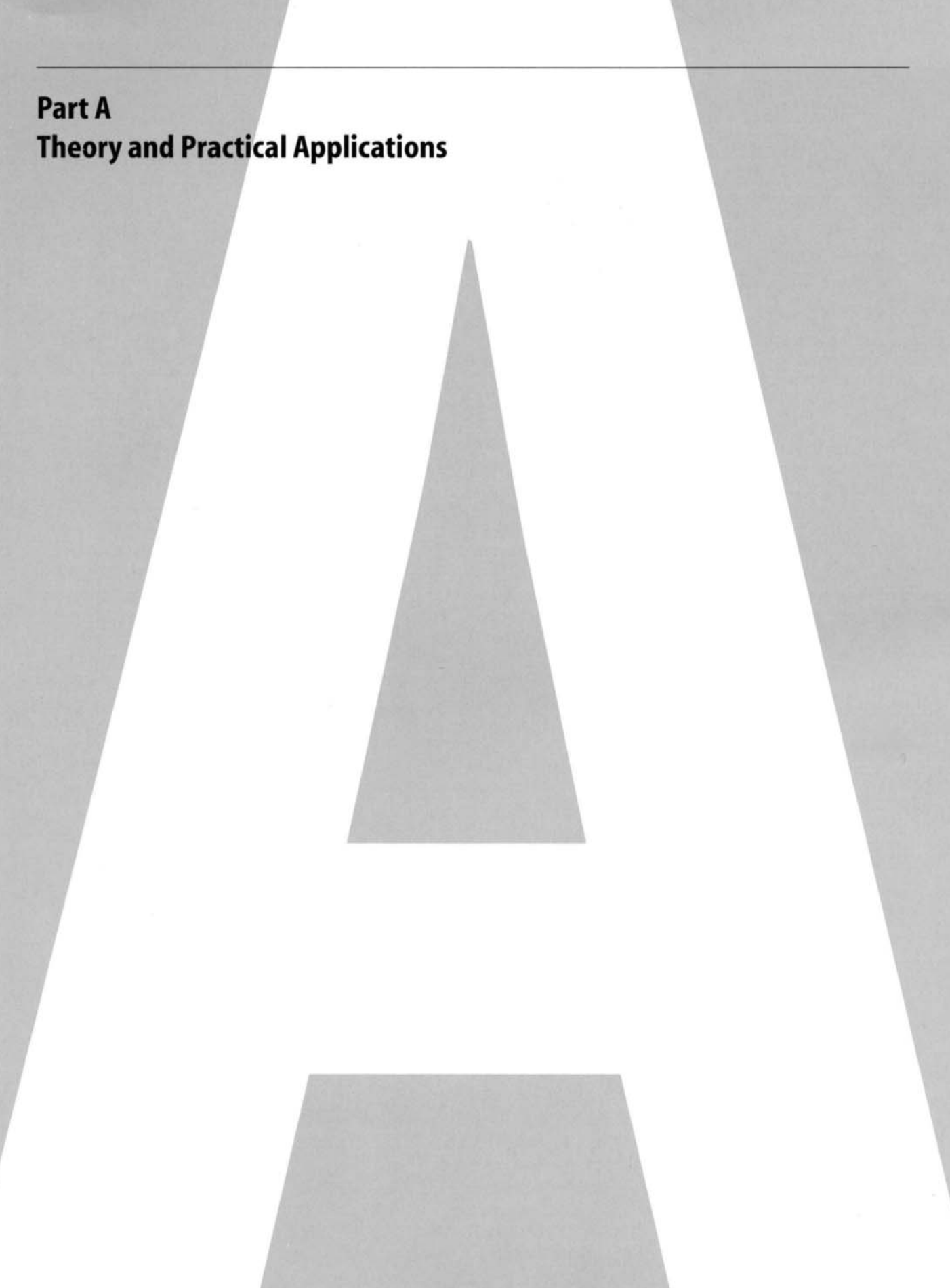


1
Introduction

About 5×10^{10} kg of polymeric materials are annually consumed by mankind. Few of these polymers can be used as produced; examples are intrinsically stabilised polyaromatics like the polypyromellitic imides or inorganic polymers like boron nitride or quartz. All organic polymers are subject to oxidative or other kinds of degradation, or they lack certain properties like elasticity or flame resistance, or they do not have the colour wanted for a certain application. Thermoplastics may degrade during processing, rubber gets brittle from ozone attack.

Here enter the additives. However, before going into details it has to be stated that many chemical and physical properties can be reached by the choice of the proper material, by copolymerisation or by polymer blending. None of these materials, however, can withstand sunlight, ionising radiation, heat, the attack of microorganisms, not to mention aggressive chemicals. (Very few may pass for stable, for instance aromatic polypyromellitic imides like Kapton.) Protective additives, in amounts between 0.02% and about 2%, are able to prolong the lifetime of polymeric materials by several orders of magnitudes. This means that optical and mechanical properties – these are the most important ones – remain almost constant for a long time.

Polymers are the most widely used materials after steel, and polymeric hydrocarbons[1] (polyethylene, polypropylene, polystyrene) together with polyvinylchloride make the majority of all industrial polymers. This explains why *antioxidants* for polyhydrocarbons and *heat-* as well as *light stabilisers* for PVC are on top of the big family of additives. To give two figures: the worldwide production of PVC in 1985 was 1.4×10^{10} kg and that of PVC stabilisers 2.5×10^{8} kg (this makes an average of 1.8% of stabiliser in PVC). The importance of all the other industrial polymers and additives is, of course, no less; this may be shown by the considerable variety of applications and chemical compositions of the latter.

The following chapters were arranged according to the instrumental techniques used in additive analysis. The bibliography, on the other hand, presents publications on special groups of additives and on the applied analytical methods. This allows rapid access to both topics – methods and materials.

The complete analysis of an industrial polymer follows this scheme:

1. *Extraction* of low-molecular material from polymer
2. *Separation* of additive mixtures into their components
3. *Identification* of polymer
4. *Identification* of additives
5. *Quantitative analysis*

In this text, only items 1 and 4 will be treated in more detail. Item 2 is thoroughly described in the book of Scholl (Hummel/Scholl vol. 3, Sect. 10.1), chemical analysis (items 4 and 5) in that of Crompton. Recent literature is found in Sect. 10.2 and in the 4th edition of Gächter/Müller.

1 We use the term *polyolefines* only for unsturated polymeric hydrocarbons like polybutadiene, polyisoprene etc.

2
Extraction, solution precipitation and separation of additives

2.1
Extraction

Most additives are soluble in the usual solvents; as a rule, a solvent can be found which extracts the additive (or the mixture of additives) and leaves the polymer undissolved. In practice, a Soxhlet-type extractor or an extractor applying the boiling solvent is used. Prior to extraction, the polymer material is reduced by milling (in the N_2-cooled mill) or chopping. An admixture of quartz sand is applied in order to avoid the lumping or sticking together of the material. Films can easily be extracted after they have been, together with a net of thin wire, rolled into a scroll. The same can be done with thin films of vulcanisates which have been obtained by microtoming. (The extracted vulcanisate can frequently be dissolved by boiling in 1,3-dichlorobenzene.)

The extract is evaporated, preferably under N_2. Knowledge of the polymer and of the additives used for this material as well as a mass or *IR* spectrum of the dry residue usually gives sufficient information on the additive system in question. A separation into components is done by chromatographic methods (see Sect. 2.3). Plasticisers are usually separated by gas chromatography. Ample information on experimental details, stationary phases and retention times can be found in the book of Scholl (l.c.).

Solvent extraction has a number of shortcomings. It is time-consuming, up to two days for almost fully regaining the additive system. (Extraction by supercritical fluids, especially CO_2, at high pressures and high temperatures may reduce the time to about 1 h.) "Polymer" additives (they are usually oligomers) diffuse slowly, need long extraction times and will not be completely extracted. Chemically unstable additives may be degraded, e.g. by oxidation. Fractionated extraction with different solvents, preferred by some authors, certainly do not make chromatographic or other methods of separation unnecessary.

Pigments are sold either in solid or in paste forms. Aqueous pastes are agitated several times with hot acetone/water 1:1; eventually, a few drops of dilute HCl are added. The pigment is isolated by filtration or in a centrifuge. Organic pastes are worked up with acetone, ether, hexane (spirit) or another suitable solvent for the dispersing agent. The same is tried with paints, printing inks and unhardened surface coatings.

Prior to extraction, hardened surface coatings and insoluble plastics are milled and afterwards extracted with $CHCl_3$ (azo pigments) or glacial acetic acid (sulfonates, carboxylates, lake pigments). Soluble plastics may be dissolved in suitable solvents, and the dispersion is centrifuged. Ester-type binders may be hydrolysed; in nice cases the pigment stays undissolved.

Table 2.1 gives a collection of solvents and materials to be extracted which have been suggested in the literature.

2.2
Solution Precipitation

Solution precipitation (or reprecipitation) has the advantage that it can be performed under protective gas from the beginning, that the separation of additives from polymer can usually be made complete, and that the time needed is less than for extraction. The prerequisite for this method is of course that the polymer be soluble in whatever solvent.

Precipitation sometimes happens simply by cooling the solution (polyethylene, polypropylene, polyoxymethylene). Oligomers (together with the additives) may stay in solution. They can be precipitated with a proper non-solvent; during subsequent chromatography they remain, together with polymer additives, at the origin. In all other cases the solution is poured into an excess (at least ten times) of non-solvent for the polymer but solvent for the additives. This is usually methanol or acetonitrile. The polymer is washed several times with the nonsolvent, and the combined solutions are evaporated. In order to check the complete separation of polymer and additives, the polymer is reprecipitated. If the liquid phase, after evaporation, does not leave a residue then the separation is considered to be complete.

The dried residue is studied by *IRS* or *MS*, before or after separation by chromatography.

Table 2.2 shows solvents/non-solvents for different polymers described in the literature.

Table 2.1.
Extraction of additives from plastics and rubber (from Wheeler, 10.1; Squirrel, 10.2.1; Freitag, 10.1)

Polymer	Extractans	Extractandum
Polyethylene	Boiling $CHCl_3$ (up to 16 h)	All additives (results with HDPE may be low)
	$CHCl_3$, CCl_3CH_3 (reflux)	Antioxidants
	Hexane	Wax, some phenolics
	Ether (24 h at r.t., dark room)	Antioxidants
	Methanol	Emulsifiers, antistatics
	H_2O	Cellulose ethers, polyvinyl alcohol
	at 70 °C, N_2	antioxidants
Crosslinked PE (after milling[a])	Boiling toluene	Most additives (extracted PE is precipitated with acetonitrile)
Polypropylene	Boiling $CHCl_3$ (up to 16 h)	All additives
	CH_2Cl_2+CCl_3COOH (reflux)	Amides, amines
Polyvinylchloride (consecutively)	Ether, CCl_4	Plasticisers, stabilisers, some antioxidants, lubricants
	Methanol, ether	Diphenylthiourea, 2-phenylindole, dicyanodiamide
	Hexane	plasticisers, lubricants
	$CHCl_3$	antioxidants, *UV*-absorbers
	Acetone	stabilisers
	Ether (8 h)	plasticisers, antioxidants
	Methanol/CCl_4 1:2 (16 h)	stabilisers, polymer plasticisers
Poly(oxymethylene) (consecutively)	$CHCl_3$	Phenolics
	Methanol	Dicyanodiamide
Cellulose esters	Ether	Plasticisers
Polyvinylacetate dispersions	Pentane/ether	Plasticisers
Rubber	H_2O	Antioxidants (partially)
	Methanol	*p*-Phenylenediamine derivatives
	Ethanol+HCl (reflux)	Amine- and phenolic antioxidants
	Acetone	Most additives, S_8, mineral oil, fatty acids
	Ether	Phenylsalicylate, resorcinol benzoate

a Some oxidation may occur

Table 2.2.
Separation of additives from polymers by solution/precipitation (from Hummel/Scholl and Gächter/Müller, 10.1; by kind permission of Carl Hanser Verlag, Munich)

Polymer	Solvent	Precipitation of polymer by
Polyethylene, polypropylene	Benzene, toluene, xylenes (boiling)	Cooling; additional precipitation by CH_3OH or CH_3CN, if necessary
Polystyrene	Benzene, toluene, tetrahydrofuran, CH_2Cl_2	CH_3OH
Crosslinked PE(mill)	Toluene (boiling)	CH_3OH or CH_3CN
Polyvinylchloride	Tetrahydrofuran	Hexane, CH_3OH
Polyoxymethylene(mill)	Dimethylformamide (140 °C)	Cooling
Polycarbonate	Cyclohexanone, CH_2Cl_2	CH_3OH or CH_3CN
Polyacrylates	Acetone	H_2O
Polyamides	$CF_3C(OH)CF_3$, HCOOH, CF_3CH_2OH	CH_3OH or CH_3CN
Polyurethanes	Dimethylformamide	CH_3OH

In aged or thermally treated samples, additives may have reacted with the polymer and then cannot be separated completely from the latter by physical methods. This is shown in Fig. 2.1 (from Schroeder, 10.2.1). PVC was stabilised with dibutyl-^{113}Sn-*bis*(methylmaleate) and subjected to heat treatment. Depending on the solvent system the radioactiv-

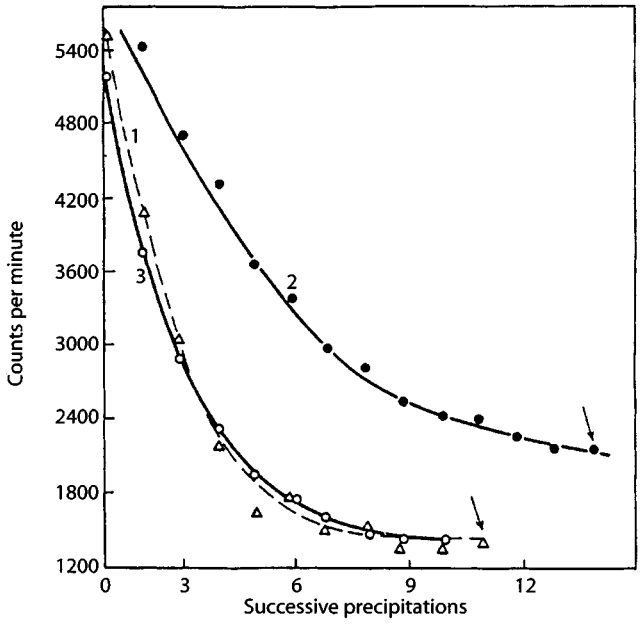


Fig. 2.1 Progress of the separation of dibutyl-^{113}Sn-*bis*(methylmaleate) from PVC by reprecipitation. Solvents: THF (*1* 3% PVC, *2* 7.5% PVC) and cyclohexanone (*3* 7.5% PVC). The PVC/stabiliser system was heat-treated prior to solution/precipitation. Technique: radiometry. (E. Schröder et al., 10.1, 10.2.1)

ity went down, after 12 reprecipitations, to about 40 or 25%; it is presumed that the PVC-stabiliser complex can partially be dissociated by certain solvents.

If the polymer material contained insoluble components like fillers, these can usually be removed by filtration (with a filter aid) or centrifuging. The insoluble material is washed several times with the solvent. It is, after drying, dispersed in tetrabromomethane (d=2.97 g cm^{-3}); this operation is simplified by pasting the solids with paraffin oil. The dispersion is centrifuged; heavy components (TiO_2, corundum, Pb compounds) subside. The lighter ones (silicates) float to the surface.

2.3 Separation of Additive Mixtures into Components

Separation of the extracted mixture of additives into fractions of defined composition is done by liquid chromatography (*LC*) in columns, thin layer (*TL*), high-performance liquid (*HPL*), gas-liquid (*GC*), gel permeation (*GP*) or supercritical fluid (*SF*) chromatography. Volatiles like plasticisers are usually separated by *GC*. The same method was applied to phenolic antioxidants and *UV* absorbers (Denning and Marshall, 10.2.2). Ample information on experimental details, stationary phases and retention times can be found in the book of Scholl (l.c.) and in the monograph of Munteanu (10.1). In addition, Scholl gives all information on *TLC* data of pigments. A thorough investigation on the chromatographic analysis of elastomer antidegradants and accelerators has been made by Vimalasiri et al. (10.1); 258 references represent older literature from 1984 back. In the following, only a few examples are given for the separation of mixtures by these methods.

A general *TLC* screening method was described by Mady et al. (10.2.2). A small amount of the dissolved material is brought upon a 0.25-mm pre-coated silica-gel 60 F-254 plate (Merck) and developed in a well-saturated tank with CH_2Cl_2/CH_3OH 49:1. For hindered phenols, phosphomolybdic acid was used for detection. *UV* absorbers like Tinuvin 328 were developed with CH_2Cl_2/heptane 7:3, the spots were detected under a *UV* lamp. Light stabilisers like Tinuvin 765 were developed with CH_2Cl_2/CH_3OH/aqueous NH_3 90:9:1 and detected by potassium diplatinate.

HPLC is successfully used for the separation of mixtures. The results can be evaluated quantitatively; the peak heights are directly proportional to the amount of the substance which produced the signal. Figure 2.2 shows the result of *HPLC* separation of a complex mixture of rubber chemicals. The amount of material per fraction is typically in the range 10–100 ng. This is at the edge or already beyond the limit of *IR* identification but well within *MS*. The assignment of the peaks to defined compounds is, however, usually done with calibration mixtures of known composition.

HPLC offers a very high separation power (up to 650 theoretical plates/cm column); thus, it is able to separate, e.g. oligomers, homologous series or even isomers. Figure 2.3 demonstrates this with phthalic acid esters used as plasticisers.

Stoveken (10.2.1) achieved the complete separation of five antioxidants, one *UV* inhibitor and three slip additives on silica gel HC-ODS/Sil-X (250 mm, 2.6 mm i.d.) at 80 °C with acetonitrile:H_2O 1:1 linear in 25 min to pure acetonitrile. The detector was LC-55 at 200 nm (Perkin-Elmer).

GPC (in columns) separates mixtures on porous gels according to the size of the molecules. Big ones traverse a *GP* column much faster than small ones – they have little chance to rest in holes of the gel. The smallest molecules come last because it is difficult to elute them from their resorts. For the detection of the eluted fractions, differential refractometers, *UV* photometers or calorimetric devices are available.

Braun and Bezdadea (10.2.8) used *GPC* for the separation of four extracted additives (2 Irgastabs, stearyl stearate and epoxidised soy-bean oil) from PVC compounds as well as the THF-soluble from plate-out produced during processing of this plate-out. The equipment was a Waters pump 6000A, a differential refractometer R 401 and μ-styragel columns. The solvent was THF.

Separation of additives by *SFC* and identification by *FTIRS* is described in Sect. 3.5.1.2.

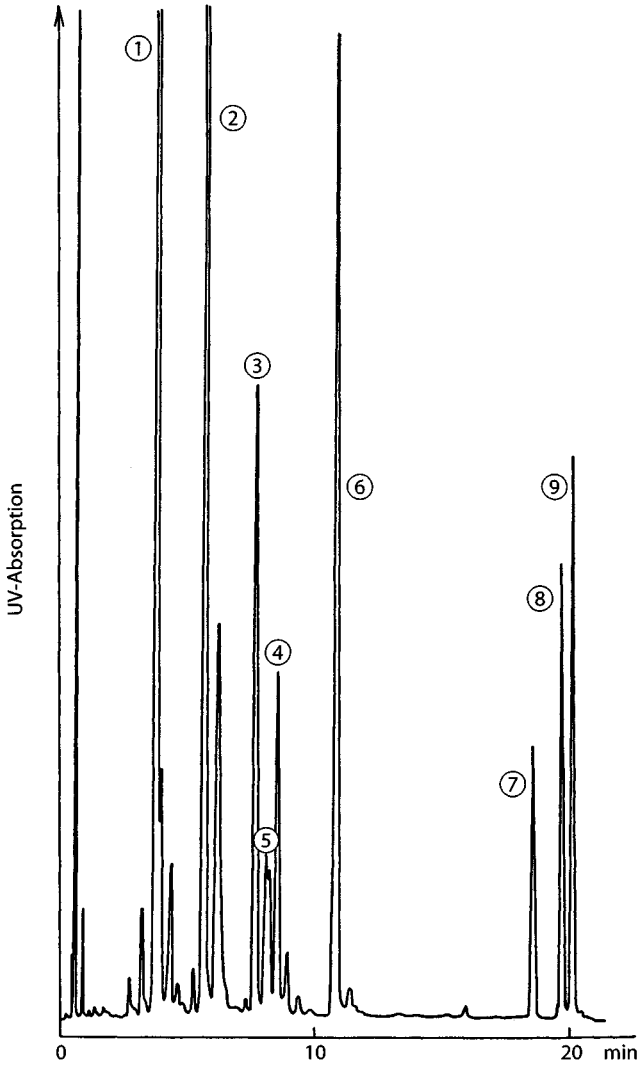


Fig. 2.2 Separation of additives by *HPLC* (J.J. Stoveken, 10.2.1, from Scholl, l.c.). Column: silica-gel HC-ODS/Sil-X, 250/2.6 mm, 80 °C. Detector: LC-55 (Perkin-Elmer). Mobile phase: acetonitrile/H_2O 1:1, 25 min linear to AN. (1) BHT, (2) oleamide, (3) Topanol CA (2,4-dimethyl-6-*t*-butylphenol), (4) UV 531, (5) stearamide, (6) erucamide, (7) dilaurylthiopropionate, (8) 2-(3,5-di-*t*-butyl-4-hydroxyphenyl)propionic pentaerythritol tetraester (Irganox 1010), β-(3,5-di-*t*-butyl-4-hydroxyphenyl)propionic octadecyl ester (Irganox 1076)

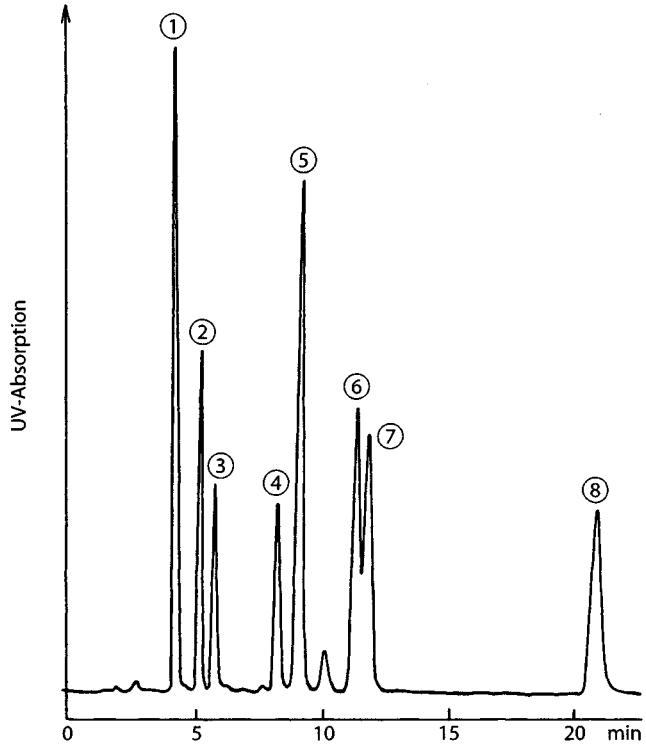


Fig. 2.3 Separation of phthalate ester plasticisers by *HPLC* (with Perkin-Elmer mod. 601, laboratory information by Scholl). Columns: 2 × ODS-SIL-X-1 (reversed phase), 250/4.6 mm; 75 °C, 2 cm^3/min, 500 bar. Mobile phase: H_2O/acetonitrile 3:2, in 80 min with convex gradient to AN. UV detector LC 55 from Perkin-Elmer. (1) dimethyl-, (2) diethyl-, (3) diallyl-, (4) diphenyl-, (5) dibutyl-, (6) dipentyl-, (7) dicyclohexyl-, (8) dioctyl-phthalate

3
Infrared Spectrometry

3.1
Fundamentals

The mid-infrared spectrum (4000–400 cm^{-1}, *IRS*) exhibits part of the vibrational behaviour of molecules, it houses their fundamental vibrations (*FV*). A *FV* is connected with a transition from the ground state of a certain vibrational mode to the first excited state. It is infrared-active if the dipole moment of the molecule in the ground state or of a (decoupled) partial structure changes during this transition. A vibrational mode is Raman-active when the polarisability of the molecule changes during the transition. The two methods are complementary. Selection rules, based on molecular symmetries, tell us which of the possible vibrations are *IR* and which ones are Raman active.

A complete picture of the vibrational behaviour of a molecule can be obtained solely by inelastic neutron scattering spectrometry (*INS*). This method does not know excitation conditions and selection rules; thus, the (few) vibrational modes being both *IR* and Raman inactive can be observed by *INS*.

The total number N_{FV} of *FV* of a molecule built of n atoms can be obtained by a simple consideration. (We set, by the way, a mechanical model of masses and springs in the stead of a molecule. The number of possible vibrations of this model are set = N_{FV}.) In 3-dimensional space, n atoms have $3n$ degrees of freedom. If the atoms are bound together, the resulting molecule, if it is non-linear, can perform 3 translations in space and three rotations around 3 axes. What is left are vibrations: $N_{FV} = 3n–6$; for linear molecules NFV = $3n–5$. Why? The rotation around the main axis of the molecule cannot be excited – the excitation energy would be higher than the dissociation energy. This is a consequence of quantum mechanics. The equations given above hold only if all vibrations in the molecule considered are coupled. We also keep in mind that doubly degenerate vibrations count twice, triply degenerate ones three times.

This model, despite the included assumptions, works quite well with small molecules. Large ones exhibit much less *IR* and Raman bands than required by $N_{FV} = 3n–6$. Quite dramatic is this band deficit in the case of polymers. The reason for this effect is the limited vibrational coupling in large molecules. This is evident in the case of strongly deviating masses or bond strengths. C and H are not sufficiently different; $\nu_s(CH_2)$ and $\nu_{as}(CH_2)$ differ by about 75 cm^{-1} and can easily be measured. The SiH_2 group produces only one stretching band with normal *IR* spectrometers. The effect of different bond strengths is also obvious. The stretching vibrations of single, double, triple bonds of CC and CN are separated by several hundred cm^{-1}. Within a chain, double and triple bonds as well as heavy atoms interrupt vibrational coupling. Finally, looking at polymers, numerous different chain conformations restrict coupling within a few monomeric units. (This is, however, sufficient to distinguish between block, statistical and alternating copolymers.) Crystalline polymers, on the other hand, show long-range coupling within a chain – regular chain conformations are the prerequisite for polymer crystallisability. This view can, *mutatis mutandis*, also be applied to smaller molecules. These, in the liquid state, may assume different conformations, being different in symmetry. This produces a broadening of the bands attributable to vibrations of the related partial structure. Crystallisation forces the molecules into the same conformation. This causes sharp bands and frequently also splitting of bands due to intra- or inter-molecular phase relations.

Due to the low symmetry of large molecules (usually just identity) most of the *IR* bands are isofrequent with analogous Raman bands. Due to the different excitation conditions, the intensities (transition probabilities) of *IR* and Raman bands belonging to the same vibrational mode may be quite different.

From these considerations we draw the following conclusions for analytical *IR* spectrometry:

- Molecular identity can be determined only for relatively small molecules.
- In a first approximation, *IR* spectra of large molecules may be considered as the superposition of partial spectra of partial structures. The term "group frequency" is inadequate.
- Some partial structures allow the assignment of substances from their spectra to certain "families" or to members of homologous series.

- Insufficient spectral differences of closely related liquid substances can be lifted by measuring the spectra of the solid materials at low temperatures.

The spectroscopist sometimes puts aside the fact that the *MIR* range not only exhibits bands belonging to *FV* but also (usually weak) bands from overtones and combination vibrations. These may sometimes be helpful in structure elucidation (substitution of aromats) and for the statement of identity. They can, however, feign *FV* once they are intensified by Fermi resonance: if an overtone or a combination vibration comes close to an intense *FV* then the former usually increases considerable in intensity. (This is a simplified presentation.)

In recent years, near-infrared spectrometry (*NIRS*) obtained renewed attention. *FT*-spectrometers are available which give easy access to the *NIR* (4000–12 500 cm^{-1}) and the Raman ranges. The former is free from *FV* as well as from overtones and combination vibrations of heavier groups; thus, it houses predominantly the 1st and 2nd overtones of XH_n groups, X being C, N, O, P... in addition to the 2nd and 3rd overtones of strong *FV* in the 1800–1500 cm^{-1} range. Their intensities are 1/10 or less of the related *FV*, film thicknesses are therefore around 0.5 mm or more. This is advantageous for quantitative determinations (less noise and false-light, averaging of possible deviations of the composition of the sample). Scattered light may produce some problems, especially with KBr dispersions; background correction with a suitable program usually solves them.

Generally, *NIR* spectra do not provide sufficient information for structure elucidation. However, there is another interesting application – it is the possibility to use the *NIRS* as a physical constant. Almost no sample preparation is necessary; the powdered material in a vessel is put into the *FT* spectrometer and the spectrum is measured in diffuse reflexion (*DRIFT IRS*). This technique is almost unique for quality control and (after calibration) for the quantitative analysis of multicomponent systems. Not the least advantage of reflexion *NIRS* is the possibility of remote control via glass fibre optics: *NIR* radiation is not absorbed by glass. Thus, the *NIR* data may be collected where additives and plastics are mixed, and immediately transported to the spectrometer. Siesler gave a number of basic contributions on technique and applications (10.1, 10.2.8). Spatafore and McDermott (10.2.1) describe the analysis of polyhydrocarbon additives by reflexion *NIRS*.

3.2 Sample Preparation and Measurement

The classical methods of sample preparation have been described in detail (Brame and Grasselli, 10.1; Günzler and Böck, 10.1 and others). We restrict ourselves to some special aspects.

The least disturbance of the plastic/additive system would be caused by a direct measurement, either by transmission or by reflexion. Unfortunately for the analyst, the concentration of additive in polymer is so low (1% or lower) that it is really difficult to find an absorption range where the additive has a strong absorption band and the polymer offers a window. Best chances provide aliphatic polyhydrocarbons, i.e. polyethylene (PE) and polypropylene.

A fine example is described by Tikuisis and Van Dang (10.2.2). Two common antioxidants, Irganox 1010 and Irgafos, were incorporated in PE. A film of 0.5 mm thickness was pressed and measured. Luckily, the ester-type Irganox 1010 absorbs at 1740 cm^{-1} where PE does not, and the phosphorus derivative Irgafos found, with a characteristic band complex at 850 cm^{-1}, another window (Fig. 3.1). It was possible to calibrate the method by measuring samples with additive concentrations between 1000 ppm and 2000 ppm. If bands of polymer and additive overlap partially then spectral subtraction of the pure polymer should be a technique to be examined.

In most cases, additives have to be separated from their matrix. Plasticisers, fillers, rubber extenders and the like can be recovered in quantities allowing conventional preparation methods. Antioxidants, stabilisers, vulcanisation agents and sometimes also pigments are applied in small concentrations and, to daunt the analyst, as mixtures. If the additives in 5g of polymer are extracted or separated by solution/precipitation, the yield will be typically 5 mg. These will be subjected to chromatographic (*TLC*, *HPLC*, *GC* – if volatile) separation; the components weigh down to 50 µg.

Fortunately, hardware companies provided micro-accessories which allow the measurement of good spectra with samples down to about 0.1 µg. The following (older) data are from Bodenseewerk Perkin-Elmer (Krohmer, Kemmner):

Sampling	Diameter of wafer	Hardware	Limit
		Microscope	<0.1 µg
Solids in KBr	0.5 mm	Micro-illuminator, ordinate expansion	0.1 µg
	0.5 mm	Micro-illuminator	0.2 µg
	1.5 mm		2 µg
	3 mm		3 µg
Solution		Micro-cuvette	8 µg
Micro-reflexion		2-mm mirror	10 µg
FMIR		*ATR* crystal	15 µg

Volatiles (plasticisers, alkylsubstituted phenolics, hindered amines, some rubber chemicals) can be analysed by the elegant combination capillary-*GC-FTIRS*. Here, the separated fractions with defined compounds are measured online in a short gas cell with low diameter. Non-volatiles (oligo- or polymers) may be thermally degraded in a pyrolyser directly attached to the gas chromatograph. Figures. 3.2–3.4 show the results obtained in our institute by D. Weber (10.2.8).

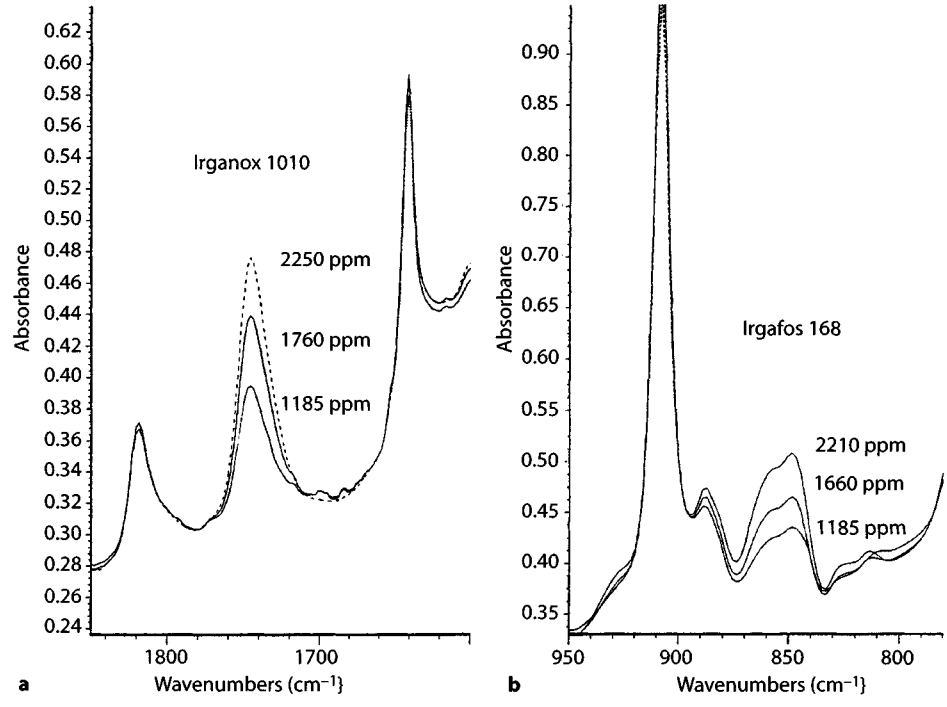


Fig. 3.1
Direct *FTIR* determination of the Ciba-antioxidants Irganox 1010 (at 1740 cm^{-1}) and Irgafos 168 (at 850 cm^{-1}) in polyethylene. Film thickness: 0.5 mm. (Tikuisis and Van Dang, 10.2.2; by kind permission of Chapman & Hall, London)

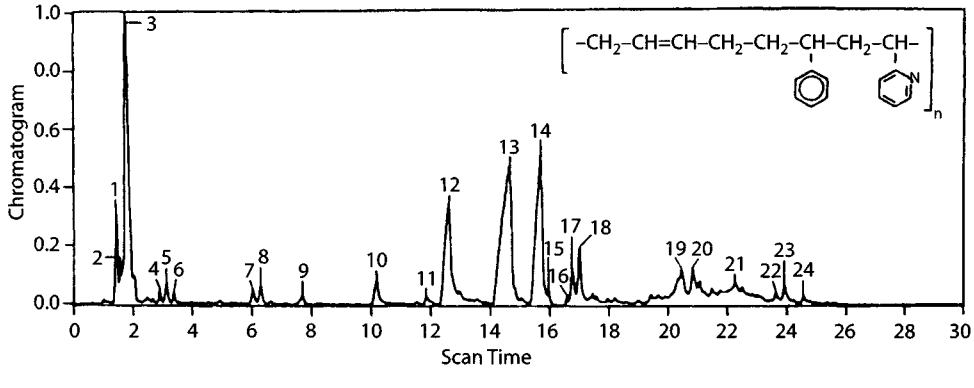


Fig. 3.2
Gram-Schmidt reconstruction of the pyrolysis-gas chromatogram of poly(butadiene-*co*-styrene-*co*-vinylpyridine) (Bunatex VP, Huels) from the pyrolysis-*FTIRS*. Isothermal pyrolysis at 700 °C, time of pyrolysis 10 s. ***1*** CO, CO_2, CH_4, C_2H_4, ***2*** H_2O, propene, ***3*** 1,3-butadiene, 1-butene, ***4*** 1,3-*E*-pentadiene, ***5*** cyclopentadiene, ***6*** cyclopentene, ***7*** benzene, ***8*** 1,3-cyclohexadiene, ***9*** 2,2,4-trimethyl-1-pentene, ***10*** toluene, ***11*** 2-methylpyridine+X, ***12*** 4-vinylcyclohexene, ***13*** styrene, ***14*** 2-vinylpyridine, ***15*** alkylaromat, ***16*** α-methylstyrene, ***17*** branched olefin, ***18*** 2,2,4,6,6-pentamethyl-3-heptene, ***19–23*** olefins, ***24*** 2-alkylpyridine (from D. Weber, 10.2.8)

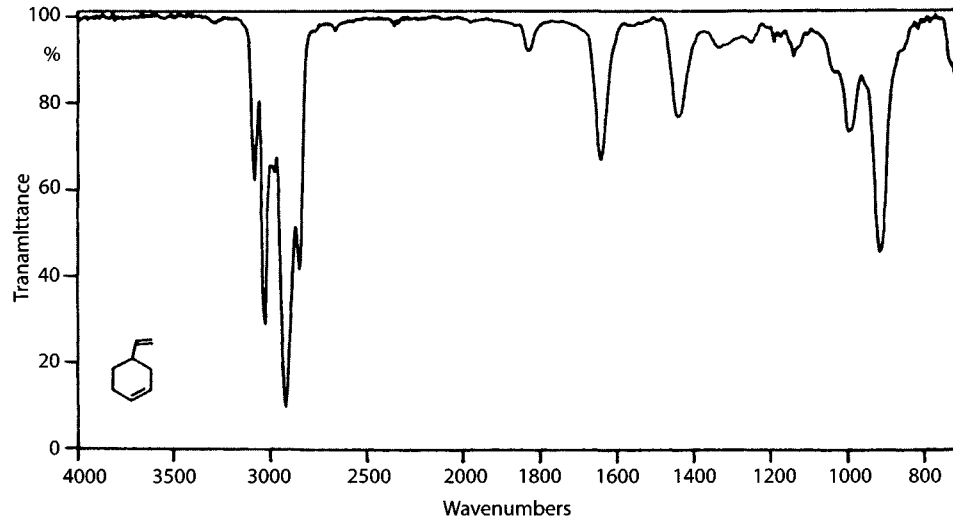


Fig. 3.3
FTIR gas-phase spectrum of 4-vinyl-1-cyclohexene from peak 12 of the Gram-Schmidt reconstruction of poly(butadiene-*co*-styrene-*co*-2-vinylpyridine) at 250 °C (from D. Weber, 10.2.8)

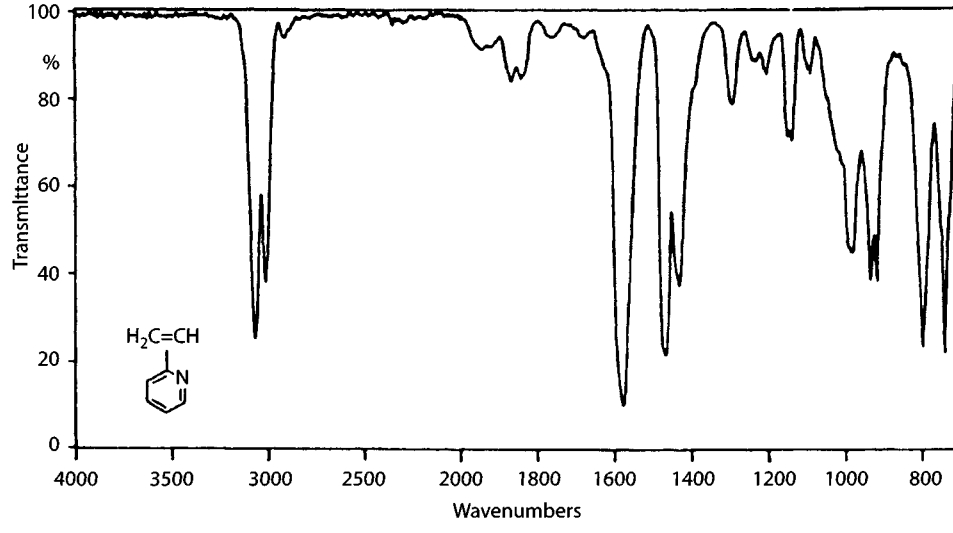


Fig. 3.4
FTIR gas-phase spectrum of 2-vinylpyridine from peak 14 of the Gram-Schmidt reconstruction of poly(butadiene-*co*-styrene-*co*-2-vinylpyridine) at 250 °C (from D. Weber, 10.2.8)

3.3 Conventional and Computer-Supported Interpretation of *IR* Spectra

Once upon a time there was a spectroscopist who sat in front of his PE model 21, waited until the cylinder had made its turn and the pen had drawn the spectrum, threw a look at the paper and said: "Oh, this is emulsion PVC with some vinyl acetate in it." The time for learning took years in those old days, books and publications were the daily bread, and experience brought knowledge. *Tempi passati.* Nobody will pay for this long period of learning, some universities stopped lectures in applied infrared spectrometry, spectral libraries are now on the hard disks of computers, and the time needed for an *IR* analysis is now a few minutes (plus sample preparation time) instead of an hour. Interpretation of spectra is frequently made only by computer-aided search for the nearest match in a digitised library.

Yet ... the unforgettable Thomas Clerc once wrote: *Today, a spectroscopist doesn't have to understand spectroscopy – though it wouldn't hurt.* So I urge everyone to keep the books of Socrates, Lin-Vien et al. and Günzler/Böck (all 10.1) to hand. The first look at a spectrum is still an adventure, and it helps immensely to have a rough knowledge of the chemistry of the analytical material in mind when studying the list of the 20 substances (produced after a search) which are spectroscopically most similar to the analyte.

The chemistry of plastics additives covers almost the whole organic and inorganic chemistry. Tables 3.1–3.23

present partial spectra (characteristic band combinations) of all important organic structures and basic absorptions of inorganic ions. The absorption ranges given do not represent the whole probability region for a vibration but rather those of highest probability. The assignments are tentative; most of the vibrations cited are coupled with other modes. The information for these tables have been taken from the literature and from our own spectral data. They can help to make some basic assignments; everything else may be done with similarity searches and by using the cited literature.

Abbreviations used in vibrational spectroscopy

s	strong	ν	stretching vibration
m	medium	δ	i.p. deformation vibration
w	weak	γ	o.o.p. def. vibration
v	very	ϱ	rocking vibration
var	variable	τ	twisting vibration
b	broad	ϖ	wagging vibration
sh	sharp	*Z*	("*cis*") configuration
sld	shoulder	*E*	("*trans*") configuration
i.p.	in plane	*FV*	fundamental vibration
o.o.p	out of plane	*cis*	close conformation (60°)
$_s$ (as subscript)	symmetric	*trans*	wide conformation (180 °)
$_{as}$ (as subscript)	antisymmetric	ϕ	phenyl

The spectroscopic literature has been used to establish computer-driven assignment programs, "artificial intelligence". Usually, they give their suggestions immediately after a spectrum has been measured. Immense work of thoroughly trained spectroscopists has been buried in these programs, and they are certainly apt to give some basic information on the chemistry of defined substances. With mixtures, and this is almost always the case in practical analytical work, these suggestions tend to be oracular.

How can, by the way, the spectroscopist distinguish between the spectrum of a defined substance and that of a mixture? If the mixture is a series of homologues (adipates, phthalates etc.) or oligomers (polyoxyethylenes etc.) he cannot. If it represents species with spectroscopically prominent components (phthalate+phosphate esters, carbonate+sulfate etc.), the expert will recognise the mixture. Generally speaking, the perception of a mixture from its spectrum is an art rather than science – in other words, it needs a large amount of experience.

3.4 Some Aspects of *FTIR* Spectrometry

3.4.1 Storage of Spectra in the Computer

The first computer-equipped *IR* spectrometers were hybrids: the spectrometer itself was double beam-dispersive, the attached computer stored the wavenumber and intensity data point by point. Programs for mathematical treatment allowed standardisation, forming of derivatives, addition or subtraction of spectral information etc.

The dispersive spectrometers are extinct (big body, little brain), the modern ones are creatures with a big brain (rapid computer for Fourier analysis, large storage room, lots of programs) and small body (interferometer). After Fourier analysis, a spectrum is digitised as a one-dimensional matrix. The step width on the wavenumber scale is found from the positions of the first and last wavenumbers in the spectrum and the number of data points. (In the abscissa-expanded spectrum on screen or as hardcopy, the steps appear as straight lines.) This information is to be found in the "header block" of each spectrum and is followed by the series of intensity values.

The specified distance of the data points on the wavenumber axis is known as the data interval. The number of data points is found from the wavenumber range chosen (usually 4000–400/cm) and the data interval. So we get 226 data points for an interval of 16 cm^{-1} and 3601 for an interval of 1 cm^{-1}, both the first and last points being counted. The smaller the data interval the larger is the amount of computer memory required; file operations then take longer. It has to be stressed that the data interval in a library considerably influences search operations and intensity measurements. If the analytical band is sharp (half band width, e.g. 4 cm^{-1}), a data interval of 16 cm–1 would almost with certainty have the consequence that the exact position of A_{max} of the band is missed – the measured value is low. The influence on the integrated intensity of the band is much smaller. Our own experience is that search operations should be done with data intervals of 4 cm^{-1}, and quantitative measurements of *A* with 2 cm^{-1}, in case of spectra with very sharp bands, even with 1 cm^{-1}. By the way, the computer printouts show intensity and wavenumber values with a ridiculously large number of decimals; apparently nothing can be done against this rubbish (it is not the computer, it is the programmer).

Intensity values are at best reproducible within a range of 2% on the *A* scale.

3.4.2 The Search for Similarity and Equality ("Identity")

In everyday speech the concepts identity, equality and similarity are often confused; here we use the scientific definitions. *Identity*, in a strict sense, means uniqueness. It can only be with a thing or organism itself: a piece of rock, a tree, a person. Identity is the elementary symmetry property. To say that two spectra were measured with the identical sample means that one and the same specimen (cell included) was measured twice. The two spectra are equal but not identical; the same is true for two eggs of the same size. *Similarity* is a term that could be applied to a cat and its kitten, or to the spectra of two adjacent members of a homologous series.

In computer-aided searches we must make a compromise. Our aim is to find for our analyte the "identical twin" in the library, say anatase for anatase. The score on the similarity scale for this case is said to be the highest one, it *defines* identity. In commercial (and proprietary) spectral libraries one and the same compound may, due to different trade names, be present several times. This is a fine opportunity to check the reproducibility of the measurement and the performance of the search system. None of these (normalised) spectra will have the same score on the similarity scale, though all of them own high scores. So we define (with *reservatio mentalis*) a certain niveau on the scale as the beginning of identity. We remain aware that real spectra are only an approach to the ideal of the *IRS* as a physical constant. The distance from this ideal depends on quite a number of factors.

As a rule, *FTIR* spectra are measured with a spectral resolution of 1 cm^{-1} or 2 cm^{-1}. Commercial libraries contain normalised (baseline, A_{max}) spectra, usually with this high resolution. To keep the storage capacity and searching time within reasonable limits, the spectra for an actual search file have data intervals of 4 cm^{-1}, 8 cm^{-1} or even 16 cm^{-1}. The optimal data interval of the library depends on the analytical spectrum; if this exhibits numerous sharp bands, a high data density in the search file may be necessary. Using an appropriate program, this interval can be chosen by the analyst if the original file is available. In our experience, a data interval of 4 cm^{-1} is good enough for all purposes, and 8 cm^{-1} is adequate for most.

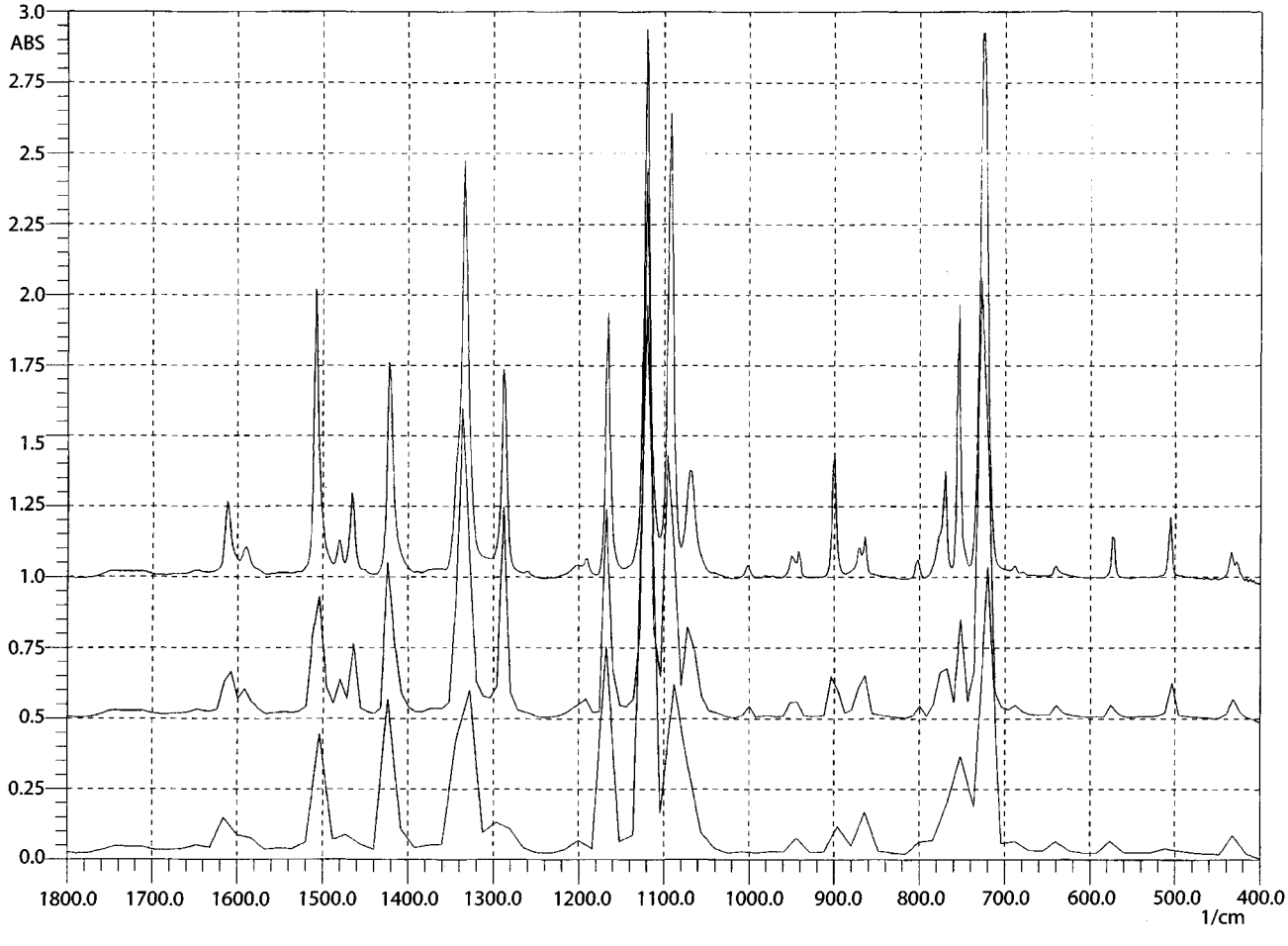


Fig. 3.5 *FTIR* spectrum of Cu phthalocyanine, influence of data reduction; from above: 2/cm, 8/cm, 16/cm (by K. Holland-Moritz)

Whether data reduction influences the appearance of a spectrum or not depends on the "sharpness" of bands, i.e. on the half-band width of the bands. (The half-band widths of the bands in a spectrum may differ considerably; we refer to the sharp ones.) The *IRS* of Cu phthalocyanine presents around 25 peaks, most of them sharp (Fig. 3.5, upper spectrum with a resolution of 2 cm^{-1}). Reduction of the data density to 8 cm^{-1} (middle) reduces the number of bands but little; thus, the splitting of the close twins at about 945 cm^{-1}, 865 cm^{-1} and 415 cm^{-1} is lifted. The relative intensities of the bands are, on the other hand, afflicted considerably. Further reduction of data density to 16 cm^{-1} leads to the disappearance of weak and sharp bands and to the fusion of neighbouring bands. At the same time, the shape of the bands approaches triangle functions. Whole-spectrum similarity searches with strongly reduced spectra, either in the library or as analytical spectrum, are useless if the spectra have sharp bands. Spectra containing exclusively broad bands (oxides, sulfides and others) are hardly influenced by data reduction. The majority of organic substances, including polymers, produces spectra with bands having half-band widths between these extremes. Figure 3.6 shows *IRS* of dinonylphthalate with data reductions of 2 cm^{-1}, 8 cm^{-1} and 16 cm^{-1}, respectively (from above). Here, the number of bands is diminished only slightly when going from 2 cm^{-1} to 16 cm^{-1}, and the band shapes aren't changed too badly.

Principally, we have the possibility to search with peak tables or with the whole spectrum (point-by-point). The first process is the oldest (half a century). It began with the mechanical evaluation of punched cards; each card contained a peak table (λ or cm^{-1}, A_{max} or transmittance) and chemical information on the related substance. All modern program packages have algorithms on the same principle (chemical information separately). *Spectacle*[2] allows four different algorithms working with *peak tables*:

$$M_{sum} = \sum_{i} p_i$$

2 Creon.Lab.Control, Max-Planck-Str. 17a, D 50858 Köln; delivered with the hardware of several companies.

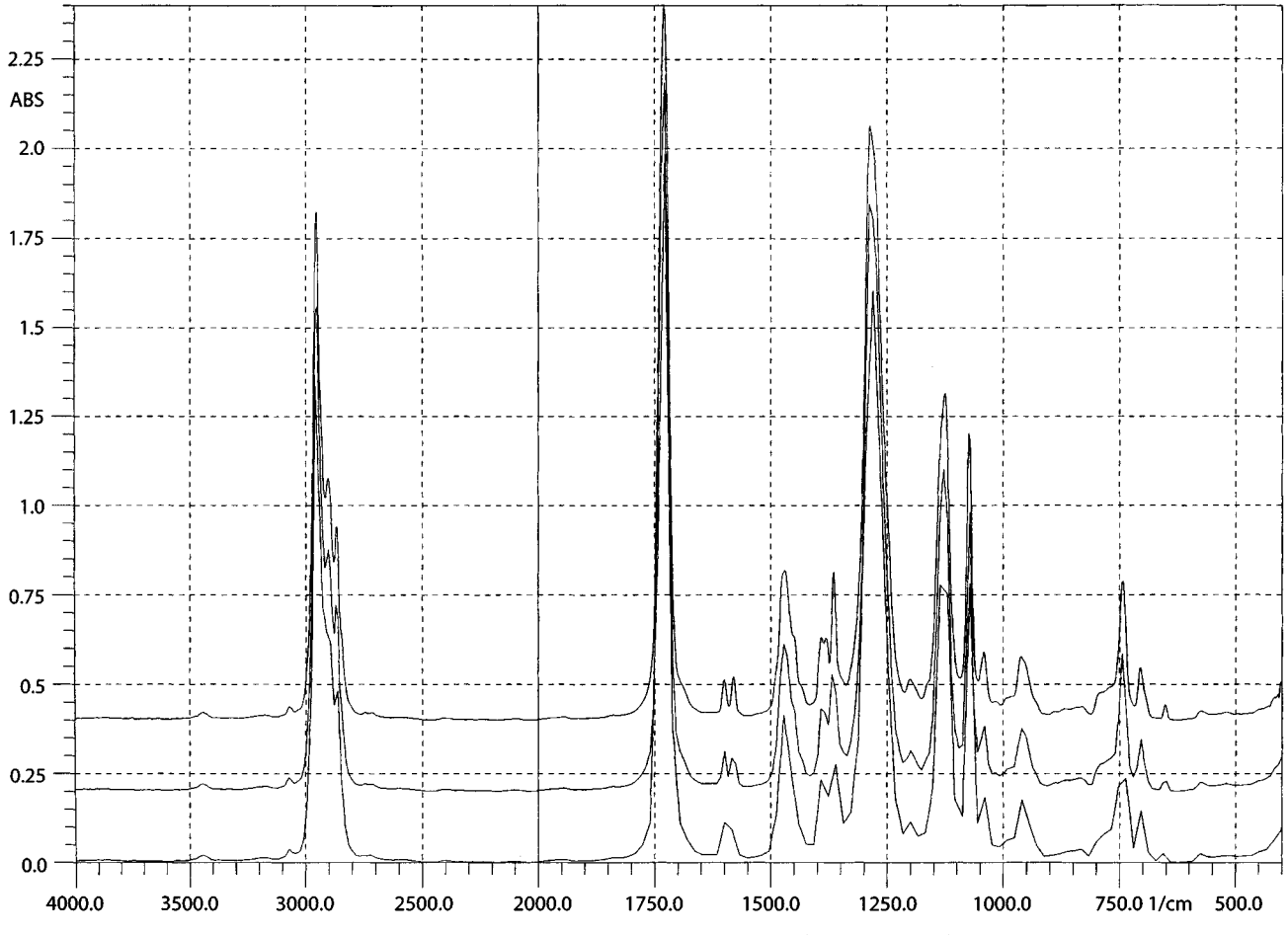


Fig. 3.6 *FTIR* spectrum of dinonylphthalate, influence of data reduction; from above: 2 cm^{-1}, 8 cm^{-1}, 16 cm^{-1} (by K. Holland-Moritz)

$$M_{wei} = \sum_i \left| R - dp_i \right| \cdot dp_i$$

$$M_{squ} = \sum_i \left(\left| R - dp_i \right|^2 \right) \cdot p_i$$

$$M_{per} = \left(\sum_i p_i / P \right) \cdot f_s$$

where p_i=1 if the band is present in both the sample spectrum and the reference spectrum, otherwise p_i=0, R is the prescribed tolerance, dp_i is the wave number difference between the band in the data file and the analytical band, P is the total number of bands in the spectrum of the analyte and f_s is a scaling factor.

The first correlation coefficient M_{SUM} lists library spectra in the order of the number of peaks that match peaks in the spectrum of the analyte. The values vary between zero (no matching pairs of bands) and the actual number of peaks in the analytical spectrum (maximum 75).

M_{WEI} (*WEI* means weighting) distinguishes between large and small discrepancies between the matching peaks of analyte and reference substance; this discrepancy lies within a predetermined tolerance range R. Large discrepancies receive extra weighting.

M_{SQU} squares the discrepancies of M_{WEI}.

M_{PER} is similar to M_{SUM}, but gives the fraction of matching peaks based on the total number of absorption bands in the unknown spectrum. The *Spectacle* software package also allows searches in a maximum of ten wavenumber ranges (characteristic band combinations).

Peak table algorithms (PTA) are simple and extremely fast; very big libraries can be searched in seconds. The results are less specific than those resulting from whole-spectrum searches. PTA have some advantages if the libraries to be searched are of relatively low quality.

Most of the commercial program packages contain the Lowry-Huppler algorithms (LH1–LH4) for whole-spectrum searches; *Spectrafile* offers these:

$$M_{AB} = \sum_i \left| s_i \cdot r_i \right|$$

$$M_{SQ} = \sum_i \left| s_i - r_i \right|^2$$

$$M_{AD} = \sum_i \left| ds_i - dr_i \right|$$

$$M_{SD} = \sum_i \left| ds_i - dr_i \right|^2$$

where s_i and r_i are the normalised absorbance values for each data point, s is sample, and r reference

LH1 (M_{AB}) calculates the difference between the analytical and the reference spectrum on the absorbance scale in the selected data interval for each wavenumber determined by the interval. The differences are then summed. A small value of M indicates a high similarity between the two spectra.

LH2 (M_{SQ}) squares the differences on the absorbance scale prior to the summation (sum of the least squares of differences). As all differences are <1, the larger differences are more strongly weighted than the smaller. A distance of one order of magnitude on the linear A scale increases to two orders of magnitude on the square scale. This conflicts with spectroscopic reality. A small number of large discrepancies produce a larger value of M (reduced similarity) than a large number of small discrepancies. The absence of weak but important bands ($\nu_{=C-H}$ of olefins and ν_{ring-H}, 3150–3000 cm^{-1}, combination vibrations of aromats, 2100–1700 cm^{-1} and others) in the reference spectrum affects the value of A but little. With the LH2 algorithm spectra are defined as identical if their dissimilarity values are $<10^3$. Since all organic matter has some structural and spectral similarity the LH2 dissimilarity for organics will not go far beyond 10^5.

LH3 and LH4 (M_{AD} and M_{SD}) use the first derivatives of the two spectra being compared. M_{AD} sums the linear differences, and M_{SD} sums the squared differences. This has the advantage that a rising or falling base line is straightened and broad, weak absorptions (mostly useless for analysis) are not considered. A disadvantage is that all the reference spectra in the library have to be differentiated. With a very noisy background these two algorithms cannot be used. It is noteworthy that these two derivative functions increase the gap on the dissimilarity scale between identical and similar spectra.

M_{EU}, a fifth algorithm, squares the absorbance values and then forms the differences:

$$M_{EU} = \sum \left(\left| s_i^2 - r_i^2 \right| \right)^2$$

i.e., Euclidian distance.

Let us, for a last time, come back to the problem of similarity and identity. It must be possible to detect, in the result of a search, whether the substance at the bottom of the dissimilarity scale is identical with the analyte; in other words, whether the spectrum of the analyte is present in the library. This is illustrated by Fig. 3.7. Naturally, each search ends with a comparison of the spectra of the first few hits with the spectrum of the analyte (visual pattern recognition).

A new algorithm specially for spectra of mixtures was developed by Fröhlich (10.2.8, included in *Spectacle*). It uses the results of similarity (usually with M_{AB}) and peak (complete table) searches in the following way:

Result of similarity search with whole spectrum	Result of peak search
Best hit	Correlation step 1
Second best hit	Correlation step 2
Search result	

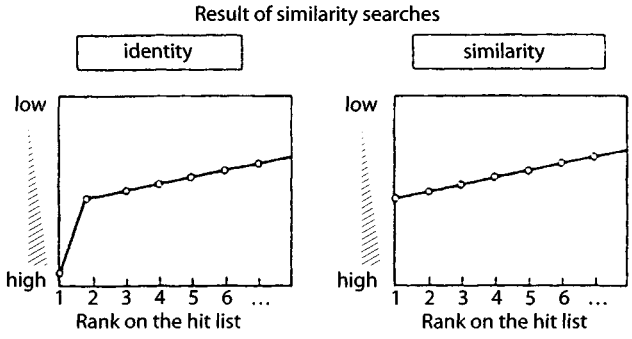


Fig. 3.7 Spectroscopic identity and similarity, a spectroscopic definition by evaluation of a spectral file and plotting the results on a dissimilarity scale. *Left*: the spectrum of the analyte is present in the file; there is a jump in the dissimilarity function between the best hit and the second one. *Right*: the spectrum of the analyte is absent in the file. The dissimilarity function begins above the identity limit and shows only hits with increasing dissimilarity

The dissimilarity value M_{comb} for the best hit is given by

$$M_{comb} = \sum\left(s^2 + p^2\right)$$

where s is the placement in the whole-spectrum similarity search and p the one in peak search. For the placement on the dissimilarity scale of the next hits the results of whole-spectrum and peak searches are ratioed with M_{comb}; the results are correlated. The values of M_{comb} are theoretically between 2 and infinity; they usually don't go beyond 500 (residual spectral and structural similarity of all organics, disregarding the structure). Spectral identity is given if M_{comb}<50.

The theoretical basis for this combination algorithm is small though reasonable. Due to the limited range of vibrational coupling in large molecules of low symmetry (famous exception: Cu phthalocyanine with its centre of symmetry) the vibrational spectrum of such molecules tends to be a superposition of the partial spectra of the decoupled partial structures. (One of the consequences of this fact is the spectral similarity of substance families.) Thus, band positions (A_{max}) tell us more about structures than band envelopes. In the case of mixtures (including copolymers and multifunctional molecules) M_{comb} puts the highest similarities, as usual, on top of the list of the best 20. The components of the mixture are heaved up from low similarities into the range of best hits.

Numerous searches in our institute have confirmed this assumption, with two remarkable irritations: (1) searching with a "wrong" (analyte: pigment, library: pyrolysates) library yields irrational results, and (2) a certain amount of artefacts (false-light, Christiansen effect, bad base-line correction) puts such a spectrum way down on a similarity scale, far apart from the (correct) library spectrum of the same substance.

3.5 Recent Work on *IR* Spectrometry of Additives

3.5.1 Additives with Preventive or Curative Properties

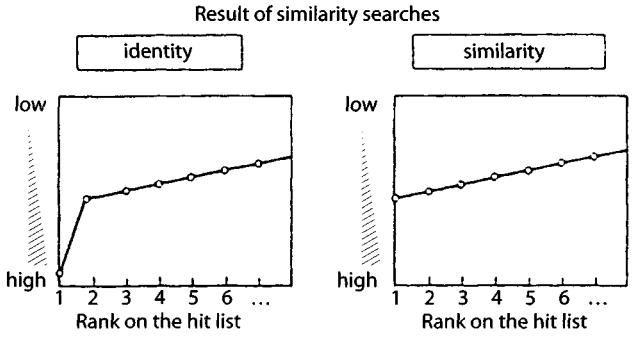
3.5.1.1 Empirical *IR* Band Assignment

The first comprehensive spectral collection of antioxidants and stabilisers was the one of Scholl (10.1). In the second edition (1981), 163 *IRS* of *UV* and PVC stabilisers and 113 *IRS* of antioxidants were presented. In the same book, the empirical assignment of *IR* bands to structures was discussed.

Most antioxidants and stabilisers belong either to the hindered-amine light stabilisers (HALS) or to the phenolic antioxidants. The former usually exhibit one or (rarely) two sharp bands, $\nu(NH_{free})$, of weak (aliphatic) or medium to strong (aromatic-aliphatic) intensity at the high-frequency end of the spectrum. ν(H-N<aliphatic) may be found around 3600 cm^{-1}, ν(H-N<aliphatic/aromatic or aromatic) around 3400 cm^{-1}. Some of the aromatic-aliphatic (di-)amines carry associated NH groups. In this case, ν(NH) produces a w-m, broad band at 3350–3400 cm^{-1}. Common to all aromatic-aliphatic and aromatic amines is a medium (associated NH) to strong (free NH) ν(Ar-N) band between 1360 cm^{-1} and 1305 cm^{-1}.

Phenolic antioxidants exhibit ν(OH) at the high-frequency end of the spectrum. If no bulky substituents are in the two *o*-positions the OH groups will associate; ν(OH) then produces a band (vs, br) at about 3250 cm^{-1}. Sterically hindered phenols exhibit a band (s-vs sh) between 3650 cm^{-1} and 3600 cm^{-1}; this may show crystal splitting (two close peaks). If the kind of substituents in *o,o'*-positions allows some association ν(OH) broadens; finally a sharp band at about 3450 cm^{-1} and a broad one with maximum at about 3250 cm^{-1} appear. Other typical bands of the HO-Ar group can be recognised by their being broader than the sharp ring vibrations, namely 1475–1440 cm^{-1} (s, associated phenols) or ca. 1430 cm^{-1} (s sh, free phenols), ca. 1200 cm^{-1}, (s-vs br, associated phenols) or ca.1160 cm^{-1} (s sh), both ν(Ar-O).

Bands characterising NH or OH, aromatic ring system and alkyl substituents usually allow (near) identifications of amine type and phenolic antioxidants. In an early publication, Carlson et al. (10.2.6) use *IR*, *NMR* and *MS* for the identification of antioxidants from rubber vulcanisates. The samples were ground in a Wiley mill and extracted at r.t. with acetonitrile. Extending oil was "freezed out" by cooling the solution at −20 °C for 2–3 h. The decanted and filtrated solution is evaporated, the residue is used for the spectroscopic analyses.



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3.5.1.2 Separation of Additives and Identification by (*FT*)*IR* Spectrometry

There is (friendly) competition between mass and infrared spectroscopists with respect to their hyphenated techniques: *GC-MS*, *MS-MS*, *GC-FTIRS*, *LC-FTIRS*, etc. We have executed both quite intensely in our institute, and I dare say that *FTIR* and *MS* techniques complement each other ideally. *MS*, depending on the kind of ionisation, yields molecular masses and fragment masses of volatile, separated species; due to well-known thermal or electronic fragmentation mechanisms it is possible to reconstruct non-volatile substances like polymers from their pyrolysates. *MS* can analyse picograms of sample; this allows the very efficient coupling of capillary *GC* with *MS*. *FTIRS*, other than *MS*, is independent on the aggregational state of the sample, "visualises" functional groups and whole structures, distinguishes between structural isomers, and finally allows quantitative analyses due to strict physical correlations between molar concentrations and absorbances. It has reached a sensitivity in the range of nanograms.

3.5.1.2.1 Separation by Liquid Chromatography (references 10.2.1)

Already in 1968, Crompton (survey article) described the (off-line) combination of thin layer, column or gas chromatography with *IR* spectrometry for the identification of additives in polymeric hydrocarbons. After the introduction of the faster *HPLC* with its much higher separation power (some 10^3 up to 5×10^4 theoretical plates), it was possible to separate multicomponent additive mixtures in a reasonably short time. Standt, in a typical investigation, described the identification of low-molecular compounds, basically additives, in the extracts of dashboard films by reversed or normal phase, gradient *HPLC* (acetonitrile/CH_3OH+H_2O). Up to 30 components were separated on preparative columns (LiChrosorb RP-8, 250 mm long, 20 mm i.d., 7 µm particle size), detected by their *UV* absorption at 260 nm and identified (still off-line) by *IRS*, employing reference spectra. Alternatively, analytical columns with 4.6 mm i.d. were used. The most time-consuming process (24 h) was the Soxhlet extraction with ether or hexane; the separation itself needed about 90 min.

HPLC, especially with preparative columns, is but a semi-micro method. With sufficient amount of analyte and off-line *IR* identification this is advantageous. However, on-line *FTIR* analysis is a challenge, and for that it is necessary to get rid of the solvent at least in a semi-continuous way. Somsen et al. extracted the additives from PVC and polypropylene samples and separated them on narrow-bore *HPLC* columns by reversed-phase chromatography. The volatile mobile-phase solvent was removed during the deposition of the effluent by a spray-jet interface onto ZnSe windows. The spots of the components (nanogram range) were small enough for micro *FTIRS*, and the spectra were good enough for library search and/or visual interpretation.

Bruheim et al., in a recent publication, turned to temperature-programmed packed-capillary liquid chromatography (let us call it *TP-CLC*), off-line coupled to *FTIRS*. (In fact, the system is on-line up to the deposition of the spots on a rotating GeAl disc; the latter has to be transferred to the *FTIR* spectrometer.) This combination is quite sensational in being related to temperature-programmed gas chromatography-*FTIRS* – with the basic difference that non-volatile substances including (to present) oligomers are separated. With true capillaries (i.d.<1 mm), only isocratic mobile phases can be used; gradual changes of the mobile phase composition cause problems with respect to the low flow-rates required as well as during the nebulisation process.

In the present investigation, the fused silica capillary columns (length 300 mm, 320 µm i.d.) were packed using supercritical CO_2 as the slurry medium. The stationary phase material was 3.5-µm Kromasil 100 ODS (HiChrom, Reading, UK). A Merck Hitachi L-7100 piston pump delivered the mobile phase (acrylonitrile, AN) with a flow rate of 5 mm^3 min^{-1}. Manual injections were performed with a Valco Model CI4 W injection valve having an internal loop of 0.06 mm^3. The column was coupled to the injection valve by a 100-mm fused silica capillary (50 µm i.d.). A 5730A gas chromatograph (Hewlett Packard) served as column oven. *UV* detection (280 nm) was performed using a Spectra Physics model 2000, using a capillary "U" shaped detector cell with 8-mm light path (UZ-LI-CAP from LC Packings, Amsterdam). A Shimadzu C-R5 A integrator was used for *UV* data sampling. To prevent the mobile phase from boiling when operating at elevated temperatures, a fused silica linear restrictor (length 400 mm, 50 µm i.d.) was connected to the end of the *UV* detector cell. The end of this restrictor capillary served as the nebuliser tip, and was subsequently mounted directly within the in-house constructed nebuliser of the modified *LC-FTIR* interface (LC Transform 200, Lab Connections, Marlborough, MA, USA). The solutes were deposited on GeAl discs, utilising the original rotation disc drive system (5° min^{-1}). The discs were routinely cleaned with AN.

The nebuliser was an important part of the arrangement. It was constructed with special attendance to minimum dead volume (optimal separation of the components of mixtures); sufficient details are given in the paper of Bruheim et al. Heated sheath gas (50 °C, 5.5 dm^3 min^{-1}) was introduced to the capillary nebuliser, surrounding the fused silica restrictor capillary. Nebuliser spray and analyte deposition (spots) on the collector discs could be observed visually. It was found that a vertical position of the nebuliser outlet 5 mm above the disc collector resulted in optimal deposits (AN as mobile phase solvent).

FTIR measurements (eight scans per spectrum, 4000–700 cm^{-1}, resolution 4 cm^{-1}) were carried out on a Nicolet Magma 550 with deuterated triglycine sulfate detector. The GeAl disc was rotated during scanning at the same rate as during the sample deposition. Reflection-absorption spectra and constructed Gram-Schmidt chromatograms were acquired with the Nicolet Omnic 2.0 software. The mass limit of detection was 40 ng (signal/noise=3). The sensitivity may be improved by a factor of ca. 5 by employing an HgCdTe detector. Mixtures of antioxidants were separated and measured with good results. In one case (Irgafos P-EPQ) even the isomers of this oligomeric phosphonic acid ester were completely separated. The *FTIRS* were good enough for library search and visual interpretation. The range beyond about 850 cm^{-1} showed very strong noise and couldn't be used for a discussion of aromatic substitution.

TP-CLC-FTIRS, as described by Bruheim et al., can also be used for the separation and identification of oligomeric additives. The same is true for the (off-line) combination of gel permeation chromatography (*GPC*) with *IRS* as described by Howard in an early publication. The molar mass exclusion limit depends on the gel used for separation; with Poragel A-1 used in this study it is 1 kg mol^{-1}. The separation power of *GPC* is much lower than in the case of *HPLC* or *CLC*; Howard reached 460 theoretical plates with nine (*sic*) 4-ft. columns filled with a tetrahydrofuran slurry. The separation of the molecules is effected by their size; small molecules will penetrate the gel deeply, big molecules do not. This is the reason why, in *GPC*, big molecules are eluted first and small ones come last. Isomers and most other isobaric molecules cannot be separated. The "bands" in a *GP* chromatogram (empirical intensity *vs* eluted volume or "elution counts") are usually broader than the peaks in *HPLC* or *CLC*; Howard used them for the quantitative determination of specific antioxidants. In addition, THF extracts from polypropylene and PVC (10 g each) of different producers were separated; the chromatograms were characteristic for their origins. In addition, the influence of ageing and processing was studied by analysing consecutive chromatograms. *IRS* was used for the identification of eluted plasticisers.

3.5.1.2.2 Separation by Supercritical Fluid Capillary Chromatography

The (off-line) combination of *SFC* with *FTIRS* is one of the most powerful methods for separation and identification of multicomponent systems. Other chromatographic techniques suffer from certain disadvantages. Thus, *GC* requires volatility and thermal stability of a system; high-molecular mass or reactive additives are therefore not apt for *GC* separation. *HPLC* has detector problems and considerably lower resolution power than capillary chromatography, and it isn't easy to couple with *IR* or *MS*. Size-exclusion (gel permeation) chromatography suffers from poor resolution and low sensitivity.

Capillary *SFC* with CO_2 as mobile phase allows high-resolution separation of nonvolatile, thermally labile, high-molecular mass compounds. It can (among others) be operated with the universal flame-ionisation detector (*FID*). The considerable compressibility of CO_2 in the supercritical state as well as its relatively low critical temperature (31 °C at 7.4 MPa) allows one to work at moderate temperatures. Densities similar to liquids can be achieved; thus, density programming can control the solvating power of the fluid and thereby also the selectivity of the arrangement.

Finally, each eluate with a defined component is directly deposited from the end of a restrictor onto a small area (ca. 0.2 mm, a few ng of substance) of an *IR* transparent support as the CO_2 evaporates immediately. The *IRS* is measured with the substance on its support in a microscope.

A thorough investigation of the application of this technique to mixtures of additives was presented by Raynor et al. (10.2.1). A schematic diagram of the *SFC/FTIR* system is shown in Fig. 3.8. A Lee Scientific 501 SFC pump controlled by LS software run on an IBM XT 286 PC was used for

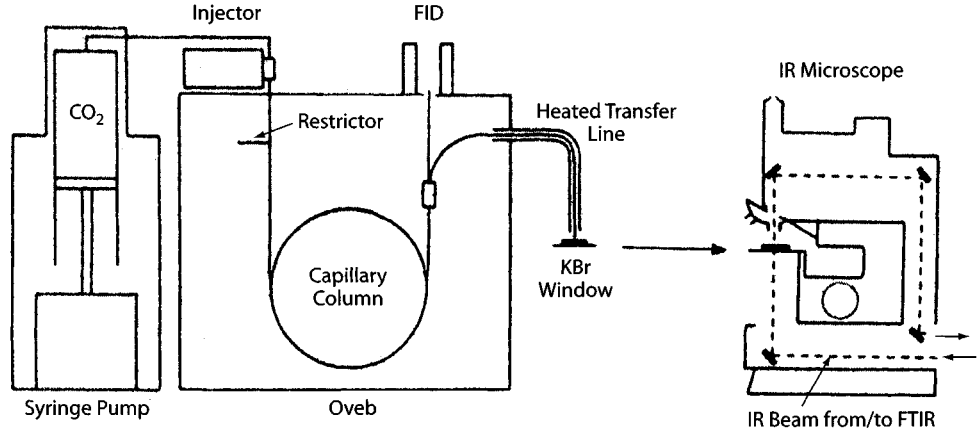


Fig. 3.8
Schematic diagram of the major instrumental components of an *SFC/FTIR* system with a microscope accessory (M.W. Raynor et al., 10.2.1)

pressure programming. CO_2 was delivered by the pump to a pneumatically actuated C14W microvalve injector (15 °C) fitted with a 0.2-mm^3 Valvo internal sample volume rotor. A 15-m fused-silica capillary column (0.1 mm i.d.) coated with a 0.5-μm crosslinked poly(methyl phenyl siloxane) was mounted in a Carlo Erba Fractovap 2150 *GC* oven with *FID* (400 °C). The column was connected to the injection valve via an inlet splitter (SGE) having a split ratio of 1:3. The column effluent was split between a tapered capillary restrictor in the *FID* and a heated transfer line by using a butt connector and a graphite ferrule (SGE). The system was maintained at 140 °C and an initial pressure of 150 atm for 12 min, before programming to 350 atm at a rate of 3 atm/min (1 atm=1.01×10^5 Pa).

The transfer line from the *SFC* to the *IR* microscope interface consisted of a 0.5-m deactivated fused-silica capillary (50 μm i.d.) with a tapered restrictor fixed at the interface end. The transfer line was threaded through a piece of stainless steel tubing, maintained at the column temperature. The tubing was inserted into the restrictor housing (140 °C). An *FID/FTIR* interface split ratio of 1:1 was set by cutting the *FID/FTIR* interface restrictors until each had a gaseous flow rate of 1.5 cm^3/min measured at r.t., and a column pressure of 150 atm. The end of the transfer line restrictor was positioned approximately 50 μm above the surface of a 13 mm KBr disc which was kept at r.t. After the elution of each peak (as detected by the *FID*) the KBr disc was placed in the microscope. The *IR* beam was reduced to an aperture of 150 μm or less depending on the size of the deposit and spectra were measured with a resolution of 4 cm^{-1}. The results were very good.

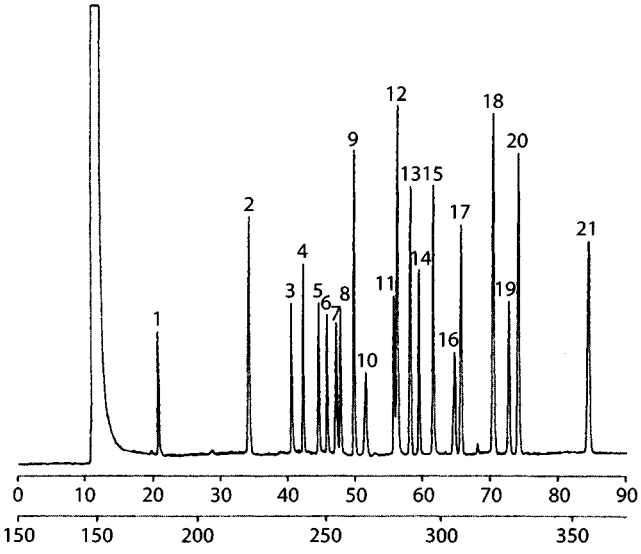


Fig. 3.9 *SFC* of 21 defined additives (M.W. Raynor et al., 10.2.1); for the structures belonging to certain trade names see Table 7.24. **1** Topanol OC, 2,4,6-tri-*t*-butylphenol, **2** Tinuvin P, 2-(2-hydroxy-5-methylphenyl)-2*H*-benzotriazole, **3** Tinuvin 292, *bis*(1-methyl-2,2,6,6-tetramethylpiperidinyl)sebacate, **4** Tinuvin 320, **5** Tinuvin 326, **6** Tinuvin 328, **7** Chimassorb 81, 2-hydroxy-4-octyloxybenzophenone, **8** Z-13-docoseneamide, **9** Tinuvin 770, *bis*(2,2,6,6-tetramethyl-4-piperidinyl)sebacate, **10** Tinuvin 440, 8-acetyl-3-dodecyl-7,7,9,9-tetramethyl-1,3,8-triazaspiro(4,5)decane-2,4-dione, **11** Irgafos 168, **12** Tinuvin 144, **13** Irganox PS800, **14** Irganox 1076, **15** Irganox MD1025, **16** Irganox 245, **17** Irganox 1035, **18** Irganox 3114, **19** Irganox PS802, **20** Irganox 1330, 1,3,5-*tris*(3,5-di-*t*-butyl-4-hydroxybenzyl)-2,4,6-trimethylbenzene, **21** Irganox 1010

The polymer additives used are listed in the legend of Fig. 3.9; additional structure informations are found in Table 7.24. A synthetic mixture containing 400 ng mm^{-3} of each of the 21 components in CH_2Cl_2 was used to find suitable chromatographic conditions, the resolution was excellent (Fig. 3.9). Commercial polypropylene samples from ICI (10 g) were Soxhlet extracted with ether for 15 h, the extracts were freed from low-molecular PP and subsequently analysed in the described way.

3.5.1.3 Solubility of Stabilisers and Antioxidants in Polymers

An interesting contribution on the solubility of HALS in low-density polyethylene (LDPE) has been published by Zehnacker and Marchal (10.2.5). The authors found that both A_{max} and the absorptivity a (m^2 mol^{-1}, not l mol^{-1}) of ν(CO) depend on the state of the investigated antioxidant, *bis*(2,2,6,6-tetramethyl-4-piperidinyl) (Tinuvin 770). Thus, A_{max} for ν(CO) of the dissolved antioxidant was 1740 cm^{-1} (in hexane) or 1736 cm^{-1} (in LDPE). The same band for the solid additive was found at 1718 cm^{-1}. The polymer solution was obtained by heating LDPE with 0.5 wt% of the additive to 190 °C, extruding to films (ca. 50 μm) and quenching. Due to the absence of absorptions of LDPE in the range of 1740 cm^{-1} the films can be measured directly. The value for a_{solid} (additive bloomed to the surface) of ν(CO) at 1718 cm^{-1} was found to be about 1/3 higher than that for $a_{dissolved}$. Quantitative measurements allowed the determination of the fractions of dissolved and solid additive, respectively.

Coleman and coworkers (10.2.2) studied the important problem of self-association *vs* inter-association (additive to polymer) for the additive poly(2,6-di-*t*-butyl-4-vinylphenol) in poly(oxytetramethylene) (poly-THF). Polymeric additives are not volatile, exhibit low diffusion rates and are resistant to leaching. They are, on the other hand, usually incompatible with the polymer they are supposed to protect. They share this property with most polymer-polymer systems. This is a consequence of the extremely small free enthalpy of mixing due to the extremely small mixing entropy. There is a chance for a negative *free* mixing enthalpy left: a negative mixing enthalpy. (This is a simplified explanation.) Weak self-association (SA) and strong inter-association (IA, by hydrogen bonds) of a phenolic antioxidant with a polymer would therefore increase the solubility of the additive in the polymer.

The authors studied the ν(OH) range of four phenolic model compounds with increasing steric hindrance (none to completion) and made the following assignments (cm^{-1}):

Non-bonded ("free") phenolic OH	3645–3610 sh
Hydrogen-bonded dimers	ca. 3570
Chain-like associates	ca. 3350 br

In order to study interactions with ester carbonyl, the four phenolic model compounds were dissolved 1:4 (w/w) in ethyl *i*-butyrate (EIB); the latter is a fine model for the monomeric unit of poly(ethylmethacrylate). Spectra were measured at r.t. from 1800 cm^{-1} to 1650 cm^{-1}. ν(CO) for neat EIB is at 1738 cm^{-1}. Hydrogen bond formation shifts ν(CO) to the red end, the more the stronger the bond. The measurements revealed that sterically unhindered phenols caused the strongest shift (28 cm^{-1}); the one for a 2,6-di-*t*-butylphenol was 10 cm^{-1}. Apparently, the oxygen of the ester carbonyl successfully competes with the oxygen of the phenolic OH; in other words, IA was, in these cases, stronger than SA. This is a bit simplified. The authors calculated the equilibrium constants for these systems from the spectra. They found out that methyl in the 2,6-position decreases SA by about 1/3, compared with 4-ethylphenol. IA is, however, in both cases reduced by about the same factor. Thus, the ratio IA/SA is in both cases the same, namely 2.5. For a 2,6-di-*i*-propylphenol, SA was reduced to about 1/10, IA/SA was 4.4. For the 2,6-di-*t*-butylphenol, SA and IA were not detectable.

The step to polymers was done with poly(2,6-di-*i*-propyl-4-vinylphenol) (PPVP) as antioxidant and poly(oxytetramethylene) (POTM) as polymer to be protected. PPVP is soluble in POTM (and many other polymers) over the whole range of compositions. In its spectrum, $\nu(OH_{free})$ is at 3622 cm^{-1} and $\nu(OH_{ass})$ at about 3550 cm^{-1}. In the spectrum of a polymer blend with 5 wt% PPVP, $\nu(OH_{ass})$ appears at about 3450 cm^{-1}; this belongs to the inter-associate.

Ageing experiments were done at 150 °C in air. Pure POTM, after 30 min, already exhibited a weak ν(C=O) band in its spectrum. After 3 h, a band at 1737 cm^{-1} (oxidation product) was even stronger than ν(CH). With 0.04 wt% of PPVP, even after 10 h at 150 °C only a very weak ν(C=O) was visible.

These results show that solubility of antioxidants (in this case polymers being able to form chain-like associates via hydrogen bridges) is an important factor in polymer stabilisation.

In a recent publication, Coleman, Mock and Painter (10.2.2) showed that carefully designed copolymers (CP) of styrene (S) with relatively small amounts of 2,6-di-*i*-propyl-4-vinylphenol (PVP) are compatible with poly(oxyethylene) (POE) and poly(vinylmethylether) (PVME). The CP used for these experiments contained 7 mol.% PVP. An amount of 10 wt% of the CP in POE and 5 wt% in PVME stabilised the polyethers in a way that even after 4 h at 150 °C in air no ν(CO) was observable in the spectra.

3.5.1.4 *ATR* Investigations of Rubber Surfaces

The surfaces of unvulcanised or vulcanised rubber mixtures differ in their composition from that of the interior. This is partially due to release agents or processing aids like silicone oil, talc, soaps, and partially due to the fact that low-molecular additives in rubber tend to diffuse to the surface[3].

Attenuated total reflectance (*ATR*) is a rather sensitive method to study surfaces. The infrared beam, coming from the medium with the higher refractive index, at the interface between the reflecting crystal and the analyte leaves the former and enters the analyte for a few microns before it is definitively reflected (this description is simplified). On its way, the *IR* beam is partially absorbed by the analyte – a spectrum can be calculated. The usual *ATR* materials are Ge, Si and KRS-5 [Tl(Br,I)]. Ge, in this order, has the highest, KRS-5 the lowest refractive index *n*; the penetration increases with decreasing *n*.

Pasch and Disselhoff (10.2.6) described possibilities and limits of *ATR* for qualitative and (in some cases) quantitative analysis of rubber surfaces. In order to overcome the problem of the strongly absorbing carbon black at least partially they used Si as reflecting crystal. By this, samples with up to 30% carbon black can be investigated. (It has to be mentioned that most vulcanisates contain higher amounts of a strengthening filler, carbon black or amorphous SiO_2. In these cases, Ge would be preferable.)

Vulcanisates with known additives were subjected to *ATR*. Substituted *p*-phenylenediamines, zinc stearate (formed during vulcanisation from ZnO and stearic acid), benzothiazolesulfenamides and paraffins were observable.

Quantitative analysis of surface components was made possible by defined surface impregnations with different additives (50–1500 μg cm^{-2}).

3.5.1.5 Quantitative *IRS* Analysis of Additives

In a historical though important publication Spell and Eddy (10.2.2) showed that *IRS* is quite apt for a (somewhat time-consuming) quantitative determination of additives in polyethylene. Standard samples containing known amounts (1–500 ppm) of 2,6-di-*t*-butyl-4-methylphenol (BMP), 4,4-thio-*bis*(6-*t*-butyl-3-methylphenol) (SBMP) and 9-octadeceneamide (OAMD) as a slip agent were milled to 50 mesh in a Braun pulveriser. Then 5 g of a sample were shaken at r.t. with 25 cm^3 of CS_2 or CCl_4 in a stoppered bottle for about 1 h; this was sufficient to extract 98% of these additives. The CS_2 extractions were filtered in a 1-cm or – for low additive con-

3 They don't know, of course, where the surface is. They diffuse in all directions and finally find the surface.

centrations – in a 3.3-cm cell and scanned between 1280 cm^{-1} and 1075 cm^{-1}. The same thickness of pure solvent was in the reference beam. The analytical bands of BMP (1156 cm^{-1}) and SBMP (1183 cm^{-1}) had absorptivities of 17.8 m^2 mol^{-1} and 50.2 m^2 mol^{-1}, respectively.

For OAMD CCl_4 was used as a solvent. Amide-I at 1695 cm^{-1} (34.6 m^2 mol^{-1}) or ν_{free}(NH) at 3450 cm^{-1} (about 3.5 m^2 mol^{-1}) served as analytical bands. Minimum detectability was about 1 ppm, precision within 4 ppm.

When interferences were present the alkylphenol was extracted by *i*-octane. The extracts were measured in the *UV* between 250 nm and 350 nm in a 1-cm or 5-cm cell. A_{max} for BMP was measured at 285 nm, the absorptivity was 208 m^2 mol^{-1}; the data for SBMP were 286 nm and 714 m^2 mol^{-1}.

The quantitative analysis of mixtures from their spectra is principally possible for spectroscopically ideal systems. This prerequisite means that the values for $A_i(\nu)$ for each component *i* are additive; simply speaking, the spectra of the components in the system add up to the spectrum of the mixture (modified Lambert-Beer law).

The first research group to solve the problem of the simultaneous determination of additives from their *IRS* was quite recently Blanco et al. (10.2.6). In their first publication the authors investigated mixtures of different compositions containing four or five additives from analytically pure components in CCl_4. The *FTIR* spectra of CCl_4 solutions were recorded in 0.15 mm NaCl cuvettes in the range 4000–600 cm^{-1} at 4 cm^{-1} intervals. The CCl_4 spectrum was subtracted from each sample spectrum; the result was converted to its first derivative.

Only the range 1800–900 cm^{-1} contained analytically useful information; also, the range of maximum absorption of CCl_4 (1650–1500 cm^{-1}) had to be disregarded.

The results of numerous measurements were subjected to a matrix treatment, using partial least-squares regression for multivariate regression. The quantitative results were quite satisfactory; the errors of prediction were generally <2% and in the worst of cases <5%.

In a second publication the same research group developed a quantitative *FTIR* method for the determination of accelerators and antioxidants in extracts of vulcanised rubber. Since additives during vulcanisation decompose, at least to some fraction, this method again does not depend on characteristic bands of the components in the system but rather on absorption ranges containing the highest information on these. In this respect, the described method resembles closely the near-infrared (*NIR*) analysis of multicomponent mixtures (Hirschfeld, Stark, 10.1; Osborne, Fearn, 10.1; Siesler, 10.2.8), though with diffuse reflectance.

The two model vulcanisates, in addition to ZnO, stearic acid, carbon black and (in one case) oil, contained three accelerators/vulcanising agents and one antioxidant (amounts as parts per hundred parts of rubber):

Vulcanisate I	Cu dimethyldithiocarbamate	0.11
	Sulfur	0.34
	Tetramethylthiuramsulfide	1.0–3.5
	1,2-Dihydro-2,2,4-tributylquinoline	0.5–4.0
Vulcanisate II	Tetraethylthiuramdisulfide	0.5–2.5
	Tetramethylthiuramdisulfide	0.5–2.5
	N-Cyclohexyl-2-benzothiazole-sulfenamide	0.5–2.5
	1,2-Dihydro-2,2,4-tributylquinoline	0.5–2.5

The polymer bases were poly(styrene-*co*-butadiene) and poly(isoprene-*co*-butadiene), respectively. Extractions were done with 5 g vulcanisate/75 cm^3 CCl_4 in a Soxhlet for 6–8 h. The extracts were reduced to 5 cm^3 and measured in a cell 0.15 mm wide. Subsequently, CCl_4 absorptions were subtracted, and the spectra were normalised. Both absorbance and first derivative spectra were used for the investigations. It turned out that the latter brought better results, very likely because underground problems are minimised.

For quantitative evaluation six different *MIR* ranges were tested; best results were obtained with 1500–900 cm^{-1}. From system I, 23 vulcanisates with different compositions of additives were prepared, 12 of them were used as calibration set and the rest as validation set (to avoid "in-breeding"). The calibration technique used was partial least-squares regression, internal validation by cross validation, using the leave-out method (literature is given). The relative standard errors of prediction, with first derivatives, were 7–8%.

3.5.2 Pigments[4] and Fillers

3.5.2.1 Organic Pigments

3.5.2.1.1 Some Basic Facts

Few other functional classes in nature and in human chemistry posses so many different functional groups and substituents as organic pigments. The reason is that the human eye distinguishes minute hues and wants them in clothes, paints and other coloured objects – and the chemist tries to follow this by adding functional groups or substituents to the pigment molecule. The spectroscopist isn't too happy about this because it is close to impossible to unravel the superimposed partial spectra (with a sum of 60–70 bands) of partial structures, and to assign an analytical spectrum to a certain

4 The term *colorants* covers *dyes* and *pigments*. In this book, we deal predominantly with pigments.

pigment family. The richness in bands makes, on the other hand, pigment spectra highly specific. This is quite advantageous in quality control and computer-aided statement of identity. (Note: pigment spectra are not strictly reproducible, especially if a pigment exhibits polymorphism. This is the case with, e.g. pigment violet 19, pigment red 122, copper phthalocyanine. For the latter, see Knudsen and Shurvell; Pinzuti, both 10.2.3.)

In addition, pigments are frequently applied as mixtures, including inorganic fillers like $BaSO_4$. Simple tests of solubility may give hints on their presence (consecutive treatment):

Solvent	Dissolved pigments
Water and ammonia	Dyes
Ethanol and concentrated CH_3COOH	Spirit and basic dyes, pigments without $-SO_3H$
Ammonia and NH_3/ethanol	Acid and lake dyes
conc. CH_3COOH	Azo pigments
Residue	Phthalocyanines, quinacridones, dioxazines

The isolation of pigments from dispersions or processed materials is described elsewhere in this chapter. Thin-layer separation of pigments is treated in the literature, especially in the book of Scholl (10.1).

Isolated pigments are usually prepared with KBr for *IRS*. In favourable cases – printing inks and prints, pigmented binder on plane surface – *ATR* may be successful (Reichert, 10.2.3).

In the following paragraphs more recent literature on the *IR* analysis of pigments will be dealt with.

3.5.2.1.2 Phthalocyanines

Phthalocyanine itself (PcH_2), its copper derivative (PcCu) and the halogenated (Cl, Br) derivatives of PcCu have attracted considerable attention both in fundamental and in applied research. Pcs own high symmetries, PcCu, for example, has a centre of symmetry. The shade of Pcs between deep blue and green depends on the central atom, on the (halogen) substitution of the four 1,2-benzenic rings and not least on the crystal structure (amorphous content, polymorphous modification).

The first *IR* investigation of Pcs was published by Cannon and Sutherland (10.2.3). Later, Knudsen found no less than five (α–ε) modifications with (slightly) differing *IRS*; Shurvell and Pinzuti studied, in addition to PcH_2 itself, the *IRS* of PcCu (probably the β modification), $PcCl_4Cu$, $PcCl_{16}Cu$, $PcNa_2$, PcAlOH and PcMo. Table 3.21 collects some of the results of these authors together with our own ones; Fig. 3.10 shows the *MIRS* of the modifications of PcCu. According to Knudsen, the modifications of PcCu may be distinguished by the following bands (cm^{-1}):

γ	722	781		
α	722	781	missing	
β	730		1173	1101
δ	730		1168	1095
ε	730	785	775	

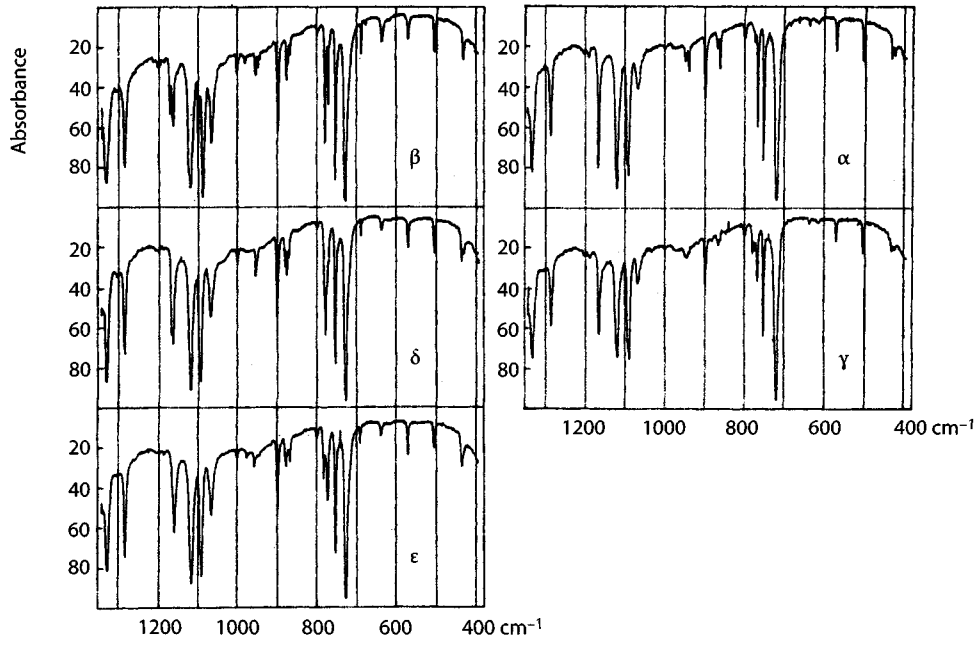


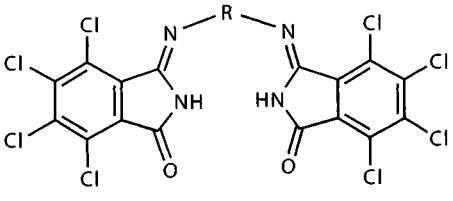
Fig. 3.10
IRS of the five polymorphous modifications of copper phthalocyanine (B.I. Knudsen, 10.2.3)

3.5.2.1.3 Increasing the Information on Structures: Combination of Spectroscopic Methods

FTIRS is certainly a powerful method for the *identification* of organic pigments, but it is not strong enough for complete *structure elucidation*. One of the reasons for this is that it is close to impossible to disentangle the superimposed partial spectra produced by a pigment structure; another is that we lose the intramolecular connections when applying this concept of spectral interpretation (we have no other choice – the coupling phenomena are too complicated).

Manukian and Lichti, a generation ago (10.2.3), gave a fine example for the combination of *IR*, mass, *NMR* and *VIS* spectrometries together with elementary analysis for a complete elucidation of the structure of the analyte. They anticipate that the family of the analytical pigment is known. This is either taken from company information or found by a characteristic *IR* band combination. Today, this is done by a similarity search with a pigment library. The task is now to identify the substituents and/or the bridges.

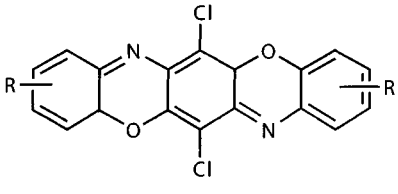
In their first example the authors investigate a dimer tetrachloroisoindolinone (TCI, Pigment Yellow 109) whose bridging group is unknown:



The *IRS* exhibited bands at 3330, 1742/1730, 1660, 798 and 720 cm^{-1}; the latter two gave a hint on three adjacent H atoms at a benzene ring.

If the two monomeric groups were directly bound the chemical formula $C_{16}H_2N_4O_2Cl_8$ would result. Elemental analysis differed considerably and suggested a hydrocarbon bridge. The (*EI*) mass spectrum exhibited series of *e/m*=372 (+2, 4, 6, 8) and 650 (+2, 4, 6, 8, 10, 12) with the typical intensity distribution of the Cl isotopes. These mass numbers had to be explained by monomer-C_7H_7 and dimer-C_7H_6. The ^{1}H-*NMR* spectrum (solvent: CF3COOD) revealed three aromatic (7.9 ppm, TMS=0) and three aliphatic (2.6 ppm) H atoms. Consequently, the bridge between the TCI units was 2,6-tolylene.

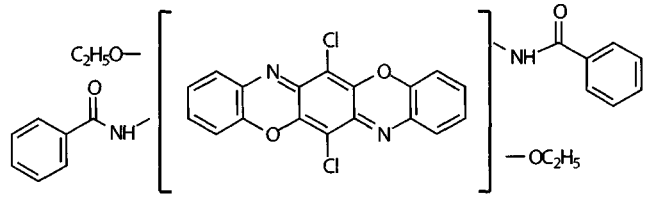
A more complicated problem was the identification of the substituents of Pigment Violet 35 (9,10-dichlorotriphenedioxazine) (DAZ) derivative:



The unsubstituted DAZ is red, the analyte is violet; consequently the structure of DAZ must be different. The *EIMS* revealed series at *m/z*=575/577/579 and 680/682/684; no higher masses were observed. With the results of an elemental analysis, a chemical formula $C_{36}H_{26}N_4O_6Cl_2$ was concluded. Since DAZ of this kind have equal substituents on the 1,2-benzo groups, each of these should have the formula $C_9H_{10}NO_2$.

The *EIMS* also exhibited a series with *m/z*=634/636/638 and 575/ 577/579. The former series can be explained by the elimination of C_2H_6O, i.e. ethanol, from the DAZ molecule. The latter series suggests the elimination of C7H5O (105), i.e. benzoyl.

The IRS shows bands of a secondary amide (3320 and 1660 cm^{-1}), of an aromatic-aliphatic ether at ca. 1190 cm^{-1}, and bands characterising the ring substitution at ca. 910, 867, 820, 773 and 700 cm^{-1}. The latter two bands characterise phenyl attached to C=O. Consequently, the substituents are C_2H_5O- and C_6H_5-CO-NH-, and the structure can be formulated like this:



(I may add that both 1,2/3,4- and 1,3-substitutions, due to the bands at 820 and 910 cm^{-1}, seem likely – adjacent H pair and isolated H.)

Admittedly, this publication is historical, and modern analytical methods would shorten the way to the correct results considerably. The systematic way of these analyses is, however, still exemplary.

3.5.2.2 Inorganic Pigments and Fillers

Substances containing carbon are called organic, and all of them are molecular. Molecules, charged or not, are held together by forces directed in space; we call these forces bonds. Inorganic substances do not contain carbon, they may form molecules, many of them do not (e.g. metal oxides and sulfides). In the latter case the forces are usually ionic and coulombic in nature (we should therefore not speak of ionic bonds). Ionic forces are distributed all over space, ideally in a spherical distribution (alkali halides). Detailed information on the *IRS* of inorganics are found in the books by Siebert, Nyquist and Kagel, and Nakamoto (10.1).

The spectroscopist treats inorganic molecules and molecular ions like organic ones, and excitation conditions and selection rules are the same for both categories. Since inorganics rarely form large structures, their molecules/ molecular ions usually possess simple symmetries. In a simplified way, we look at the following possibilities:

Form	Vibration	Activity	Remark
3-Atomic sticks	ν_s	*R*	Y-X-Y[a]
Examples: CO_2, CS_2	ν_{as}	*IR*	
	δ	*IR*	Doubly degenerate
HCN	ν_s	*IR, R*	Y-X-Z
	ν_{as}	*IR*	
	δ	*IR*	
Bent sticks	ν_s	*R*	Y-X-Y
Examples: H_2O, NO_2	ν_{as}	*IR, R*	
	δ	*IR, R*	
3-Tipped stars	ν_s	*R*	
Examples: CO_3^{2-}, NO_3^{2-}	ν_{as}	*IR*	Doubly degenerate
	δ	*IR*	Doubly degenerate
	γ	*IR*	Out of plane
Trilateral pyramids	ν_s	*R*	
Examples: PH_3, $AsCl_3$	ν_{as}	*IR, R*	Doubly degenerate
	δ_s	*IR*	
	δ_{as}	*IR, R*	Doubly degenerate
Tetrahedrons	ν_s	*R*	Central-symmetric
Examples: CCl_4, SiF_4,	ν_{as}	*IR*	Triply degenerate
SO_4^{2-}, PO_4^{3-}, CrO_4^{2-}	δ_{as}	*R*	Doubly degenerate
	δ_{as}	*IR*	Triply degenerate
Octahedrons			
Examples: SF_6, SiF_6^{2-},	ν_s	*R*	Central-symmetric
$PtCl_6^-$, centres of symmetry[a]	ν_s	*R*	Antisymmetric, degenerate
	ν_{as}	*IR*	Triply degenerate
	δ_s	*R*	Triply degenerate
			6 inactive vibrations

The superscript a denotes the Rule of mutual exclusion: *IR* active vibrations are Raman inactive and vice versa.

Interestingly, the *IRS* of a molecule or ion becomes simpler with increasing symmetry. Thus, the frequent XY_4 species possess nine FV; due to selection rules and degeneracy only two *IR* bands should be observable. Owing to a distortion of the equilibrium potential energy field by, e.g. cations a degeneration may be lifted. This is quite frequent in the case of sulfates; the band around 1100 cm^{-1} is then split into three components. In addition, weak to medium bands may show up where Raman active *FV* exist. This is due to a distortion of the symmetry of the molecular ion by, among other causes, the (metallic) cations and allows, e.g. the distinction between salts with the same anion. In the case of solids, the crystallographic elementary cell serves for the calculation of the *FV*; this is the reason why polymorphous modifications frequently can be distinguished by their *IRS*.

Both effects, together with the one of the cation on bond strengths (ν_{as} !) can be studied with XO_4^{2-} and CO_3^{2-} (Table 3.22).

Non-molecular inorganics generally do not exhibit bands in the *NIR* and *MIR* ("internal" vibrations; they absorb, however, strongly in the *FIR*. These lattice or "external" vibrations may be considered as hindered translations and rotations. The sum of internal and external vibrations is 3*N*.

A thorough investigation of the *IRS* of metal oxides was published by McDevitt and Baun (10.2.3); results which may be relevant for pigments and fillers are included in Table 3.23.

In most cases, by the way, the presence of an inorganic substance can be derived from the absence of CH bands ($\nu, \delta, \omega, \gamma$) in the spectrum.

3.5.2.3 Pigments and Other Components in Fine Art and Historical Objects

FTIRS including micro-techniques has brought considerable progress in the field of the analysis of painting materials. A major advantage is the small amount of material needed; this is a few mg for normal *FTIRS* and 50–10 µg for micro-techniques. Table 3.24 shows characteristic band combinations for pigments and pigment mixtures used in paints.

There is no standardised procedure for the separation of binder and fillers. In the case of pasty or liquid paint systems a series of possible solvents are applied, e.g. water, C_1-C_3 alcohols, acetone, esters, chloroform, white spirit; usually, at least one works. The same is true for fresh coatings. Separation is done by a centrifuge, the solution is evaporated in a Petri dish. Some of the concentrated solution is distributed with a glass rod onto a pre-warmed KBr disk; care has to be taken that the solution does not collect as a ring at the edge of the disk. After drying in vacuo, the binder is identified by its *IR* spectrum.

Most organic pigments dissolve in conc. H_2SO_4; carbonates (evolution of CO_2) and some oxides will dissolve too. Most of the inorganics (sulfates, silicates, others) will stay undissolved; separation can be done by a sintered frit.

Hardened (crosslinked) paints are boiled in dioxane or 1,3-dichlorobenzene or immersed in hexafluoro-2-propanol (1–2 h). If they will not dissolve, boiling alcoholic KOH is applied. The unsaponifiable is filtered off, dried and again treated with solvents. The residue is considered to be pigments and fillers; the *IRS* will give the answer. If the residue is white it is heated in a crucible; if it turns black it still contains organic (non-pigment) matter. The digestion and identification of hardened paints challenges the skill and imagination of an analyst.

3.5.3 Plasticisers

Plasticisers were the earliest additives to be analysed by *IRS*: they present little problems in preparation and have "beautiful spectra". This means that the spectra are characteristic, easy to interpret and appropriate for quantitative analysis. Two limitations have to be kept in mind: (1) the spectra usually reveal the acid component but the alcoholic one only with difficulties; (2) plasticisers are frequently applied as mixtures. When the plasticiser has been separated from the polymer it has to be established whether it is a mixture or not. This can usually be done by simple column chromatography.

Coming back to the problem of the alcoholic component of ester-type plasticisers: it is worthwhile to take a closer look at the spectra. The following ranges will permit conclusions on the kind of alkoxy group present (cm^{-1}):

- 3050–2700, ν(CH);
- 1395–1365, $\delta_s(CH_3)$;
- 1150–1000, ν(C-C);
- 1000–900, $\varrho(CH_3)$;
- 760–720, $\varrho(CH_2)n$;
- 650–400, δ(skeleton).

Generally speaking, low members of a homologous series can easily be distinguished, the higher ones are spectroscopically very similar. In the latter case, intensity considerations may be helpful.

The first (1958) spectral collection of plasticisers was probably my own (69 spectra) (10.1). Meise and Ostromow (10.2.4) described the *IR* identification of plasticisers in extracts of plastics and exhibited 39 *IRS*. The 3rd volume (of F. Scholl) of the 2nd edition of the Atlas (Hummel, Scholl, 1971) already presented the spectra of 313 *IRS* of plasticisers with all known compositions. This book also contains all desirable information on the extraction of plastics and their separation by chromatographic methods.

Table 3.1
Characteristic absorption band combinations/partial spectra of saturated aliphatic hydrocarbons

Vibrating group	Assignment	Range/cm^{-1}	Intensity	Remark
$-CH_3$	ν_{as}	2975–2950	m-s	sh, violet shift by adjacent aromat, N or O
	ν_s	2885–2865	m	Same
	δ_{as}	1465–1440	m	Same
	δ_s	1390–1370	m-s	Same
$-CH_2-$ open	ν_{as}	2940–2915	m-s	Same
	ν_s	2870–2840	m	Same
$(CH_2)_3$ cyclic	ν_{as}	3100–3070	m	
	ν_s	3040–2995	m	
$(CH_2)_4$ cyclic	ν_{as}	3000–2975	m	
	ν_s	2925–2875	m	
$(CH_2)_5$ cyclic	ν_{as}	2960–2950	m	
	ν_s	2870–2850	m	
-CH<	ν	2890–2880	w	
		2830+2770	m	In aldehydes, Fermi resonance
$-CH_3$	δ_{as}	1475–1465	m	High-frequency side of $\delta(CH_2)$
	δ_s	1390–1380	m-s	sh
$-C(CH_3)_2-$	δ_s	1385, 1370	m-s	Doublet by coupling, almost equal intensity, sh
$-C(CH_3)_3$	δ_s	1395, 1365	m, m-s	Doublet by coupling, sh
$-CH_2-$	δ	1470–1450	m	Overlaps with $\delta_{as}(CH_3)$
-CH<	δ	ca. 1340	w	Rarely identifiable
$(CH_2)_3$ cyclic	$\delta(CH_2)$	1420–1400	s	Varies with substitution
	ν_{as}(ring)	1365–1295	s	Varies with substitution
$(CH_2)_4$ cyclic	$\delta(CH_2)$	1450–1440	s	
	ν_{as}(ring)	1245–1220	m-s	Varies with substitution
$-CH(CH_3)_2$	ν(C-C)	1175–1165	m	No H on central C: 1190
$-C(CH_3)_2-$	$\varrho(CH_3)$	1150–1130	m	
	$\omega(CH_3)_2$?	840–790	w	
		495–490	w	
$C-CH_3$	$\varrho(CH_3)$	ca. 970	m	
$C-CH_2-CH_3$	$\varrho(CH_3)$	ca. 925	m	
$-CH(C_2H_5)_2$	δ(CCC)	510–505	w	
$-(CH_2)_n-$ n >3	$\varrho(CH_2)$	725–720	w-m	Splits in crystalline chains
$-(CH_2)_3-$		735–725	w-m	
$-(CH_2)_2-$		745–735	w	
$-CH_2-$		785–770	w	

Table 3.2
Characteristic absorption band combinations/partial spectra of alkyl-X groups with X # C

Vibrating group	Assignment	Range/cm^{-1}	Intensity	Remark
$R-O-CH_3$	$\nu_{as}(CH_3)$	2995–2955	m-s	
	$\nu_s(CH_3)$	2900–2865	s	
		2835–2815	s	Fermi resonance
	$\delta_{as}(CH_3)$	1470–1430	m	
	δ_s	1445–1430	s	
	ν_{as}(C-O-C)	1120–1100	vs	
$Ar-O-CH_3$	$\nu_{as}(CH_3)$	2840–2820	w-m	
	ν_{as}(Ar-O-C)	1260–1245	vs	

Table 3.2 Continue

Vibrating group	Assignment	Range/cm^{-1}	Intensity	Remark
R-N-CH_3	$\nu_s(CH_3)$	2805–2780	s	Fermi resonance?
	$\delta(CH_3)$	ca. 1460	m	Merges with $\delta(CH_2)$
R-N$(CH_3)_2$	$\nu(CH_3)$	2825–2810	s	Fermi resonance?
	$\nu(CH_3)$	2775–2765	vs	
Ar-N-CH_3	$\nu(CH_3)$	2820–2810	w-m	
Ar-N$(CH_3)_2$	$\nu(CH_3)$	2800	m	
P-CH_3	$\delta_s(CH_3)$	1320–1280	w-m	
	$\varrho(CH_3)$	960–830	m	
S-CH_3	$\delta_s(CH_3)$	1325–1300	w-m	
	$\varrho(CH_3)$	1030–950	m	
O-Si-CH_3	$\nu_{as}(CH_3)$	ca. 2960	s	In polysiloxanes
	$\nu_s(CH_3)$	ca. 2910	w	Same
	$\delta_s(CH_3)$	1260	vs	Same

Table 3.3
Characteristic absorption band combinations/partial spectra of alkynes and alkenes

Vibrating group	Assignment	Range/cm^{-1}	Intensity	Remark
-C≡CH	ν(≡ C-H)	3340–3300	m	
	ν(C≡C)	2130–2110	w-m	
-C≡C-		2210–2190	var	Inactive with equal substituents
R-C≡CH	δ(CC-H)	640–625	s	
	δ(HCC-C)	355–335	var	
R-vinyl	$\nu_{as}(=CH_2)$	ca. 3080	w-m	
	ν(=C-H)	ca. 3000	vw	Merges with $\nu_{as}(CH_3)$
	overtone	ca. 1820	weak	
	ν(C=C)	ca. 1640	m	
	$\delta_s(=CH_2)$	ca. 1415	vw	
	$\varrho(C=CH_2)$	ca. 1300	vw	
	ωE(HC=CH)	ca. 990	m	
	$\omega(=CH_2)$	ca. 910	s	
	ωZ(HC=CH)	ca. 630	w-m	
Z R-CH=CH-R′	ν_{as}(HC=CH)	3020–3000	m	
	ν(C=C)	1660–1650	w-m	
	γ_s(HC=CH)	ca. 690 (...750)	m, br	Frequency depends on substitution
E R-CH=CH-R′	ν_{as}(HC=CH)	ca. 3015	w	
	ν(C=C)	ca. 1660	var	Inactive with equal substituents
	γ_s(HC=CH)	ca. 970	s	
RR′>C=CH_2	$\nu_s(=CH_2)$	ca. 3080	m	
	overtone	ca. 1785	w-m	
	ν(C=C)	ca. 1650	s	
	$\gamma(C=CH_2)$	895–885	s	
RR′>C=CHR″	ν(C=CH)	ca. 3020	w	
	ν(C=C)	ca. 1675	vw	
	γ(C=CH)	840–790	m-s	Frequency depends on substitution
RR′C=CR″R‴	ν(C=C)	1675–1665	zero-w	Inactive with equal substituents

Table 3.4
Characteristic absorption band combinations/partial spectra of aromats

Vibrating group	Assignment	Range/cm^{-1}	Intensity	Remark
All aromats	ν(ring-H)	3080–3010	w-m	Several peaks[a]
	combination vibration	2000–1700	vw-w	Number and position depend on substitution
	ν(ring)	ca. 1600	w-s[b]	Sometimes split[c]
	ν(ring)	1510–1470	w-s[d]	Wavenumber depends on substituent[e]
	δ(ring-H)	1150–1000	var	Difficult to identify
Benzene derivatives (-substituted)				
mono-	γ(ring-H)[f]	750±15	s	Five adjacent H atoms
	γ(ring)	697±11	m-s	
	δ(ring	625–605	w-m	
1,2-di-	γ(ring-H)	750±10	vs	Four adjacent H atoms
	δ(ring)	550–500	w-m	
1,3-di-	γ(ring-H)	780±10	vs	Three adjacent H atoms
	γ(ring)	690±15	m-s	
1,4-di-	γ(ring-H)	815±20	vs	
1,2,3-tri-		780–760	s	Three adjacent H atoms
		745–705	var	
1,2,4-tri-		885–870	m	
		830–800	m-s	Two adjacent H atoms
1,3,5-tri-		865–810	s	Isolated H atoms
	δ(ring)	730–675	m	
1,2,3,4-tetra-	γ(ring-H)	810–800	m	Two adjacent H atoms
	δ(ring)	585–565	m-s	
1,2,3,5-tetra-	γ(ring-H)	850–840	m	
	δ(ring)	580–505	m-s	
1,2,4,5-tetra-	γ(ring-H)	ca. 805	w	
		870–855	m-s	
penta-		ca. 870	m	Single H atom
	δ(ring)	580–555	m-s	

a Decreasing in number with increase in substitution
b Strong in aromats with electronegative substituents and in aromatic heterocyclics, absent in benzene
c With substituents having double or triple bonds conjugated to the ring
d Strong with polar substituents
e ca. 1510/cm for electron donors and ca. 1470/cm for electron acceptors
f First order substituents (alkyl, other groups with no double or triple bond conjugated to the ring)

Table 3.5
Characteristic absorption band combinations/partial spectra of five-membered heterocyclics and their aromatically condensed derivatives

Vibrating group	Assignment	Range/cm^{-1}	Intensity	Remark
Pyrroles, furans, thiophenes	ν(ring)	ca. 1580		
		ca. 1490		
		ca. 1400		
Pyrroles	ν(NH)	3500–3400	var sh	In dilute solution
		3400–3000	s br	In condensed state
	ν(ring-H)	3100–3010	m	Several peaks
	ν(ring)	1580–1545	w-m	N substituted: 2 bands
		ca. 1470	w-m	
		1430–1390	vs	
	γ(ring)	ca. 480	m-s	Not greatly influenced by substit.

Table 3.5 Continue

Vibrating group	Assignment	Range/cm^{-1}	Intensity	Remark
1-substituted	γ(ring-H)	ca. 1070	s	Four adjacent H atoms
		1035–1015	m	
		ca. 925	m	
	δ(ring) ?	ca. 725	vs	
2-substituted	δ(NH)	ca. 1115	w-m	Three adjacent H atoms
	γ(ring-H)	1105–1070	m-s	
		ca. 1030	m-s	
		ca. 925	w	
		ca. 880	w-m	
1,2-disubstituted		ca. 1090	m	
		1065–1050	var	
1,2,5-trisubstituted		ca. 1035	m	Two adjacent H atoms
		980–965	w	
	δ(ring)	ca. 755	vs	
1,3,4-trisubstituted	γ(ring-H)	ca. 1055	s	Isolated H atom
		ca. 930	m	
Indoles	ν(ring)	1630–1615	m	
		1600–1575	m	
		1565–1540	var	
		1520–1470	m	
Furans	ν(ring-H)	3180–3000	m	
	ν(ring)	1610–1560	m-s	
		1520–1470	m-s	
		1400–1390	m-s	
	δ(ring)	595–515	s	
2-substituted	δ(ring-H)	1085–1070	m	
	γ(ring-H)	885–880	w-m	
3-substituted	δ(ring-H)	1025–1000	vs	
	γ(ring-H)	ca. 875	s	
	δ(ring)	790–720	s	Usually two bands
2,5-distituted	ν(ring) ?	1255–1225	w-m	
		1165–1140	w-m	
	δ(ring-H)	990–960	m	
Thiophenes	ν(ring-H)	3120–3000	m	
	ν(ring)	1555–1480	var	
		1445–1390	var	
		1375–1340	var	
		1240–1195	var	
	γ(ring)	530–450	var	
2-substituted	ν(ring)	1535–1515	var	
		1455–1430	var	
		1360–1345	var	
	γ(ring)	470–430	var	
3-substituted		540–515	m	Sometimes only one band present
		500–465	var	
Imidazoles	ν(ring)	1660–1610	var	
		1605–1585	w-m	
		1560–1520	s	
	γ(ring)	670–625	s	
4-substituted		630–605	s	
		360–325	m	
4,5-disubstituted		645–610	m-s	
1,4,5-trisubstituted		660–640	m-s	
		420–390	w-m	

Table 3.5 Continue

Vibrating group	Assignment	Range/cm^{-1}	Intensity	Remark
Benzimidazoles	ν(ring)	1560–1520	m	In addition to the benz-bands
Oxazoles	ν(ring)	1585–1555	m	
1,2,4-Oxadiazoles		1590–1560	m-s	1,2,5-Oxadiazoles (furazanes) have
		1470–1430	m-s	similar ν (ring)
		1390–1360	m-s	
	δ(ring-H)	1070–1050	m	
		915–885	m-s	
	γ(ring) ?	750–710		
Pyrazoles				
N-alkyl substituted	δ(ring-H)	ca. 1090	m-s	
	γ(ring-H)	ca. 755	m-s	
3-alkyl substituted	δ(ring-H)?	ca. 935	s	
	γ(ring-H)	ca. 770	s	
4-alkyl substituted	δ(ring-H)?	1010–1000	s	
	γ(ring-H)	ca. 860	s	
		ca. 805	s	

Table 3.6
Characteristic absorption band combinations/partial spectra of six-membered aromatic heterocyclics

Vibrating group	Assignment	Range/cm^{-1}	Intensity	Remark
Pyridines	ν(ring-H)	3090–3000	w-m	Several bands
	ν(ring)	1615–1575	m-s	
		1575–1555	m	Intensity depends on substitution
		1500–1465	var	
		1430–1410	m	
	δ(ring-H)	1055–990	m-s	
	δ(ring)	635–600	m-s	Not with *p*-substitution
2-substituted	ν(ring)	1300–1270	w-m	
		ca. 1150	w-m	
	δ(ring-H)	1055–1040	w-m	
	γ(ring-H)	770–740	vs	Four adjacent H
		740–720	m	
	γ(ring)	410–385	m	
3-substituted	ν(ring)	1200–1180	var	
		ca. 1125	w	
		ca. 1105	w	
	δ(ring-H)	1045–1030	m	
		920–890	w	
	γ(ring-H)	820–770	m-s	Three adjacent H
		730–690	m-s	
	δ(ring)	630–615	w	
	γ(ring)	410–385	m	
4-substituted	ν(ring)	ca. 1600	vs	Intensity is characteristic
		1230–1210	var	
	δ(ring-H)	ca. 1070	s	
	γ(ring-H)	830–790	s	Two adjacent H
		730–720	m	
2,3-disubstituted	γ(ring-H)	815–785	m	Two adjacent H
		740–690	m-s	
2,5-disubstituted		825–810	m-s	Two adjacent H
		735–725	m-s	

Table 3.6 Continue

Vibrating group	Assignment	Range/cm^{-1}	Intensity	Remark
2,6-disubstituted		815–770	m-s	Three adjacent H
		750–720	m-s	
3,4-disubstituted		860–840	m	Two adjacent H
Pyrimidines	ν(ring-H)	3100–3010	m	Several bands
(1,3-diazabenzenes)	ν(ring)	1640–1620	w	
		1580–1520	m-s	
		1410–1375	var	
	δ(ring-H)	1000–960	m-s	
	γ(ring-H)	825–775	m-s	
2-pyrimid.	δ(ring)	650–630	m-s	
4-pyrimid.		685–660	var	
Pyrazines	ν(ring-H)	3080–2980	w	Several bands
(1,4-diazabenzenes)	ν(ring)	1600–1575	var	Not pyrazine itself
		ca. 1500	w-m	
		1420–1370	s	
sym-Triazines	ν(ring-H)	3100–3000	m	
	ν(ring)	1580–1520	vs	At least one band
	γ(ring) ?	860–775	w	At least one band
Melamines	ν(NH_2)	3500–3100	m	Several bands
	δ(NH_2)	1680–1640	m	
	ν(ring)	ca. 1550	s	
		1450–1350	var	Several bands
	γ(ring) ?	825–800	m	Only one of these present
		795–750	m	

Table 3.7
Characteristic absorption band combinations/partial spectra of -C≡N, >C=N, -N=N-, -N=C=N- and -N=C=O compounds

Vibrating group	Assignment	Range/cm^{-1}	Intensity	Remark
Nitriles				
alkyl-	ν(CN)	2260–2230	m	
-CH_2-CN	δ(CH_2CN)	580–555	w-m	CN trans to C
		560–525	w-m	CN trans to H
>CH-CN		580–550	var	Depends on conformation
		545–530	var	
>CR-CN		ca. 595	m	Depends on conformation
		ca. 575	m	
conjugated with C=C	ν(CN)	2250–2200	m-s	
aryl-	ν(CN)	2240–2220	m-s	
	δ(Ar-CN/γ(ring)	580–540	s	
	δ(Ar-CN)	430–380	m	
Imines	$\nu(NH)_{free}$	3400–3300	var sh	Dilute solution
	$\nu(NH)_{ass.}$	3400–3100	s br	Condensed state
R_2C=NH	ν(C=N)	1650–1640	s sh	
ArCR=NH		1635–1620	m sh	
R_2C=NR		1665–1645	w-m sh	
ArCH=NAr		1645–1605	var	Often 2 bands
Oximes	$\nu(OH)_{free}$	3650–3500	m sh	Dilute solution
	$\nu(OH)_{ass.}$	3450–3100	m br	Cond. state, several bands
aliphatic	ν(C=N)	1680–1660	m	

Table 3.7 Continue

Vibrating group	Assignment	Range/cm^{-1}	Intensity	Remark
conj.-olefin. and aromatic		1650–1620	m	
	δ(OH)	1500–1400	m	br, 2 bands ?
	ν(N-O)	960–930	s	
Azo compounds	ν(N=N)	1575–1500	var	Inactive or weak
alkyl		1575–1555	w	
Z-aryl		ca. 1510	m	
E-aryl		1440–1410	w	Mixed vibration
Carbodiimides, aromatic				
	ν_{as}(N=C=N)	ca. 2170	vs	Broader than ring vibrations
Isocyanates				
aliphatic	ν_{as}(N=C=O)	ca. 2275	vs	
aromatic		ca. 2265	vs	
	ν_{s}(N=C=O)	1460–1340	w	

Table 3.8
Characteristic absorption band combinations/partial spectra of amines

Vibrating group	Assignment	Range/cm^{-1}	Intensity	Remark
Amines, aliph.				
primary	$\nu_{as}(NH_2)$	ca. 3330	m sh	Crystalline
		ca. 3250	w-m br	Noncryst. phase
	$\nu_{s}(NH_2)$	ca. 3170	w-m br	Noncryst. phase
	$\nu_{as}(NH_2)$	3370–3330	w-m br	Liquid
	$\nu_{s}(NH_2)$	3290–3270	w-m br	State
	$\delta(NH_2)$	ca. 1600	w-m br	Condensed state
	ν(C-N)	1140–1080	w-m	Depends on substitution
		1090–1020	w-m	
	$\gamma(NH_2)$	940–800	m-s vbr	Max. ca. 850
		950–870	m-s sh	Cryst. phase, multiply split
secondary	ν(NH)	ca. 3300	w br	Liquid
	δ(NH)	ca. 1650	vvw	Liquid
	ν(C-N)	1145–1130	m	$-CH_2-NH-CH_2-$
		1190–1170	m	$-CH_2-NH-CH<$
	γ(NH)	750–710	m-s	Liquid
tertiary	ν(C-N)	1210–1150	m	$N(-CH_2-)_3$
		1100–1030	m	Same
		ca. 1040	m-s	$-CH_2-N(CH_3)_2$
Aromatic				
primary	$\nu_{as}(NH_2)$	3470–3385	m-s sh	Crystalline phase
	$\nu_{s}(NH_2)$	3380–3325	m-s sh	
	$\nu_{as}(NH_2)$	3300–3280	m br	Non-crystalline phase
		3210–3180	w-m	
	$\nu_{as}(NH_2)$	ca. 3430	w	
	$\nu_{s}(NH_2)$	ca. 3350	w-m	
		ca. 3200	w	
	$\delta(NH_2)$	ca. 1630	m-s	
	ν(Ar-N) ?	ca. 1280	m-s br	Possibly $\omega(NH_2)$
	$\gamma(NH_2)$	800–600	m, vvbr	

Table 3.8 Continue

Vibrating group	Assignment	Range/cm^{-1}	Intensity	Remark
secondary				
Ar-NH-R	ν(NH)	ca. 3400	m-s br	Liquid
	δ(NH) ?	1330–1320	s	Liquid
		ca. 1260	s	
Ar-NH-Ar	ν(NH)	ca. 3400 (doublet)	m-s	Solid, crystal splitting
	δ(NH) ?	ca. 1310	s	
	γ(NH)	430–400	vbr	
tertiary				
Ar-NR_2	ν(Ar-N) ?	ca. 1300		

Table 3.9
Characteristic absorption band combinations/partial spectra of OH compounds and ethers

Vibrating group	Assignment	Range/cm^{-1}	Intensity	Remark
Alcohols	$\nu(OH)_{free}$	3670–3580	m sh	Dilute solution
	$\nu(OH)_{ass.}$	ca. 3300	m br	Solid state
		ca. 3330	m-s br	Liquid
	$\gamma(OH)_{ass.}$	ca. 650	w-m br	Liquid
primary	ν(C-O)	1080–1050	s	Several bands, strongest 1070
secondary		1160–1100	m-s	Several bands
tertiary		ca. 1200	m-s	
Phenols	$\nu(OH)_{free}$	3620–3590	m sh	Dilute solution
		ca. 3650	m-s sh	Sterically hindered
	$\nu(OH)_{ass.}$	3400–3300	vbr	
	δ(OH)	ca. 1350	s	
	ν(Ar-O)	ca. 1250	s br	Assoc. OH
		ca. 1240	s sh	Free OH
Ethers, aliph.				
R-O-CH_3	$\nu_{as}(CH_3)$	3000–2970	w-m	
	$\delta_s(CH_3)$	ca. 1450	w-m	Together w. $\delta(CH_2)$
-O-CH_2-O-	ν(CH)	ca. 2780	m	
R-O-R	ν_{as}(C-O-C)	ca. 1110	vs br	Splits in cryst. ethers
vinyl ethers		1225–1200	s	
epoxides	ν(ring)	1260–1230	m-s	
monosubst.	δ(ring)	ca. 850	m-s	
trisubst.		770–750	m	
oxolane and oxane deriv.	ν_{as}(ring)	1090–1070	vs	Tetrahydrofurane Tetrahydropyrane
peroxides	ν(C-O)	1150–1030	m	
	ν(O-O)	900–830	vw	May be inactive
aliphatic-aromatic	ν_{as}(ring-O-C)	1270–1230	vs	Donors shift red
		ca. 1250		
aromatic	ν_{as}(ring-O-ring)	ca. 1230	vs	
peroxides	ν(C-O)	ca. 1000	m	

Table 3.10
Characteristic absorption band combinations/partial spectra of CHO-carbonyl compounds: ketones and quinones

Vibrating group	Assignment	Range/cm^{-1}	Intensity	Remark
Ketones, aliph.				
sat., open	2x ν(C=O)	ca. 3410	vw	First overtone
	ν(C=O)	ca. 1715	vs	
	δ(CH_2CO)	ca. 1415	w-m	
	δ_s(CH_3CO)	ca. 1360	m-s	Acetyl band
	δ(C-CO)	530–510	w	Also with aldehydes
cyclic				
cyclobutanone	ν(C=O)	1790–1765	vs	Derivatives
cyclopentanone		1750–1740	vs	Derivatives
cyclohexanone		ca. 1715	vs	Derivatives
conj. unsatur.		ca. 1690	vs	
Z-config.	ν(C=C)	ca. 1620	s	
E-config.	ν(C=O)	ca. 1675	vs	
	ν(C=C)	ca. 1635	s	
Aliph.-aromatic				
Ar-CO-CH_3	ν_{as}(CH_3)	ca. 3000	vw-w	
	ν(C=O)	1700–1680	vs	
	δ_s(CH_3)	ca. 1360	s	Acetyl band
	δ(ring-CO-C)	600–580	s	
	ν(ring-C)	1275–1250	s	
Ar-CO-CH_2-R	ν(C=O)	ca. 1690	vs	
Ar-CO-Ar	2x ν(C=O)	ca. 3280	vw	First overtone
	ν(C=O)	1670–1650	vs	
	ν(ring-C)	ca. 1275	s	
	δ(C-CO-C)	ca. 640	s	
***p*-Quinones**	ν_{as}(C=O)	1680–1655	vs	Sometimes split
p-benzoquinones	γ(CH)	915–900	w-m	
monosubst.		865–825	m-s	
2,3-disubst.		860–800	s	
2,5/2,6-disub.		920–895	s	
anthraquinones (no OH or NH)	ν_{as}(C=O)	1680–1650	vs	
anthraquin.-NH_2	ν_{as}(NH_2)	ca. 3410	m	
	ν_s(NH_2)	ca. 3300	m	
	ν_{as}(C=O)	ca. 1600	s	Multiply split
anthraquin.-OH	ν(OH)	ca. 3450	vw vbr	
		ca. 1630	s	Split

Table 3.11
Characteristic absorption band combinations/partial spectra of CHO-carbonyl compounds: aldehydes, carboxylic acids, carboxylates

Vibrating group	Assignment	Range/cm^{-1}	Intensity	Remark
Aliphatic-CHO				
saturated	2x ν(C=O)	ca. 3430	vw sh	First overtone
	ν(C-H)	2845–2820	m	Fermi resonance
		2735–2720	m	Broader than ν(CH_2)
	ν(C=O)	1730–1720	vs	
	δ(CH_2-CO)	ca. 1410	w	

Table 3.11 Contunie

Vibrating group	Assignment	Range/cm^{-1}	Intensity	Remark
conjug.-unsat.	2× ν(C=O)	3370–3320	vw sh	First overtone
	ν(C-H)	2845–2780	w	Fermi resonance
		2755–2700	vw-w	
	ν(C=O)	1695–1680	vs	
	ν(C=C)	1640–1615	s sh	
Aromatic-CHO	ν(C-H)	2865–2820	w	Additl. weak bands in this range
		2760–2720	w sh	
	ν(C=O)	1705–1695	vs	
	ν(ring-C)	ca. 1200	m-s sh	Not always present
Aliphatic-COOH	All bands of the 8-memb. ring of dimers are broad			
saturated	$\nu(OH)_{free}$	3580–3500	m	Dilute solution
	$\nu(OH)_{ass.}$	3400–2500	s vbr	Overlappg. of several H-bond species
		2700–2500	w-m br	Two bds.of defin.associates
	ν(C=O)	ca. 1710	vs	Medium broad
	ν(CO)δ(OH)	ca. 1410	w-m	Combination band
	γ(O-H...O)	ca. 950	m br	
conj.unsatur.	ν(C=O)	1705–1690	vs	*E*-configuration
	ν(C=C)	1650–1635	s	Intensif. by conj.
Aromatic-COOH	$\nu(OH)_{ass.}$	3150–2500	m br	Mult. overlapping bands
		ca. 2650	m br	Defined
		2550–2520	m br	Associates
	ν(C=O)	1690–1680	vst	
	ν(CO)δ(OH)	1420–1400	m-s	Combination band
	γ(O-H...O)	940–905	m-s br	
Carboxylates				
aliphatic -CO_2^-	$\nu_{as}(CO_2)$	1560–1520	vs	Sometimes split
	$\nu_s(CO_2)$	ca. 1425	w-m br	Sometimes split
	$\delta(CO_2)$	ca. 700	w-m	Red flank of $\varrho(CH_2)_n$
aromatic -CO_2^-	$\nu_{as}(CO_2)$	1565–1530	vs	
	$\nu_s(CO_2)$	1390–1360	s-vs	

Table 3.12
Characteristic absorption band combinations/partial spectra of CHO-carbonyl compounds: esters, anhydrides

Vibrating group	Assignment	Range/cm^{-1}	Intensity	Remark
Aliphatic esters				
saturated	ν(H-C=O)	ca. 2880	w	Formates
	ν(C=O)	ca. 1740	vs	
	$\delta(CH_2\text{-}C{=}O)$	ca. 1420	vw-w	
	$\delta_s(CH_3\text{-}C{=}O)$	ca. 1375	s	Acetyl band
	$\nu_{as}(C\text{-}O\text{-}CO)$	ca. 1245	s	Acetates
		ca. 1200	s	Butyrates
		ca. 1190	s	Formates
		ca. 1190	s	Propionates
		ca. 1175	s	Stearates, adipates
		ca. 1170	s	Sebacates
		ca. 1165	s	Fatty glycerates
	δ(C-O-CO)	ca. 635	w-m	Acetates
		ca. 605	w-m	Acetates

Table 3.12 Continue

Vibrating group	Assignment	Range/cm^{-1}	Intensity	Remark
carbonates aliphatic	ν(C=O)	1755–1745	vs	
	ν_{as}(O-CO-O)	1280–1260	vs	Higher carbonates: 1260
	δ(O-CO-O)	800–790	m	
R-O-CO-O-Ar	ν(C=O)	1790–1755	vs	
Ar-O-CO-O-Ar	ν(C=O)	ca. 1775	s	
	ν_{as}(O-CO-O)	ca. 1230	vs	Multiply split
		1180–1160	s	Split
	δ(O-CO-O)	ca. 790	m	
lactones, aliph.	ν(C=O)	1840–1815	vs	Four-membered ring
		1780–1765	vs	Five-membered ring
	ν_{as}(ring)	1175–1170	s-vs	
		1060–1020	s	
Unsaturated aliphatic esters				
conjug. to C=O	ν(C=O)	1730–1720	vst	
	ν(C=C)	1660–1630	m-s	Intensif. by conjugation
Z-vinylene	ν(=C-H)	ca. 3010	m sh	Isolated
fatty esters	ν(C=C)	ca. 1655	w br	
	γ(HC=CH)	ca. 730	m br	
		below ρ(CH_2) of long chains		
E-vinylene	ν(=C-H)	ca. 3010	w	Shoulder
fatty esters	ν(C=C)	1660–1650	vw	
	γ(HC=CH)	ca. 970	m	Isolated
		ca. 985	w-m	-CH=CH-CH=CH-
		ca. 995	m-s	Three conjugated -CH=CH-
Esters of aromatic carboxylic acids with alcohols				
benzoates	ν(C=O)	1720	vs	
	ν(ring)	1600/1580	w-m	Double band
	ν_{as}(C-O-CO)	1280–1260	s-vs	Broader than neighbour
		ca. 1110	m-s	ring vibrations
o-phthalates	ν(C=O)	1728	vs	All bands are rather constant and
	ν(ring)	1600/1580	w	broader than neighb. ring vibr.
	ν_{as}(C-O-CO)	1287	s-vs	
		1123	m	
		1074	m	
isophthalates	ν(C=O)	ca. 1733	vs	
	ν(ring)	1610	w-m sh	
		ca. 1300	m-s br	Fused with 1260
	ν_{as}(C-O-CO)	1235–1230	s br	
		1095–1075	m-s	Frequently double band
	γ(ring-H)	730	s sh	
terephthalates	ν(C=O)	1720	s-vs	
	ν(ring)	ca. 1575	w-m	
		ca. 1410	s	
	ν_{as}(C-O-CO)	1265/1245	vs	Fused double band
		1120/1100	vs	Fused double band
	γ(ring-H)	725	s	
	γ(ring)	505	w-m	
trimellitates	ν(C=O)	1730	vs	
	ν(ring)	1600/1570	w-m	Twin bands
	ν_{as}(C-O-CO)	1280	s	Fused with 1240
		1240	vs	
		1115	s	

Table 3.12 Continue

Vibrating group	Assignment	Range/cm^{-1}	Intensity	Remark
	δ(ring-H)	1065	m-s	
	γ(ring-H)	750		
Esters of aromatic acids with phenols	ν(C=O)	1735–1730	vs	
	ν_{as}(C-O-CO)	1260–1255	s	
		1200–1195	s	
		1065–1050	vs	
Carboxylic anhydrides				
aliphatic open	ν_{as}(CO-O-CO)	1827–1810	s	Coupled ν(C=O)
	ν_{s}(CO-O-CO)	1756–1743	m-s	Weak in *trans*-conformation
	δ_{s}(CH_3-CO)	1770	m	In H_3C-CO-O-CO-R
	ν_{as}(CO-O-CO)	1043–1031	vs	1125 in acetic anhydride
	ν_{s}(CO-O-CO)	945–910	m br	Only in higher alkyl anhydrides
aliphatic cyclic	ν_{as}(CO-O-CO)	ca. 1810	m-s	Succinic: 1863 w
	ν_{s}(CO-O-CO)	ca. 1755	vs	Succinic: 1784 vs
	ν(ring)	1235–1210	m br	
		ca. 1090	s br	Succinic: 1060
		935–920	m-s br	
	δ(ring)	665–650	w-m br	
Ar-CO-O-CO-Ar	ν_{as}(CO-O-CO)	ca. 1780	s-vs	Coupled ν(C=O)
	ν_{s}(CO-O-CO)	ca. 1715	m-s	
	ν_{as}(C-O-C)	ca. 1210	vs	

Table 3.13
Characteristic absorption band combinations/partial spectra of CHNO-carbonyl compounds: amides and lactams

Vibrating group	Assignment	Range/cm^{-1}	Intensity	Remark
Aliphatic amides R-CO-NX-R				
primary -CO-NH_2	$\nu_{as}(NH_2)_{free}$	3540–3480	m-s sh	Dilute solution
	$\nu_{s}(NH_2)_{free}$	3420–3380	m-s sh	
	$\nu_{as}(NH_2)_{ass.}$	3370–3330	m-s br	Solid state
	$\nu_{s}(NH_2)_{ass.}$	3210–3180	m-s br	
	$\nu(C{=}O)_{ass.}$	1680–1660	vs	Amide band I
		1650–1620	w-m br	Fused with ν(CO)
	ν(C-N)	1420–1400	m-s br	Amide band III
	$\gamma(NH_2)_{ass.}$	700–600	m vbr	
secondary -CO-NH-	$\nu(NH)_{free}$	3460–3420	m-s sh	Dilute solution
	$\nu(NH)_{ass.}$	3350–3290	m	*trans* conformation
		3100–3070	w	2×amide II
	$\nu(C{=}O)_{ass.}$	1670–1640	vs	Amide band I
	δ(NH)ν(CO)	1570–1540	m-s	Combin., amide II
	ν(C-N)	1300–1240	w-m	*trans*, amide III
		1350–1310	w-m	*cis*, amide III
	δ(NH...OC)	750–660	m vbr	Amide V
		630–600	w	Amide IV
teriary -CO-N<	ν(C=O)	1660–1630	vs	Amide I
		ca. 1675	vs	Dialkylformamides
		1650–1640	vs	Dialkylamides
	δ_{s}(CH_3-CO)	1355–1350	w-m	Acetyl band
lactams				
3-propane-	$\nu(NH)_{ass.}$	ca. 3260	m	*cis* conformation
	ν(C=O)	ca. 1750	vs	

Table 3.13 Continue

Vibrating group	Assignment	Range/cm^{-1}	Intensity	Remark
4-butane-[a]	$\nu(NH)_{ass.}$	ca. 3250	m br	*cis* conformation
	$\nu(C{=}O)$	ca. 1690	vs	
	$\nu(C\text{-}N)$	1300–1285	m	
	δ(ring)	ca. 1000	w sh	
	$\delta(NH\ldots OC)$	850–600	m vbr	
5-pentane-[b]	$\nu(NH)_{ass.}$	3225	m br	*cis* conformation
	$\nu(C{=}O)$	1670	vs	
	$\nu(C\text{-}N)$	ca. 1310	m	
		1120	w-m	
	δ(ring)	990	w	
	$\delta(NH\ldots OC)$	900–700	m vbr	
ε-capro-	$\nu(NH)_{ass.}$	3215	m br	*cis* conformation
	$\nu(CO)+\delta(NH)$	3090	w-m	Combination vibration

a 2-pyrrolidone
b 2-piperidone

Table 3.14
Characteristic absorption band combinations/partial spectra of CHNO-carbonyl compounds: ureas

Vibrating group	Assignment	Range/cm^{-1}	Intensity	Remark
Urea and defined urea derivatives				
urea	$\nu_{as}(NH_2)_{ass.}$	3435	vs br	
	$\nu_{s}(NH_2)_{ass.}$	3330	s-vs br	
	$\nu(C{=}O)$	1673	s-vs	
		1630–1590	vs	Merged doublet
	$\delta(NH_2)\nu(C\text{-}N)$	1458	s	Coupled vibration
	$\nu(C\text{-}N)$	1147	m-s	
	$\delta(NH\ldots OC)$	700–300	m-s vbr	
ethyl-	$\nu_{as}(NH_2)_{ass.}$	3425	s br	
	$\nu_{s}(NH_2)_{ass.}$	3355	s br	
	$\nu(NH)_{ass.}$	3215	m br	
	$\nu(C{=}O)$	1661	vs	Amide I
		1598	vs sh	
	$\delta(NH)\nu(C\text{-}N)$	1565	s br	Amide II
	$\nu(C\text{-}N)$	1160	s sh	
	$\delta(NH\ldots OC)$	605	s br	
1,3-dimethyl-	$\nu(NH)_{ass.}$	3345	s-vs br	
	$\nu(CO)+\delta(NH)$	3175	m	Combination vibration
	$\nu(C{=}O)$	1630	vs	
	$\delta(NH)\nu(C\text{-}N)$	1585	s	Amide II, merged w. amide I
	$\nu(C\text{-}N)$	1270	s br	
		1175	m sh	
	$\delta(NH\ldots OC)$	675	s br	
1,3-diethyl-	$\nu(NH)_{ass.}$	3340	s br	
	$\nu(CO)+\delta(NH)$	3140	w-m br	Combinataion vibration
	$\nu(C{=}O)$	1627	vs	Amide I
	$\delta(NH)\nu(C\text{-}N)$	1585	s	Amide II, merged w. amide I
	$\nu(C\text{-}N)$	1260	s br	
		1158	m sh	
	$\delta(NH\ldots OC)$	660	s br	
1,3-diaryl-	$\nu(C{=}O)$	ca. 1640	s	Amide I

Table 3.15
Characteristic absorption band combinations/partial spectra of CHNO-carbonyl compounds: isocyanates, urethanes and imides

Vibrating group	Assignment	Range/cm^{-1}	Intensity	Remark
-N=C=O				
aliphatic		3680–3630	w-m	Combination vibration
	ν_{as}(NCO)	2270–2240	vs	
	ν_{s}(NCO)	1375–1350	m	
	δ(NCO)	ca. 585 (peak)	m-s br	Fused band on the violet side
aromatic		3690	w	Combination vibration
	ν_{as}(NCO)	ca. 2270	vs	
	ν(ring)	ca. 1525	s	Intensified by coupling with NCO
	δ(NCO)	570–560	m-s	Neighbouring ring vibrations
H_2N-CO-O-	ν(CO)δ(NH_2)	1630–1620	vs	"Amide" I
-NH-CO-O-				
aliphatic	ν(NH)	ca. 3310	s sh	
	ν(C=O)	ca. 1690	vs	"Amide" I
	ν(C-N)δ(NH)	ca. 1535	s	"Amide" II
	ν_{as}(C-O-CO)	ca. 1260	s	
	δ(NH...OC)	ca. 655	m br	
Ar-NH-CO-O-R	ν(NH)	ca. 3300	m-s sh	Broad shoulder on the violet side
	ν(C=O)	ca. 1695	vs	"Amide" I
		ca. 1540	s	"Amide" II
	ν_{as}(C-O-CO)	ca. 1240	s-vs	
	ν_{s}(C-O-CO)	ca. 1070	s	
>N-CO-O-	ν(C=O)	1690–1680	vs	"Amide" I
R-CO-NH-CO-R	ν(NH)	3280–3200	m	*trans-trans*[a]
		3245–3190	m-s	*cis-trans*
	ν(C=O)	ca. 1735	vs	*trans-trans*
		ca. 1700	vs	*cis-trans*
	Unknown	ca. 1650	m	
		ca. 1630	m	
		1510–1500	s	*trans-trans*
		1235–1165	m	
	δ(NH...OC)	835–815	m	*cis-trans*
	δ(NH...OC)	740–730	m br	*trans-trans*
Succinimides	ν(NH)	ca. 3150	m br	
	ν_{s}(C=O)	ca. 1775	m	$_{s}$ and $_{as}$ relate to
	ν_{as}(C=O)	ca. 1700	vs	coupled C=O vibration
	ν(ring)	ca. 1190	s	
Aspartimides	ν_{s}(C=O)	ca. 1780	w-m	
	ν_{as}(C=O)	ca. 1705	vs	
Maleimides	ν(NH)	ca. 3200	m br	
	ν_{s}(C=O)	ca. 1775	m	Weak in maleimide
	ν_{as}(C=O)	ca. 1700	vs	
	ν(C=C)	1650–1630	m	Not in maleimide
	ν(ring)	1365–1340	m br	
	δ(ring-H)	1080–1040	m sh	
	δ(NH...OC)	850	m br	Maleimide
Phthalimides	ν(NH)	ca. 3200	m br	
	ν_{s}(C=O)	1790–1735	m-s sh	ca. 1770
	ν_{as}(C=O)	1745–1670	vs	ca. 1750, several merged bands

Table 3.15 Continue

Vibrating group	Assignment	Range/cm^{-1}	Intensity	Remark
Trimellitic amide-imides, aromatic, N,N′-substituted				
	2 x ν(C=O)	3480	w sh	Overtone
	ν(NH)	ca. 3360	w-m	Asymmetric
	ν_s(C=O)	ca. 1780	m sh	Imide ring
	ν_{as}(C=O)	ca. 1720	vs	Imide ring
	ν(C=O)	ca. 1665	s	Aromatic amide I
	δ(NH)ν(C-N)	ca. 1530	m	Aromatic amide II merged w. ν(ring)
	ν(C-N)	ca. 1225	s	Aromatic amide III
Pyromellitic imides, aromatic, N,N′-substituted				
	2×ν(C=O)	ca. 3480	w sh	Overtone
	ν_s(C=O)	ca. 1775	m-s sh	
	ν_{as}(C=O)	ca. 1720	vs	
	ν(ring)	ca. 1370	s-vs	Imide ring
	ν(C-N)	ca. 1240	s-vs	

a The conformations relate to the carbonyl groups

Table 3.16
Characteristic absorption band combinations/partial spectra of CHNO compounds: amine oxides, nitroso and nitro compounds, nitrite and nitrate esters

Vibrating group	Assignment	Range/cm^{-1}	Intensity	Remark
Amine oxides				
aliphatic	ν(N→O)	970–950	m	
	δ(N→O)	ca. 775	m	
pyridine→O		1320–1230	m-s	Depends on ring substitution; pyridine→O: 1250 s
		1190–1150	m-s	Pyridine→O: 1172
	δ(N→O)	895–840	m	
Monomer -N=O				
aliphatic	ν(N=O)	1590–1540	s	Usually at 1550
aromatic		1515–1480	s	
Dimer (-N=O)$_2$				
aliphatic	ν(N-O)	1425–1330	m-s	*Z* configuration
		1290–1175	s	*E* configuration
aromatic		ca. 1390	s-vs	*Z* configuration, three fused bands
		1300–1250	m-s	*E* configuration
-NO$_2$				
aliphatic	ν_{as}(O=N=O)	1555–1545	vs	CH_3NO_2: 1563
tertiary		1550–1530	vs	
	ν_s(O=N=O)	1395–1360[a]	m	CH_3NO_2: 1404
CH_2-NO_2	δ(O=N=O)	620–600	m br	CH_3NO_2: 657
>CH-NO_2		630–610	m	
aromatic	ν_{as}(O=N=O)	1535–1510	vs	
	ν_s(O=N=O)	1350–1335	vs	
	δ(O=N=O)	680–655	w-m	
-O-N=O	ν(N=O)	1680–1650	vs	*E* configuration
		1625–1610	vs	*Z* configuration
	ν(N-O)	850–810	s	*Z* configuration
		815–750	vs	*E* configuration

Table 3.16 Continue

Vibrating group	Assignment	Range/cm^{-1}	Intensity	Remark
	δ(O-N=O)	690–615	s	*Z* configuration, $C_2H_5NO_2$: 690
		625–565	s	*E* configuration
-O-NO$_2$ aliphatic	$\nu_{as}(NO_2)$	1660–1625	vs	
	$\nu_s(NO_2)$	1285–1270	vs	
	ν(N-O)	870–855	vs br	
	$\delta(NO_2)$	760–755	w-m	
	$\gamma(NO_2)$	710–695	w-m	

a May be adjacent or superimposed to $\delta_s(CH_3)$, 1380/cm

Table 3.17
Characteristic absorption band combinations/partial spectra of sulfur-organic compounds

Vibrating group	Assignment	Range/cm^{-1}	Intensity	Remark
-SH thiols				
aliphatic	ν(S-H)	2560–2554	w-m	
	$\delta(CH_2\text{-S})$	ca. 1430	w	Merges with $\delta(CH_2\text{-C})$
	$\omega(CH_2\text{-S})$	1278–1247	m-s	
	$\nu(CH_2\text{-S})$	655–650	w	
	ν(>CH-S)	620–610	w	
aromatic	ν(S-H)	2560	w-m	
	δ(SH)	1099–1082	m-s	
	ν(ring-S)	630–620	w	Thiophenol: 700
	γ(SH)	482–477		Thiophenol: 465
R-S-R	$\delta_{as}(CH_3\text{-S})$	1435–1430	m	$H_3C\text{-S-}CH_3$: 1433s
	$\delta(CH_2\text{-S})$	1425–1420	w-m	Merges with $\delta(CH_2\text{-C})$
	$\delta_s(CH_3\text{-S})$	ca. 1310	m-s	
	$\omega(CH_2\text{-S})$	1270–1255	m	
	$\nu_{as}(C\text{-S-C})$	ca. 690	w-m	Not in $S(C_4H_9)_2$
Ar-S-CH$_3$	$\delta_{as}(CH_3\text{-S})$	ca. 1440	m	Merged with ν(ring)?
	$\delta_s(CH_3\text{-S})$	ca. 1315	w	
	$\nu_{as}(C\text{-S-C})$	615	vw	δ(ring) ?
	$\nu_s(C\text{-S-C})$	475	m	γ(ring) ?
Ar-S-Ar	$\nu_{as}(C\text{-S-C})$	617	vw	Diphenylsulfide
	$\nu_s(C\text{-S-C})$	463	m	
>S=O sulfoxides				
aliphatic	$\nu_{as}(CH_3\text{-S=O})$	2995	w-m	
	$\delta_s(CH_3\text{-S=O})$	ca. 1310	w-m	
	ν(S=O)	1070–1040	vs	
		1055–1010	vs	Hydrogen-bonded
	ν(C-S)	ca. 700	w-m	
	δ(C-S=O)	395–360	var	
aromatic	ν(S=O)	1040–1020	vs	Split
>SO$_2$ sulfones				
aliphatic	$\nu_{as}(CH_3\text{-}SO_2)$	ca. 3025	m	
	$\nu_{as}(SO_2)$	ca. 1315	vs	Split
	$\nu_s(SO_2)$	1150–1135	vs	
alkylaryl-	$\nu_{as}(SO_2)$	1335–1325	vs	
	$\nu_s(SO_2)$	1160–1150	vs	
diaryl-	$\nu_{as}(SO_2)$	ca. 1310	s-vs	Split
	$\nu_s(SO_2)$	ca. 1160	vs	

Table 3.17 Continue

Vibrating group	Assignment	Range/cm^{-1}	Intensity	Remark
-SO_2-OH sulfonic acids				
aliphatic				
anhydrous[a]	ν(OH)	ca. 2900	s br	
		ca. 2400	w-m br	
	$\nu_{as}(SO_2)$	1350–1340	s	
	$\nu_s(SO_2)$	1200–1100	s	
	ν(S-O)	1165–1150	s br	
	δ(OH...OS)	910–890	s	
hydrated	ν(OH)	3500–2600	s vbr	
		2440–2400	m br	
	$\nu_{as}(SO_2)$	1350–1340	s-vs br	
	$\nu_s(SO_2)$	1165–1155	s-vs	
		910–900	s br	
aromatic	ν(OH)	3300–2600	m-s vbr	
		2460–2400	w-m br	
	$\nu_{as}(SO_2)$	ca. 1350	m br	
	$\nu_s(SO_2)$	ca. 1175	s-vs	Complex of usually three bands
	δ(OH...OS)	ca. 910	s br	
-SO_3^-				
aliphatic	$\nu_{as}(-SO_3^-)$	1200–1170	vs br	
	$\nu_s(-SO_3^-)$	ca. 1050	s-vs	
	$\delta(-SO_3^-)$	ca. 620	m	
		ca. 550	m br	
R-SO_2-O-R	$\nu_{as}(CH_3-SO_2)$	3025	w	
	$\nu_{as}(SO_2)$	ca. 1350	s-vs	
	$\nu_s(SO_2)$	ca. 1175	s-vs	
	ν_{as}(C-O-S)	1010–1000	m-s	
	ν_s(C-O-S)	ca. 815	m-s	
	δ(O=S=O)	ca. 530	m-s	
R-SO_2-O-Ar	$\nu_{as}(SO_2)$	ca. 1360	s	
	ν(Ar-O)	ca. 1200	s	
	$\nu_s(SO_2)$	ca. 1150	vs	
		ca. 870	vs	
Ar-SO_2-OR	ν_{as}(O=S=O)	1365–1335	m-s	
	ν_s(O=S=O)	1200–1185	vs	
R-O-SO_2-O$^-$$Na^+$	ν(OSO_2O)	ca. 1250	s	Linear alkyl
		ca. 1220	vs	Linear alkyl
		ca. 1230	vs	Merged double band
		1085–1080	s sh	Linear alkyl
		1070	s sh	Branched alkyl
	ν(C-O-S)	ca. 835	m	Fused band on red side
	δ(OSO_2O)	ca. 690	m-s	
R-O-SO_2-O-R	ν_{as}(O=S=O)	ca. 1390	s	
	ν_s(O=S=O)	1200–1190	vs	
Ar-SO_2-NH_2	$\nu_{as}(NH_2)$	3350–3325	m-s	
	$\nu_s(NH_2)$	3270–3240	m-s	
	$\delta(NH_2)$	1570–1550	w-m br	
	ν_{as}(O=S=O)	1335–1325	s-vs	
	ν_s(O=S=O)	1160–1150	vs	
	δ(O=S=O)	540–530	m-s	
Ar-SO_2-NH-R	ν(NH)	ca. 3290	s	
	ν_{as}(O=S=O)	ca. 1325	s-vs	

Table 3.17 Continue

Vibrating group	Assignment	Range/cm^{-1}	Intensity	Remark
	ν_s(O=S=O)	ca. 1160	vs	
	δ(O=S=O)	590–570	m-s	Fused with δ (ring)?
(R,Ar)-SCN	ν(CN)	2155	vs	
	ν(S-C)	ca. 685	w-m	
	$\nu(C_\alpha\text{-S})$	680–580	m	
	same	625–590	m	Aliphatic substituent
	δ(SCN)	ca. 410	m	

a Sulfonic acids are very hygroscopic; spectra obtained under normal laboratory conditions represent usually the hydrated form

Table 3.18
Characteristic absorption band combinations/partial spectra of organic phosphorus compounds

Vibrating group	Assignment	Range/cm^{-1}	Intensity	Remark
$(RO)_3P{=}O$	ν(P=O)	ca. 1275	s	Two components
	ν_{as}(P-O-C)	1050–1000	vs	Max. 1050, 3 components
$(ArO)_3P{=}O$	ν(P=O)	ca. 1300	s	Two components
	ν(Ar-O)	1170–1150	s	
		ca. 970	vs	Broader than ring vibrations
	$\delta(PO_3)$	530–510	m	
$(\Phi O)_2ROP{=}O$	ν(P=O)	1295	s	
	ν(Ar-O)	1200	vs	
	ν_{as}(P-O-C)	ca. 1025	s-vs	Two components
	ν(O-P-O)	950	vs	
	$\delta(PO_3)$	530–510	m	Two components
$(RO)_2(HO)P{=}O$	ν(P=O)	1250–1210	vs	
	γ(OH...O=P)	590–460	m br	
		400–380	w	
$(ArO)_2(HO)P{=}O$	ν(P=O)	ca. 1275	s	
	$\delta(PO_3)$	600–580	s	Dependent on ring substitution
		565–535	s	
		515–500	s	
		490–470	s	
		400–380	w	
$(RO)(HO)P(O)O^-$ surfactant	ν(OH)	ca. 3220	s vr	
		ca. 2400	m vbr	
	δ(OH)	1670	w-m vbr	
	ν(P=O)	1233	m sh	
		1192	m sh	
	ν(P-O-C)	1115+1090	vs	Merged
		980	m-s	
		900	m-s	
		533	s	
$(RO)_2RP{=}O$	ν(P=O)	1265–1230	vs	
		800–750	w-m	
		570–500	m br	
		490–410	m br	
		440–400	w	
$(RO)_2ArP{=}O$	ν(P=O)	ca. 1250	vs br	
		ca. 1050	vs br	
	ν(P-O-C)	970	s br	
		920	m br	

Table 3.18 Continue

Vibrating group	Assignment	Range/cm^{-1}	Intensity	Remark
	ν(P-C)	830+800	s+m	
		585–565	s	
		530–520	s	
$(ArO)_2ArP{=}O$	ν(P=O)	1265–1230	vs	
		620–600	m	
		535–515	s	
$P(OR)_3$	$\nu_{as}(PO_3)$	ca. 1000	vs br	Several components
	$\delta(PO_3)$	ca. 750	s br	Three components
$P(OAr)_3$	ν_{as}(P-O-Ar)	1220–1210	vs	Double band
		1200–1175	s-vs	
		875–850	vs	
$P(O\Phi)_3$	ν_{as}(P-O-Φ)	1200	vs	
		1165	s sh	
	δ(P-O-Φ)	875	vs	Double band
		765	m-s	
		725	m	
R-P-H	ν(P-H)	2285–2265	m	
	δ(H-P-H)	1100–1085	m	
	δ(P-H)	1065–1040	w-m	
	ω(H-P-H)	940–910	m	
Ar-P-H	ν(P-H)	2285–2270	m	
	δ(P-H)	1100–1085	m	

Table 3.19
Characteristic absorption band combinations/partial spectra of organic silicium compounds

Vibrating group	Assignment	Range/cm^{-1}	Intensity	Remark
SiH derivatives				
$RSiH_3$	ν(SiH)	2155–2140	s	Reduced coupling
	$\delta_{as}(SiH_3)$	945–930	m-s	No splitting
	$\delta_s(SiH_3)$	930–910	m-s	in asymmetric and sym. modes
	$\varrho(SiH_3)$	680–540	s	
R_2SiH_2	ν(SiH)	2140–2115	s	
	$\delta(SiH_2)$	950–930	m-s	
	$\omega(SiH_2)$	895–885	m-s	
R_3SiH	ν(SiH)	2100–2090	s	
	ω(SiH)	845–800	s	
$ArSiH_3$	ν(SiH)	2160–2150	s	
	$\delta_{as}(SiH_3)$	945–930	m-s	
	$\delta_s(SiH_3)$	930–910	m-s	
Ar_2SiH_2	ν(SiH)	2150–2130	s	
	δ(SiH)	950–925	m-s	
	ω(SiH)	870–840	m-s	
Ar_3SiH	ν(SiH)	2135–2110	s	
	ω(SiH)	845–800	s	
-O-Si(CH_3)H	ν(SiH)	ca. 2230	s	
SiC derivatives				
C-Si$(CH_3)_{1-3}$	$\nu_{as}(CH_3)$	2980	s-vs sh	May be merged with $\nu_{as}(CH_3$-C)
	$\delta_s(CH_3)$	ca. 1250	s sh	
O-Si$(CH_3)_{1-3}$	$\nu_{as}(CH_3)$	2980	s-vs sh	
		ca. 1265	s sh	

Table 3.19 Continue

Vibrating group	Assignment	Range/cm^{-1}	Intensity	Remark
(C,C)>Si(CH_3)$_2$	ν(Si-C)	ca. 830	vs	
		815–800	s	
(O,O)>Si(CH_3)$_2$		ca. 800	vs	
C-Si(CH_3)$_3$	ν(Si-C)	ca. 830	vs	
		770–750	m-s	
O-Si(CH_3)$_3$		ca. 860	s	
C-SiΦ$_2$-C	ν(ring-H)	3080+3070	w sh	
	ν(ring)	1430	s sh	All bands due to ring vibrations are sharp
	ν(Si-ring)	1110	s-vs sh	
		ca. 820	m	
	γ(ring-H)	700	vs sh	
	δ(ring)	540	m-s sh	
	γ(C-Si-Φ)	465	w-m sh	
Ar-SiΦ$_2$-Ar	ν(ring-H)	3085+3075	w sh	
	ν(ring)	1430	m-s sh	
		1400	m-s sh	
	ν(Si-ring)	1110	s sh	
	δ(ring-H)	1015	m-s sh	
	ν(Si-ring)	830	m-s sh	
	γ(ring-H)	700	vs sh	
	δ(ring)	530–515	m	
>SiΦ-O-	ν(ring-H)	3080	w-m sh	
	ν(ring-H)	3070	w sh	
	ν(Si-ring)	1130	s sh	May be merged with ν(O-Si-O)
	γ(ring-H)	ca. 735	m-s sh	
		700	m-s sh	
	δ(Φ-Si-O)	ca. 480	m sh	
-O-SiΦ$_2$-	ν(ring-H)	3080+3070	w sh	
	δ(ring-H)	995	m sh	May be merged with 1030
		740	w sh	
		720	w-m sh	
	γ(ring-H)	700	m-s sh	
	δ(Si-O-Φ)	ca. 520	m	
		ca. 490	w-m	
Si-OH and Si-O derivatives				
Si-OH	ν(OH)	3800–3600	m br	Silanols
-Si(CH_3)$_2$-O- siloxanes	ν_{as}(Si-O-Si)	1100	vs br	Fused double band
		1025	vs br	
	δ(Si-O-Si)	400	m br	
Si-O-R silylethers	ν_{as}(Si-O-C)	1110–1000	vs br	Frequently around 1050
	δ(Si-O-C)	ca. 500	m br	
Si-O-Ar	ν_{as}(Si-O-Ar)	1250–1180	s-vs	Broader than ring vibr.
		1000–900	s br	2–3 components
	δ(Si-O-Ar)	520–500	m-s br	
Si(OR)$_{1-3}$ silyl esters				
>Si(OCH_3)$_2$	γ(Si-O-C)	390–360	s	
-Si(OCH_3)$_3$	ν_{as}(CH_3)	ca. 2850	s-vs sh	
		1410–1400	w-m sh	
	ν_{as}(Si-O-C)	1190	s-vs	
	ν_{as}(OSiO)	ca. 1090	vs br	
	δ(Si-O-C)	645–620	w-m sh	

Table 3.19 Continue

Vibrating group	Assignment	Range/cm^{-1}	Intensity	Remark
-Si(OC_2H_5)$_3$	overtone	2770	w sh	Important for identification
	overtone	2740	w-m sh	
	ν_{as}(Si-O-C)	1170	m-s	
	ν_{as}(O-Si-O)	1110+1080	vs br	Merged twin band
		645–635	w-m	
($RO)_3$Si-CH=CH_2	ν(HC=CH_2)	3060	m sh	
	ν(C=C)	1600	m-s sh	
	δ(HC=CH_2)	1010	s sh	
		550–540	m-s sh	

Table 3.20
Characteristic absorption band combinations/partial spectra of organic halogen compounds

Vibrating group	Assignment	Range/cm^{-1}	Intensity	Remark
C-F[a] aliphatic				
R-CH_2-F	δ(**CH_2**F)	ca. 1430	w-m	
	ν(CF/CC)	ca. 1055	m-s	coupled vibration
	ν(CF/CC)	ca. 1015	s	coupled vibration
	ν(CCF/CF)	ca. 915	m	coupled vibration
-CH_2-CHF-CH_2-	δ(**CH_2**F)	ca. 1420	m-s	
	ν(CF/CC)	ca. 1090	vs br	coupled vibration
	ν(CCF/CF)	ca. 1030	s-vs br	coupled vibration
	ν(CCF)δ(CHF)	ca. 830	s-vs	
-CH_2-CF_2-CH_2-	ν_{as}(CH_2)	3020	w-m sh	
	ν_s(CH_2)	2980	w sh	
	δ(**CH_2**-CF_2)	1400	s-vs	
	ν_{as}(CF_2)	ca. 1180	vs br	
	ν(CCF)δ(CF_2)	880	s-vs	
CF_3-CH_2-	δ(CH_2)	ca. 1415	w	
	ν_{as}(CF_3)	ca. 1280	vs	
	ν_s(CF_3)	1165+1145	vs	
	δ(CF_3)	ca. 665	m sh	
CF_3-CO-	ν(C=O)	ca. 1785	s-vs	
	ν_{as}(CF_3)	ca. 1230	s	
	ν_s(CF_3)	ca. 1170	vs	
	δ(CF_3)	ca. 690	m sh	
CF_3-Ar	ν_{as}(CF_3)	1335–1320	vs	
	ν_s(CF_3)	1140–1130	vs	
	δ(CF_3)	700–600	m-s sh	dependent on substitution
Ar-F	ν(Ar-F)	1265–1200	s-vs	dependent on substitution
		550–500	var	dependent on substitution
		455–440	w-m sh	ΦF: 405m
CCl[b] aliphatic				
R-CH_2-Cl	$\omega CH_2Cl\nu CCCl$	1300–1240	var sh	*i*-alkyl: vs
	ν(C-Cl)	ca. 650	m	
β-branched		ca. 730	s	
		ca. 690	w-m	
($CH_2)_2$>CH-Cl	$\nu CCCl\omega CH_2Cl$	ca. 1250	s-vs br	
		ca. 960	m	
	ν(C-Cl)	760–740	m	
		690–660	var	

Table 3.20 Continue

Vibrating group	Assignment	Range/cm^{-1}	Intensity	Remark
		ca. 640	var	
		ca. 610	var	
R_3C-Cl	ν(C-CCl)	1240–1225	m sh	
		1160–1145	s-vs	
	ν(C-Cl)	ca. 620	w-m	
		570–560	m-s	
Ar-Cl	δ(ring-H)/	1100–1090	s	*p*-substitution[c]
	ν(ring-Cl)	1080–1070	m	*m*-substitution[c]
		1060–1030	m-s	*o*-substitution[c]
	ν(ring-Cl)	ca. 680	m-s	*o*- and *m*-substitution
		640–630	m-s	*p*-substitution
C-Br aliphatic				
R-CH_2-Br	νCCBrωCH_2Br	1255–1225	s-vs	numerous acti-
	ν(C-Br)	650–640	m	vated skeleton
		570–555	m	vibrations
Ar-Br	δ(ring-H/	1085–1070	m-s	*m*- and *p*-substitution
	ν(ring-Br)	1030–1020	m-vst	*o*-substitution[c]
		680–655	m-s	*o*- and *m*-substitution
		605–595	m-s	*p*-substituted
R-I aliphatic				
n-alkyl	ν(C-CI)	1250–1185	m-vs	dependent on chain length
		1190–1170	m-s	not always present
	ν(C-I)[d]	600–590	vw-m	C_2H_5I: 500
		505–500	w-vw	
i-alkyl numerous activated skeleton vibrations				
Ar-I	ν(Ar-I)	655–640	m-vs sh	
		465–430	w-s sh	

a CF groups are vibrationally strongly coupled with neighbouring structures. Thus, it is not feasible to speak simply of ν(CF), δ(CF) etc. In addition, the electronegative nature of F activates vibrations of adjacent C-C bonds by an inductive effect (electric coupling)
b Mechanical coupling of CCl groups with adjacent structures is less than in the case of CF. On the other hand, CCl band frequencies are dependent on both configuration and conformation of adjacent groups. In the case of *i*-alkyl, a number of additional bands are observed in the ν(C-C) range
c Other w-m sharp bands may appear between 1100 and 1000
d Dependent on conformation

Table 3.21
IR absorption bands (cm^{-1}, intensity) of phthalocyanine (Pc) and some of its derivatives (Shurvell and Pinzuti, Knudsen, 10.2.3, abridged; own data)

PcH_2	Copper phthalocyanine, modifications			$PcCl_4Cu$	$PcCl_{16}Cu$
	α	β	δ		
3290 m-s					
3074 sld		3082 sld		3058 vw	
3064 sld		3059 sld			
3050 m-s	3050 w-m	3050 w			
3030 sld	2649 w	3030 vw			
	2571 w			2954 sld	2954 sld
2922 vw	1954 vw-w			2920 m	2925 w
	1896 w				
	1815 vw				
1616 m	1611 m	1611 w		1606 s	1610 vw
1608 m				1606 s	1610 vw

Table 3.21 Continue

PcH_2	Copper phthalocyanine, modifications α	β	δ	$PcCl_4Cu$	$PcCl_{16}Cu$
1580 w	1590 w-m	1590 w			1553 w
1523 s		1509 sld		1511 sld	
1501 s	1508 s	1505 m		1502 s	1497 m
1578 w	1480 w-m	1480 w		1462 sld	
1458 w	1465 m			1445 s	
1438 s	1421 m-s			1391 s	1391 vs
1402 w					
1362 m					1365 vw
1335 s	1332	1333	1332	1335 sld	1327 s
1320 s				1335 sld	1320 s
1303 m				1315 vs	1306 vs
1277 s	1286	1287	1286	1293 sld	1276 s
1252 vw				1254 m	
		1201 w	1201 w		1211 vs
1189 m	1189 w	1173		1187 w	1194 vw
1160 m	1167 w	1167 w	1168 w	1161 sld	1154 vs
		1164	1163	1134 s	
1120 vs	1120	1120	1119		
1111 vs		1101			
1095 s	1091	1090	1095	1097 s	1097 s
				1083 s	
1068 vw	1068	1068	1068		
1045 w				1046 s	
1006 vs	1002	1002	1001		
		982 w			
		956	955		
949 w	949	949		959 m	949 vs
943 w	940			959 m	949 vs
	900	900	900	920 s	929 sld
			882		
		879			
		876 w	877	884 m	
875 s	870	870	871		
	863				
841 vw	802	800	800	824 s	
				800 vw	804 vw
	776 w	781	779		779 s
		772	772 w		
767 s	769			774 m-s	772 sld
	754	755	755	764 m-s	
				742 s	749 s
736 vs					
731 vs		730	729	724 m	
716 vs	722				
686 m	689 w	690	689	692 m	
	679 w				
642 m	640 w	639	638	640 vw	649 vw
620 m-s				627 vw	620 vw
	573	573	572		
558 m	506	507	506		
494 m				520 m	510 s
490 m				520 m	510 s
	434	434		429 m	
421 w	426			421 w	421 w

Table 3.22
Lift of degeneration and selection rules as shown with XO_4^{2-} and CO_3^{2-} (data from Newman, 10.2.3); values in cm^{-1}

Name	Formula	ν_{as}[a]	ν_s[b]	δ_{as}[a]
	$SrCrO_4$	927/912/887	845	431/410
Yellow Ultramarine	$BaCrO_4$	936/899/859		418
Crocoite	$PbCrO_4$	905/858/833		Not determ.
Anhydrite	$CaSO_4$	1159/1130		676/616/579
Gypsum	$CaSO_4 \cdot 2H_2O$	1150/1120	1010	673/605
Baryte	$BaSO_4$	1179/1120/1084	983	637/614
Assignment for CO_3^{2-}		ν_{as}[c]		δ_{as}[c]
Calcite	$CaCO_3$	1425		872
Aragonite	$CaCO_3$	1460	1082	860
Cerussite	$PbCO_3$	1440/1404	1055	841
Hydrocerussite	$2PbCO_3 \cdot Pb(OH)_2$	1430/1400/1360	1090	850/834
Azurite	$2CuCO_3 \cdot Cu(OH)_2$	1490/1415	1090	837/817
Malachite	$CuCO_3 \cdot Cu(OH)_2$	1500/1400	1095	820/803

a Triply degenerate
b Forbidden
c Doubly degenerate

Table 3.23
Characteristic absorption band combinations/partial spectra of inorganic compounds (arranged according to symmetries)

Vibrating group	Assignment	Range/cm^{-1}	Intensity	Remark
Sticks				
C≡N in complexes				
$Fe^{2+}(CN)_6^{4-}$	ν(CN)	2041	vs sh	
		2024	s sh	
	ϱ(CN)	584	m-s sh	Hindered rotation
$Fe^{3+}(CN)_6^{3-}$	ν(CN)	2112	vs sh	
		2024	s sh	
	ϱ(CN)	572	w	Hindered rotation
CN^-	ν(CN)	2130–2000	s sh	
KCN		2080	vs sh	
		664	w	Hindered rotation
NaCN		2088	vs sh	
		688	w	Hindered rotation
C≡O in complexes	ν(CO)	2100–1800	vs sh	
$N{\equiv}O^+$ free nitrosonium				
	ν(NO)	2370–2230		
in complexes		1860–1720		
Bent sticks				
H_2O (l)	ν_{as}	ca. 3000	vs vbr	All vibrations concern the associate
	δ	1640	m	
	γ	700	m vbr	
D_2O	ν_{as}	ca. 2520	vs vbr	
	δ	1650	w-m vbr	
		1210	m	
		ca. 1100	m vbr	Merged with 1210
		ca. 530		
O=N-O⁻	ν_{as}	ca. 1265	vs	
	δ	ca. 825	m sh	

Table 3.23 Continue

Vibrating group	Assignment	Range/cm^{-1}	Intensity	Remark
CNO^-				
CNO^-Na^+	ν(C≡N)	2160	vs sh	
	ν(N-O)	1300	m sh	
		1208	m sh	
	δ(CNO)	636	m-s sh	
		628	m sh	
^-NCO	ν(N≡C)	2250-2190	var sh	
NCS^-Na^+	ν(N≡C)	2048	vs sh	
	ν(C-S)	748	m-w sh	
	δ(NCS)	484	m-w sh	
Three-tipped stars (planar)				
CO_3^{2-}				
Na_2CO_3	$\nu_{as}(CO_3)$	1460	vs	
		1408	m sh	
	$\delta_{as}(CO_3)$	868	m sh	May be split in 876+860
Calcite	$\nu_{as}(CO_3)$	1450	vs br	
	$\delta_{as}(CO_3)$	878	s sh	
		712	m sh	
Aragonite	$\nu_{as}(CO_3)$	1460	vs br	
		1085	m sh	
	$\delta_{as}(CO_3)$	860	m-s	
		715	m-s sh	
		702	m sh	Merged with 715
$BaCO_3$	$\nu_{as}(CO_3)$	1445	vs	
	$\delta_{as}(CO_3)$	853	m-s	
		690	m-s sh	
$PbCO_3$	$\nu_{as}(CO_3)$	ca. 1400	vs br	
		1040	w sh	
	$\delta_{as}(CO_3)$	677	m-s sh	
NO_3^-				
$NaNO_3$	overtone	1792	w sh	
	$\nu_{as}(NO_3)$	1383	vs sh	
	$\delta_{as}(NO_3)$	836	m sh	
KNO_3	overtone	1764	w-m sh	
	$\nu_{as}(NO_3)$	1384	vs	
	$\delta_{as}(NO_3)$	826	m-s sh	
NH_4NO_3	overtone ?	2393	m-w sh	
	$\nu_{as}(NO_3)$	1383	vs	
	$\delta_{as}(NO_3)$	824	w sh	
		712	w-m sh	
$Ba(NO_3)_2$	overtone	1777	w sh	
		1418	m	
	$\nu_{as}(NO_3)$	1383	vs	
		1368	m	
	$\delta_{as}(NO_3)$	820	w-m	
		730	w-m	
$Pb(NO_3)_3$	overtone	1769	vw	
	$\nu_{as}(NO_3)2$	1383	vs sh	
	$\delta_{as}(NO_3)$	828	vw	Double band with 808
		808	vw	
		728	w sh	

Table 3.23 Continue

Vibrating group	Assignment	Range/cm^{-1}	Intensity	Remark
Tetrahedron				
SO_4^{2-} 1140–1100 (several comp.) vs 670–600 (2 bands) m-s				
Na_2SO_4	$\nu_{as}(SO_4)$	1125	vs br	
	$\delta_{as}(SO_4)$	633	m sh	
		610	s-vs	
$CaSO_4 \cdot 2H_2O$	ν(HO)	3550+3400	s br	
	$\delta(H_2O)$	1680	m	
		1615	m-s	
	$\nu_{as}(SO_4)$	1140	vs br	Merged with neighbour
		1110	vs br	
	$\delta_{as}(SO_4)$	665	s	
		ca. 602	s	
$BaSO_4$	$\nu_{as}(SO_4)$	ca. 1180	s br	
		ca. 1120	s-vs br	
		ca. 1080	vs br	
		985	m sh	
	$\delta_{as}(SO_4)$	630	m	
		605	s	
$PbSO_4$	$\nu_{as}(SO_4)$	1130	vs	
		1095	s-vs	
		1035	vs	
		960	m sh	
	$\delta_{as}(SO_4)$	607	s	Merged neighbours
		595	s	
CrO_4^{2-}	$\delta_{as}(CrO_4)$	888	vs	Two satellites
PO_4^{3-}	$\nu_{as}(PO_4)$	1040	vs	$Ca_3(PO_4)_2$
	$\delta_{as}(PO_4)$	604	m	
		568	m-s	
ClO_4^-	$\nu_{as}(ClO_4)$	976	vs	Two satellites
	$\delta_{as}(ClO_4)$	620	m	$NaClO_4$
		488	m-s	
Lower symmetries				
$HP(O)O_2^{2-}$	ν(P-H)	2340	m-s sh	Pb phosphite
	$\nu_{as}(PO_3)$	1068	vs	
	$\delta_{as}(PO_3)$	554	m sh	
SO_3^{2-}	$\nu_{as}(SO_3)$	1116	vs	Pyramid
	$\nu_s(SO_3)$	975	s-vs	
	$\delta_{as}(SO_3)$	620	m	
		495	m	
Oxides with different symmetries (if any)				
MgO		ca. 520	s br	Merged bands
		ca. 430	vs br	
ZnO		530	m	
		490	vs br	
		430	vs br	
Al_2O_3		ca. 750	s vbr	Merged bands
		ca. 570	vs vbr	
SiO_2 α-quartz		ca. 1180	m	
	ν(-O-Si-)	1085	vs br	Chain vibration
		800	s	
	δ(-O-Si-)	780	m-s	Chain vibration
		695	m sh	

Table 3.23 Continue

Vibrating group	Assignment	Range/cm^{-1}	Intensity	Remark
SiO_2 amorph.	ν(-O-Si-)	1100	vs br	Chain vibration
	δ(-O-Si-)	800	m br	Chain vibration
	γ(-O-Si-)	470	m-s br	Chain vibration
TiO_2 rutile	δ(-O-Ti-)	680	vs vbr	Merged bands
		525	s vbr	
		420	m	
		350	m	Lattice vibration
Anatas	δ(-O-Ti-)	680	vs vbr	Merged bands
		530	s br	
		360	m	Lattice vibration

Table 3.24
Characteristic absorption band combinations/partial spectra of pigments and pigment mixtures for paints; spectral range sometimes does not cover 4000–400 cm^{-1} (Newman, 10.2.3, own measurements)

Color/name	Formula	Bands: cm^{-1}, intensity					
Blue							
Cu phthalocyanine	$C_{32}H_{16}N_8Cu$	1611	1587 w-m	1507 s	1466 m	1422 m-s	1334 s
		1288	1167 m	1120	1093 s-vs	1068 w	901 w-m
		863 w-m	802 w	772 w-m	753 m-s	723 s-vs	572 w-m
Berlin blue	$Fe_4[Fe(CN)_6]_3$	2080–2070 m					
Ultramarine	$Na_8[Al_6Si_6O_{24}]S_{2-4}$	3700 w sh	3614 w sh	1017 vs[b]	693 m	666 w-m	585 w
		539 w-m	454 s				
Green							
Chromium green	Cr_2O_3	635 w-m sld	555 vs	481 vs	420 sh		
Viridian	CrO(OH)	690 s sld	632 vs	566 vs	443 m sh	416 s sh	
		3601 w sh	3557 w sh	3534 w sh	1105 m	1075 m	972 vs
		845 w	800 w-m	746 w	681 m	494 s	457 vs
Ferric celadonite		442 m-s	427 m				
(or seladonite)		3606 w-m sh	3564 m sh	3535 w-m sh	1625 w	1115 m-s	1077 m-s
		975 vs	959 vs	847 w	797 m	682 m	495 m-s
Terre verte[a]		457 s	440 s				
(green earth)							
Terre verte Paciosi[a]		115 m	1077 m	975 vs	959 vs	841 w	800 w-m
		682 m	662 m sh	495 s	454 vs	440 m-s	
Glauconite	K Fe(II) Al silicate	992 vs	838 w	816 w	797 w	493 w-m	457 m
		437 w					
		3560 w-m	3535 w-m	1625 w	992 vs	838 w	673 w
		662 w	493 m-s	457 s	437 m		
Red							
Lead chromate	$PbCrO_4$	1110–1050 m vbr	863 vs	627 w sh	600 vw		
Sicomin red	$PbCrO_4$+$PbSO_4$	1187 w-m sld	1106 m	1067 m	863 vs		
Yellow							
Sicomin yellow	$PbCrO_4 \cdot PbSO_4$	1102 m	1067 m	971 w	867 vs	627 m sh	600 w-m sh
Sicotan yellow	$TiO_2 \cdot Cr_2O_3 \cdot Sb_2O_3$	680 vs	577 s	408 m-s			
White							
Anhydrite	$CaSO_4$	1159 m-s	1130 vs	676 m	616 m	579 m	515 w-m
Heavy spar	$BaSO_4$	1175 s	1117 s	1082 vs	982 m sh	801 w	778 w
		693 vw	635 m	608 s	512 vw	462 w-m	
Blanc fixe	$BaSO_4$	1437 w sh	1402 w sh	1171 s-vs	1117 s-vs	1079 s-vs	982 m sh
		631 m-s sh	608 s				

Table 3.24 Continue

Color/name	Formula	Bands: cm^{-1}, intensity					
Talc[c]	$Mg_3(OH)_2Si_4O_{10}$	3676 w-m sh	1445 m-s	1017 vs	882 w-m	670 s sh	531 w sld
		458 s[b]	419 w				
Kaolin	$Al_4(OH)_8Si_4O_{10}$	3700 m-s sh	3653 w-m sh	3624 m sh	1100 s	1032 vs	1009 s
		917 s	793 w	755 w	701 m	539 s	431 m
Zinc white	ZnO	535 m-s sld	ca.400 vs				
Rutile	TiO_2	689 vs br	540 m-s br sld	4423 m sh			
Anatas	TiO_2	678 s br	520 vs br				

a seladonite, Fe(II) Ca Mg Al layer silicate
b Close twin band
c Colourless to light greenish

4
Raman Spectrometry

4.1
Fundamentals

The inelastic scattering of light by molecular systems was predicted by Smekal and discovered by Raman. Outside of resonance absorption, most of the light interacting with matter is scattered elastically (Rayleigh scattering). A small fraction, typically 10^{-8} to 10^{-9}, of the light is shifted to the red (Stokes) or to the violet (anti-Stokes):

$$h\nu_R = h\nu_i \pm (E_m - E_n),$$

where ν_i is the frequency of the incident light, ν_R the one of the Raman-scattered light; E_m and E_n are vibrational energy states of the interacting system[5]. ΔE is usually much smaller than $h\nu_i$. At room temperature, most of the molecules of our system remain in the vibrational ground state. If a larger fraction of the molecules is excited to the first level above ground ("hot" systems in a direct or indirect sense) then a molecule may transfer its vibrational energy to the colliding photon. This is the reason why Stokes is much more frequent than anti-Stokes shift. Commercial Raman spectrometers scan the red-shift ($\Delta\nu$) as a two-dimensional intensity/wavenumber plot.

The *excitation condition* for the Raman effect is that, during the induced vibration, the polarisability of the molecule changes. *Selection rules* tell us which of the possible modes are active in one or the other effect or in both (or in none). The vibrational modes of molecules with only identity as symmetry element are active in both effects. Increasing symmetry of a molecule splits, so to speak, the activity of the modes: an increasing number of modes is either *IR* or Raman active. If a molecule has a centre of symmetry *IR*-active modes are Raman inactive and *vice versa* (rule of spectroscopic exclusion). Examples for this are some polycyclic pigments. Figure 4.1 shows the Raman spectrum of Cu phthalocyanine; the true bands on the low-wavenumber side, despite the long-wavelength excitation, are almost outshone by the strong fluorescence (candle in sunshine). This background can partially be removed by mathematical treatment, and some more Raman bands will come up (Fig. 4.2). None of these appear in the *IRS* (compare Fig. 3.5).

Fluorescence, the main problem of Raman spectrometry (*RS*), is possible if the system absorbs radiation by resonance and owns a number of energy levels between the ground state and the excited state considered. An excited electron may then, rather than falling straight down, prefer the detour along steps. The radiation emitted between each step is called fluorescence or phosphorescence (the latter if the step is a triplet state). It is, in the case of simple molecules without chromophoric groups, easy to find an exciting wavelength far from absorption ranges, and therefore obtain spectra with little or no fluorescence. Most organic pigments have several chromophoric and auxochromic groups, absorb over wide ranges and allow many transitions from the near *UV* to the *NIR*. They are definitely no pleasure for a spectroscopist.

RS has a number of advantages over *IRS*: it covers a broad range of vibrational frequencies (4000–30 cm^{-1}), it doesn't incur the problem of sample thickness, the exciting vibration traverses glass (capillaries or vessels for substances) and water (investigation of solutions), it allows the study of samples with sizes of a few micrometers (Raman microscopy), and the (maximal or integral) intensity of a band is directly proportional to the concentration of the vibrating group or molecule. These advantages are almost compensated by serious disadvantages: the equipment is about twice as expensive as a (modest) *FTIR* spectrometer, the laser radiation may heat the sample and change its physical or chemical state, the reproducibility of the spectra is still not satisfactory, and fluorescence.

The latter problem has partially been solved by the use of *NIR* lasers, by resonance *RS* or by other techniques.

4.2
Applications of *RS* in the Field of Plastics Additives

This would be a fine and interesting chapter; unfortunately, there are no general publications in this field and only few

5 For condensed systems, we neglect rotational states.

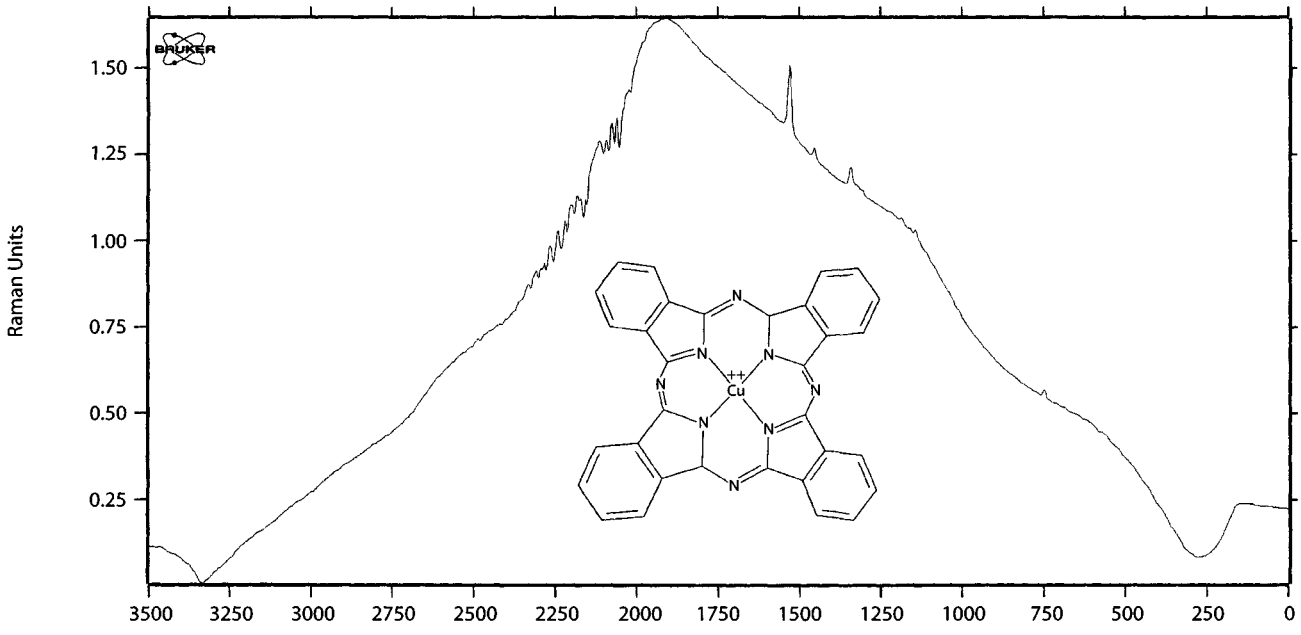


Fig. 4.1
Raman spectrum of Cu phthalocyanine with defocused Nd:YAG 1.064 μm laser excitation (100 mW). High-frequency side of the fluorescence maximum: rotational-modified first overtone of $\nu(H_2O)_{gas}$, low-frequency side: Raman bands. (Measurement by B. Schrader, University of Essen)

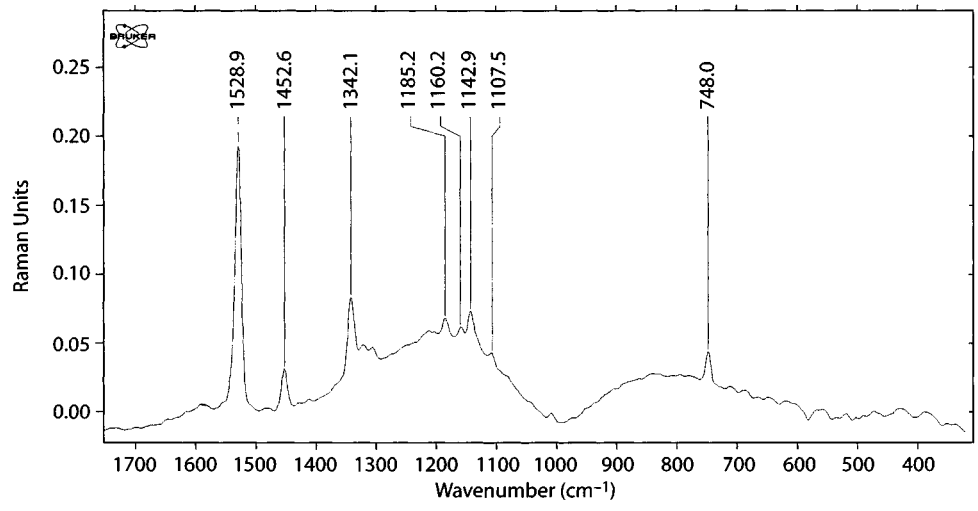


Fig. 4.2
Raman spectrum of Cu phthalocyanine, conditions as in Fig. 4.1. The fluorescence was mathematically subtracted (B. Schrader). Real bands are the ones at (cm^{-1}) 1529, 1453, 1342, 1185, 1143 and 748. None of these coincides with bands in the *IRS* (see Fig. 3.5)

ones dealing with special applications[6]. This looks strange in view of the large number of literature on *IRS* of additives. The farther-reaching question is why the enthusiastic welcome of laser-excited *FT* Raman spectrometers wasn't followed by a flood of papers on the application of this method in all fields where *IRS* keeps the fortress. Some of the reasons have been discussed toward the end of the preceding chapter, but there are some more:

- Poor Raman scattering of certain substance categories
- Unsatisfying reproducibility of spectra with one and the same instrument
- Differences in spectral quality when comparing results of different laboratories (even with the same make of instrument)
- Lack of digitised specific Raman libraries (which is partially due to the above arguments)

A number of these problems can be overcome by experimental tricks like changing the laser wavelength, cooling the samples (to reduce laser heating or to induce crystallinity), using resonance Raman etc., but all this needs skill and time and

6 I used the CA search algorithm and appropriate key words.

makes the price of a good Raman spectrum several times higher than the price of a good *FTIR* spectrum.

However, there are a few really impressive advantages of laser *RS* over *IRS*: to measure down to about 30 cm^{-1} (lattice vibrations), to measure aqueous solutions, to have a very fine space resolution (down to 1 μm) by the extremely narrow laser beam, and to be able to couple *RS* with *VIS* microscopy. The latter technique will fill most of the next chapter.

In order to exemplify possibilities and limits of *RS* in the field of plastics additives three befriended institutes[7] measured a number of selected additives under adjusted conditions. Colourless, liquid or solid samples generally presented few problems. The *RS* of triphenylphosphite (colourless liquid, Fig. 4.3) exhibits almost exclusively vibrations of the phenyl groups. The strongest *IR* bands of TPP, 1490 (ν_{as} ring), 1196 (ν_{as} PO_3), 861 (δ PO_3), and 690 cm^{-1} (γ PO_3) are Raman inactive. The *RS* of the colourless solid 2,6-di-*t*-butylphenol (Fig. 4.4) is again almost free from fluorescence; due to the low melting point of this substance (36 °C) the sample melted during the measurement. ν(OH) (3640 cm^{-1} in the *IR*) is Raman inactive, and so is ν (ring-O) (1430 cm^{-1} in the *IR*). The *RS* is quite characteristic for the aliphatic-aromatic system. Tetramethylthiuramdisulfide (vulcanisation accelerator) is a colourless solid. Its *RS* (Fig. 4.5) shows $\nu_s(CH_3)$ as second-strongest band (2927 cm^{-1}); in the *IRS*, this is weak. ν(C=S), in the *IRS* (1500 cm^{-1}), is very strong; in the *RS*, it is weak (1463 cm^{-1}) or inactive. Here 973 cm^{-1} is active in both *IR* and Raman (ϱ CH_3, ν C-S). The strongest band in the *RS* (559 cm^{-1}) is active also in the *IR* (563 cm^{-1}, medium). Thus, ν(S-S) as an assignment is unlikely; ϱ(C=S) is more likely.

1,3-Diphenylguanidine (accelerator) is a colourless solid; despite this, the *RS* exhibits short-wavelength fluorescence of medium intensity; this reduces the information of the *RS* but little (Fig. 4.6). Due to the low symmetry of the molecules (different types of association) about a dozen bands coincide in Raman and *IR*. Interestingly, both in Raman and *IR* several bands appear in the ν(C=N)/δ(NH range (1660–1530 cm^{-1}).

Almost all organic pigments are aromatic, many of them condensed. Consequently, they own numerous electronic states in *UV/VIS* and therefore, with *UV/VIS* laser excitation, produce extremely strong fluorescence which drowns all Raman-shifted lines. By using red (785 nm) or near *IR* (1064 nm) excitation and subtraction of the background, reasonable *RS* may be obtained in the medium and long-wavelength range. This is shown by Figs. 4.7–4.9. Despite these successful investigations, *IRS* is faster, cheaper and more specific than *RS* in the identification of organic pigments.

7 B. Schrader, University of Essen; K.-J. Eichhorn, D. Fischer, Institut für Polymerforschung, Dresden; P. Reich, K.-W. Brzezinka, BAM, Berlin-Adlershof

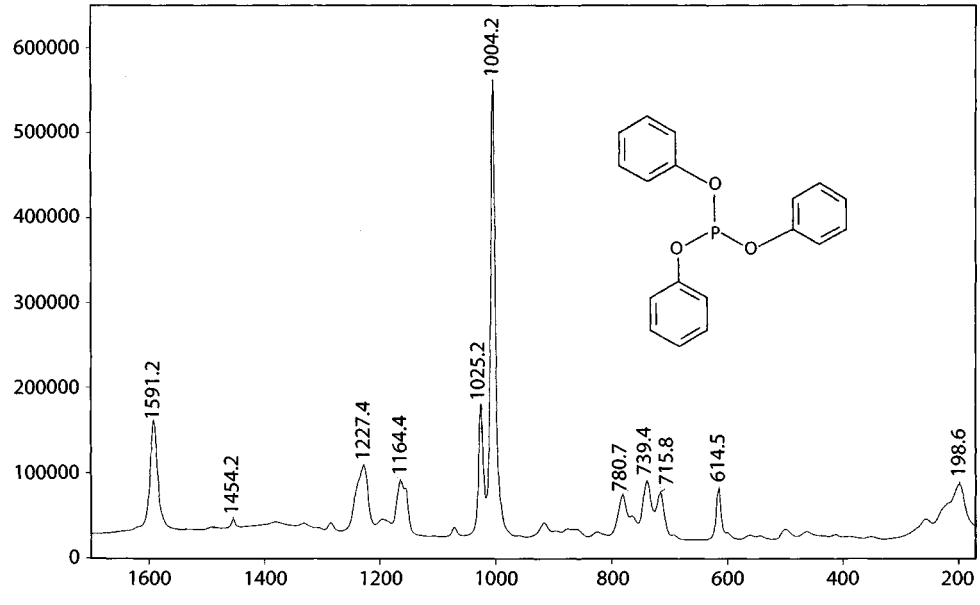


Fig. 4.3
Raman spectrum of triphenylphosphite (Ciba-Geigy). Conditions: Holoprobe, Kaiser Optics, 785 nm laser, resolution 0.6 cm^{-1}, 5-mm quartz cell, 2 s exposure, 20 scans. (Measurement by K.-J. Eichhorn and D. Fischer, IPF Dresden)

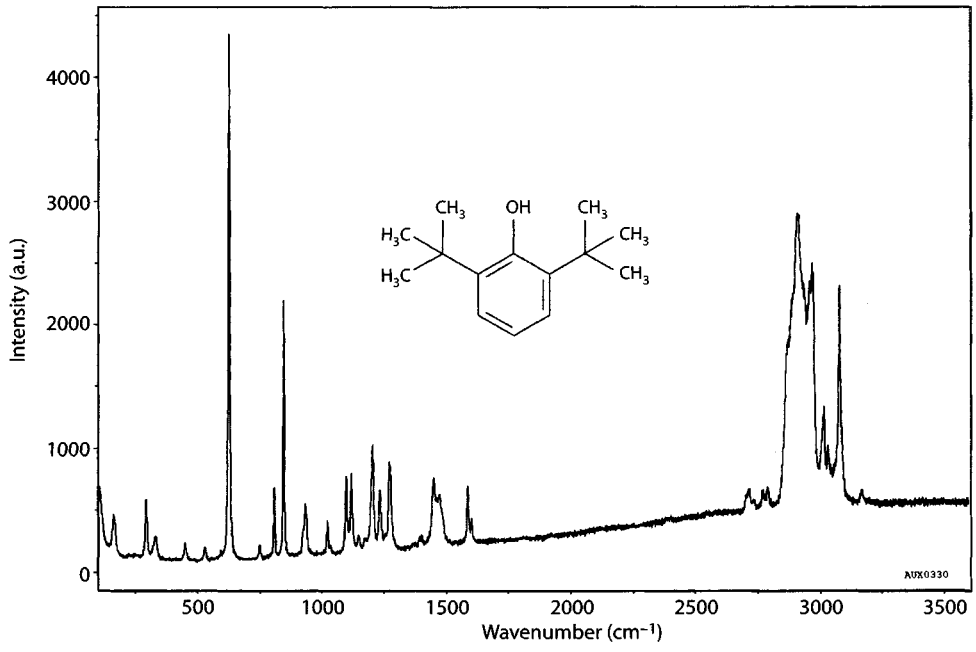


Fig. 4.4
Raman spectrum of 2,6-di-*t*-butylphenol (Ethyl). Conditions: DILOR-XY spectrometer with LN_2 *CCD* camera and BH2 Olympus microscope, 514.5 nm 10 mW laser. Peaks (cm^{-1}): 158, 288, 324, 445, 525, 622, 805, 843, 930, 1016, 1142, 1168, 1231, 1269, 1394, 1444, 1582, 1598, 2886, 2968, 3006, 3013, 3077. (Measurement by K.-W. Brzezinka, BAM, Berlin-Adlershof)

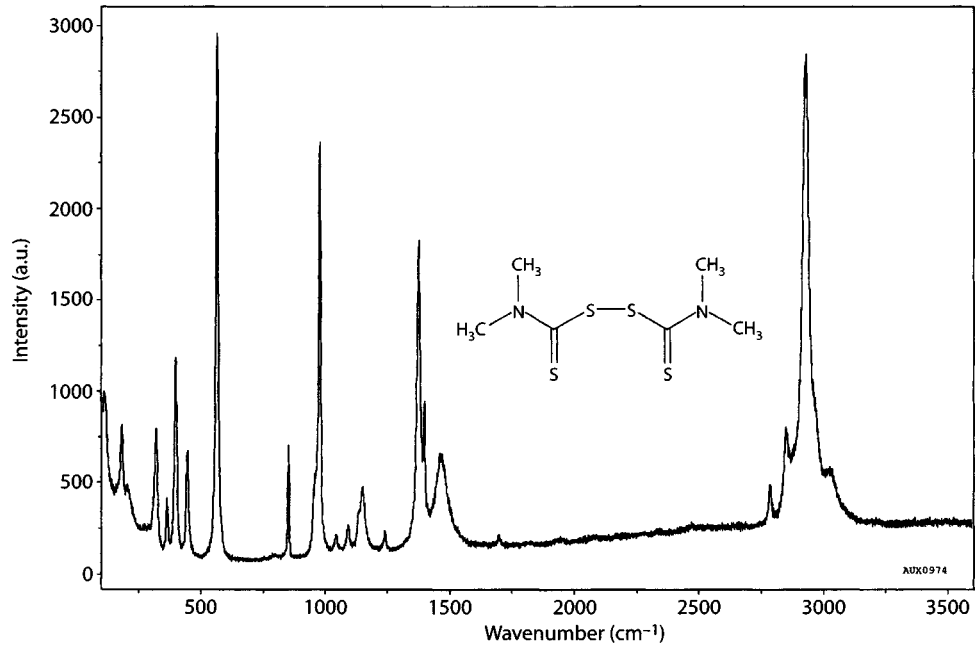


Fig. 4.5
Raman spectrum of tetramethylthiuramdisulfide (Perkazit TMTD, Akzo). Conditions as in Fig. 4.4. Peaks (cm^{-1}): 177, 317, 360, 393, 442, 559, 849, 973, 1040, 1088, 1147, 1234, 1371, 1395, 1463, 1694, 2783, 2847, 2927

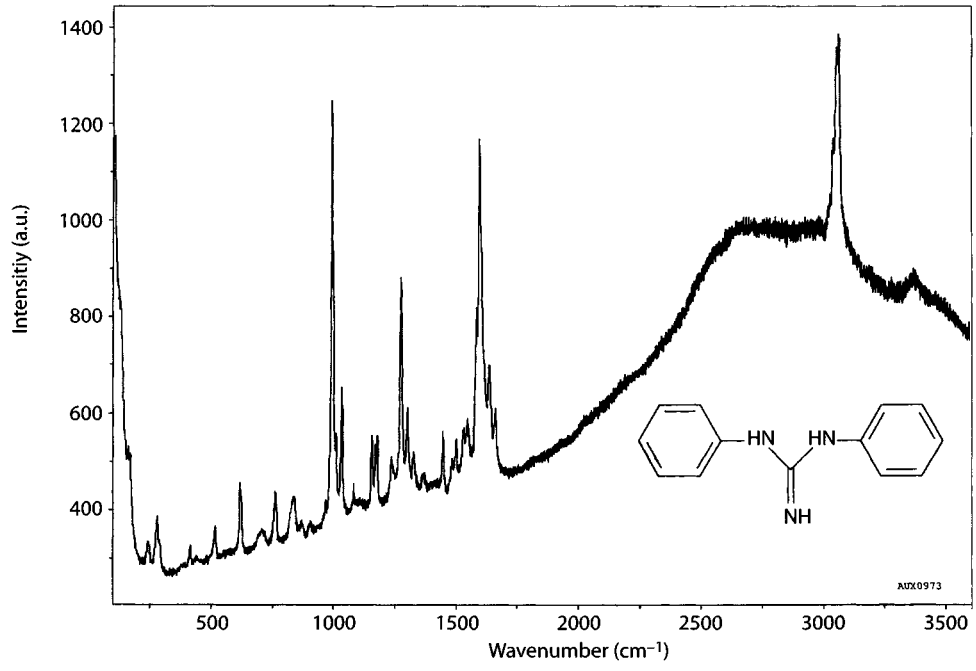


Fig. 4.6
Raman spectrum of 1,3-diphenylguanidine (Perkacit DPG, Akzo), fluorescence uncorrected. Conditions as in Fig. 4.4. Peaks (cm^{-1}): 241, 276, 513, 703, 760, 833, 1007, 1079, 1175, 1233, 1272, 1298, 1324, 1364, 1443, 1482, 1497, 1543, 1581, 1633, 1658, 3061

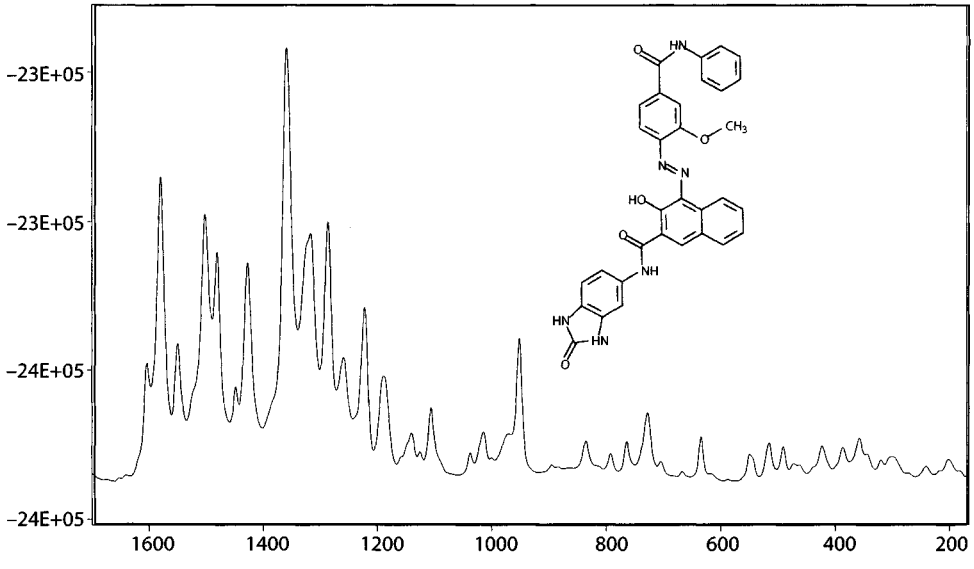


Fig. 4.7
Raman spectrum of pigment red 12515 (Novoperm Carmin HF3 C, Hoechst), background subtracted. Conditions as in Fig. 4.3, glass tube, exposure time 5 s. Peaks (cm^{-1}, strong and medium bands in the medium range): 1604, 1581, 1551, 1503, 1482, 1428, 1360, 1318, 1287, 1260, 1223, 1189, 1107, 952, 729, 634

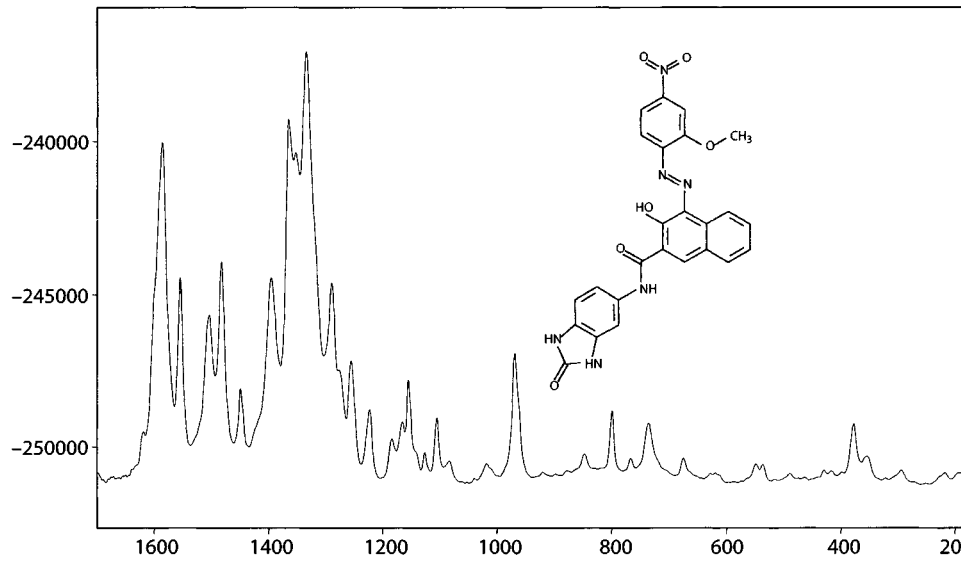
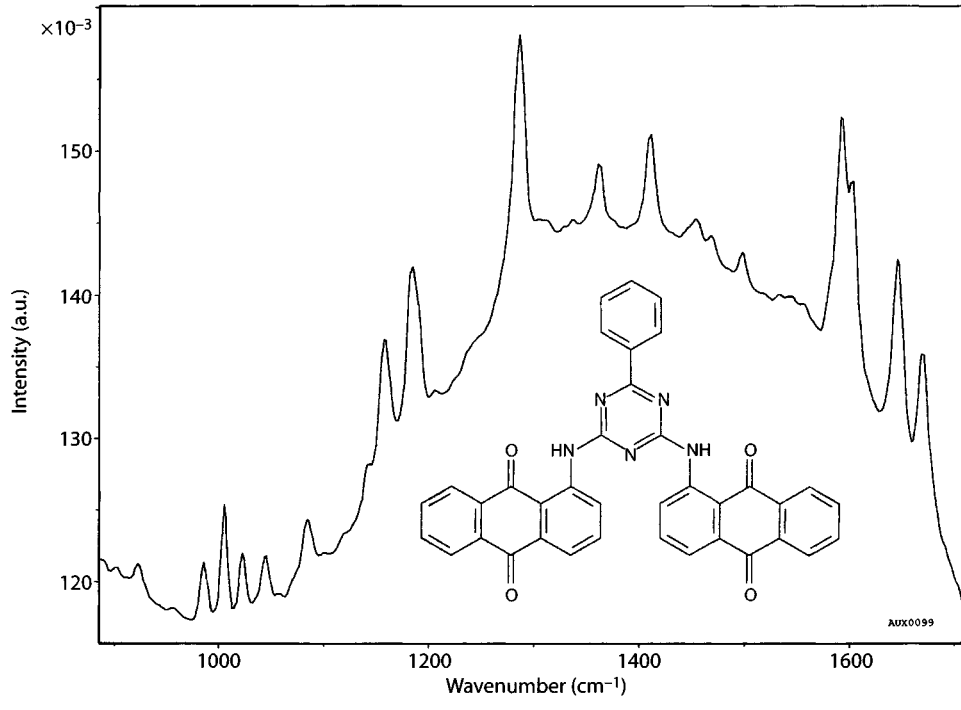


Fig. 4.8
Raman spectrum of pigment red 12512 (Novoperm Marron HFM01, Hoechst), background subtracted. Conditions as in Fig. 4.3, glass tube, exposure time 5 s. Peaks (cm^{-1}, only strong and medium bands): 1586, 1555, 1505, 1483, 1449, 1395, 1364, 1334, 1289, 1255, 1223, 1155, 1106, 969, 800, 736, 378



File:	H99g	Power:	75 mW, 1 mm	Time:	4195 sec	Detector:	D 418-S
Sample:	AUX0099	Filter:	Rayleigh	Accum:	2500 scans	LabelHor:	Wavenumber (cm^{-1})
Date:	10-10-2000	Spectro:	900 – 1750 cm^{-1}	Objectiv:	–	LabelVer:	Intensity (a.u.)
Operator:	Brzezinka	Slit:	–	Grating:	–	Hole.	6 mm
Excit_line:	1064 nm	Spec. width:	–	Remark:	217/00		

Fig. 4.9
Raman spectrum of pigment yellow 147 (Cromophtal Gelb AGR, Ciba-Geigy), *N, N'* -(5-phenyl-1,3-triazine)-*bis*(1-amino-9,10-anthraquinone), fluorescence uncorrected. Conditions: Bruker IFS66 V spectrometer, *FT*-Raman module FRA106, 75-mW 1064-nm laser, 2500 scans. Peaks in the medium range (cm^{-1}): 984, 1003, 1021, 1042, 1082, 1285, 1360, 1409, 1592, 1604, 1645, 1669. (Measurement by K.-W.Brzezinka, BAM, Berlin-Adlershof)

4.3 Raman Spectrometry Combined with Information-Enhancing Techniques for the Identification of Dyes and Pigments[8]

4.3.1 Subtracted Shifted Resonance Raman Spectrometry

Before we turn to so-called Raman microscopy (*RS* combined with optical microscopy) an interesting paper recently published by Bell et al. should be discussed. The authors, when investigating a Chinese, yellow-dyed, 9th century manuscript (*Diamond Sutra*), found Raman signals buried in fluorescence and noise. Known strategies (among others) to circumvent these problems were:

- Enhancing the Raman signal by, e.g. resonance *RS* or surface-enhanced *RS*
- Shifting of the exciting wavelength in a way that the Raman signals are remote from the range of fluorescence (which is rarely possible)
- Shifting of the exciting wavelength into a range where it would (hopefully) not generate fluorescence (Nd:YAG laser at 1.064 μm)

Surface-enhanced *RS* was not acceptable since the unique manuscript would have to be pressed on the reflecting metal surface and possibly be damaged. Shifting of the exciting wavelength (out of the near-resonance condition) was not possible since resonance *RS* was necessary to enhance the signals of the dye from the ones of the paper substance. Finally, *NIR*-excitation didn't promise success (and wasn't available).

The solution of the problem by the authors is impressive. The 100 mW 363.8 nm radiation of an Ar^+ laser was close enough to the *UV* absorption of the paper dye to perform resonance *RS*. The acquisition protocol was then first to record a spectrum under normal conditions, then shift the optics of the spectrometer by δ cm^{-1} (21 cm^{-1}) and record a second spectrum, and then move to the third position (2δ) for the final data acquisition of the cycle. These shifts are chosen to be sufficiently small that the background fluorescence remains approximately constant while the Raman bands follow the shifted spectrometer grating positions. To minimise the effect of changes in background fluorescence, this cycle was repeated several times. Typical accumulation times were 1–2 h. Subsequently, each of the shifted spectra is subtracted from the original *RS* thus yielding derivative-like spectra from which fluorescence and noise background has been almost eliminated. Curve-fitting of the difference data using a double-Lorentzian function (GRAMS 386 software) finally allows the reconstruction of *RS* in the usual presentation. (The results with shifts of δ and 2δ were quite similar.) The *RS* shown in this publication of two isolated dyes from *Phellodendron amurense* as well as of three different dyed papers are excellent and allow qualitative and semi-quantitative characterisations of dyes on organic carriers.

4.3.2 Raman Spectrometry Combined with Light Microscopy

The *VIS*-lasers used to excite Raman lines emit usually at 514.5 nm or 647.1 nm. This radiation is not absorbed by glass, and a Raman spectrometer can therefore be combined with conventional microscopic equipment including studies with polarised light. Microscopically small samples (down to a diameter of ca. 1 μm and a sample weight of a few nanograms) can first be localised and subsequently measured without remounting. This non-sampling method is unique for the identification of materials in, e.g. paintings, coloured manuscripts and forensic material.

In a pioneering work, Andersen accentuated the considerable increase in analytical reliability of Raman results by employing other physical or physico-chemical methods with the same sample. These techniques should be complementary in yielding information (elementary composition, crystal structure, chemistry of binders, etc.) the *RS* does not comprise. Andersen used, in addition to *RS*, scanning electron microscopy with energy-dispersive X-ray analysis for the identification of Naples yellow of different provenance. He found, in addition to $Pb_3(SbO_4)$ (the supposed constituent of Naples yellow), bindheimite, valentinite, cerussite and crocoite (see Table 4.1). In a delustered spandex fibre he found rutile as a pigment.

Ten years later, Clark, Best and coworkers started a series of fascinating publications on the identification of pigments in mediaeval paintings and manuscripts.

The result of these elaborate investigations was the identification of pigments in coloured initials or in other illuminated parts of choir books (13th and 16th century), in a 13th century Lucka bible (Paris), in an Icelandic law code, in a Byzantine/Syriac gospel lectionary (13th century) and in other old manuscripts, in paintings of Titian and Veronese.

Table 4.1 (taken from these papers, together with some information from other sources) presents colour, name and chemical composition of commonly used inorganic pigments, whitenings and fillers. These authors also made a study of the performance of accompanying methods which is interesting enough to be reproduced as Table 4.2.

In a few cases I do not agree. Specificity is, at least basically, excellent for both *IRS* and *RS*; they are twins. In *RS* the intensity of a Raman line depends not only on the change of polarisability of a molecule or a chemical group during a

8 Literature: 10.2.3

Table 4.1
Inorganic pigments of artistic, forensic and industrial importance (after Best et al., 10.2.3/1, Andersen, ibid., Clarc, ibid. 1, own sources)

Colour	Common name	Chem. formula	Remark
Black	Charcoal, carbon	C	
Blue	Azurite	$2CuCO_3 \cdot Cu(OH)_2$	Basic copper carbonate
	Cerulean blue	$CoO \cdot nSnO_2$	Cobalt stannate
	Cobalt blue	$CoO \cdot Al_2O_3$	Co-doped alumina glass
	Egyptian blue	$CaCuSi_4O_{10}$	Cuprorivaite
	Lazurite (from lapis lazuli)	$Na_8(Al_6Si_6O_{24})S_n$	S radical anions in a Na Al-silicate matrix
	Manganese blue	$Ba(MnO_4)_2$+$BaSO_4$	
	Posnjakite	$CuSO_4 \cdot 3Cu(OH)_2 \cdot H_2O$	
	Prussian blue (Berlin blue)	$Fe_4[Fe(CN)_6]_3 \cdot 14H_2O$	
	Smalt	$CoO{\cdot}nSiO_2$(+K_2O+Al_2O_3)	Co silicate
	Verdigris	$Cu(CH_3CO_2)_2 \cdot 2Cu(OH)_2$	Basic Cu acetate
Green	Green earth (celadonite+glauconite)	$K[Al^{3+},Fe^{3+})(Fe^{2+},Mg^{2+})] \cdot$	Hydrous alumosilicate of Mg, Fe and K
		$Al(Si_3/Si_4O_{10})(OH)_2$	Mg, Fe and K
	Malachite	$CuCO_3 \cdot Cu(OH)_2$	Basic Cu carbonate
Orange to	Cadmium orange	Cd(S,Se)	Cadmium selenosulfide
Brown	Ochre (goethite)	$Fe_2O_3 \cdot H_2O$+clay	
Red	Cadmium red	CdSe	
	Litharge	PbO	Lithargyrum
	Realgar	As_4S_4	
	Red lead	Pb_3O_4	Minium, Pb orthoplumbate
	Vermilion	HgS	Cinnabar
White	Anatase	TiO_2	
	Baryte	$BaSO_4$	
	Bone white	$Ca_3(PO_4)_2$	Ca orthophosphate
	Cerussite	$PbCO_3$	
	Chalk	$CaCO_3$	Calcite, whitening
	Gypsum	$CaSO_4 \cdot 2H_2O$	
	Kaolin	$Al_2(OH)_4Si_2O_5$	Layer alumosilicate
	Lead white	$PbCO_3$	
	Lithopone	ZnS+$BaSO_4$	
	Rutile	TiO_2	
	Vienna lime	(Ca,Mg)CO_3	Dolomite
	Zinc white	ZnO	
Yellow	Bindheimite	$Pb_2Sb_2O_6$(O,OH)	Cubic
	Cadmium yellow	CdS	
	Chrome yellow	$PbCrO_4$	
	Cobalt yellow	$K_3[Co(NO_2)_6]$	
	Crocoite	$PbCrO_4$	
	Lead antimonate yellow	$Pb_2Sb_2O_7$ or $Pb_3(SbO_4)_2$	
	Lead tin yellow	Pb_2SnO_4	
	Massicot	PbO	
	Monimolite	$Pb_3(SbO_4)_2$	
	Naples yellow	$Pb_3(SbO_4)_2$	May also be valentinite or cerussite+crocoite
	Orpiment	As_2S_3	Auripigment, royal yellow
	Valentinite	Sb_2O_3	Orthorhombic

Table 4.2
Strengths and weaknesses of the main techniques available for pigment analysis (Best, Clark, Withnall, 10.2.3)

Technique	In situ	Specificity	Sensitivity	Spatial resolution	Immunity to interference
SEM[a]	?	Bad[b]	Good	Excellent	Good
XRF[c]	?[d]	Good	Good[e]	Good	Good
XRD[f]	-	Good	Fair[g]	Poor	Poor
PIXE/PIGE[h]	Yes	Good	Good[i]	Poor	Good
Raman	Yes	Excellent	Good [x]	Excellent	Fair[j,l]
IR	Yes	Excellent[l]	Good	Fair	Fair[l]
Optical microscopy	Yes[k]	Poor	Good	Fair	Fair

a Scanning electron microscopy
b Except where used in conjunction with an energy-dispersive *X*-ray analysis attachment
c X-ray fluorescence
d With appropriate modifications *in situ* studies may be performed, but with a loss of spatial resolution
e Elements heavier than K
f X-ray diffraction
g Increases with atomic number
h Particle-induced X-ray emission
i Simultaneous analysis of all elements with atomic number >9; Li, Be, B and N can also be detected with high sensitivity
j Fluorescence can be an interference
k Polarisation studies require samples to be removed
l My judgement

vibration but also on the state of the system. To give just one example: one and the same substance in the amorphous state may produce a poor *RS* which may even be drowned by fluorescence (e.g. certain natural and synthetic resins) whereas, in the crystalline (pure!) state, this substance produces a fine *RS* with sharp bands. Another problem is presented by strongly emitting groups. Substances with long aliphatic or ethyleneoxide chains exhibit an extremely simple *RS*; it consists only of the very intense $\nu(CH_2)$ pair whereas other structural details can hardly be seen. Polar groups, in the *RS*, make weak bands whereas, in the *IRS*, they produce strong ones. The situation is *vice versa* for nonpolar groups or molecules. To express it as simple as possible: *if* a good *IRS* or *RS* can be obtained both are highly specific.

Immunity to interference is another point of discussion. If the analyst wants to identify a pigment by *RS* and the binder fortunately is a "weak emitter" he feels lucky. If he wants to identify the binder he has bad cards. Certainly, minor constituents below 5–10% are difficult to "see" in the *IRS*. Each component contributes, however, with its own partial spectrum to the *IRS*. A drop in the similarity score of the *IRS* of the analyte as compared with the *IRS* of the main component reveals the mixture and allows tricks like subtraction of the *IRS* of the main component.

The technique of Raman microscopy (Fig. 4.10) is described in more detail by these authors (slightly changed text). The incident laser beam is passed through a beamsplitter (B_1), converted into a parallel beam by lens L_1 and focused on the sample using a microscope objective. The Raman radiation retraces the path of the incident laser beam as far as the beamsplitter B_1, where half of the radiation is directed into the monochromator.

Two aspects of the optical configuration are of particular importance for pigment analysis. First, collinear with the final leg of the path of the incident laser beam is the white-light beam of a conventional microscope. Thus, selection of the particle to be examined is achieved in the same way as in optical microscopy. Selection of either white-light or laser illumination is accomplished using the swing-away mirror. Second, in the optical train between the microscope and the

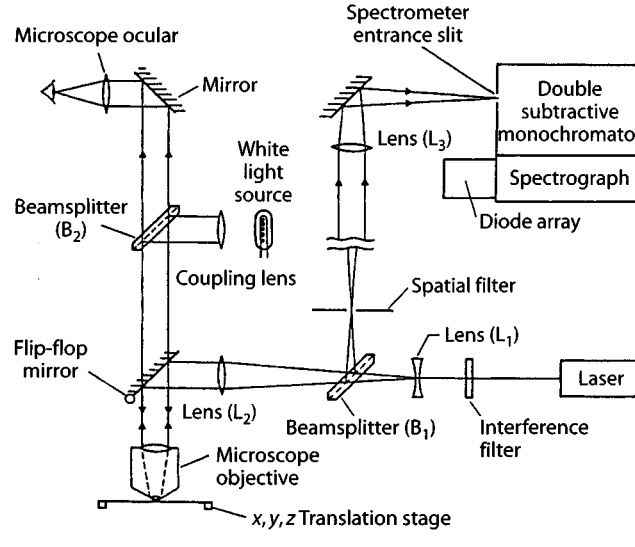


Fig. 4.10 The optical configuration of a Raman microscope (S.P. Best et al., 10.2.3/2)

spectrometer is a secondary focus. The accurate location of an aperture at the focal point improves the spatial resolution of the experiment, and this has allowed the collection of Raman spectra at different depths within the sample (depth profiling) in favourable cases. In circumstances where the Raman signal due to the pigment is swamped by fluorescence an enormous reduction in the fluorescent signal can be achieved by use of the aperture at the secondary focus.

Another group around B.W. Singer (Davey et al.; Singer and Cahaner) used Raman microscopy for the identification of pigments used in water-colour works on paper and in Indian miniature paintings. The first paper is realistic in showing also Raman spectra where fluorescence almost drowns the Raman signals. The authors expect that red and near-infrared lasers will reduce fluorescence due to media or organic pigments. They announce a library of Raman data on both traditional and modern pigments (which is highly desirable). Table 4.3 shows Raman data of inorganic pigments collected from the literature.

Finally, a recent paper of Edwards et al. should be mentioned which deals with the identification of pigments from wall paintings. Small samples ("about the size of a pin-head")were measured with a Fourier-transform Raman spectrometer equipped with a near-infrared Nd:YAG laser (1064 nm). The spectra shown are excellent and free from fluorescence.

Table 4.3
Raman bands (cm^{-1}) of selected inorganic pigments in alphabetic order (from Best et al., 10.2.3/1 and 2; Clark et al.; Davey et al., ibid.)

λ_{excit}/nm	Pigment	Band maxima (intensity)
514.5	Azurite	248(w) 404(vs) 770(m) 838(vw) 1098(m) 1424(w) 1578(w)
	Azurite, different	182(w) 251(m) 256(m) 408(m)
514.5	Bone white, $Ca_3(PO_4)_2$	965(m)
	Lapis lazuli	259(w) 549(vs) 807(w) 1096(m) 1355(vw) 1641(w)
514.5	Lead-tin yellow, Pb_2SnO_4	131(s) 197(m) 276(w) 291(w) 386(w) 458(w) 552(w, br)
514.5	Lead-tin yellow I, Pb_2SnO_4, other source	35(w-m) 58(w) 80(m) 129(vs) 196(m) 274(w) 291(w-m) 379(w) 454(w-m) 524(w) 613(w)
514.5	Lead-tin yellow II, $PbSn_{1-x}Si_xO_3$	40(m) 66(m) 85(sld) 138(vs) 324(w-m,br) 444(w,br)
514.5	Lead yellow, PbO, massicot	73(w) 88(m) 144(s) 291(m) 385(w) 425(w)
514.5	PbO, orthorhombic	385 (m) 424(w)
647.1	PbO, litharge, tetragonal (reddish)	81(s) 147(vvs) 322(vw) 338(s)
	Malachite	225(w) 274(w) 355(w) 437(m) 516(vw) 540(w) 724(w) 757(vw) 1064(w) 1104(w) 1372(w) 1498(m)
647.1	Minium, Pb_3O_4	121(vs) 152(m) 223(w) 232(w) 313(w) 391(w) 477(w) 549(s)
	Orpiment, As_2S_3	136(m) 154(m) 179(w) 203(m) 293(s) 311(s) 355(s) 384(m) 587(vw)
647.1	Orpiment, different sources	23(w) 34(w) 60(w) 67(w) 104(w) 134(m) 152(m) 177(w) 200(m) 290(m) 308(m) 352(s) 357(m) 364(w) 380(w)
647.1	Realgar, As_4S_4	140(vw) 150(vw) 186(w) 201(w) 227(m) 231(m) 271(w) 340(w)
	Realgar, different sources	124(vw) 143(m) 166(w) 172(w) 183(s) 193(s) 214(w) 222(s) 329(w) 345(m) 355(s) 370(w) 376(w)
	Red lead	121(vs) 152(m) 223(w) 232(w) 313(w) 391(w) 477(w) 549(s)
647.1	Red ochre	224(w) 290(w) 295(w) 406(vw)
	Red ochre, diff.s.	225(w) 295(m) 413(m) 621(w-m)
514.5	Tin(IV) oxide	634(w)
647.1	Vermilion	40(vs) 251(s) 281(vw) 340(w)
	Vermilion, different sources	254(s) 281(w) 344(m) 253(s) 283(w) 343(m)

5
Spectrometry in the Ultraviolet and Visible Regions

5.1
Fundamentals

Resonance absorption in the ranges 200–400 nm (50,000–25,000 cm^{-1}, near *UV*) and 400–800 nm (25,000–12,500 cm^{-1}, *VIS*)[9] is caused by electronic transitions. Formally, these are accompanied by vibrational and rotational transitions; the whole spectrum can, however, be resolved only for free (gaseous) molecules and with high-resolution instruments. The *UV/VIS* spectra of condensed matter exhibit few and broad bands (non-resolvable vibrational broadening) which are hardly substance-specific. (Citation from D.A. Wheeler, 10.2.2: Ultraviolet spectroscopy is not a good tool for the identification of unknown constituents since it is non-specific and subject to many interferences.) The bands in the near *UV* belong to electronic transitions of chromophoric groups like double or triple bonds and aromatic ring systems. Certain other (bathochromic) functional groups shift the absorption of chromophoric groups into the visible range. This is important for coloured pigments and dyes. (The reason why *UV* measurements below 190 nm are only possible with evacuated spectrometers is the absorption of atmospheric O=O.)

There is (at least) one distinct advantage of *UV/VIS* over *IR* spectrometry – the very high molar absorptivities. These may go up to 10^3 m^2 mol^{-1} which is about 100 times higher than the molar absorptivities of medium intense *IR* bands. ν(C=O), e.g. may reach 50 m^2 mol^{-1}. This is the reason why *UV/VIS* is frequently used for the quantitative analysis of dissolved, absorbing species (spectrometry, colorimetry). Care has to be taken, however, that a moderately absorbing component (to be determined) is not superimposed by a strongly absorbing impurity.

Another important point is the integrating nature of *UV* bands. Thus, members of homologous species carrying the same chromophoric group produce the same absorption band(s), though with different molar absorptivities; consequently, they can be analysed as a "family". Closely related compounds like 2,4,6-alkylsubstituted phenols (alkyl does not absorb in the *UV/VIS* ranges) have at least one common band and can also be determined jointly. If molar absorptivities are related only to the band of the analytical group, they may be equal or very close.

The third and final point is that more qualitative and especially quantitative information can be extracted from *UV/VIS* spectra by calculating higher derivatives. This is made possible by the large signal-to-noise ratio of these spectra. By forming derivatives shoulders may become peaks and weak peaks grow into a quantitative range. Absorption peaks, in derivatives with odd number, become points of inflection; in derivatives with even number they remain peaks but with increasing sharpness (with negative satellites on both sides).

5.2
Antioxidants

A review of methods proposed for the analysis of antioxidants in polymeric materials, cast in the form of a step-by-step examination of the problems involved in any scheme of analysis, with a critical appraisal of the published procedures designed to overcome them was published by D.A. Wheeler (10.2.2[10]) in 1968. It contains chapters on Analysis *in situ*, Analysis after separation, Identification of separated antioxidants, Quantitative analysis and no less than 132 citations up to 1967. The *UV/VIS* paragraph is short and concentrates mainly on quantitative analysis by (spectroscopic) colorimetry.

Scholl (Hummel/Scholl, 10.1/2), in a chapter on *UV* spectrometry of antioxidants (AO), referred to the high absorptivities of phenols and aromatic amines which makes them apt for quantitative determination in the presence of additives without chromophoric groups. For the same reason aromatic additives in optically clear films of aliphatic polyhydrocarbons can be determined without extraction (see below). The fact that phenolates absorb 20–40 nm higher (red shift) than the respective phenol allows the distinction of phenolic AO with different degrees of steric hindrance (see below). AO

9 This partition is wholly for instrumental reasons.

10 Same for all following citations.

without *o,o'*-substitution are deprotonated already by very weak methanolic alkali; *o,o'*-di-*t*-butylphenols need up to 3 N alkali, and even then the deprotonation is a slow process. In the case of 4,4'-methylene-*bis*(2,6-di-*t*-butylphenol) the deprotonation by methanolic N alkali is not yet complete even after 20 h. Also, 2,6-di-*t*-butyl-4-methylphenol needs methanolic 3 N KOH to be (almost) completely deprotonated. Table 5.1 shows the values of A_{max} for a number of phenolic AO and their phenolates (from Scholl, l.c.).

The direct *UV* analysis of an AO in molten polyethylene (PE) was described by Albarino. PE is free of *UV* absorptions but, in its partially crystalline state, scatters *UV/VIS* (low signal-to-noise ratio). The author therefore investigated molten PE samples at temperatures around 130 °C and, depending on the concentration of 2,6-di-*t*-butyl-4-methylphenol (AO1), film thicknesses between 30 μm (0.1% AO1) and 780 μm (0.01% AO1). The analytical wavelength was 280 nm, the concentration measure was the absorbance A_{an} between A_{max} and the intersection with the baseline. For 30 μm/0.10% AO, A_{an}=0.180, for 780 μm/0.01% AO1, $A_{an.}$=0.42. The quantitative evaluation for A_{an} *vs* film thickness was very good. The molar absorptivities at 280 nm were between 815 m^2 mol^{-1} and 795 m^2 mol^{-1} with an average of 807 m^2 mol^{-1}. The method described here will (to my opinion) be applicable to other (*UV* non-absorbant) and non-scattering (amorphous) polymers. Prerequisite is of course that the AO withstands thermal treatment and will not evaporate.

The first to employ derivative spectrometry for the determination of phenolic antioxidants (AO) in low-density PE were Pump and Woltjes. Contrary to the technique of Albarino, these authors used high-temperature (140 °C) pressed and quenched (amorphous) pellets for their measurements. The AO were 2,6-di-*t*-butyl-4-methylphenol (I), 4,4'-thio-*bis*(2-*t*-butyl-5-methylphenol) (II) and 1,1,3-*tris*(2-methyl-4-hydroxy-5-*t*-butylphenyl)butane (III). The chromophoric groups were similar, and consequently the analytical band for I–III was almost at the same wavelength, namely 280 nm. The interesting point is that in the second derivative these AO were easily distinguishable, and even the second derivative of the spectrum of a mixture of II and III allowed a quantitative evaluation.

The authors showed in the same publication that second derivatives also in the case of *VIS* spectra can be of considerable advantage. As examples, the "tedious" spectra of blue, yellow and orange transparent LDPE films gain considerable information in the second derivative.

Soon afterwards, Nuyken and Talsky followed with a paper on high-resolution higher-order *UV/VIS* derivative spectrophotometry (*HODS*) for copolymer composition, determination of unconverted monomer in polymers and analysis of polymer additives. In the latter case, the analytical system was Irganox 1010 (AO1, see above) down to 0.05% in polystyrene (!). AO1 reveals itself only by a weak shoulder at the red flank of a very intense PS band. In the fourth and fifth derivative, the band of AO1 is well separated from the PS absorption and can be used for quantitative analyses; the calibration lines show very good linearity.

Soucek and Jelínková investigated a case where the *UV* spectra of the two investigated AO (2,6-di-*t*-butyl-4-methylphenol, AO1, and a 4-alkylsubstituted 2,6-xylenol, AO2) were qualitatively so similar that also the second derivatives of the spectra were indistinguishable. (The molar absorptivity of AO1 at 283 nm was 195.6 m^2 mol^{-1}, the one of AO2 50.6 m^2 mol^{-1}.) The problem was solved by the bathochromic effect

Table 5.1
Values of A_{max} in the *UV* for a number of phenolic antioxidants (in methanol) and their phenolates (in 0.1 *N* methanolic KOH). Concentrations: 0.25–1.0 mg cm^{-3}

Chemical name	Trade name	A_{max}/nm
2,6-Di-*t*-butyl-4-methylphenol	ASM KB	278, 283
phenolate[a]		306
4,4'-Dihydroxydiphenyl	ASM DOD	266
phenolate		ca. 296
4,4'-Methylene-*bis*(2-methyl- 6-*t*-butylphenol)	Antioxidant 720	283
phenolate		309
2,2'-Methylene-*bis*(4-methyl-6-*t*-butylphenol)	CAO 5	278
phenolate[a]		303 sld
4,4'-Thio-*bis*(3-methyl-6-*t*-butylphenol)	Santowhite crystals	248, 282
phenolate		262
2,2'-Thio-*bis*(4-methyl-6-*t*-butylphenol)	CAO 4	294
phenolate		296, 316
N-Lauroyl-4-aminophenol	Suconox 12	248
phenolate		266

a Incomplete deprotonation

of deprotonation of the phenolic group of AO2. AO1, due to the steric hindrance by the *t*-butyl groups, is difficult to deprotonise by weak bases. AO2 is deprotonated already by weak alkali; the band maximum shifts from about 280 nm to 298 nm. This works also with mixtures of the two AO.

Polypropylene was stabilised with the following mixtures: 0.03–0.15% AO1 and 0.1–0.2% AO2. Stabilised sheets (0.5 mm thick) were cut into pieces of 50×50 mm^2, weighed and refluxed 3 h in 50 cm^3 of boiling heptane; >98% of AO were extracted by this procedure. The heptane extract was transferred quantitatively into a 50-cm^3 calibrated flask and made up to the mark with heptane (solution A). The solution of phenolics (B) was made from 8 cm^3 A and 2 cm^3 2-propanol. Solution of phenolate (C) was made from 8 cm^3 A and 2 cm^3 of 0.005 mol dm^{-3} KOH in 2-propanol. Concentrations of the solutions used for measurement corresponded to extraction of AO from 1 g of a stabilised sheet into 50 cm^3 of heptane.

The principle of the analytical procedure was as follows. First, AO2 is determined by second derivative difference spectrometry of the bathochromically shifted, basified extract using the non-basified extract as a reference. The second derivative spectral amplitudes of non-basified extracts are additive for both AO. The contribution of AO2 to the total second derivative amplitude is then subtracted, and the residual corrected amplitude corresponds to AO1.

5.3 Light Stabilisers

Light stabilisers are frequently hindered amines (HALS). The aliphatic ones usually do not absorb in the *UV*. Some HALS, however, contain aromatic groups. For the polymeric HALS Chimassorb 944 (LS1, CIBA-Geigy), e.g. the chromophore is a melamine derivative (2,4,6-aminosubstituted 1,3,5-triazine). This is used for the light stabilisation of polypropylene (PP).

Freitag (10.2.2) investigated the system PP/LS1 by *UV* spectrometry. Extraction of a polymer additive by solvents is inefficient; the author preferred therefore the separation of LS1 by solution precipitation.

Decalin – with 0.1% *tetrakis*[methylene-3-(3′,5′-di-*t*-butyl-4′-hydroxyphenyl)propionate]methane as an antioxidant – was used as solvent. Here 1.00 g of the LS1-stabilised PP was dissolved in 100 cm^3 solvent at 150 °C bath temperature during max. 40 min with stirring. The solution was allowed to cool down to room temperature without stirring, PP precipitated. The suspension was agitated ultrasonically for 5 min, then quantitatively transfered to a separatory funnel and extracted with 100.0 cm^3 N sulfuric acid containing 0.5% diethanolamine. The latter proved to be useful in preventing the adsorption of LS1 on the glass walls. Phase separation takes several hours, the aqueous phase was used for the *UV* measurement. A_{max} at 245 nm was compared with the same band of the calibration solution. The latter was prepared by dissolving 1.00 mg LS1 in 100.0 cm^3 N sulfuric acid containing 0.5% diethanolamine. The measurements were made between 200 nm and 350 nm using a 1 cm quartz cell and N sulfuric acid in the reference beam; the absorbance range was 0–2.

As a standard, PP was mixed with 0.3 wt% LS1 and extruded. Here 96% of the LS1 was found by the process described; down to 0.01% (or even somewhat less) of LS1 can be determined quantitatively. *UV* absorbers and phenolic antioxidants in the usual range of 0.05–0.5% do not interfere as they are separated off during the extraction step.

5.4 Pigments

Vibrational spectrometry (*IR* and Raman) is unsurpassed in the identification of organic and inorganic pigments. Raman microscopy in combination with scanning electron microscopy and X-ray analysis is excellent in the identification of micro-particles of pigments in objects of fine art or in forensic objects. It seems that *UV/VIS* spectrometry has little chance against these giants. Reflective[11] microspectrophotometry in the *VIS* range together with a computer program based on the Kubelka-Munk theory was, however, quite effective for the identification of pigments in small, forensic paint samples (Cousins et al., based on work by Laing et al., 10.2.3). The computer program allowed the prediction of the reflectance spectra of pigment mixtures from the reflectance spectra of individual components by the following equation: where $(K/S)_\lambda$=ratio of absorption to scatter at wavelength λ and R_λ=reflectance at wavelength λ expressed as a decimal

$$(K/S)_\lambda = \frac{(1-R_\lambda)^2}{2R_\lambda}$$

The *K/S* values are additive. To combine two individual spectra, *K/S* is calculated for both spectra and these are added together for each wavelength. The appertaining reflectances can then be calculated from the transposition of the equation given above.

The following wavelength ranges (nm) were observed in the reflectance spectra of some blue and green pigments:

11 A minimum in the reflectance curve corresponds to a maximum in the absorbance curve.

	Major peak	Minor peak(s)
Cu phthalocyanine blue	466–490	660–674
Metal-free phthalocyanine blue	486	670 sld
Prussian blue	450–470	
Indanthrone blue	430	740–746
Cu phthalocyanine green	498–518	710–714 762–770 sld

The equipment consisted of a Nanospec spectrophotometer (370–900 nm) combined with a Leitz microscope. (The former produced an artificial peak at 800 nm which sometimes disappeared or turned negative.) Different concentrations of the pigments were obtained by mixing the original paint with a rutile-based respray paint; the diluted paints were spread on glass microscope slides and dried. (Dilution usually yields reflection spectra with more details.) Pigment squares with known concentrations from the Hoechst catalogue were measured without further preparation.

Fuller (10.2.3) combined thin-layer chromatography with direct reflectance microspectrometry in the visible range. This allows the identification of soluble mono-azo pigments (red, some yellow) in tiny forensic objects. The pigments were extracted with CH_2Cl_2, 1,2-dichlorobenzene or dimethylformamide, spotted on Merck DC aluminium sheets, pre-coated with silica gel 60F254 (activated 1 h at 110 °C), and developed with chlorobenzene/1,2-dichloroethane/toluene 1:1:1 (by volume). R_f values were given for a few pigments:

Pigment red	2	0.15
	3	0.13
	4	0.39
	5	0.00
	6	0.24
	10	0.14
	11	0.13
	12	0.09
	112	0.12
Pigment orange	5	0.24
Pigment yellow	1	0.30
	3	0.49
	12	0.26
	17	0.25
	73	0.28
	74	0.16

The *VIS* spectra (380–900 nm) were measured directly in remission from the plates[12]. They are good (with the exception of a constant artefact at 803 nm) and are apt for a characterisation of (soluble) pigments.

The majority of the 72 pigments investigated were insoluble. Spots of the suspended material were applied to *TLC* plates – even though no elution was possible – and measured in reflection.

Bacci et al. (10.2.3/1) investigated the inorganic pigments in frescoes by *VIS* (400–800 nm) reflection spectrometry. The spectral characteristics of pigment standards are presented in Table 5.2. The spectra showed usually one intense and broad band, sometimes with a shoulder or a weaker neighbouring band. Band width and to some extent also λ_{max} of a pigment depended on whether this pigment was measured as pure sample (powder) or in a fresco. The intensities along a reflection curve depended on grain sizes. In a second publication Bacci et al. applied fibre optic reflectance spectroscopy (400–1000 nm) for the identification of inorganic pigments used in paintings. The use of first derivatives of the reflection curves increased somewhat the possibility to distinguish different pigments.

5.5 Plasticisers

Chromophoric groups in plasticisers are almost exclusively benzo-aromatic systems. Esters of aliphatic alcohols with a defined aromatic acid form families with very similar *UV* spectra, i.e. phthalates, isophthalates, trimellitates etc. The same is true for phenolic esters of phosphoric acid. The following small compilation may be helpful (values in nm):

Dialkylphthalates	215	274	280	
Dialkylisophthalates	215	274	281	288
Trialkyltrimellitates	235	283	290	
Triphenylphosphate	254	259	266	
Tricresylphosphate	263	269		
Trixylenylphosphate	255	262		

12 This method resembles the (superior) measurement of *TLC* spots directly with Raman microscopy by Adams and Gardner and later by von Czarnecki (both 10.2.8).

Table 5.2
Spectral characteristics (400–800 nm in reflection) of pigments used in the fresco technique (Bacci et al. 10.2.3/1)

Colour	Pigment name	Chemical composition	Reflectance peaks (nm)
Red	Sinopia	Fe_2O_3	660 sld 750
	Haematite	Fe_2O_3	650 sld 745
	Pozzuoli red	Fe_2O_3	640 sld 746
	Red bole	Aluminosilicate with Fe_2O_3	650 sld 750
	Cinnabar	HgS	<630: strongly reduced reflectance
	Minium	Pb_3O_4	<620: strongly reduced reflectance
Yellow	Yellow ochre	Alumosilicate with (Fe_2O_3,H_2O)	450 600 760
	Orpiment	As_2S_3	790<600: strongly reduced reflectance
Green	Green earth	Alumosilicate with Fe^{3+}/Fe^{2+}	556 680>800
	Verona earth green	same	550 610
	Malachite	$CuCO_3 \cdot Cu(OH)_2$	518
Blue	Azurite	$2CuCO_3 \cdot Cu(OH)_2$	454
	Ultramarine blue, lapis lazuli	Alumosilicate	460 610 sld 770
Brown	Brown ochre	Alumosilicate with (Fe_2O_3,H_2O)	460 610 sld 770
	Sienna	Same	450 sld 620 sld 760

6
Nuclear Magnetic Resonance (*NMR*) Spectrometry

6.1
Fundamentals

All nuclei whose mass number is not divisible by 4 have a nuclear magnetic spin (*NMS*) moment. The magnitude of this moment depends on the kind of nucleus. If a chemical system containing equal nuclei with an *NMS* is brought into a strong magnetic field, then the direction of these moments is (at least partially) aligned. When a tunable microwave source is arranged perpendicular to the magnetic field, the spins of the aligned nuclei will flip over at a defined micro-wavelength. (This is not a periodic process. With intense microwave radiation we observe spin saturation.) The exact value of this wavelength is influenced by the chemical neighbourhood of the nucleus in question (chemical shift) as well as by adjacent nuclear spins (spin-spin coupling). The position of a resonance is given on the abscissa relative to a standard, usually tetramethylsilane (= 0). The (maximal or integrated) intensity of a resonance peak is proportional to the amount of nuclear spins being in resonance. This is important for quantitative analyses.

In order to get highly resolved *NMR* spectra with sharp resonances, the sample has to be liquid or dissolved in a liquid (randomly oriented spins). The solvent itself should have a simple *NMRS* with but few resonance lines ($CDCl_3$ is rather optimal). This reduces the applicability of *NMRS* for additive analyses to some extent. A way out would be the use of magic angle spinning *NMRS*.

A wealth of empirical *NMR* data has been collected over the years; this helps in assigning the resonance lines in (the sometimes quite complicated) *NMRS*. Mixtures can be analysed quantitatively if a typical resonance line can be found for each component.

Most frequently used nuclei are ^{1}H and ^{13}C; ^{31}P is important for phosphate ester plasticisers, phosphite antioxidants, flame inhibitors and other P-containing additives. ^{13}C is a rare C-isotope; however, modern *NMR* spectrometers are sensitive enough to produce good resonances. These are very sharp since it is close to impossible that two adjacent ^{13}C nuclei are found in a molecule. *NMR* spectrometers have to be tuned for each analytical nucleus.

6.2
Applications

Literature on *NMRS* of additives is scarce. Freitag and Lind (10.2.2) extracted the following antioxidants exhaustively from polypropylene plaques (5 g) with $CHCl_3$ and determined them quantitatively by analytical proton resonances: 2,6-di-*t*-butyl-4-methylphenol (BHT, 7.0 ppm, aryl-H), 3,3′-thio-*bis*(propanoic acid didodecyl ester) (DLTDP, 4.1 ppm, -CH_2-COO-), octadecyl-3-(3′,5′-di-*t*-butyl)-4′-hydroxyphenyl-propionate (Irganox 1076, 7.0 ppm), and *tetrakis*(methylene-3-(3′,5′-di(*t*-butyl-4′-hydroxyphenyl)-propionate)methane (Irganox 1010, 7.0 ppm). A polymeric light stabiliser of the hindered amine class (Tinuvin 622) was separated from a low-density polyethylene blown film by the following process: 5 g of the film were dissolved in boiling toluene. The solution was allowed to cool to room temperature, LDPE precipitated. The analytical resonances were 2.5 ppm (-OCO-CH_2-CH_2-CO-O-) and 2.8 ppm (>N-CH_2-). In both cases, the solution was evaporated to dryness, and 1,4-dinitrobenzene (2 mg) in $CDCl_3$ (2 cm^3) was added as an integration standard. The solutions were concentrated to about 0.5 cm^3 and spectra were recorded at 100 MHz. At least three integrations were run. Owing to the presence of extracted atactic or low molar mass polymer, only signals at lower field than 2.5 ppm were considered.

The additive contents were calculated using the formula

$$\%\ additive = \frac{(W_{st} \cdot N_{st} \cdot I_a \cdot M_a)}{(W_p \cdot N_a \cdot I_{st} \cdot M_{st})}$$

with W_{st} the weight (mg) of integration standard applied, W_p the weight (mg) of polyolefin, N the number of protons corresponding to the integrated signal, I the peak area and M the molar mass of additive($_a$).

The error observed was 5–10%.

The method is useful for the determination of complex stabiliser mixtures in a single run. Furthermore, it is suitable for the analysis of polymeric stabilisers which are difficult to determine otherwise.

NMRS is frequently employed together with other physicochemical techniques for the analysis of complex polymer-ad-

ditive systems. Pierre and van Bree (10.2.8) used pyrolysis mass spectrometry (*MS*) together with[13] C-*NMRS* for the analysis of moulding compounds. The *NMR* spectra of complex additive mixtures were not disentangled for defined constituents but rather considered as "fingerprints". Examples were epoxidised soybean oil and chlorinated paraffins.

The authors report also on a ^{31}P *NMR* investigation of the behaviour of phosphite antioxidants during processing of the styrene-butadiene-acrylonitrile compound. The extract of the finished compound did not show the resonances of nonylphenol phosphite (as an example) but rather P-containing decomposition products.

Braun and Bezdadea (10.2.8) employed a combination of physico-chemical methods including ^{1}H-*NMRS* for the elucidation of the formation of plate-out[13] during the extrusion of PVC compounds. Typically, a compound being likely to produce plate-out had the following composition:

Substance	Action	Weight parts
Hard PVC		100
TiO_2 (Kronos A)	Pigment	4
Irgastab BC-29	Ba-Cd soap stabiliser	3
Irgastab CH-300	(R/Ar) phosphite co-stabiliser	0.5
Reoplast 39	Epoxidised soybean oil plasticiser	1.5
Irgawax 370, stearyl stearate	Slip additive	0.8
$CaCO_3$ (Omyalite)[a]	Filler	3

[a] $CaCO_3$ was added only to some mixtures.

Three parts of PVC compound or plate-out were refluxed for 8 h in 97 pts. of tetrahydrofuran, centrifuged for 2 h and decanted. The polymer was precipitated from the solution by gradually adding petrol ether. All additives with the exception of the inorganics and part of the main stabiliser Irgastab BC-29 stayed in solution. For the gravimetric determination, the insoluble was treated with 32% aqueous HCl, $CaCO_3$ went into solution. After washing and drying, the residue was treated with 98% H_2SO_4, metal soaps went into solution.

The ^{1}H-*NMRS* were measured with a 100-MHz instrument, solvent was THF-d_8. According to the spectra, the THF-soluble part of the compound and the plate-out were chemically quite similar. The assignments for quantitative determinations are given in the following compilation:

- Epoxy plasticiser/stabiliser
  5.26 ppm quintet, β-glyceryl protons
- Irgastab CH-300, isodecylphenylphosphite
  7.17 ppm, phenyl protons; aromatic: methylene protons = 1:4.5
- Irgastab BC-29
  6.76 ppm, one of the two doublets (the other one produces 7.06) from bisphenol A (4 protons), component of this stabiliser; pentaerythritol interferes
- Lauroyl
  1.2 ppm $(CH_2)_9$, 0,95 ppm CH_3 triplet
- Irgawax 370, >90% stearylstearate
  4.00 ppm, methylene-oxycarbonyl; other substances with this group interfere.

13 Plate-out is the deposit of organic matter from a polymer compound during extrusion or calendering on metallic surfaces of the machinery.

7
Mass Spectrometry

7.1
Fundamentals

7.1.1
Mass Separation

Modern mass spectrometry (*MS*) began around 1920 with the work of Aston, Mattauch, Herzog and Dempster: the (positive) ions, produced by electron impact on the molecules of the (volatile) analyte, were – in a high vacuum of $<10^{-4}$ Pa – accelerated in an electrical field and separated according to their m/z values in a magnetic sector field (m=relative molecular mass, z=number of elementary charges, usually 1, sometimes 2). Afterwards they were caught successively in Faraday cages, and the electrical ion currents were measured. The single-focusing mass spectrometers of today have the same principle. Their resolution, $m/\Delta m$ is about 10^3; this means that the mass numbers 1000 and 1001 (10% valley) can be determined separately. Double-focusing spectrometers have, after the accelerating field, an additional homogeneous electrical field; their resolution is 10^5–10^6. The time needed for the scanning of a highly resolved *MS* is of course longer than that needed for a single-focus *MS*. The considerable advantage of high-resolution *MS* is the possibility to distinguish between (almost) isobaric masses having different atomic compositions.

Quadrupole mass spectrometers need no magnetic field. Their separating principle ("mass filter") is a quadratic arrangement of four charged bars producing a complicated electrical field. Only ions with a certain m/z can traverse this system, others are discharged at the bars.

The last mass separation principle to be mentioned is the time-of-flight (*TOF*) mass spectrometer. Here, the speeds of the isoenergetic but – due to their different masses – differently fast ions are measured. One of the advantages of quadrupole and *TOF-MS* is the possibility to measure mass numbers up to a few 10^4 m/z.

7.1.2
Ionisation

Until about 1970, mass spectrometers were equipped solely with *electron impact* (*EI*) ion sources. The standard accelerating voltage was 70 V; this is far beyond bond energies and above the highest ionisation energy (He, 24.5 eV). The yield of radical ions $\cdot M^+$ is high. The primary species are long enough (ca. 10^{-6} s) in the ion source to undergo dissociation and rearrangement reactions. (Vibrational energy transferred during ionisation is dissipated in a molecule within the time of a few vibrations, i.e. within 10^{-12} s.) With *EI*, CH(O,S) fragments usually have uneven mass numbers. The fragmentation pattern is typical for a certain molecule, and it is sufficiently reproducible. Digitised libraries simplify the interpretation of 70 V *EI* results. *EIMS* is less or not at all applicable for mixture analysis: it is difficult or impossible to unravel superimposed fragmentation patterns. (See, however, *MS* with preseparated mixtures.)

Reduced accelerating voltage (20–10 V) is accompanied with lower ion yield but allows the analysis of mixtures as well as on-line identification of *GC* fractions.

Normally, volatile substances (including pyrolysates) are first collected in a heatable chamber attached to the *MS* and then enter the *MS* through a perforated diaphragm. Chemically unstable substances are (in a suitable vessel) fixed at the tip of a shifting rod and moved close to the electron source within the *MS*.

Field ionisation (*FI*) *MS* was developed by Beckey and others as a low-fragmentation method for the determination of relative molecular masses of large molecules and for the analysis of mixtures. It was, for the first time by Schüddemage, Düssel and others in our institute, combined with isothermal and temperature-controlled pyrolysis for the analysis of non-volatile substances, especially polymers.

The essence of *FIMS* is the action of a strongly inhomogeneous field (5×10^7 V/cm) at the tips of microscopic needles on the molecules of the analyte. These are polarised and drawn towards the tip of a needle. Directly above the surface, they lose an electron by tunnelling and are, as positive ions, pushed out of the field right into the mass separator. Alterna-

tively, a proton is transfered from H_2O, tenaciously sticking to the surface of the cathode, and the molecule leaves with the mass $m+1$. The ionising Wollaston wire (Pt or W, ca. 10 µm) is activated in the spectrometer (under 10 kV) with acetonitrile, benzonitrile or acetone. By this process the wire is covered with a dense fur of fine needles, containing the metal and C, and then looks like a brush for microbottles. The ionisation probability is much lower (about 1/100) than for *EI*; this is partially compensated by the fact that the *FIMS* frequently exhibits only the very intense peaks M^+ and $M+1^+$ (with some weak peaks due to field fragments). The analyte, if necessary after pyrolysis, enters the *MS* from the heated inlet system or is pyrolysed close to the ionisation wire. (Caution, the wire may break in the storm of the pyrolysis gases!)

Field desorption (*FD*) *ionisation* is closely related to *FI*, with two exemptions. (1) The sample, usually in solution, is deposited directly onto the (W) ionising wire. (2) The ionisation itself happens during desorption of the analyte by controlled heating of the wire or by cationisation (addition of cations like H^+, Na^+ etc. from impurities on the surface of the emitter or from deliberately added substances); it is higher than with *FI*. *FDMS* was frequently used for the investigation of chemically unstable substances.

CH(O,S) compounds, with *FI* or *FD*, predominantly form ions or radical ions with even mass numbers. CHN/P(O) compounds with uneven number of N/P atoms tend to form ions or radical ions with uneven mass number.

Chemical ionisation (*CI*) is quite different from the methods described above. The volatile analyte A (partial pressure $<10^{-4}$ Pa) is mixed with a large excess of a highly pure (>99.5%) gaseous reactand X (10–100 Pa) having a higher ionisation potential (*IP*) than A. The mixture is then transfered into a special *EI* source; the electrons (50–100 V) ionise almost exclusively X molecules. Still within the source, the following two categories of processes are possible:

- $X^+ + A \rightarrow A^+ + X$ charge transfer (1)
- Chemical processes (2)

$X^+ + A \rightarrow AH^+(X-H)$ protonation
$\rightarrow (A-H)^+ + XH$ hydride abstraction
$\rightarrow (AX^+)$ addition

In both cases (1 and 2) ionisation fragmentation will occur. This increases with increasing differences in the *IPs*. When *IP*(X) reaches additional 5 eV, the *CIMS* becomes similar to a 70-V *EIMS*. Among the standard reactands, CH_4 is a "hard" one (high *IP*), *i*-butane a "soft" one. With approximately equal *IPs*, fragmentation of A is minimised and the *CIMS* presents almost exclusively A^+, AH^+, $(A - H)^+$ and AX^+. This allows qualitative and quantitative analyses of mixtures. With decreasing *IP*(X) selective gas-phase chemistry becomes possible: some substance categories are ionised, others are not. With the comparably soft $C_6H_5^+$, e.g. unsaturated fatty esters are ionised, saturated are not. In cases where a high output of AH^+ or AX^+ ions is wanted protonating gas mixtures are employed, e.g. CH_4 with a few percent of NH_3. Here, NH_4^+ is almost exclusively the acting ion.

Fast atom bombardment (*FAB*) is an interesting alternative to the other mild ionising techniques for the investigation of chemically unstable and/or scarcely volatile substances. The analyte is mixed with a dispersive liquid, usually glycerol, and eventually a salt (NaCl), brought upon a target and exposed to fast (hot) Ar or Xe atoms. In a sputtering process, supported by an electric field, molecular cations A^+ or simple derivatives like AH^+ or ANa^+ are expelled from the surface and measured as usual. This technique was successful in cases where others fail, i.e. with organic cations and anions (e.g. surfactants), free acids, sugars and oligopeptides.

7.1.3 Ion-Detection

Originally the ions hit a photographic plate which they blackened. These plates were replaced by Faraday cages and later by secondary-electron multipliers (*SEM*). A sophisticated and very successful selective separator/detector is another mass spectrometer, on-line coupled with the first one. This technique is called tandem *MS* or *MS/MS*. It has been developed by Beckey and Levsen and described in details by Schwarz (10.1). More information is found in Sect. 7.5.

7.2 Mass Spectrometry with Electron Impact Ionisation (*EIMS*)

Scholl (Hummel/Scholl vol. 3, 10.1), in the early 1970s, made a thorough investigation on *EIMS* of plastics additives. The technique was standard: heated inlet system and ion source, 70 V acceleration, single-focusing sector-field *MS* (resolution ca. 10^3), *SEM* detection.

Figure 7.1 shows the results of an investigation on additives in vulcanised rubber. The microslices were evaporated at different temperatures directly in the *MS* and close to the ion source. The observed *m/z* have to be interpreted in the following way:

1. *N*-Nitrosodiphenylamine (Vulkalent A), M=198.2 g/mol

38	Benzyne/2
83.5	M–HNO/2
84.5	Diphenylamine/2
168	Diphenylamine – H
169	Diphenylamine

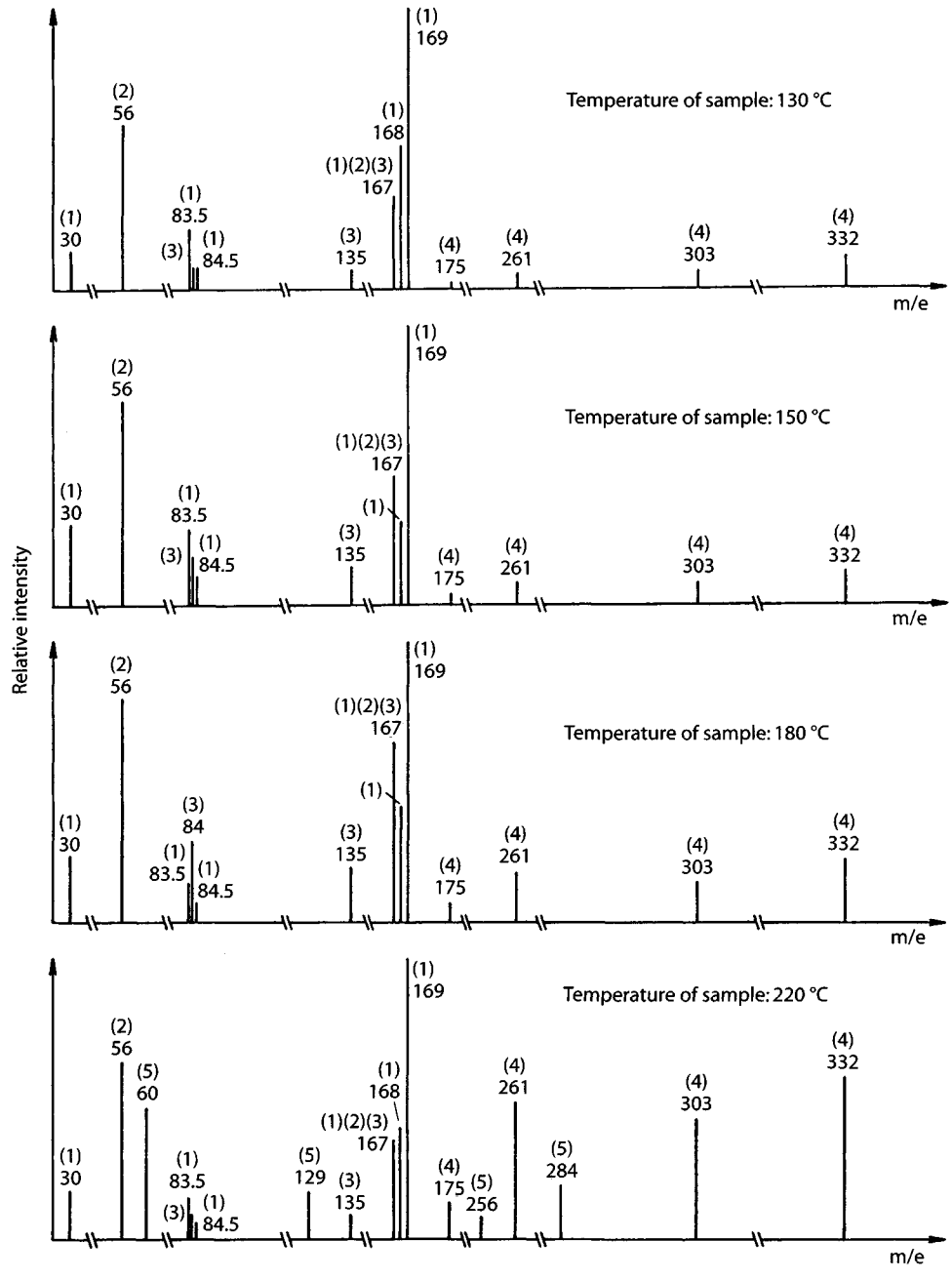


Fig. 7.1
Mass spectra of rubber additives. The vulcanisate was positioned directly in the mass spectrometer, the samples were heated to different temperatures; ionisation at 70 V. (F. Scholl, laboratory information.) Characteristic mass numbers M/z, usually $z=1$; sometimes, for aromats with a strong mass current, $z=1$ and 2

2. *N*-Cyclohexyl-2-benzothiazolesulfenamide (Vulkacit CZ), *M*=264.4 g/mol

57	C_4H_9
167	2-Mercaptobenzothiazole

3. Di-(2-benzothiazole)disulfide (Vulkacit DM), *M*=332.4 g/mol

64	S_2
135	Benzothiazole
167	2-Mercaptobenzothiazole

4. Di-2-octyl-*p*-phenylenediamine (UOP 288), *M*=332.5 g/mol

175	N-Cyclohexenylphenylenediamine
261	M - C_5H_{11}
303	M - C_2H_5
332	M

5. Stearic acid, *M*=284.2 g/mol

60	CH_3COOH
129	$C_6H_{13}COO$
256	M - C_2H_4
284	M

All compounds containing isotopes ($^{12}C/^{13}C$, $^{35}Cl/^{37}Cl$...) produce split signals for one and the same fragment or molecule. If a species contains *n* atoms with two isotopes, its signal is split into *n*+1 lines. Pentachlorothiophenol is an impressive example for this situation. It is used for the mastication (partial depolymerisation, solubilisation of vulcanisates) of rubber. Due to the five Cl-atoms in the molecule, the molecular peak is split into six components with a typical intensity distribution. This is shown by Fig. 7.2; the peak for 5 ^{37}Cl atoms (290) is too weak to be observed.

The first and until today largest collection of *EIMS* of additives was published in the book of Scholl (l.c.). The samples were completely volatilised into the glass container (150–250 °C) attached to the *MS*. The spectra were measured with a single-focusing instrument RMU 6-D (Hitachi-Perkin Elmer) with 70-V ionising electrons and an ion-source temperature of 150–200 °C; they were standardised and represented in tables. For the present book these were freed from some errors and evaluated with respect to fragment structures (Tables 7.1–7.22).

Yoshikawa et al. (10.2.1) published the first paper on the identification of plastics additives by evaporating these from the polymer matrix in a heated tube connected directly to the inlet system of a mass spectrometer. Reprecipitated polypropylene was mixed with solutions of additives in CCl_4, dried

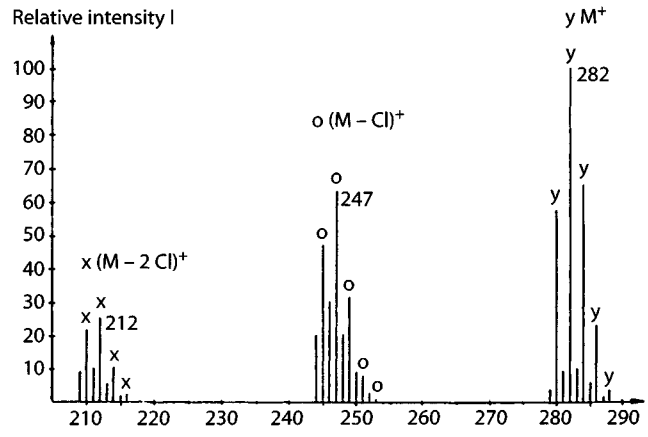


Fig. 7.2 Mass spectrum of pentachlorothiophenol. The four molecular peaks represent the following species; the one with 5 ^{37}Cl atoms is too weak to be observed; *m/z* 280 282 284 286 288; ^{35}Cl 5 4 3 2 1; ^{37}Cl 0 1 2 3 4

and compression moulded for 1 min at 190 °C into films of 1 mm thickness. The mass spectra were measured with a Hitachi RMU-6 single-focus spectrometer under the following conditions: ion-source temperature 250 °C, ionisation energy 80 eV, ionising current 80 μA, accelerating potential 1.2 kV. The temperature of the inlet system was kept, depending on the volatility of the additives, between 250 °C and 350 °C. The vapors produced by additive (20 mg) or polymer samples (0.2 g) were collected in a heated reservoir (1 dm^3) and subsequently transfered into the spectrometer. PP produced hydrocarbon fragments from C_2 to C_{14}; additive fragments with *m/z*<200 were therefore not considered.

All of the investigated phenolic compounds as well as a selection of commercial additives showed the parent/molecular peak *M* in their mass spectra with intensities between 100 (strongest peak) and 15. Table 7.23 exhibits mass numbers and relative intensities of the peaks observed by the authors in the *EIMS* of commercial additives. The limits of detection from the polymer matrix were between 0.02% and 0.1%.

With the described method the authors were able to identify the additives in 14 commercial PP samples.

7.3 Mass Spectrometry with Low-Fragmentation Ionisation

7.3.1 (Pyrolysis-) Field Ionisation (*FI*) and Field Desorption Mass Spectrometry (*Py-FIMS, FDMS*)

Czybulka et al. (10.2.6, thesis and publication) investigated, in our institute, the isothermal degradation of both vulcanisates (extracted or not) and vulcanisation accelerators by *Py-FIMS*. The mass spectrometers used were the CH4 and CH5/DF

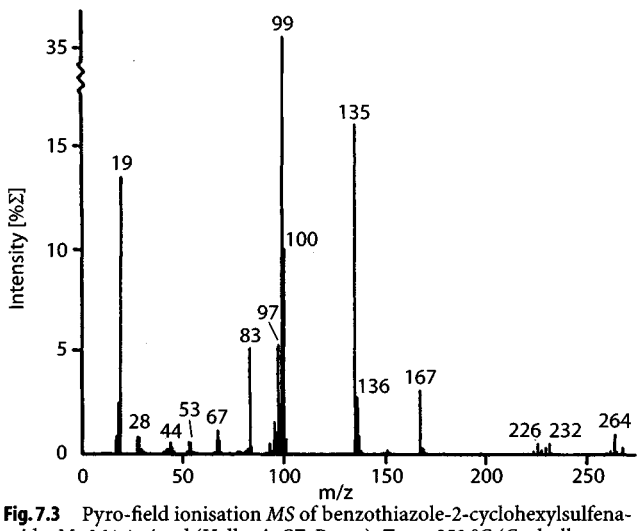


Fig. 7.3 Pyro-field ionisation *MS* of benzothiazole-2-cyclohexylsulfenamide, M=264.4 g/mol (Vulkacit CZ, Bayer), T_{max}=250 °C (Czybulka et al., 10.2.6)

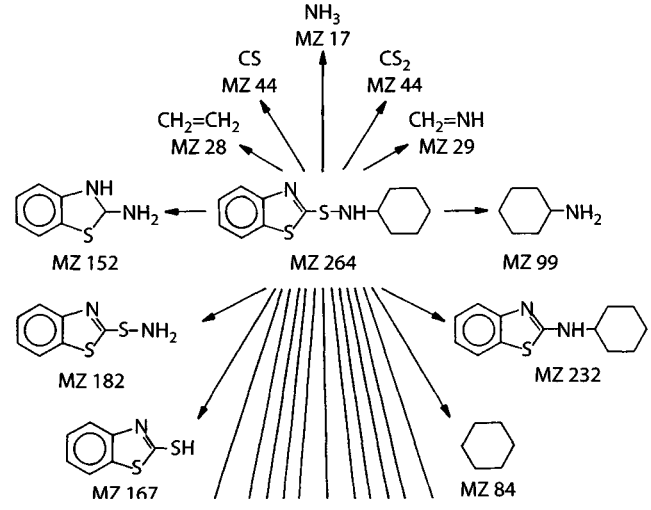


Fig. 7.4 Schematic diagram of the thermal degradation of benzothiazole-2-cyclohexylsulfenamide at 250 °C (Czybulka et al., 10.2.6)

(Varian MAT) with combined *EI/FI* sources (activated Pt Wollaston wire for the latter). The samples (rubber or accelerator, ca. 0.2 mg) were collected in a small quartz vessel at the top of a vacuum-tight shifting rod and pyrolysed in the vacuum (<1 Pa) of the high-temperature (250 °C) inlet system (glass, 800 cm^3). The gaseous pyrolysates diffused through a perforated metal screen into the high vacuum of the *MS*.

Typical examples were tetraethylthiuramdisulfide (TET) and benzothiazole-2-cyclohexylsulfenamide (CBS). Earlier studies with polymers had shown that, under the conditions chosen, field fragmentation was negligible; in other words, the fragments observed were true thermal ones. The pyrolytic reactions occur when the sample is still in the condensed state (time of pyrolysis ca. 10 s).

TET proved to be thermally labile; already at 290 °C no molecular peak with *m/z* 296 was observable. Strongest peak was 87 (ethylisothiocyanate) followed by 73 (diethylamine) and 76 (CS_2). The heaviest peak was 232, dithiooxalic-*N,N'*-tetraethylamide which is formed by the combination of two $(C_2H_5)_2N$-C=S radicals. The latter originate when S_2 is abstracted from TET. (The masses at 322 and 354 are probably unidentified condensation products of TET.)

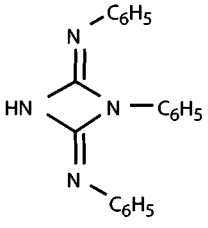
Figure 7.3 shows the *Py-FIMS* of CBS at 250 °C. The molecular peak at 264 is observable though weak. The strong peaks at 99 (cyclohexylamine) and 135 (benzothiazole) show that separation of the ring systems by N-S and S-ring is predominant over cleavage of the rings themselves. Figure 7.4 depicts the structures belonging to the observed mass numbers. (Here, 19 is H_3O^+ from water adsorbed on the surface of the Wollaston wire.)

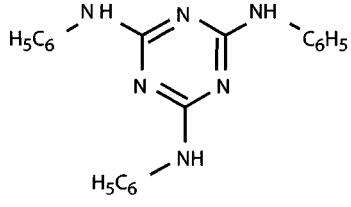
Using these results, the authors were able to identify fragments of accelerators in extracted and non-extracted vulcanisates. Model vulcanisates were made with 100 parts polymer, 40 parts carbon black, 2 parts sulfur and 0.6 parts benzothiazole-2-cyclohexylsulfenamide (Vulkacit CZ). The rubbers were poly(*Z*-butenylene) (BR), natural rubber SMR-5 (NR), synthetic poly(2-methyl-*Z*-butenylene) (IR), poly(butadiene-*co*-styrene) (SBR) and poly(butadiene-*co*-acrylonitrile) (NBR). Pyrolysis was effectuated at 500 °C. In addition to the fragments of the polymer chains, masses were observed which were characteristic for the accelerator as well as CHS compounds resulting from reactions between the polymer chain and the sulfur in the blend (tentative assignments):

m/z	Fragment	BR	NR	IR	SBR	NBR
71	CH_2=CH-$(CH_2)_2$-NH_2		+	+		
93	Aniline	+			+	+
135	Benzothiazole	+			+	+
34	H_2S	+	+	+	+	+
48	CH_3SH	+	+	+	+	+
60	CH_2=CH-SH	+			+	
62	C_2H_5SH	+			+	
74	CH_2=CH-CH_2-SH	+	+	+	+	+
86	CH_2=CH-S-CH=CH_2	+			+	
88	CH_2=CH-S-C_2H_5	+			+	

Interestingly, BR and SBR on the one hand and NR as well as IR on the other showed the same accelerator/sulfur fragments; this may be explained by specific vulcanisation behaviours. (None of these *m/z* values matched with strong hydrocarbon masses.)

Soon afterwards the thermal degradation of guanidine accelerators was described by Hummel et al. (10.2.6); the experimental equipment was the same. Figure 7.5 shows the (relatively simple) *Py-FIMS* (290 °C) of 1,3-diphenylguanidine (DPG), Fig. 7.6 the assignment of the observed *m/z* values (including the molecular mass 211). Main decomposition product is aniline, followed by diphenylcarbodiimide. HCN, which should be formed in considerable amounts, produces only a weak signal (*m/z* 27). This is very likely due to a low ionisation probability. Interestingly, dimerisation and trimerisation must have happened when DPG was still in the condensed phase; the masses at 312 and 354 can be assigned to 1-phenyl-2,4-*bis*(phenylimino)-1,3-diazetidine and *sym*-triphenylmelamine:





In the same publication, pyrolysis of di-*o*-tolylguanidine is described. It is quite analogous to that of DPG, including the dimerisation and trimerisation (*m/z* 354 and 396, respectively.)

Lattimer et al. (10.2.6/2 and 3; the publications are very similar) studied the analytical efficiency of different ionisation techniques for the identification of rubber additives in uncured rubber compounds and in vulcanisates: *EI*, *FI*, *FD*, *CI* and *FAB* with compounds (high-vacuum evaporation near the ion source) and with extracts. Standard compounds were made with natural (NR), butadiene-styrene (SBR) and *Z*-1,4-polybutadiene (BR) rubber; all of them contained carbon black, aromatic processing oil, paraffin wax, ZnO, stearic acid, *t*-octylphenol-formaldehyde resin and sulfur as well as three or four of the additives shown in Fig. 7.7.

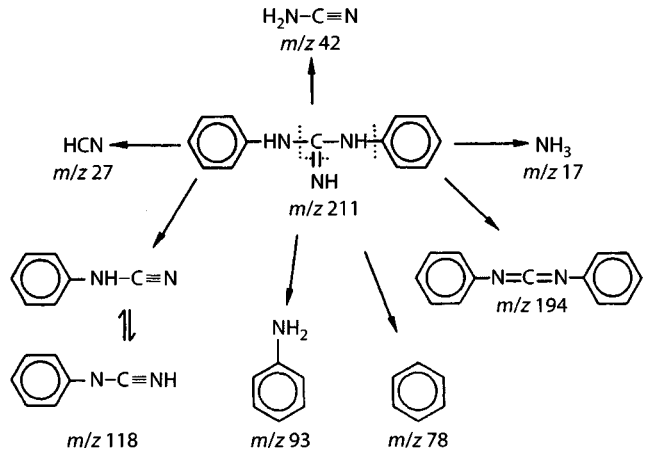


Fig. 7.6 Schematic diagram of the thermal degradation of 1,3-diphenylguanidine (without the constructive masses 312 and 354) at 290 °C (Hummel et al., 10.2.6)

For *direct* (*evaporation*) *rubber analysis* small pieces were cut from ASTM sheets, placed in an Al crucible and introduced into the *MS*. *EI* and *CI* spectra were measured with a Finnigan MAT 311A/Incos 2400 having a mass range up to *m/z* 1450. The ion source temperature was 250 °C, the accelerating potential 3 kV, and the resolution 1000 (10% valley). The ionisation potential for *EI* was 70 V, the *CI* gases were CH_4 or *i*-butane. CH_4 yields a somewhat larger abundance of fragment ions than *i*-butane. The temperature of the sample was increased from 50 °C to 300 °C.

For direct *FAB* analysis the rubbers were cut into strips (8×3×2 mm^3) which were attached to the *FAB* probe with Scotch 924 transfer tape.

For *FI* analysis a Finnigan MAT 731/SS200 system with a combined *EI/FD/FI* ion source was used. The source temperature was 50 °C, the accelerating potential 8 kV, the extraction plate potential 3 kV, and the resolution was 2000. The heated direct probe (AMD Intectra, D-Beckeln) was used for sample introduction. It employs a quartz crucible that is positioned within 2 mm of the emitter, and the temperature is programmable with a maximum of 800 °C.

For *extract analysis* the samples were extracted with acetone, acetonitrile or CH_2Cl_2 either in a Soxhlet (24 h) or by

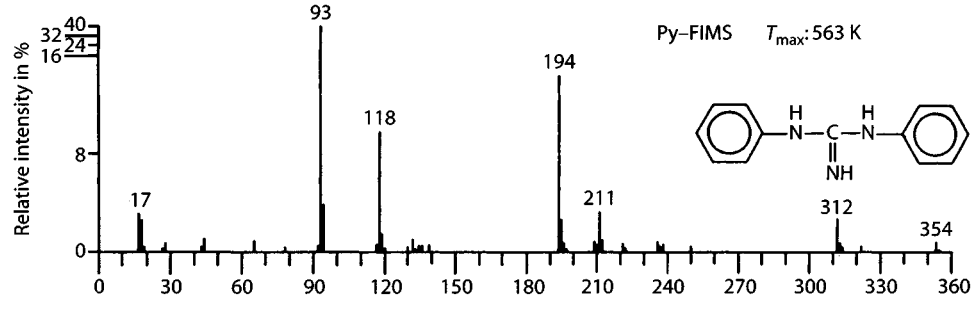


Fig. 7.5
Pyro-field ionisation *MS* of 1,3-diphenylguanidine, *M*=211.3 g/mol (Vulkacit D, Bayer), T_{max}=290 °C (Hummel et al., 10.2.6)

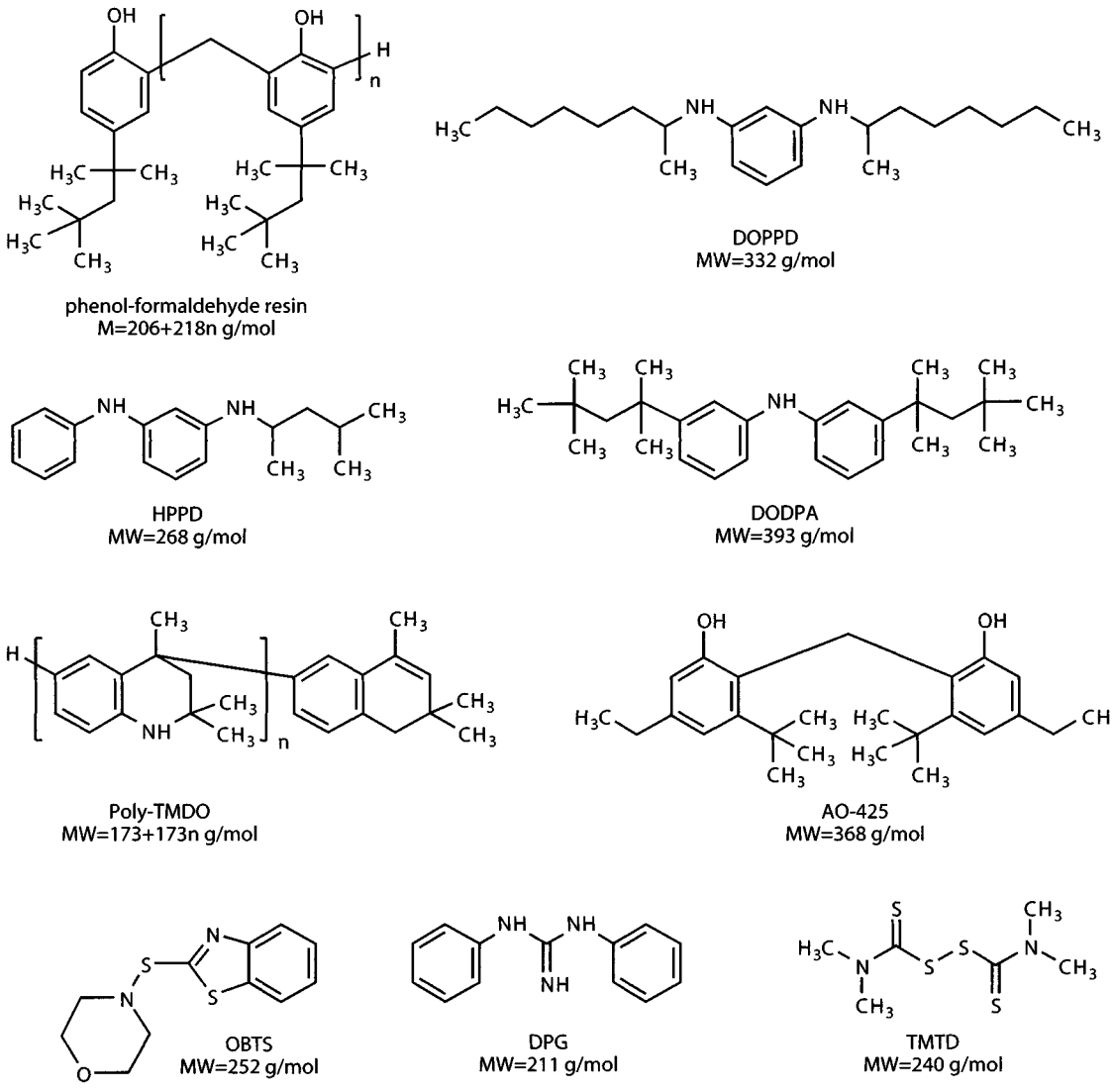


Fig. 7.7 Structures of rubber additives (Lattimer et al., 10.2.6/3)

placing a small piece of rubber (5×5×2 mm^3) with 1 cm^3 of solvent in a vial and letting it stand for at least 1 h. The results were the same. A Finnigan MAT 311A was used for the analyses (details given above). Samples in the direct probe (Al crucible) were heated from 50 °C to 300 °C. For *FD* analysis, about 1 mm^3 of the extract was applied directly to the emitter wire. The ion source temperature was 90 °C, the acceleration potential 3 kV, the extraction plate potential 6 kV, and the resolution 600. The emitter was heated manually with up to 30 mA.

For *FAB* analysis, 1 mm^3 of the extract was deposited onto the stainless steel *FAB* probe containing some thioglycerol as liquid matrix. The ion-source temperature was 70 °C and the resolution 1000. The IonTech *FAB* gun provided Xe atoms at an energy of 8.0 keV. The conditions for *FI* were the same as described above.

The characteristic mass numbers found by the authors using different ionisation techniques were, for comparison with the results of other authors, collected in Table 7.23. Lattimer et al. stated that *FI/FD* is the most efficient method for identifying organic additives in rubber stocks; this confirms our own findings in *Py-FIMS*.

Just a few examples of the many given in the papers of Lattimer et al. will demonstrate the specificity of *FIMS* both with direct (evaporation) and extract analysis. Figure 7.8 shows the *FIMS* produced by an (unvulcanised) SBR compound when heated in the vacuum of the *MS* to 300 °C. All organic additives in the compound (with the exception of DPG) are present as molecular peaks: HPPD (268), poly-TMDQ (386 and 346, two of the many components), OBTS (252), S_8 (256) and stearic acid (284). The multiple-mass underground ("mass memory") looking like the back of a hedgehog certainly is not caused by the rubber.

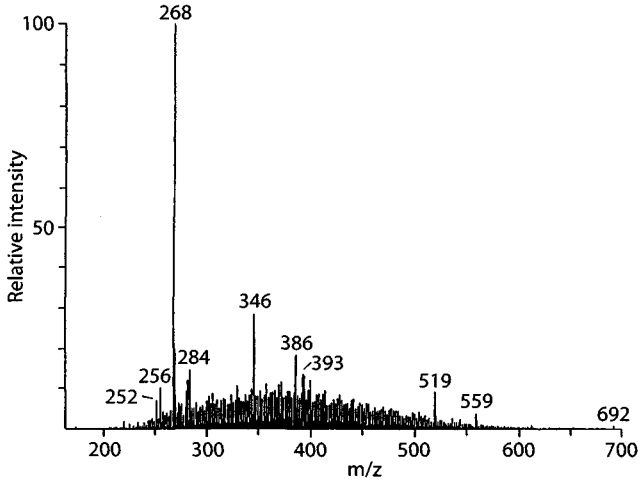


Fig. 7.8 *FIMS* (direct analysis) of a butadiene-styrene standard rubber containing HPPD, poly-TMDQ, OBTS and DPG (see Fig. 7.7) as organic additives (Lattimer et al., 10.2.6/2+3)

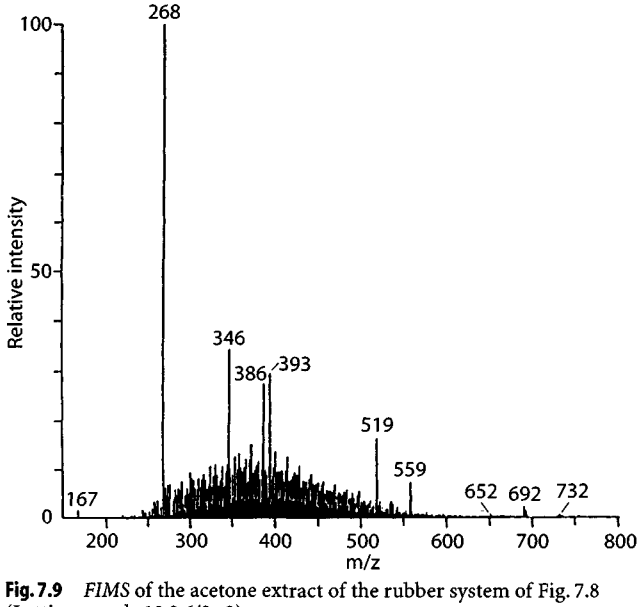


Fig. 7.9 *FIMS* of the acetone extract of the rubber system of Fig. 7.8 (Lattimer et al., 10.2.6/2+3)

Figure 7.9 exhibits the *FIMS* of the acetone extract of the same SBR compound. It presents (together with a considerable mass-memory effect) additional poly-TMDQ components with relative molecular masses of 652, 692 and 732. The very weak masses 252 and 256 are swallowed by the mass noise. The peak of stearic acid (284) is missing; this additive is not extracted by acetone.

Figure 7.10 shows (this time without the mass-memory effect) the direct-analysis *FIMS* of the NR compound. All organic additives (and sulfur) in the compound are present as molecular peaks: DOPPD (332), DODPA (393), OBTS (252, very weak), stearic acid (284) and S_8 (256). The peak at 256 very likely belongs to palmitic acid. Other peaks being separated by 28 mass numbers (CH_2) belong to saturated

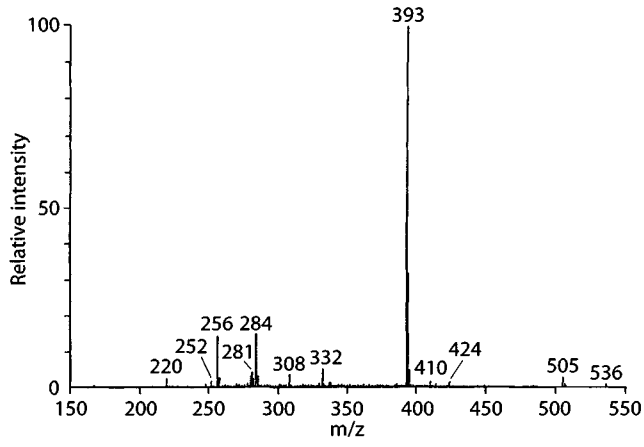


Fig. 7.10 *FIMS* (direct analysis) of a natural rubber compound containing DOPPD, DODPA and OBTS (see Fig. 7.7) as organic additives (Lattimer et al., 10.2.6/2+3)

and unsaturated hydrocarbons from extender oil and wax (252, 280, 308, 332).

We keep in mind that these thorough investigations had the aim to identify rubber additives with an optimal method and not to study the degradation behaviour of additives as such or – during vulcanisation – in the rubber.

7.3.2 Chemical Ionisation Mass Spectrometry (*CIMS*)

Hunnemann (10.2.4) demonstrated the differences between *EI* and *CI* with dipentylphthalate (DPP, Fig. 7.11). M^+ is missing in the *EIMS*; instead, 237 (M^+- C_5H_{10}), 167 (phthalic acid+H), 149 (phthalic anhydride) and 71 ($C_5H_{11}^+$) give sufficient evidence for DPP. The *CI*(CH_4) shows M+H^+ in addition to the known fragments. In the *CIMS* of the "soft" *i*-butane all fragment peaks are weak (but still helpful for identification).

In the publications of Lattimer et al. (see above), *CI* with CH_4 was also employed for the identification of the components in the evaporating gas of rubber compounds. Figure 7.12 shows the result with a natural rubber mix. M+H^+ is strongest peak, followed by 333 (M^+- C_4H_{10}) and lighter fragments produced by the impact of the "hard" CH_4 on the molecules in the gaseous mixture. The *FIMS* of the same system under analogous conditions (Fig. 7.10) is easier to interpret.

CIMS with "soft" ionisation gases is the prefered method for multicomponent volatile systems. Rudewicz and Munson (10.2.1) demonstrated this with the determination of antioxidants in polypropylene without prior separation. The equipment was a *CI*-modified Du Pont 492B mass spectrometer with Hewlett-Packard 21-MX computer. The PP slices (1–2 mg) containing 0.5–5 µg additive/g PP or a small amount of the pure additive were placed in the well of a heatable glass probe which itself was placed in the *CI* ion source. The source temperature was kept at 225 °C for the pure additives

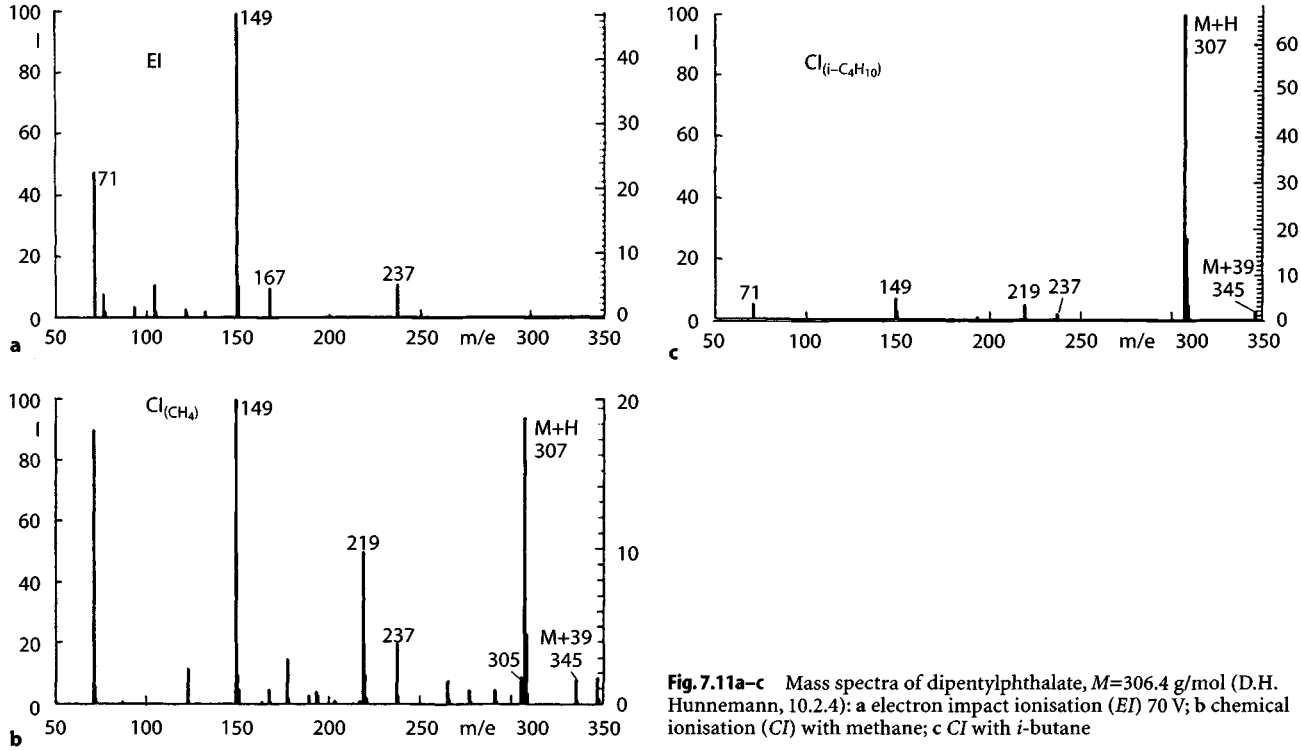


Fig. 7.11a–c Mass spectra of dipentylphthalate, M=306.4 g/mol (D.H. Hunnemann, 10.2.4): a electron impact ionisation (*EI*) 70 V; b chemical ionisation (*CI*) with methane; c *CI* with *i*-butane

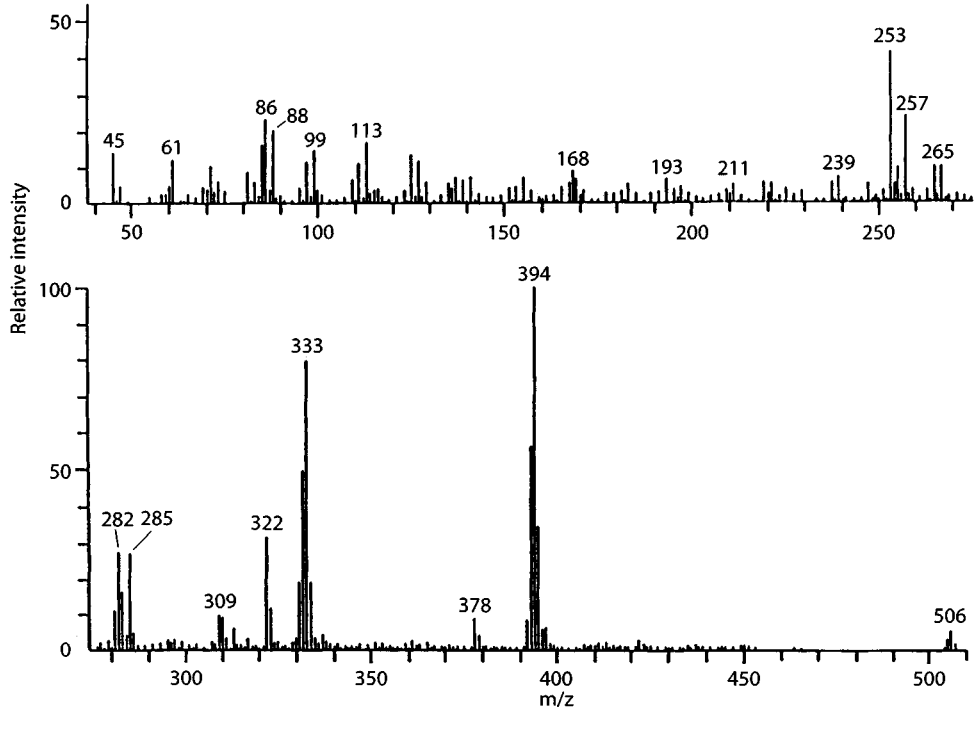


Fig. 7.12
CIMS (CH_4, direct analysis) of the NR compound of Fig. 7.10 (Lattimer et al., 10.2.6/2+3)

and 240 °C for the polymer samples. The heating programs (30–350 °C) were 20 °C/min or 30 °C/min. The accelerating potential was 1750 V, the source repeller potential was kept at 0 to maximise the ionic residence times. A mixture of 1.1% NH_3 in CH_4 at 67 Pa was used as the reagent gas. The reason for this composition is that NH_3/CI H^+-sensitivities of CHO(X) compounds having a smaller H^+ affinity than that of NH_3 (854 kJ/mol) increase with decreasing partial

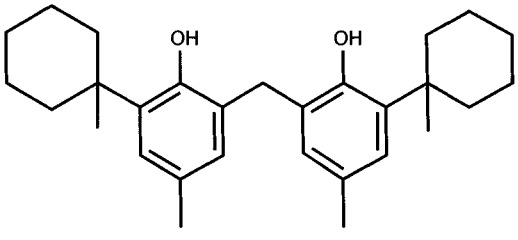
pressure of NH_3 in CH_4. Under the conditions chosen NH_4^+ makes 85% of the reactant ionisation. If the H^+ affinity of the analyte exceeds that of NH_3, AH^+ ions will be formed by H^+ transfer from NH_4^+; if it is smaller but contains polar groups, NH_4^+ will be attached to form $(A+NH_4)^+$ ions. Thus, Ionox 330 (a hindered triphenol) formed the NH_4^+ adduct (*m/z* 792), Irganox 168 (an aliphatic-aromatic phosphite) and UV-531 (a substituted benzophenone) formed AH^+ (*m/z* 647 and 327, respectively). The background from the polymer was very low.

The evolution of additives from PP usually begins suddenly around 190 °C, i.e. above the melting point of PP. From the area under the peaks of the ion currents of AH^+ or $(A+NH_4)^+$ calibration curves can be made for quantitative determinations. The authors quote a short-term reproducibility of peak areas of 6%.

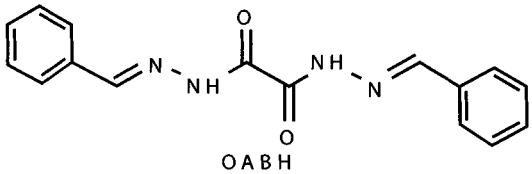
More recently, Vit et al. (10.2.1) made direct quantitative analyses of additives in polyethylene (XDK 183, ICI) employing a Finnigan 3300F quadrupole *MS* kept at 200 °C and multiple ion detection (*MID*) *CIMS* with CH_4 instead of CH_4/NH_3 reactant gas (0.12 Pa in the source). It was found by the authors that, with CH_4, the instrument showed greater stability (for the measurements of one day) and a significant increase in sensitivity. (Anyway, 15% NH_3 in CH_4 seems to be very high.) The probe was heated from 30 °C to 350 °C at a rate of 120 °C/min and spectra were collected at 3-s intervals by a SuperIncos data system.

Great pains were taken to prepare PE/additive samples with defined compositions and shapes. It turned out that also reproducible dimensions (in this case 0.25×0.40×1.50 mm^3, 0.15 mg) are important for reproducible results. (In fact, compact samples with minimal surface area were found to be ideal.) The samples were placed in a glass vial on a direct insertion probe and placed into the ion source.

Analytical samples were the antioxidant Permanax WSP (CIL) and the Cu deactivator OABH (Eastman):

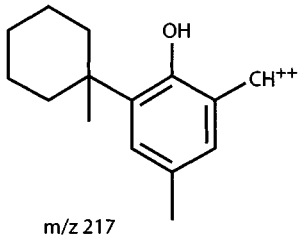


Permanax
WSP
$C_{29}H_{40}O_2$ M = 420



OABH
$C_{16}H_{14}N_4O_2$ M = 294

Analytical (thermal) fragment of the former was its dissociation product:



m/z 217

As an internal standard (1 µg per analytical sample) phenolphthalein ($M+H^+$=225) served right . This has a similar evaporation temperature range in PE as the two additives and its base peak is close to the analytical peaks. The *MID* mass chromatograms (specific ion currents/relative intensities as functions of time/temperature) exhibited quite symmetric peaks whose area was used for the construction of calibration curves, ratio analytical peak/peak of standard vs µg of analytical additive in PE; the linearity was quite satisfying. The relative standard deviation was 7% or less in most cases.

Great care had to be taken to ensure that accurate and reproducible results were obtained regarding the state of the mass spectrometer. The instrument was allowed to equilibrate at the experimental settings before starting an experiment; this improves the peak area stability. At times, the sensitivity of the instrument dropped markedly after several hours of measurement.

7.3.3 Fast-Atom Bombardment Mass Spectrometry (*FAB-MS*)

Feistner et al. (10.2.4) studied the performance of no less than seven different *MS* techniques in the identification and semi-quantitative determination of carboxylic and phosphoric acid esters:

- Gas chromatography coupled with electron-impact *MS* (*GC-EIMS*), *EIMS/MS* or chemical ionisation *MS* (*CI-MS* or *CI-MS/MS*)
- *CI-MS/MS* without *GC* pre-separation
- *FAB-MS* and *FAB-MS/MS*

The plasticiser-type esters were found as contaminants in commercial alcohol and proved – incidentally – to be almost ideal for such a critical investigation:

- Di(2-ethylhexyl)phthalate (DOP)
- Hexanoic, octanoic and decanoic mono- and diesters as well as mixed esters of tri(oxyethylene)diol (TEG-C_8, TEG-C_{10}, TEG-$2C_8$, TEG-$2C_{10}$, TEG-C_6C_8, TEG-C_8C_{10})
- Triphenylphosphate (Φ_3P)

- Three isomeric/isobaric *i*-propylphenyl diphenyl phosphates ($C_3\Phi$-Φ_2P)
- Two isomeric/isobaric tri(*i*-propylphenyl) phosphates [$(C_3\Phi)_3P$]
- Di(*i*-propylphenyl) phenyl phosphate [$(C_3\Phi)_2P\Phi$, possibly a mixture of isomers]

GC separation was achieved on a 10-m or 30-m/0.25-μm DB-5 column (J&W Ass., Folsom, Cal.). Low-resolution spectra were measured with an HP-5985B *GC/MS*, a VG-ZAB-SE spectrometer was used for high-resolution spectra. The latter instrument also served for *FAB* and *FAB* collisional activation (*CA*) *B/E*-linked scan analyses of authentic compounds. *FAB* and *FAB-CA* mass analysed ion kinetic energy (*MIKE*) spectra were obtained on a three-sector mass spectrometer linked to a Kratos DS-55 computer system. *FAB* was performed with 8 keV Xe atoms using either glycerol-acetic acid (5:1), thioglycerol, or dithioerythritol-dithiothreitol (1:5) matrices.

Protonated molecular ions of the TEG esters are not present in *EIMS* but can be detected with either *CI* or *FAB* (*m/z*): TEG-C_8 277, TEG-C_{10} 305, TEG-$2C_8$ 403, TEG-$2C_{10}$ 459, TEG-C_8C_{10} 431. Fragments arise from cleavage at the TEG ether linkages. Fatty acyl oxyethyl ions are observed in *EI, CI, FAB* and *MIKE* spectra, fatty acyl ions in *FAB CA MIKE* and in *EI CA* spectra. Protonated DOP (391) is present both in *EIMS* and *FABMS*.

Protonated molecular ions of phosphate esters are present both in *EIMS* and *FABMS* (*m/z*): Φ_3P 327, $C_3\Phi$-Φ_2P 369, $(C_3\Phi)_3P$ 453, $(C_3\Phi)_2P\Phi$ 411.

The classical *GC/EIMS* still appears to be the method of choice whenever ultimate sensitivity and specificity are needed. Pre-separation with *GC* (*HPLC* etc.) is obligatory when isomers have to be identified. Employing this technique we should keep in mind that certain additives are chemically instable and wouldn't leave the *GC* unchanged.

FAB can also be applied for solid or resinous substances. Here, the material is finely dispersed in the matrix or, if this is not possible, it is covered with a layer of the matrix. This has been shown by Lay and Miller (10.2.4) for phthalate plasticisers in PVC (baby pacifiers). DOP reveals itself in the *FAB-MS* by its protonated molecular ion (*m/z* 391). A quantitative determination is possible if a standard phthalate (e.g. didecylphthalate) is added to the analyte. The relative standard deviation amounts to a few percent but may go up to about 10%. It has to be kept in mind that physiological properties of substances depend also on the isomeric composition. In the present case, all di-C_8H_{17} phthalates would produce *m/z* 391. A pre-separation (usually *GC-MS*) is necessary if a specification is wanted.

7.3.4 Laser-Desorption Mass Spectrometry

Laser radiation has long been employed for the evaporation of substances with low volatility directly within the mass spectrometer; it replaces thermal devices like the Pt coil. A prerequisite for its action is that the laser radiation is absorbed by the sample; thus, the laser has to be chosen with respect to the absorption behaviour of the sample. In addition, the intensity of the radiation has to be controlled carefully; otherwise the sample is heated, changes its state of aggregation or decays. The latter may be desirable with samples having defined mechanisms of pyrolysis like a number of polymers.

Tremendous progress has been achieved by the invention (Hillenkamp and Karas) and development of a technique where the absorption behaviour of a matrix, usually in the *UV*, allows the investigation of a broad variety of analytes, regardless of whether they absorb the laser radiation or not. This will be the subject of the following paragraph.

7.3.4.1 Matrix-Assisted Laser-Desorption Ionisation Time-of-Flight (*MALDI-TOF*) Mass Spectrometry

The essence of this technique is a low-molecular, strongly *UV*-absorbing, usually hydroxyaromatic matrix which dissolves or disperses the analyte; the absorption behaviour of the latter doesn't matter. Examples for matrix substances are 2,5-dihydroxybenzoic acid, 1,8,8-trihydroxyanthracene or 4-hydroxy-α-cyanocinnamic acid. Frequently, the analyte is cationised with Li^+, Na^+ or K^+, or it is protonated in the matrix during desorption. The matrix substance is usually applied as concentrated solution, the concentration of analyte in the common solvent is low, 1–0.1%. Around 1/4 mm^3 solution for each spot, containing about 100 ng solute, are placed on a metallic target thus forming spots with a diameter of about 2 mm. After evaporation of the solvent, the target is introduced into the mass spectrometer. *UV* light excites the matrix electronically, the energy is transfered to the analyte molecular ions and both analyte and matrix molecules are desorbed from the surface. Very little fragmentation happens to the molecular ions, and it is therefore possible to analyse even molecules which are thermally instable. The *MS* signal(s) of the analyte should be well above that of the matrix.

Pasch et al. (10.2.5) presented an interesting study on the direct identification of *UV* stabilisers in plastics by *MALDI-TOF-MS*. The measurements were made with a Kratos Compact MALDI 3, Urmston, UK; the mass number precision was, in the mass ranges studied, ±1. 4 mg of material were dissolved in 1 cm^3 solvent, 10 mg of 1,8,9-trihydroxyanthracene were dissolved in 1 cm^3 THF. Then 15 mm^3 of the two solu-

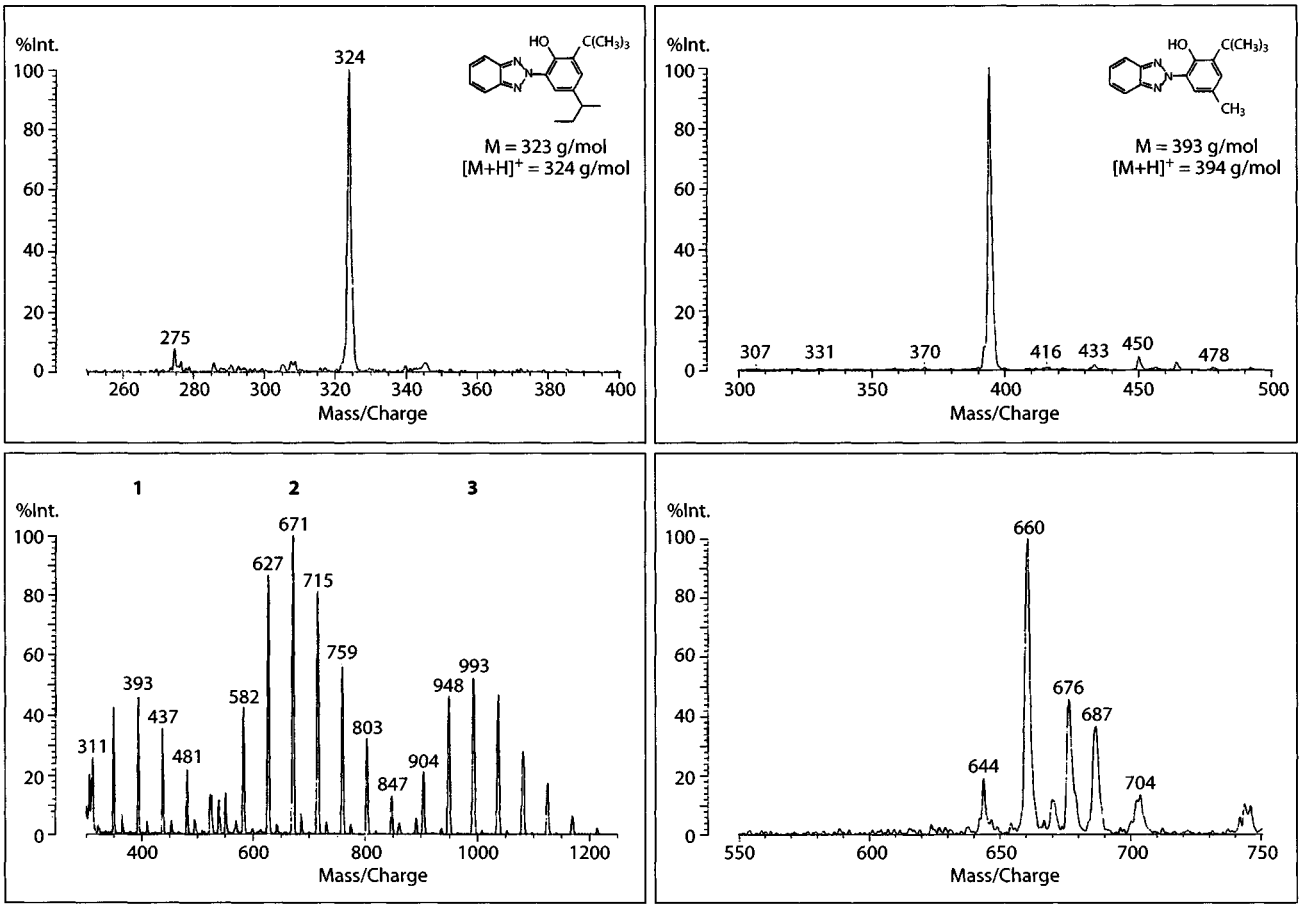


Fig. 7.13 *MALDI-TOF-MS* of *UV* stabilisers (Pasch et al., 10.2.5): **1** (*above left*) Tinuvin 350, Ciba; **2** (*above right*) 2-(2-hydroxy-3-dodecyl-5-methyl)-phenyltriazole; **3** (*below left*) 2-(2-hydroxy-3-*t*-butyl-5-carboxypropionic)phenyltriazole-EO adduct; **4** (*below right*) mixture of hindered phenols with aliphatic-aromatic phosphite (see Fig. 7.15)

tions were mixed, 0.5 mm^3 of solution per spot were applied. For each *MS* the sample was irradiated with 150 laser pulses. Figure 7.13 shows the spectra of four different *UV* stabilisers and antioxidants. Each of the benzotriazoles **1** and **2** (above) produced only one strong signal which was easily assigned to $M+H^+$. The spectrum of **3** (below left) shows three series with a typical distribution of peak intensities and peak distances of 44 mass numbers. This is typical for ethyleneoxide adducts, and **3** is in fact the EO adduct of a benzenetriazole derivative, together with poly(oxyethylene) (Fig. 7.14). The peaks are not signals of degradation products but those of defined adducts. Then **4** is a mixture of a hindered phenol and an aliphatic-aromatic phosphite (Fig. 7.15). The interesting thing here is that the two kinds of molecules grabbed the omnipresent alkali ions Na^+ and K^+.

The investigations were continued with samples of polyethylene (HDPE) and polypropylene being stabilised with different concentrations of a hindered phenol or a hindered amine (Fig. 7.16). These stabilisers absorb strongly in the *UV*, the polymers do not. The authors therefore left out the matrix and simply deposited thin films from a hot toluene solution on the target. The result is quite spectacular (Fig. 7.17). Down to a concentration of 0.1% of stabiliser, the species $M\text{-}Na^+$ govern the spectra. Interestingly, the chances of K^+ to unite with M decrease rapidly with decreasing concentration of the latter.

7.3.4.2 Laser-Desorption *FT*-Ion Cyclotron Resonance (*LD/FT-ICR*) Mass Spectrometry

This sophisticated technique seems to unite the specific advances of other *MS* techniques discussed to now. *FT-ICR* can achieve both high resolution and high mass accuracy. Switching from positive to negative ion mass spectral acquisition can be done simply through a software command. At low laser power density, predominantly molecular ions (with addet H^+, Na^+, K^+) are formed while, with higher power density, extensive fragmentation can be obtained for addi-

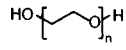
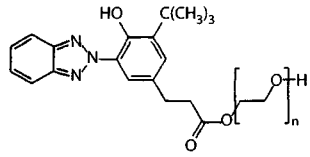
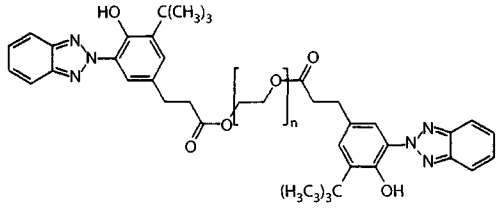
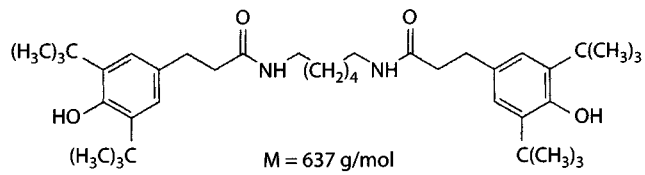
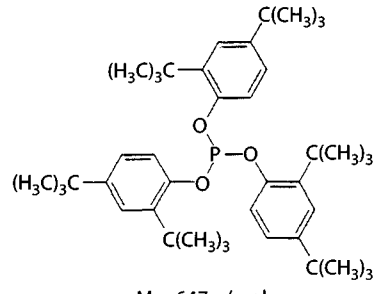
Peak series	Structure
1	 M = (18.01 + n · 44.05) g/mol
2	 M = (339.39 + n · 44.05) g/mol
3	 M = (660.77 + n · 44.05) g/mol

Fig. 7.14 Structures of the three peak series in the *MALDI-TOF-MS* of the EO adduct (3) in Fig. 7.13 (Pasch et al., l.c.)



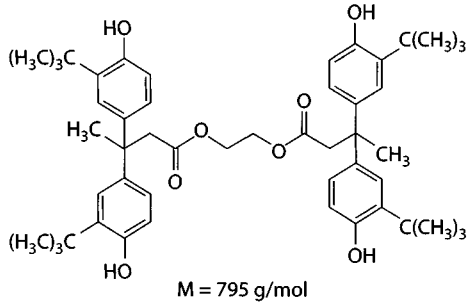
M = 637 g/mol
$[M+Na]^+$ = 660 g/mol
$[M+K]^+$ = 676 g/mol



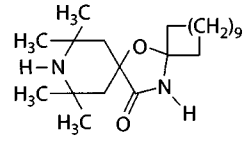
M = 647 g/mol
$[M+Na]^+$ = 670 g/mol
$[M+K]^+$ = 686 g/mol

Fig. 7.15 Structures of the two components of 3 in Fig. 7.13 (Pasch et al., l.c.)

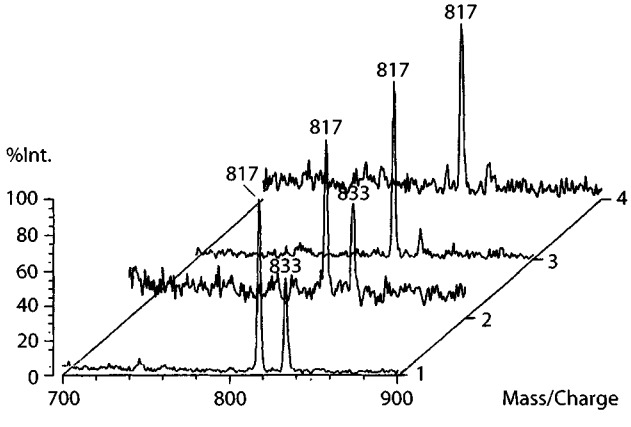
Fig. 7.16
Structures of the stabilisers in HDPE (see Fig. 7.17); *left*: Hostanox O_3, *right*: Hostavin N_{20} (both Hoechst)(Pasch et al., l.c.)



M = 795 g/mol
$[M+Na]^+$ = 818 g/mol
$[M+K]^+$ = 834 g/mol



M = 364 g/mol
$[M+Na]^+$ = 365 g/mol
$[M+K]^+$ = 387 g/mol



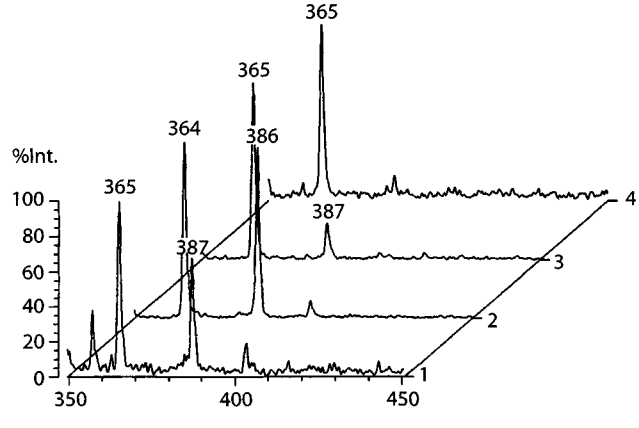


Fig. 7.17 *Left*: *MALDI-TOF-MS* of HDPE, stabilised with Hostanox O3; 1: 0.4 wt%, 2: 0.2 wt%, 3: 0.1 wt%, 4: 0.01 wt% additive; *right*: same, stabilised with Hostavin N20; 1: 1.0 wt%, 2: 0.2 wt%, 3: 0.1 wt%, 4: 0.01 wt% additive (Pasch et al., l.c.)

tional structural information. It is also possible to select a particular parent ion for fragmentation by collision-induced dissociation. Asamoto et al. describe this in their basic and highly informative paper (10.2.1) giving details on the procedure and presenting reference spectra of 18 antioxidants, 7 *UV* absorbers and 4 amide waxes (Table 7.24). In addition, they identified the additives extracted from three different polyethylenes (wash bottle, garbage can, tarp).

The polymer samples (10–15 g) were Soxhlet extracted for 8 h with around 150 cm^3 of ether. (It seems preferable to separate the additives by solution/precipitation.) The residue (50–150 mg) was dissolved in $CHCl_3$, part of the low-molecular PE was precipitated with acetone. The precipitate was filtered out with a 0.5-μm Teflon filter. The filtrate was evaporated, redissolved in CH_2Cl_2 and deposited on the probe tip with a nebuliser.

From commercial additives, probe samples were prepared by dissolving 10–20 mg in 1 cm^3 of CH_2Cl_2 or methanol. Approximately 30 μl of solution were placed on the probe tip and evaporated in air. Alternatively, ca. 0.3 mg of additive was deposited on the probe tip with a nebuliser.

The spectra were measured with a Nicolet FTMS-2000 fitted with a Tachisto model 216 pulsed CO_2 laser. The energy is in the mid-infrared (10.6 μm) where most organic compounds absorb; it was varied between 2 mJ and 20 mJ per pulse, typically 10 mJ. The power density at the sample was varied by moving the probe tip in or out along the magnet axis, which focuses or defocuses the beam at the probe tip while not changing the total energy. The spot sizes correspond to maximum power densities of some 10^8 W/cm^2. The amount of sample vaporised per shot was on the order of 100 ng. Several spectra were obtained at each of four conditions, X^+ and X^-, focused and defocused.

Table 7.25 shows the *LD-FTMS* (we prefer now this easier-to-read acronym) of the additives measured by Asamoto et al. Fragmentation of the molecules was, as expected, dependent on the laser power. With a defocused laser (low power), H^+, Na^+ and K^+ adducts were the most abundant, and sometimes the only observable ions. (These three cations are omnipresent, they were not added to the systems.) With focused beam, the intensity of the quasi-molecular ions decreased and that of fragment ions increased. Carbon clusters and other non-characteristic fragment ions were not observed.

From the spectra of additives with the same composition (6, 9, 14, 23), it can be seen that positive molecular additive species and the negative species $[M-H]^-$ and M^- are almost always present and well reproducible. Fragments, possibly formed by laser splitting of M, are much less reproducible though always typical for the original molecule. This may be explained by the presence of several "weak links" in a molecule.

Johlman et al. (10.2.1) made an interesting comparison of laser-desorption/ionisation Fourier transform (*LD-FT*) with *FAB-MS* for non-volatile additives. Their results (as they state) supplement and extend the thorough study by Asamoto et al.

LD-FT spectra were measured with a Nicolet FTMS-1000 spectrometer, coupled to a Tachisto 215G pulsed TEA CO_2 laser with 300–400 mJ per 40 ns at 10.6 μm. A ZnSe lens with a 7.5 cm focal length was used to focus the laser beam through the trapped ion cell into a 1 mm spot size on a stainless steel probe tip. There, power density was in the range of 10^8–10^9 W/cm^2. The measurement was initiated by a computer-controlled trigger of the laser pulse and was followed by a 3–10-s delay prior to data acquisition in order to permit a return to base pressure. During this time, uncharged species may escape the ion trap.

Alternatively, spectra were measured with a modified Nicolet FTMS-2000, coupled to a Spectra Physics DRA 11 Nd:YAG laser providing an unfiltered 30 mJ per 9-ns pulse at 1064 nm (9398 cm^{-1}). This is in the range of the third overtone of CH/NH/OH stretching vibrations and thus will allow good radiation absorption. With a spot size of 0.5 mm diameter, power densities were 10^7–10^9 W/cm^2, depending on initial laser energy. Spectra were acquired 2–5 s after the laser pulse.

FAB spectra were acquired with a double-sector *MS* (VG-ZAB-HF, 8 kV accelerating potential, 8 kV *FAB* source, 1 mA) or a Finnigan TSQ-70 triple-quadrupole mass analyser. Here, the *FAB* source was operated at 8 kV with a 0.2-mA discharge current. For measurements with both instruments the sample matrix was 3-nitrobenzyl alcohol.

Both pure samples (Table 7.26) and extracts were prepared in the same manner. Other than in the experiments of Asamoto et al., KBr was applied to the stainless steel probe tip either by dissolving it in CH_3OH and depositing it dropwise, or by burnishing the tip directly with the salt. Approximately 1 μg of a sample was dissolved in CH_2Cl_2 and added dropwise to the probe tip. A thin uniform coating will usually remain after evaporation of the solvent.

The results may be summarized as follows.

For all additives that were analysed, *LD* is superior to *FAB*. Since the latter has a strong tendency to fragmentise analyte molecules, the *FAB-MS* of these high-molecular mass additives present weak parent peaks or none at all. In all cases, *LD* spectra showed $[M+K]^+$ as the strongest peak. CO_2-*LDMS* exhibit more fragment peaks and thus allow the verification of structures. Nd:YAG-*LD* produces very little fragmentation and is therefore apt for multicomponent analyses. This has been established by the analysis of a five-component mixture of DLTDP, DSTDP, Goodrite 3114, Seenox 4125 and Irganox 1010; the $[M+K]^+$ of each are observed. On the other hand, spectra obtained with this laser are more dependent on a variety of factors including laser energy, laser power, sample preparation (and possibly chemical constitution of the analyte).

7.4 Mass Spectrometry with Pre-Separated Mixtures (*GC-, HPLC-, TLC-MS*)

7.4.1 On-Line Coupling of *GC* with Mass Spectrometry (*GC-MS*)

Capillary gas chromatography has an excellent separation efficiency (some 10^5 theoretical plates), and its on-line coupling with *MS* yields optimal analytical information on multicomponent systems. Unfortunately, *GC-MS* is restricted to volatile systems, and most polymer additives are non-volatile or volatilise under decomposition. One of the few exceptions are plasticisers; ample information on *GC* and *MS* data are found in the book of Scholl (l.c.; for *MS* data see Tables 7.1–7.22).

An interesting possibility is the on-line coupling of *GC* with single-ion monitoring *EI-MS*. Here, chemically similar molecules, even isomers, having a key fragment in common, are first separated by *GC* and subsequently introduced into the mass spectrometer. The magnetic field of the latter is stabilised on the *m/z* value of this key fragment. Any time a certain species is eluted, the spectrometer scans a peak with the mass number chosen. Ulsaker and Hoem (10.2.4) applied this technique for the determination of phthalate contaminants in intravenous solutions stored in PVC bags. Phthalic anhydride (*m/z* 149), as an example, is a key fragment for most phthalate esters.

In certain, lucky cases the analyst may circumvent missing volatility of a system (large molecules, polymers) by employing pyrolysis-*GC-MS*. For many years, *Py-GC* has been a comparably cheap though not too effective method for the identification of troublesome systems (crosslinked polymers like thermosetting materials and rubber, copolymers etc.). Relative retention times are not sufficient for identification; the on-line coupling of *Py-GC* with *FTIRS* or *MS*, however, brought a real jump in analytical reliability.

Literature on *Py-GC-MS* for the direct identification of additives or fragments of additives in polymers is scarce. Geissler (10.2.1) investigated additives in polymers and rubber and announced a library of *Py-EIMS* of additives. Recently, Meyer-Dulheuer et al. (10.2.1) published more details on the identification of neat additives and those in plastics by coupling conventional pyrolysis(550 °C)-*GC* with a quadrupole mass spectrometer (QP-5000, Shimadzu), *EI* with 70 V, *m/z* range 45–700. For each analysis, 0.1 mg of additive or polymer were weighed into a platinum vessel and introduced into the pyrolyser.

The wide-bore column had an i.d. of 0.32 mm and a length of 60 m (Restek, Bad Soden), and the oven was programmable up to 300 °C. A stream of He (0.8 cm^3 min^{-1}) carried the pyrolysate through the column to the *MS* interface (split ratio 1:30). A computer calculated the mass spectra (1000 scans min^{-1}) and total ion chromatograms (*TIC*).

The *EI-MS* of neat additives were typical enough for identification. It was even possible to distinguish between isomeric additives. This is shown in Fig. 7.18 with species having the same molar mass and differing only in aliphatic substituents; they differ, however, in their fragmentation behaviour under electron impact. These experiences encouraged the authors to establish a library with the *MS* of meanwhile 174 additives; an expedient program allows the comparison of analytical spectra with the library.

The identification of additive fragments in pyrolysates of stabilised polymers is possible if these fragments are big enough, i.e. heavier than the biggest fragment of the polymer. This is frequently the case, here just two examples. It was possible to identify the phenolic antioxidant Irganox 3052 FF in poly(methylmethacrylate) by fragments with *m/e* 161, 263, 339, 361 and 394. Irganox 3114, an isocyanurate with 4-hydroxy-3,5-di-*t*-butylphenyl substituents, and Hostanox O3 (see Fig. 7.15 above) in PP can be identified by *m/z* 91, 161, 175, 189, 203 and 119, 175, 309, 324, respectively. In another typical case (Hostavin N20 in PP) the identification of this HALS in the pyrolysate was not possible.

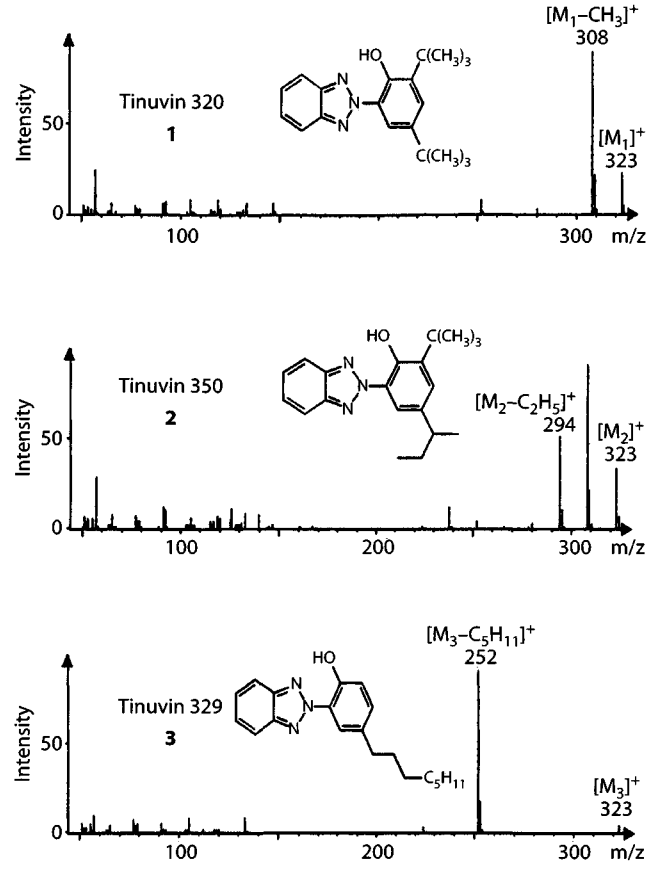


Fig. 7.18 Pyrolysis-*EI-MS* of three isomeric stabilisers (Meyer-Dulheuer et al., 10.2.1)

7.4.2 On-Line Coupling of Separation Techniques for Non-Volatile Substances with Mass Spectrometry

On-line coupling of non-destructive separation methods for large molecules with *MS* is quite promising; some interfaces are commercially available. Experimental or commercial techniques may be categorised as follows:

- Direct liquid introduction (*DLI*)
- Thermospray interfaces
- Mechanical transport (belt) interfaces
- Supercritical chromatography-*MS* interface

Probably the best-developed technique is *HPLC-MS*. Separation power of *HPLC* is lower than that of capillary *GC*; this is compensated by employing a low or medium fragmentising *MS*.

DLI of the eluate through a capillary into the ion source followed by *CI-MS* with the accompanying *HPLC* solvent seems to be the simplest technique. It often produces, however, the poorest results. Better ones are achieved by removal of the solvent in a desolvation chamber which, at the same time, produces a finely dispersed jet of the sample. Alternatively, a He nebuliser can be used as interface. *DLI* under *CI* conditions is usually operated together with quadrupole-*MS*.

Similar to *DLI* is the *thermospray interface*. The *HPLC* eluate passes a stainless steel capillary which is pre-heated to 200–300 °C. Opposite to the orifice of the capillary (and after the ion source) is a rotation pump which keeps the pressure in the ion source in an optimal range (ca. 800 Pa). The pump is equipped with a cooled trap. The high pressure difference between capillary and ion source produces a high-speed jet of nebulised sample. Ionisation is effectuated, e.g. by *CI* in the presence of ammonium acetate in the eluate. This mechanism ionises preferably polar molecules.

The *belt-interface* is a well-established and very sensitive technique (10 ng for a complete mass spectrum). The basic component of this interface is an endless belt made of stainless steel or Kapton [poly(pyromellitic imide) of oxy-*bis*(4-phenol)]. The eluate is sprayed continuously onto the moving band. It is essential that a thin, uniform film is formed. In case the eluate contains a higher concentration of H_2O (>50%) droplets may form on the belt. This is disadvantageous for the *MS*, but can be avoided by applying 2-propanol together with the eluate. In a first heated chamber most of the solvent is evaporated under normal pressure. The rest of the solvent is removed in two differently heated and evacuated chambers. In the ion source, the sample on the belt is flash-evaporated (direct *CI*). Alternatively, *EI* is possible. On the way back, the belt passes a clean-up heating stage and a washing chamber. This is just one version of the different commercial belt interfaces. It allows *HPLC* gradient elution and flow-rates up to 1 cm^3/min. The eluent has to be salt-free. Frequently, *HPLC* is run with a *UV* detector in a way that the two detectors (*MS* is the second one) operate in series.

7.4.3 A Typical Investigation

Vargo and Olson (10.2.2) identified antioxidants and *UV* stabilisers in plastics by on-line coupling of a dual-pump-gradient *HPLC* system (Waters Ass.), a Kratos 773 detector fixed at 280 nm and equipped with a 0.5 cm^3 flow cell (Kratos Analytical Instruments), and a Finnigan-MAT 4615 quadrupole mass spectrometer with a polyimide moving belt *LC/MS* interface.

The *HPLC* column (250 mm long, 2.1 mm i.d.) was packed with 5-µm ODS particles (Alltech Ass.). Sample injections were made with a Valco injection valve equipped with a 10-cm^3 loop. A pre-column filter (Upchurch Scientific) was used to remove particulate material from the injection sample. Solvent A (acetonitrile/H_2O 3:1) and solvent B (acetonitrile/THF 1:1) were applied according to the following gradient elution scheme:

min	% A	% B
0	100	
10	60	40
20		100
30		100
32	100	

The gradient controller was set for a flow rate of 0.2 cm^3/min. The column effluent was deposited on the belt in a fine spray using a nebuliser. When the *UV* detector and the *MS* were operated in series, a stainless steel tubing (200 mm long, 0.25 mm i.d.) connected the absorbance detector outlet with the interface. There was no significant loss of resolution or efficiency in going from the *UV* detector to the *MS*.

The ion source (120 °C) of the *MS* was pressurised to 40 Pa with CH_4 reagent gas; this was ionised with 70 V electrons. Solutes were desorbed from the belt at 230 °C. *CI* spectra were recorded repetitively at 3 s/scan from *m/z* 200–1200, *EI* spectra from *m/z* 50 to 800.

A mixture (in THF) of nine commonly used antioxidants and *UV* light stabilisers was used to develop a general gradient elution scheme and to optimise the *HPLC/MS* parameters. Detection was achieved with *UV* and *MS* detectors in series. The resolution was excellent (near base-line); an aliphatic stabiliser (distearyl thiodipropionate) was not detected by *UV* absorption but easily by *MS*. The sensitivity was in the region of 10^{-6} g. The 280 nm *UV* absorbance for selected aromatic-aliphatic additives was in the region of a few ng. Reconstructed mass chromatograms from selected ion cur-

rents improved the *MS* detection limit (*S/N*=3) to about the same level.

Two polypropylene samples with unknown additive contents were cut into small shavings with a drill bit. Approximately 1 g of these was extracted overnight at r.t. with 5 cm^3 of acetonitrile in a sealed vial with constant stirring (complete extraction was not intended). The solution was filtered and analysed as described above. By evaluating total ion and selected ion currents, it was possible to identify most of the substances producing the peaks. Standard addition and absorbance detection allowed the determination of the concentrations (between 0.07 mg/g and 0.95 mg/g) of some additives in the two PP samples.

7.5 Mass Spectrometry with a Second Mass Spectrometer as Analyser (*MS-MS*, Tandem-*MS*)

7.5.1 Fundamentals

It seems strange to operate two mass spectrometers on-line – it is not. With one of them we have the choice between two, may be three possibilities of ionisation: a soft one (*FI, FD...*), a hard one (*EI*) or something in between (*CI, FAB...*). Soft ionisation gives us molecular peaks but little information on structure. Hard ionisation yields many fragment peaks with structural information, but frequently no information on the molecular mass. The intermediate ionisation techniques are a compromise but have other disadvantages.

Separating multicomponent systems with *GC* and analysing them on-line with *MS* is already a classical and not too expensive method. Why then *MS-MS*?

The answer is (simplified): it is the considerably reduced time for an analysis, and the increased sensitivity (and a lot more). Many thousand publications prove the almost explosive development of *MS-MS* into one of the strongest analytical methods. Details are given in an excellent book of McLafferty et al. and later in a monography of Schwarz (both 10.1).

Figure 7.19 (from Schwarz, l.c.) shows the principle of *MS-MS* for direct analysis of a multicomponent system. ABC, DEF etc. symbolise molecules being composed of functional groups A, B, C etc. The first mass spectrometer (*MS*I) operates with soft ionisation (*FI, FD, CI, LD*) and thus produces an ensemble of molecular ions (or $M+H^+$, $M-H^+$, or adducts). It is assumed that we want to identify ABC. Then, the fields of *MS*I are fixed in a way that only ABC^+ enters the interface where it is excited by collisional activation, laser radiation or surface-induced dissociation. Within the time of one vibration (10^{-13} s), ABC^+ dissociates into fragments characterising the original molecule. These are separated and detected by *MS*II.

The sensitivity of *MS-MS* is generally in the pg range, sometimes even lower. The time needed for a complete analysis of a multicomponent system normally doesn't exceed 20 min. The quality of the spectra is high (Fig. 7.20). There are, however, shortcomings. Soft ionisation with *FI/FD* produces much lower ion yields (ca. 1/100) than *EI*. This may be not sufficient for *MS-MS*. Here, *EI* with reduced ionisation voltage, typically 20 V, or the experimentally demanding liquid secondary ion (*LSI*) technique may solve the problem. Mixtures with an extremely high number of components (some 10^2) and isomeric/isobaric species should be analysed with *GC-MS* – if the samples are volatile. (Meanwhile, *GC-MS/MS* is a well-introduced technique.) Non-volatile samples cause the same difficulties as with other *MS* techniques; laser desorption ionisation (*LDI*) or pyrolysis-*GC-MS* with soft ionisation may solve the problem. Finally, it shouldn't be forgotten that *MS-MS* is very expensive and needs highly skilled analysts.

7.5.2 *MS-MS* of Additives

Jackson et al. (10.2.1) recently contributed a fundamental and scientifically oriented paper on the analysis of (equimolar)

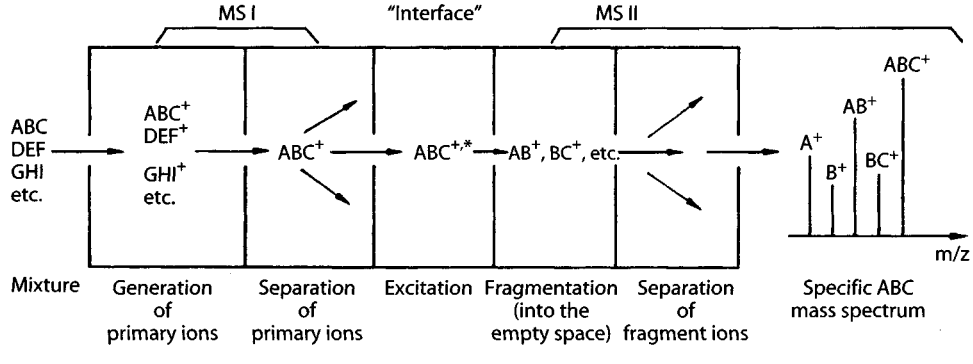


Fig. 7.19
Direct analysis of a mixture to identify the molecule ABC by *MS-MS* (schematic; from Schwarz, 10.1).

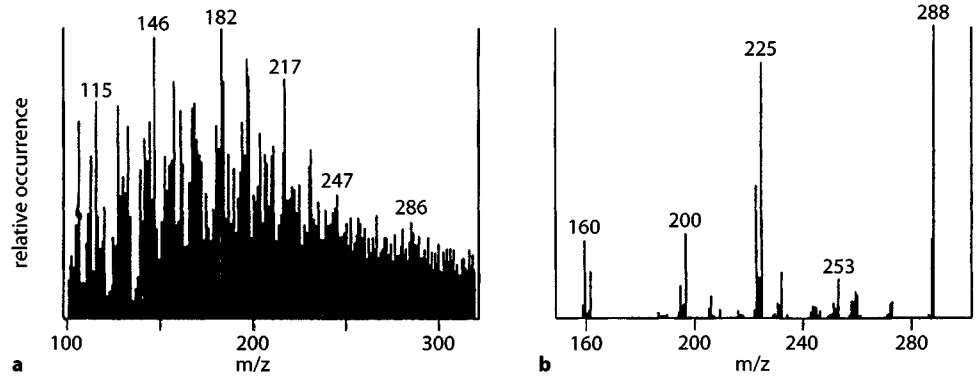


Fig. 7.20
a *CI* spectrum of trichlorodibenzodioxin (*m/z* 288) adsorbed on carbon;
b *MS-MS* of the same sample (from Schwarz, l.c., after R.G. Cooks) ordinates: relative intensity/counts

mixtures of five high-molecular weight additives (Table 7.27) by means of high-energy *MS* and tandem *MS*. (This work also proves the highly demanding nature of *MS-MS*.)

UV-MALDI spectra were measured with a time-of-flight *MS* (Micromass) operated in linear mode with an accelerating potential of 25 kV. Approximately 50 laser shots were employed to obtain the mass spectra under control of the OPUS data system. *EI, CI, LSI* and *FD* spectra were acquired by means of a ZAB-T (Micromass) four-sector *MS* of reverse geometry operating at an accelerating potential of 8 kV.

No less than five different ionisation techniques (first *MS*) were employed:

- *EI, CI, FD,* liquid secondary ionisation (*LSI*)
- *UV* matrix-assisted laser desorption (*MALD*)

The matrix employed for *LSI-MS/MS* experiments was *m*-nitrobenzyl alcohol. (The choice of the optimal matrix was crucial for these experiments.)

The collision-induced dissociation (*CID*) spectra of molecular ions were then obtained by means of tandem *MS*. The optimal fragmentation method for *MS-MS* was *LSI* (which is similar to *FAB*). Table 7.28 exhibits the fragments observed with a Cs ion gun operated at 35 kV and a gun current of 1 μA. Benzonitrile-activated W wires (13 μm) were used in *FD* experiments. The fragment with *m/z* 219 was identified as 2,6-di-*t*-butyl-*p*-cresol (minus H) and is considered as characteristic for the investigated Irganox additives. Possible structures are also discussed for the other fragments presented in Table 7.28.

To sum up: mixtures of non-volatile additives with high molar masses can preferably be analysed by *LSI-MS/MS*. This technique gives strong molecular ion signals as well as fragment ions for structural information. *FD* is also well-suited but the analysis is time-consuming and experimentally challenging. The *FD* ion currents are generally two orders of magnitude lower than those obtained by *LSI*.

It is quite a step from defined multi-component systems to dirty ones – the daily toil of the analyst. Few macromolecular systems contain, in addition to the polymer, so many wanted and a few non-wanted additives and other components than vulcanised elastomers do. In a recent and very informative publication (10.2.6), Lattimer described the practically complete (qualitative) analysis of three vulcanisates by a combination of the following techniques:

1. (Pyrolysis) *FI* of the mixture evaporating at temperatures up to 300 °C in order to win a survey *MS* with predominantly molecular species
2. Selection of prominent or otherwise interesting peaks/species and subjecting these to collision fragmentation and tandem *MS*. Evaluation of the production scan by experience
3. High resolution atomic composition (*AC*) *MS*. A computer program calculates the most likely atomic composition from the measured *m/z* (7 decimals).

The *MS-MS* system employed was a Finnigan MAT 95Q hybrid arrangement. A small slice (0.2–0.4 mg for 70 V *EI* and isobutane *CI*, 1.0–1.5 mg for *FI*) in an Al crucible was introduced into the spectrometer via the direct probe, and heated with 15–20 °C/min. The collision-induced dissociation for *MS/MS* was effectuated with air (50 eV, 0.2 Pa) in the "collision octapole". The pressure in the quadrupole analyser was 8×10^{-4} Pa.

High-resolution *MS* (*EI* or *CI* mode) was carried out by computerised peak-matching with perfluorokerosene reference peaks. Accuracy was 3–5 ppm or better.

In the following, the results of one of the three analyses are given in detail. Figure 7.21 shows the *i*-butane *CI-MS* survey scan of an unknown polyurethane below the thermal decomposition of the polymer (<200 °C). The numerous molecular peaks (odd, $M+H^+$) suggest CHO or CHN(O) compounds, the latter ones with even number of N atoms. From the strongest one, a high-resolution *CI-AC-MS* yielded *m/z* 363.28. A computer program calculated as closest hit the formula $C_{25}H_{35}N_2$ (*M*= 363.56 g/mol). This was identified as *bis*(2,6-di-2-propylphenyl)carbodiimide (Stabaxol P, Bayer). *m/z* 419 is an adduct ion $(M+C_4H_9)^+$ and *m/z* 188 is a fragmention $(NC\text{-}C_6H_4\text{-}C_6H_{12})^+$.

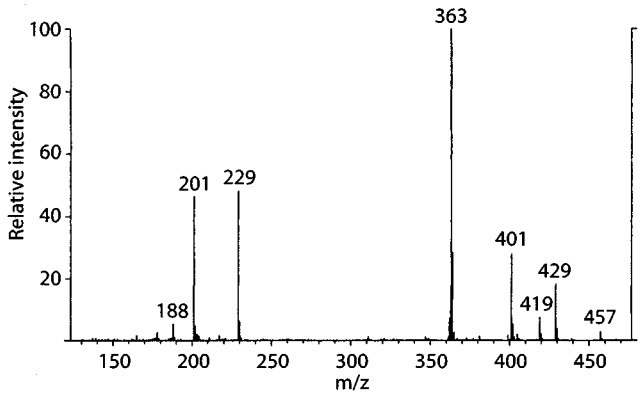


Fig. 7.21 *i*-Butane *CI-MS* survey scan of an unknown polyurethane evaporated between 20 °C and 200 °C (from Lattimer, 10.2.6/4)

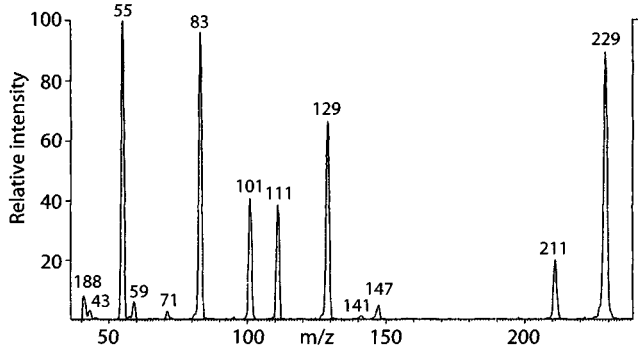


Fig. 7.22 Product-ion scan (*CI-MS/MS*) of MH^+ 229 from unknown polyurethane (from Lattimer, 10.2.6/4)

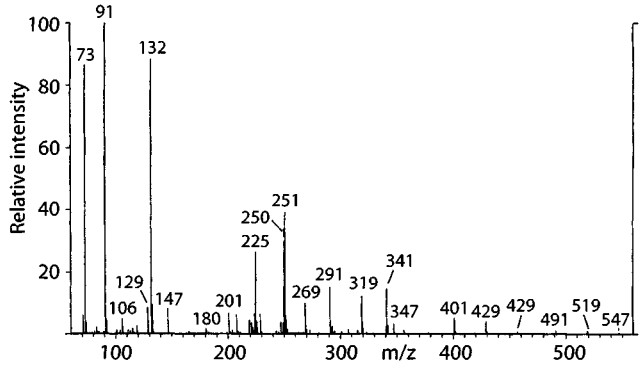


Fig. 7.23 Pyrolysis *CI-MS* survey scan (200–300 °C) of unknown polyurethane (from Lattimer, 10.2.6/4)

There are a number of peaks left for identification. The one at 229 was subjected to *CI-MS/MS* (Fig. 7.22); this revealed, as collision fragments MH^+, exclusively fragments of adipic acid, butanediol and hexanediol as well as cyclic adipate oligomers with the C_4 and the C_6 alcohol.

In order to reveal the polymer structure, the polyurethane was pyrolysed between 200 °C and 300 °C. The *i*-butane *CI-MS* survey scan (Fig. 7.23) was assigned as follows: 250/251, 4,4′-methylene-*bis*(phenylisocyanate), MDI; 341, protonated MDI-butanediol; 269, protonated MDI – H_2O; 225, OCN-C_6H_4-CH_2-NH_2; 132, OCN-C_6H_4-CH_2; 91 and 73 (fragments of the chain extender butanediol, MH and C_4H_9O). The peaks at 201, 229, 401, 429 and 457 can be derived from protonated cyclic adipic oligoesters.

Thus, the system is identified as a poly(ester urethane) on the basis of MDI, a mixed adipic C_4-C_6 polyester and butanediol as chain extender. Stabaxol P was added as a stabiliser.

Egsgaard et al. (10.2.2) proved that *MS-MS* with off-line *HPLC* is a powerful technique for the identification of antioxidants in crude extracts of polymers (orthopaedic bandages and protective gloves). Here 5.0 g of the (finely cut) material was extracted with 50 cm^3 THF for 16 h at r.t. The solution was decanted and evaporated to 5 cm^3. Then 50 cm^3 CH_3OH were added to precipitate dissolved polymer. The supernatant was evaporated to 5 cm^3, and the precipitation procedure was repeated. The solution was evaporated to a small volume.

The *MS-MS* analyses were carried out using a Varian MAT CH5 D double-focusing spectrometer equipped with an *EI/FI/FD* ion source. *FI/FD* spectra were obtained with a 10-µm W wire emitter, activated in benzonitrile vapor. Collision-induced dissociation (*CID*) was carried out by introducing He as a target gas in the second field-free region (interface). Samples were introduced in Al crucibles via the direct inlet system or dipping the emitter into the extract (for *FD*).

HPLC was performed with a Spherisorb 3-µm C_{18} column (120 mm long, 4.6 mm i.d.) and CH_3OH/H_2O (4:1) as eluent (1 cm^3/min). *UV* detection was done at 280 nm.

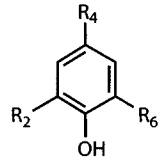
The *FD-MS* of the extract of a bandage material exhibited *m/z* 226 as strong signal, a few signals of lighter fragments were weak. *CID* by accelerated electrons of the substance causing this parent peak produced fragments with *m/z* 211 (– CH_3), 183 (– C_3H_7), 169 (– C_3H_7N), with decreasing intensity. The original molecule was identified as *N*-(2-propyl)-*N*-phenyl-*p*-phenylenediamine (IPPD). Quantitation with *HPLC* revealed a concentration of 0.1% IPPD in the polymer.

HPLC simplifies the identification of *FI-MS* components by providing relative retention times. The *FI-MS* of the extract of surgeon gloves exhibited *m/z* 358 as strongest mass (with a weak companion at 360). *CID-MS* of the 358-substance produced a strong peak at 343 (– CH_3) and numerous much weaker peaks, among them the more prominent ones at 195 and 163. These differ by the mass of ^{32}S, their sum is 358; ^{34}S would explain 360. The central splitting leaves the sulfur with either fragment. This makes it quite likely that the original molecule is a symmetrically built, *t*-butyl-substituted thiobisphenol. (*t*-Butyl easily splits off CH_3; directly ring-attached CH_3 will not be split off, neither thermally nor by radiation.) The mass of 358 requires an additional CH_3 group on each ring. Thio-*bis*(*t*-butylcresol) forms three isomers with equally substituted rings. *CA* and *HPLC* of the authentic compounds verified thio-*bis*(4-phenol) with *t*-butyl in 3- and CH_3 in 6-position. By *HPLC*, the concentration of this additive in the polymer was determined to be 1%.

Table 7.1

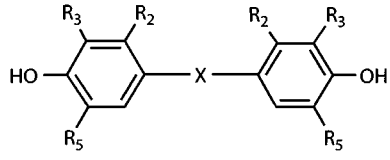
EI (70 V) mass fragments of CHO-phenolic antioxidants (without additional functions); strongest mass (base peak) := 100 (selection of Scholl data, after correction)

Monophenols



Substance			Molar mass g/mol	Base peak *m/z*	Mass numbers (*m/z*) (*relative intensities*)						
R_2	R_4	R_6									
CH_3	$C(CH_3)_3$	H	164	163	39	41	77	91	121	135	178?
					9	*13*	*10*	*14*	*11*	*39*	*32*
$C(CH_3)_3$	CH_3	$C(CH_3)_3$	220	205	41	57	81	105	145	206	220
					8	*17*	*7*	*6*	*8*	*16*	*34*
$C_{18}H_{37}$	CH_3	$C_{18}H_{37}$	612	43	41	55	57	69	71	83	97
					91	*98*	*99*	*72*	*57*	*63*	*56*
2,5-Di-*t*-pentyl-hydroquinone			250	221	29	41	43	71	192	222	250
					8	9	15	9	8	17	27

p-Bisphenols

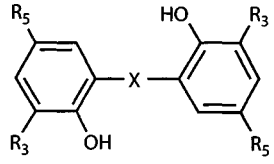


(the first representative very likely was mixed with a hydrocarbon oil)

Substance				Molar mass g/mol	Base peak *m/z*	Mass numbers (*m/z*) (*relative intensities*)						
R_2	R_3	R_5	X									
H	H			186	186	41	43	55	57	157	170	187
						10	*16*	*16*	*18*	*11*	*38*	*14*
H	$C(CH_3)_3$	$C(CH_3)_3$		410	410	41	57	162	176	190	396	411
						7	*35*	*5*	*5*	*10*	*14*	*31*
H	H	H	$C(CH_3)_2$	228	213	39	65	91	99	119	214	228
						27	*25*	*33*	*22*	*49*	*30*	*56*
H	$C(CH_3)_3$	CH_3	CH_2	340	340	127	161	177	283	325	326	341
						28	*19*	*35*	*34*	*92*	*24*	*27*
H	$C(CH_3)_3$	$C(CH_3)_3$	CH_2	424	424	57	197	219	368	409	410	425
						41	*17*	*24*	*15*	*55*	*18*	*33*
CH_3	$C(CH_3)_3$	H	HCC_3H_7	382	339	41	57	149	176	203	340	382
						9	*15*	*12*	*8*	*10*	*27*	*11*

Table 7.1 Continue

o-Bisphenols



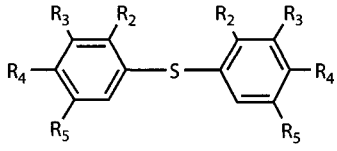
Substance			Molar mass	Base peak	Mass numbers (*m/z*) (*relative intensities*)						
R_3	R_5	X	(g/mol)	*m/z*							
$C(CH_3)_3$	CH_3	CH_2	340	177	41	57	121	149	161	164	340
					24	*37*	*30*	*44*	*75*	*66*	*53*
$C(CH_3)_3$	C_2H_5	CH_2	368	191	57	163	175	178	311	368	369
					23	*35*	*59*	*71*	*24*	*82*	*24*
$C_6H_{11}CH_3$	CH_3	CH_2	420	204	55	121	135	148	161	217	420
					69	*93*	*49*	*43*	*42*	*97*	*91*

Table 7.2

Tentative assignment of *EI* fragments of CHO-phenolic antioxidants to structures (without additional functions; for molecular masses, m.m., see Table 7.1), Mass numbers 29, 39, 41, 43, 55, 57, 65, 69, 71: unsaturated and saturated hydrocarbons (even) or hydrocarbon radicals (odd). Molecular masses: 186, 220, 228, 250, 340, 368, 382, 420, 424. Molecular masses are usually accompanied by the protonated, sometimes by the deprotonated, species

77	Phenyl	157	Phenylcyclohexene	206	*t*-Butylpropyl hydroquinone
81	Cyclohexene – H	162	Propylvinylphenol	213	Ethyldihydroxydiphenyl – H
83	Cyclohexane – H	163	*t*-Butylcresol	214	Ethyldihydroxydiphenyl
91	Benzyl	170	Hydroxydiphenyl	217	Heptenylxylenol – H
97	Methylcyclohexene	175	*t*-Butylvinylphenol – H	221	Pentylpropylhydroquinone – H
99	Methylcyclohexane	176	*t*-Butylvinylphenol	222	Pentylpropylhydroquinone
105	Styrene + H	177	*t*-Butylxylenol – H	283	Methylenebisphenol + C_6H_{11}
119	Allylbenzene + H	178	*t*-Butylxylenol	311	Methylenebisphenol + C_8H_{15}
121	Ethyltoluene + H Xylenol – H	190	*t*-Butylpropylphenol	325	Methylenebisphenol + C_9H_{17}
127	Phenyldiacetylene + H Phenylcyclobutadiene – H	192	Dipropylhydroquinone	326	Methylenebisphenol + C_9H_{18}
135	Ethylcresol – 1	197	?	339	m.m. – C_3H_7
				340	m.m. – C_3H_6
145	Butynylphenol – H Cyclobutenylphenol – H	203	*t*-Butylpropylcresol – H	396	m.m. – CH_2
149	Propylcresol – H	205	*t*-Butylpropylcresol + H	409	m.m. – CH_3
				410	m.m. – CH_2

Table 7.3
EI (70 V) mass fragments of thiobisphenol antioxidants; strongest mass (base peak):=100 (selection of Scholl data)



R_2	R_3	R_4	R_5	Molar mass g/mol	Base peak *m/z*	Mass numbers (*m/z*) (*relative intensities*)						
OH	H	H	$C(CH_3)_3$	330	135	107	150	167	182	259	315	330
						31	*37*	*64*	*20*	*31*	*47*	*60*
OH	$C(CH_3)_3$	H	CH_3	358	164	41	57	136	146	149	150	358
						19	*24*	*20*	*17*	*53*	*16*	*42*
CH_3	H	OH	$C(CH_3)_3$	358	358	121	149	164	181	196	343	359
						20	*72*	*27*	*72*	*38*	*20*	*23*
H	$C(CH_3)_3$	OH	CH_3	358	358	136	150	164	179	195	343	359
						13	*60*	*7*	*6*	*10*	*12*	*25*

Table 7.4
Tentative assignment of *EI* fragments of thiobisphenol antioxidants to structures (for molecular masses see Table 7.3)

41	C_3H_5	150	Propylcresol	259	(*t*-)Butylhydroxydiphenylthioether + H
57	C_4H_9	164	(*t*-)Butylcresol	315	*o,o'*-Dihydrox-3-*t*-butyl-3'-propyldiphenylthioether – H
107	Ethylbenzene + H	167	(*t*-)Butylthiophenol + H	330	Molecular mass
121	Ethyltoluene + H	179	Ethyl(*t*-)butylphenol + H	343	Thio-*bis*(4-phenol) + 2 CH_3+C_3H_7+C_4H_9
135	Ethylcresol – H	181	Methyl(*t*-)butylthiophenol + H	358	Molecular mass
136	Ethylcresol	182	(*t*-)Butylhydroxythiophenol	359	Molecular mass+H
146	Cyclobutenylphenol butynylphenol	195	Methyl(*t*-)butylhydroxythiophenol – H		
149	Propylcresol – H	196	Methyl(*t*-)butylhydroxythiophenol		

Table 7.5
EI (70 V) mass fragments of phenolic antioxidants with additional hetero functions; strongest mass (base peak):=100 (selection of Scholl data)

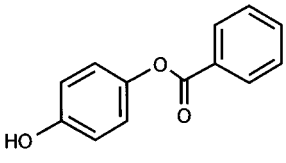
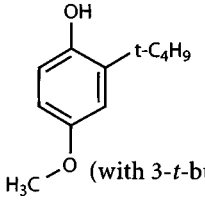
Molecule	Molar mass g/mol	Base peak *m/z*	Mass numbers (*m/z*) (*relative intensities*)						
	214	91	27	39	51	53	65	92	200
			3	*41*	*91*	*39*	*12*	*8*	*11*
(contains hydrocarbon)									
 (with 3-*t*-butyl)	180	165	39	41	77	91	137	166	180
			8	*10*	*10*	*9*	*42*	*11*	*59*

Table 7.5 Continue

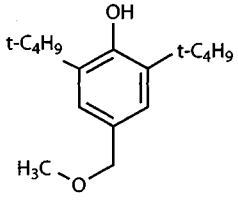
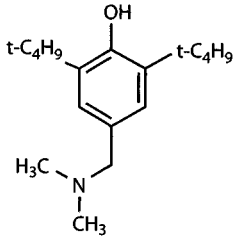
Molecule	Molar mass g/mol	Base peak *m/z*	Mass numbers (*m/z*) (*relative intensities*)						
	250	235	41 *33*	45 *24*	57 *82*	161 *20*	197 *40*	219 *66*	250 *40*
	263	161	41 *37*	44 *90*	45 *45*	163 *38*	175 *41*	203 *69*	218 *56*

Table 7.6
Tentative assignment of *EI* fragments of etherphenol and aminophenol antioxidants to structures (for molecular masses, m.m., see Table 7.5)

27	C_2H_3	161	Butadienylhydroquinone – H, butenylbenzylamine
39	C_3H_3	163	(*t*-)Butylbenzylamine
41	C_3H_5	165	Propylanisole – H
44	$N(CH_3)_2$	166	Propylanisole
45	$HN(CH_3)_2$ H_3C-O-CH_2	175	Methyl(*t*-)butylbenzylamine
51	Cyclobutadiene – H, diacetylene + H	180	m.m.
53	Cyclobutene–H butadiene – H	197	?
57	C_4H_9	200	m.m. – CH_2
65	C_5H_5, cyclopentadiene	203	?
91	Toluene – H	218	2-Butenyl-6-*t*-butyl-*p*-cresol
92	Toluene, hydroxybenzyne	219	2-Butenyl-6-*t*-butyl-*p*-cresol + H
137	Methoxycresol – H	250	m.m.

Table 7.7
EI (70 V) mass fragments of aromatic amine antioxidants; strongest mass (base peak): = 100 (selection of Scholl data)

Molecule R_1-NH-C_6H_4-NH-R_2 R_1	R_2	Molar mass g/mol	Base peak *m/z*	Mass numbers (*m/z*) *relative intensities*						
$-CH(CH_3)C_2H_5$	Same	220	191	81	107	161	163	192	205	220
				20	*16*	*7*	*7*	*13*	*13*	*44*
$-CH(CH_3)C_6H_{13}$	Same	332	332	43	81	107	161	247	248	333
				11	*26*	*14*	*11*	*90*	*17*	*26*
$-CH(CH_3)_2$	Phenyl	226	211	105.5	167	169	183	212	226	227
				14	*12*	*11*	*35*	*18*	*80*	*14*
$-C_8H_{17}$	Phenyl	296	211	105.5	183	184	212	281	296	297
				14	*16*	*15*	*17*	*9*	*64*	*15*
Cyclohexyl	Phenyl	266	266	41	111.5	130	183	184	223	267
				11	*12*	*18*	*27*	*20*		
Phenyl	Phenyl	260	260	77	130	167	168	169	183	261
				11	*9*	*19*	*13*	*23*	*15*	*22*

Table 7.8
Tentative assignment of *EI* fragments of aromatic amine antioxidants to structures. Molecular masses (see Table 7.7): 220, 226/227, 260/261, 266/267, 296/297, 332/333

41	C_3H_5
43	C_3H_7
77	Phenyl
81	C_6H_9
105.5 (m/2)	4-Amino-4′-ethyldiphenylamine
107	1,4-Diaminobenzene – H
111.5 (m/2)	4-Amino-4′-propyldiphenylamine
130 (m/2)	1,4-Diphenylaminobenzene (m) NH-C_6H_4-C_3H_3
161	4-Pentenylaniline
163	4-Pentylaniline
167	*N*-Benzynylaniline
168	Diphenylamine – H
169	Diphenylamine
183	4-Aminodiphenylamine – H
191	*N,N′*-1,4-Dipropyldiphenylamine – H
192	*N,N′*-1,4-Dipropyldiphenylamine
205	1-Propyl-4-(*t*-)butyldiphenylamine – H
211	*N*-4-(4′-Ethylphenyl)diphenylamine – H
212	*N*-4-(4′-Ethylphenyl)diphenylamine
223	*N*-4-(4′-Propenylphenyl)diphenylamine – H
247	*N,N′*-1,4-Dipentyldiphenylamine – H
248	*N,N′*-1,4-Dipentyldiphenylamine
281	4-Heptylaminodiphenylamine

Table 7.9
EI (70 V) mass fragments of other CHN (O, S) antioxidants, strongest mass (base peak): = 100 (selection of Scholl data)

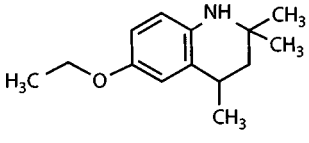
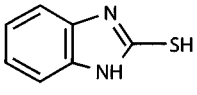
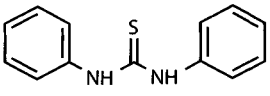
Molecule	Molar mass g/mol	Base peak *m/z*	Mass numbers (*m/z*) *relative intensities*						
	217	202	144	145	173	174	175	203	217
			7	*15*	*12*	*37*	*4*	*15*	*13*
	150	150	63	65	75	118	122	151	167
			9	*11*	*11*	*10*	*10*	*11*	*9*
	228	135	39	51	65	66	77	93	136
			11	*23*	*16*	*26*	*58*	*89*	*10*

Table 7.10
Tentative assignment of *EI* fragments of CHN(O,S) antioxidants (other than amines) to structures; molecular masses (see Table 7.9): 150/151, 217, 228

39	C_3H_3	135	*N*-Phenylthiourea
51	C_4H_3	136	*N*-Phenylthiourea+H
63	$H_2N\text{-}CH_2\text{-}SH$	144	?
65	SO_2H	145	?
66	SO_2H_2 C_5H_6	167	Benzimidazole-2-sulfoxide
75	Benzyne – H	173	Ethoxyphenylbutadiene – H
77	Phenyl	174	Ethoxyphenylbutadiene ethoxyphenylcyclobutene
93	Aniline	175	EPB/EPCB+1
118	Benzimidazole	202	2,4-Dimethyl-6-ethoxydihydroquinoline – H
122	*N*-Methyldiaminobenzene	203	2,4-Dimethyl-6-ethoxydihydroquinoline

Table 7.11
EI (70 V) mass fragments of adipate and sebacate plasticisers; strongest mass (base peak) : = 100 (selection of Scholl data)

	Molar mass g/mol	Base peak *m/z*	Mass numbers (*m/z*) *relative intensities*								
Adipate											
Dimethyl-	174	55	15	27	29	41	43	59	74	101	114
			59	*39*	*34*	*54*	*41*	*80*	*36*	*38*	*58*
Diethyl-	202	29	27	55	60	73	88	101	111	128	129
			64	*76*	*54*	*57*	*59*	*57*	*68*	*68*	*73*
Di-*i*-butyl	258	57	29	41	55	56	100	101	111	129	185
			5o	*55*	*59*	*62*	*26*	*32*	*48*	*94*	*88*
Di-2-ethylhexyl-	370	129	29	41	43	55	57	70	71	112	147
			44	*63*	*70*	*62*	*79*	*61*	*52*	*52*	*25*
Butylbenzyl-	292	91	55	65	83	92	101	107	111	129	235
			16	*12*	*9*	*11*	*19*	*10*	*25*	*82*	*11*
Sebacate											
Dimethyl-	230	55	15	41	43	59	74	84	98	125	157
			55	*72*	*53*	*48*	*91*	*45*	*57*	*46*	*39*
Diethyl-	258	29	41	55	69	88	97	98	125	171	213
			63	*93*	*39*	*36*	*39*	*33*	*34*	*35*	*42*
Dibutyl-	314	29	41	43	55	56	57	69	98	185	241
			98	*33*	*61*	*76*	*59*	*26*	*28*	*42*	*54*
Di-*i*-butyl-	314	57	27	29	41	43	55	56	98	185	241
			20	*68*	*71*	*26*	*39*	*52*	*18*	*42*	*37*
Di-2-ethylhexyl-	426	57	29	41	43	55	56	64	65	149	185
			35	*56*	*55*	*38*	*30*	*37*	*30*	*51*	*29*
Dibenzyl-	382	92	39	51	63	65	74	76	91	93	107
			18	*21*	*9*	*27*	*26*	*34*	*92*	*16*	*28*

Table 7.12
Tentative assignment of *EI* fragments of adipate and sebacate ester plasticisers to structures. Mass numbers 15, 27, 29,41, 43, 55, 56, 57, 69, 71, 97: unsaturated and saturated hydrocarbons (even) or hydrocarbon radicals (odd)

59	H_3C-COOH – H	93	Toluene+H phenol – H	128	Ethylcyclohexanol
60	H_3C-COOH, C_3H_7OH, $HCOOCH_3$	98	Cyclohexanone, cycloheptane	129	Ethylcyclohexanol + H
73	C_2H_5COOH – H	100	C_4H_7COOH,$C_5H_{11}CHO$,$HCO(CH_2)_3CHO$	147	Octanediol + H
74	C_2H_5COOH, C_4H_9OH, CH_3COOCH_3	101	C_4H_7COOH + H, $C_5H_{11}CHO$+H	157	Nonanoic acid – H
76	Benzyne	107	Benzylalcohol – H	171	Decanoic acid–H $HCO(CH_2)_8CHO$ + H
84	Cyclopentanone, cyclohexane	111	Hydroquinone + H, cycloheptanone – H	185	$HCO(CH_2)_4COOC_4H_9$ – H
88	C_3H_7COOH, $CH_3COOC_2H_5$, $C_5H_{11}OH$	112	Dihydroxycyclohexadiene	213	$HCO(CH_2)_8COOC_2H_5$ – H
91	Toluene – H	114	Dihydroxycyclohexene, methylcyclohexanol	235	C_6H_5–CH_2–$OCO(CH_2)_4COOH$ – H
92	Toluene	125	Cyclooctanone – H		

Table 7.13
EI (70 V) mass fragments of phthalate plasticisers; strongest mass (base peak): = 100 (selection of Scholl data, corrected)

Phthalate	Molar mass g/mol	Base peak *m/z*	Mass numbers (*m/z*) *relative intensities*								
Dimethyl-	194.1	149	15	50	76	77	92	104	135	164	194
			15	*16*	*16*	*24*	*11*	*8*	*9*	*12*	*14*
Diethyl-	222.2	149	50	65	76	77	93	104	105	150	177
			12	*15*	*15*	*7*	*6*	*9*	*9*	*13*	*26*
Dipropyl-	250.3	149	27	39	41	43	76	104	191	209	
			11	*6*	*12*	*11*	*8*	*8*	*8*	*10*	
Dibutyl-	278.4	149	29	41	56	57	76	104	150	205	223
			21	*17*	*8*	*8*	*6*	*6*	*11*	*6*	*8*
Dioctyl-	390.6	112	29	41	43	55	57	71	150	279	
			15	*25*	*29*	*15*	*28*	*17*	*17*	*23*	
Di(2-ethylhexyl)-	390.6	57	55	57	70	71	83	113	149	167	261
			34	*42*	*49*	*37*	*35*	*40*	*52*	*56*	*49*
Dicyclohexyl-	330.4	149	29	41	54	55	64	83	150	167	248
			7	*28*	*7*	*36*	*10*	*14*	*15*	*41*	*10*

Table 7.14
Tentative assignment of *EI* fragments of phthalate ester plasticisers to structures. Mass numbers 15, 27, 29, 39, 41, 43, 50, 54, 55, 57, 65, 67, 70, 71, 83, 113: unsaturated and saturated hydrocarbons (even) or hydrocarbon radicals (odd)

50	Diacetylene	164	Methoxycarbonylbenzaldehyde
76	Benzyne	167	Phthalic acid + H
77	Phenyl	177	Ethoxycarbonylbenzaldehyde – H
92	Toluene	191	Propoxycarbonylbenzaldehyde – H
93	C_7H_9 phenol – H	194	Dimethylphthalate
104	Styrene C_7H_4O	209	Propylphthalate + H
105	Benzaldehyde – H	223	Butylphthalate + H
135	Hydroxymethylbenz-aldehyde – H	248	Cyclohexylphthalate
149	Phthalic anhydride + H	261	Heptylphthalate – H
150	Carboxybenzaldehyde	279	Octylphthalate + H

Table 7.15
EI (70 V) mass fragments of phosphate, thiophosphate and phosphonate plasticisers; strongest mass (base peak): = 100 (selection of Scholl data)

	Molar mass (g/mol)	Base peak *m/z*	Mass numbers (*m/z*) *relative intensities*								
Phosphate											
Triethyl-	182	99	27	29	45	81	82	109	125	127	155
			23	*29*	*16*	*56*	*32*	*41*	*23*	*58*	*92*
Tributyl-	266	99	27	29	39	41	55	56	57	155	211
			10	*20*	*10*	*34*	*11*	*11*	*18*	*27*	*23*
Tri-*i*-butyl-	266	99	27	29	39	41	43	55	57	112	155
			29	*41*	*21*	*63*	*41*	*14*	*43*	*14*	*17*
Tri(2-ethylhexyl)-	434	99	41	43	55	57	69	71	112	113	211
			12	*13*	*13*	*23*	*9*	*15*	*8*	*23*	*11*
Triphenyl-	326	326	39	51	65	77	94	170	215	233	325
			25	*27*	*42*	*55*	*22*	*27*	*18*	*21*	*68*
Tricresyl-	368	77	39	65	78	79	91	107	165	354	368
			33	*67*	*31*	*37*	*68*	*33*	*39*	*34*	*43*
Cresyldiphenyl-	340	77	39	51	65	66	94	107	325	326	340
			72	*44*	*90*	*49*	*98*	*23*	*34*	*54*	*26*
Trixylenyl-	410	410	77	79	91	104	105	179	193	209	396
			99	*53*	*73*	*51*	*52*	*54*	*77*	*53*	*54*
Thiophosphate											
Triethyl-	198	121	27	29	45	65	93	97	109	115	198
			36	*56*	*35*	*68*	*77*	*60*	*48*	*42*	*98*
Tributyl-	282	227	29	41	55	56	57	99	115	129	171
			54	*56*	*50*	*39*	*65*	*40*	*94*	*69*	*96*
Phosphonate											
Diethyl-ethyl-	166	111	27	29	31	45	65	93	138	139	166
			37	*46*	*50*	*35*	*45*	*71*	*32*	*58*	*30*
Dibutyl-butyl-	250	139	29	41	55	57	83	97	121	153	195
			54	*59*	*50*	*63*	*37*	*83*	*54*	*83*	*100*
Di(2-ethylhexyl)-2-ethylhexyl-	418	195	41	43	55	57	69	71	97	209	307
			43	*45*	*47*	*53*	*35*	*38*	*75*	*41*	*50*

Table 7.16
Tentative assignment of *EI* fragments of phosphate, thiophosphate and phosphonate ester plasticisers to structures. Mass numbers 27, 29, 39, 41, 43, 55, 56, 57, 69, 71, 83, 113: unsaturated and saturated hydrocarbons (even) or hydrocarbon radicals (odd). Molecular masses (see Table 7.15): 166/165, 182, 198, 326, 340, 368, 410

31	CH_3O, P	105	Styrene + H	171	$S=P(OH)_2\text{-}OC_4H_9$
45	C_2H_5O	107	Ethylbenzene + H	179	?
65	H_2PO_2	109	$S=P(H)\text{-}OC_2H_5$, $O=P(OH)\text{-}OC_2H_5$	193	?
66	H_3PO_2	111	$(HO)_2P(H)\text{-}OC_2H_5$	195	$O=PH(OC_4H_9)_2 + H$
77	Phenyl	112	$(HO)_2P(H)\text{-}OC_2H_5 + H$	209	$O=POH(CH_3)\text{-}OC_8H_{17} + H$
78	Benzene	115	$S=P(OH)_3 + H$	211	$O=P(OH)_2\text{-}OC_8H_{17} + H$
					$O=POH(OC_4H_9)_2 + H$
79	Benzene + H	121	$S=P(CH_3)\text{-}OC_2H_3$	227	$S=POH(OC_4H_9)_2 + H$
	PO_3		$O=P(H)\text{-}OC_4H_9$		
81	H_2PO_3	125	$HO_3P\text{-}OC_2H_5$	233	$O=P(OC_6H_5)_2$
82	H_3PO_3	127	$O=P(OH)_2\text{-}OC_2H_5 + H$	307	$O=P(OH)(C_8H_{17})(OC_8H_{17}) + H$
91	Benzyl	129	$S=P(OH)_2\text{-}OCH_3 + H$	325	$O=P(OC_6H_5)3 - H$
93	$O=P(OH)\text{-}C_2H_5, C_6H_5O$	138	$O=PH(OC_2H_5)_2$	396	Molecular mass – CH_2
94	Phenol	139	$O=PH(OC_2H_5)_2 + H$		
			$O=P(OH)(H)\text{-}OC_4H_9 + H$		
97	$S=P(OH)_2, H_2PO_4$	153	$HO_3P\text{-}OC_4H_9$		
99	H_3PO_4+H	155	$O=POH(OC_2H_5)_2 + H$		
	$S=PH(OH)_2$		$O=P(OH)_2\text{-}OC_4H_9 + H$		
104	Styrene	170	$O_2P\text{-}O\text{-}C_6H_4\text{-}CH_3$		

Table 7.17
EI (70 V) mass fragments of anhydride hardeners; strongest mass (base peak): = 100 (selection of Scholl data, after correction and rearrangement)

Substance (-anhydride)	Molar mass g/mol	Base peak *m/z*	Mass numbers (*m/z*) *relative intensities*						
Phthalic	148	104	50	51	52	76	77	148	149
			40	*3*	*14*	*85*	*8*	*47*	*6*
Tetrahydrophthalic	152	79	27	39	51	77	78	80	124
			8	*14*	*8*	*13*	*8*	*42*	*48*
Tetrachlorophthalic	284 286 288 290	242	107	142	212	214	240	244	286
			57	*54*	*70*	*63*	*62*	*53*	*61*
Hexahydrophthalic	154	67	27	39	41	44	54	79	82
			63	*52*	*76*	*83*	*98*	*65*	*97*
Methyltetrahydrophthalic	166	79	39	77	80	91	93	94	118
			79	*74*	*49*	*65*	*81*	*82*	*47*
Methylhexahydrophthalic	168	81	39	44	54	55	67	82	96
			38	*38*	*85*	*44*	*30*	*29*	*89*
Endodichloromethylenetetra-chlorophthalic	368,370...380	43	26	41	54	56	57	70	71
			72	*87*	*66*	*84*	*88*	*71*	*88*
Endomethylmethylenetetra-hydrophthalic	178	79	26	39	51	54	77	78	80
			98	*91*	*45*	*93*	*93*	*76*	*94*
Trimellitic	192	148	50	75	76	102	103	104	120
			44	*55*	*31*	*33*	*33*	*45*	*53*
Pyromellitic	218	174	37	51	73	74	101	102	175
			60	*21*	*35*	*81*	*14*	*79*	*17*
Dodecenylsuccinic	266	43	41	55	57	69	83	97	109
			99	*89*	*92*	*90*	*85*	*90*	*83*

Table 7.18
Tentative assignment of *EI* fragments of anhydride hardeners to structures (for molecular masses see Table 7.17). Mass numbers 26, 27, 39, 41, 43, 44, 50, 51, 52, 54, 55, 56, 57, 67, 69, 70, 81, 82, 83, 96, 97, 109: unsaturated and saturated hydrocarbons (even) or hydrocarbon radicals (uneven)

37	1/2 74 ?	77	C_6H_5 benzene –H	101	C_8H_5 phenyl-acetylene – H	142	C_6Cl_2	242	X+2H
44	C_3H_8 or CO_2	78	C_6H_6 benzene	102	Phenylacetylene	148	Phthalic anhydride (PAH)	244	X+4H
56	C_3H_4O	79	C_6H_7 benzene + H	103	Phenylacetylene + H	149	PAH+H	286	Molecular mass
70	C_5H_{10} or C_4H_6O	80	C_6H_8 cyclohexadiene	104	Styrene	174	Endocarbonyl phthalic anhydride		
73	C_4H_9O	83	C_6H_{11} or C_5H_7O	107	1/2 214? C_8H_{11}	175	EPAH+H		
74	$C_4H_{10}O$	91	C_7H_7	118	Indane	212	Tetrachloro-benzyne		
75	$C_4H_{11}O$ or C_6H_3	93	C_6H_5O	120	Tolualdehyde	214	Tetrachloro-benzene		
76	C_6H_4 benzyne	94	C_6H_5OH	124	Methylcyclohexyl-aldehyde	240	Endocarbonyl-tetrachlorobenzene (X)		

Table 7.19
EI (70 V) mass fragments of amine and heterocyclic activators; strongest mass (base peak): = 100 (selection of Scholl data, after correction and rearrangement)

Substance	Molar mass g/mol	Base peak *m/z*	Mass numbers (*m/z*) *relative intensities*						
Diethylamine	73	30	27	28	29	42	44	56	58
			85	*99*	*91*	*92*	*81*	*94*	*95*
Triethylamine	101	28	27	30	42	56	84	86	99
			78	*78*	*82*	*96*	*78*	*79*	*82*
Trimethylcyclohexylamine	141	70	39	41	43	44	55	56	84
			32	*72*	*84*	*49*	*49*	*28*	*99*
Ethylenediamine	60	28	26	27	29	30	41	43	55
			32	*97*	*73*	*97*	*19*	*13*	*20*
Diethylenetriamine	103	44	19	27	28	30	42	56	73
			18	*15*	*15*	*34*	*11*	*15*	*59*
Triethylenetetramine	146	28	30	41	42	43	44	56	73
			97	*80*	*90*	*81*	*99*	*97*	*82*
Trimethylhexamethylenediamine	158	41	30	55	56	69	82	96	124
			98	*89*	*97*	*91*	*93*	*87*	*95*
N,N′,N′′,N′′′-Hexamethyltri-ethylenetetramine	173	58	15	28	30	42	43	44	45
			53	*75*	*55*	*97*	*67*	*87*	*57*
N,N,N′,N′-Tetramethylethylenedi-amine	116	58	15	28	30	42	43	44	56
			25	*34*	*48*	*71*	*17*	*14*	*17*
N,N,N′,N′-Tetramethyl-1,3-butanediamine	144	58	42	44	56	71	72	84	99
			99	*71*	*80*	*76*	*98*	*71*	*70*
Isophoronediamine	170	124	30	55	68	109	123	138	141
			90	*90*	*98*	*98*	*90*	*84*	*87*
Dicyanodiamide	84	16	17	18	28	42	43		
			99	*97*	*61*	*14*	*22*		
Triethylenediamine	112	42	29	55	56	57	58	70	112
			52	*99*	*85*	*87*	*77*	*58*	*85*
N,N-Dimethylbenzylamine	135	58	42	44	65	91	134	135	136
			18	*11*	*14*	*59*	*44*	*83*	*39*

Table 7.19 Continue

Substance	Molar mass g/mol	Base peak *m/z*	Mass numbers (*m/z*) *relative intensities*						
Methylene-*bis*(4-aniline)	198	197	77	104	106	180	182	198	199
			55	*43*	*98*	*69*	*70*	*99*	*61*
2-Methylimidazole	82	28	27	40	41	42	54	81	82
			50	*48*	*80*	*83*	*95*	*85*	*97*
Morpholine	87	29	27	28	30	42	56	57	87
			20	*80*	*47*	*27*	*59*	*84*	*45*

Table 7.20

Tentative assignment of *EI* fragments of amine and heterocyclic activators to structures (for molecular masses, m.m., see Table 7.19). Mass numbers 15, 26, 27, 28, 29, 30, 41, 42, 43, 44, 55, 56, 58, 65, 68, 70, 82, 84, 86, 96, 123, 124: unsaturated and saturated hydrocarbons (even) or hydrocarbon radicals (uneven). Some of these may also belong to N-containing fragments (see Table)

16	NH_2	58	C_3H_7NH or diaminoethene	96	$C_6H_{10}N$	136	m.m. + H
17	NH_3	70	C_4H_8N or azacyclopentane – H	99	$C_6H_{11}NH_2$	138	Trimethylcyclohexenylamine – H
18	H_2O	73	$C_4H_9NH_2$	104	$H_2C\text{-}C_6H_2\text{-}NH_2$	141	Trimethylcyclohexylamine
27	HCN	77	Benzene – H	106	$H_2C\text{-}C_6H_4\text{-}NH_2$	180	?
28	HCNH	81	Azacyclohexadiene	109	$H_3C\text{-}C_6H_6\text{-}NH_2$ or C_8H_{13}	182	Aminodiphenylmethane – H
30	CH_2NH_2	82	C_5H_8 N or $C_4H_6N_2$, diazacyclohexadiene	112	m.m.	198	m.m.
31	CH_3NH_2	84	C_5H_{10} N or $C_4H_8N_2$, diazacyclohexene	123	Trimethylcyclohexene–H	199	m.m. + H
44	$C_2H_4\text{-}NH_2$	86	$C_4H_{10}N_2$, piperazine	124	Trimethylcyclohexene		
45	$C_2H_5\text{-}NH_2$	87	$C_5H_{11}NH_2$ or C_4H_9NO, morpholine	134	m.m. – H		
57	C_3H_7 N or azacyclobutane	91	Toluene – H	135	m.m.		

Table 7.21

EI (70 V) mass fragments of aminoalcohol activators; strongest mass (base peak): = 100 (selection of Scholl data, after correction and rearrangement)

Substance	Molar mass g/mol	Base peak *m/z*	Mass numbers (*m/z*) *relative intensities*						
Ethanolamine	61	30	15	27	28	29	41	42	43
			35	*46*	*98*	*46*	*47*	*63*	*32*
Diethanolamine	105	74	28	30	36	38	42	45	56
			11	*48*	*43*	*13*	*8*	*16*	*53*
Triethanolamine	149	118	15	41	42	43	44	45	56
			8	*14*	*56*	*25*	*27*	*60*	*69*
2-Propanolamine	75	30	15	28	29	31	42	43	56
			37	*96*	*40*	*40*	*38*	*65*	*50*
N,N-Dimethylethanolamine	89	58	15	28	30	42	43	44	56
			63	*50*	*87*	*86*	*51*	*80*	*49*
N,N-Di(2-propyl)ethanolamine	145	70	30	41	42	43	72	84	114
			88	*93*	*98*	*96*	*93*	*92*	*93*

Table 7.21 Continue

Substance	Molar mass g/mol	Base peak *m/z*	Mass numbers (*m/z*) *relative intensities*						
N,N-Dimethyl-2-propanolamine	103	58	15	30	41	42	44	70	85
			45	*74*	*55*	*94*	*65*	*46*	*54*
N-Methyldiethanolamine	119	42	44	43	58	29	86	15	30
			86	*85*	*75*	*74*	*67*	*62*	*59*

Table 7.22

Tentative assignment of *EI* fragments of aminoalcohol activators to structures (for molecular masses, m.m., see Table 7.19). Mass numbers 15, 27, 28, 29, 30, 41, 42, 43, 44, 56, 58, 70, 72, 84, 85, 86: unsaturated and saturated hydrocarbons (even) or hydrocarbon radicals (uneven). Some of these may also belong to N- or O-containing fragments

30	CH_2NH_2	74	$H_3C\text{-}NH\text{-}C_2H_4O$
36	?	75	$H_3C\text{-}NH\text{-}C_2H_4OH$
38	?	84	$C_5H_{10}N$ azacyclohexane – H
43	$C_2H_3NH_2$	85	$C_5H_{11}N$ azacyclohexane
44	C_2H_3OH	86	$C_4H_{10}N_2$, piperazine
45	C_2H_4OH, $C_2H_5NH_2$	114	$H_2C\text{-}N(C_3H_7)_2$
70	C_4H_8N azacyclopentane – H	118	$H_3C\text{-}N(C_2H_4OH)_2$ – H
72	$C_4H_{10}N$ azacyclopentane + H		

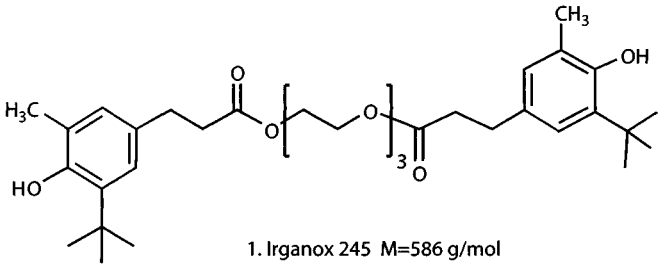
Table 7.23

Mass numbers (*m/z*>200) and relative intensities (italics) of fragments in the *EIMS* of commercial additives (from Yoshikawa et al., 10.2.1)

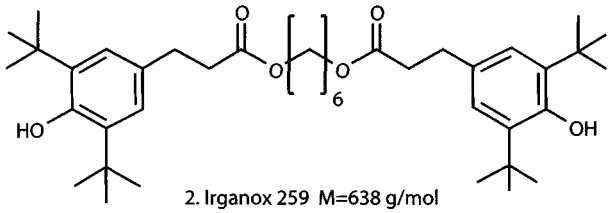
Substance[a]	Trade or chemical name	M (g/mol)	Mass numbers (*m/z*) *relative intensities* (strongest one: = 100)									
1	BHT	220	205	220	206							
			100	*25*	*15*							
2	DLTDP	514	346	329	514	273	347	330	241	300	515	441
			100	*95*	*62*	*40*	*37*	*35*	*30*	*28*	*27*	*3*
3	Irganox 1010	1176	309	323	342	219	410	425	227	355	292	351
			100	*95*	*66*	*50*	*44*	*44*	*33*	*33*	*25*	*25*
4	Irganox 1076	530	530	219	515	225	277	203	210	217	262	307
			100	*89*	*39*	*8*	*6*	*3*	*1*	*1*	*1*	*1*
5	Topanol CA	544	339	340	205	544	353	323	206	309	365	545
			100	*25*	*24*	*3*	*2*	*2*	*2*	*1*	*1*	*1*
6	Antioxidant	340	340	284	341	283	269	228	227	255	265	325
	2246		*100*	*51*	*30*	*26*	*8*	*6*	*3*	*1*	*1*	*1*
7	Santowhite	382	339	340	382	341	323	383	367	309	203	219
			100	*25*	*75*	*5*	*3*	*2*	*2*	*1*	*1*	*1*
8	Tinuvin 327	357	342	344	357	343	359	358	287	309	315	301
			100	*33*	*28*	*25*	*10*	*5*	*4*	*3*	*3*	*2*
9	erucamide	337	337	320	338	294	240	212	226	521	254	210
			100	*33*	*28*	*25*	*10*	*5*	*4*	*3*	*3*	*2*
10	oleic amide	281	281	225	264	238	212	226	253	210	220	222
			100	*37*	*33*	*25*	*25*	*25*	*22*	*10*	*10*	*10*

a 1=2,6-di-*t*-butyl-*p*-cresol,
2=dilaurylthiodipropionate,
3=pentaerythritol tetraester of 2-(4-hydroxy-3,5-di-*t*-butylphenyl)propionic acid,
4=octadecyl-3-(3,5-di-*t*-butyl-4-hydroxyphenyl)propionate,
5=1,1,3-*tris*(2-methyl-4-hydroxy-5-*t*-butylphenyl)butane,
6=2,2′-methylene-*bis*(4-methyl-6-*t*-butylphenol),
7=4,4′-butylidene-*bis*(3-methyl-6-*t*-butylphenol),
8=2-(2-hydroxy-3,5-di-*t*-butylphenyl)-5-chlorobenzotriazole

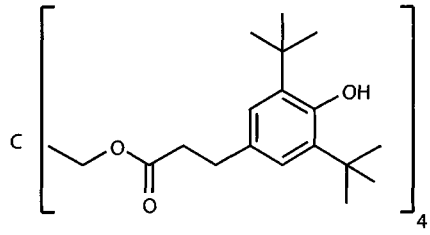
Table 7.24
Trade names, structures and molecular masses of the additives investigated by Asamoto et al. (10.2.1).



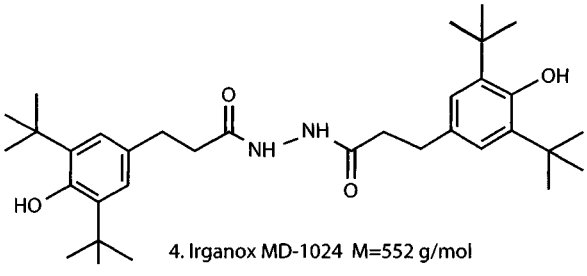
1. Irganox 245 M=586 g/mol



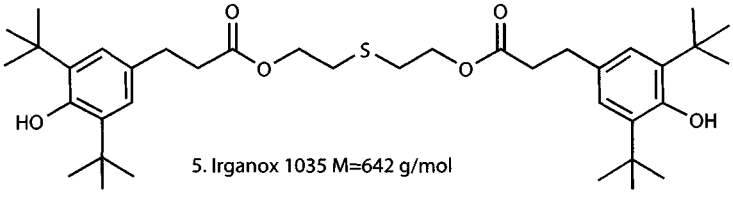
2. Irganox 259 M=638 g/mol



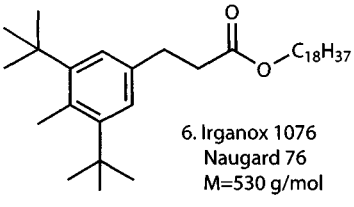
3. Irganox 1010 M=1176 g/mol



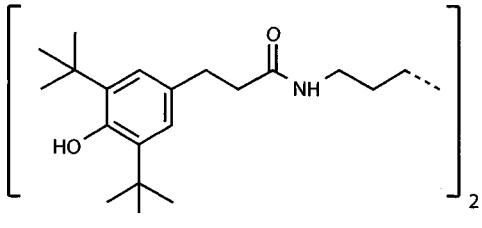
4. Irganox MD-1024 M=552 g/mol



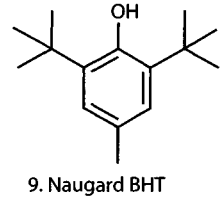
5. Irganox 1035 M=642 g/mol



6. Irganox 1076
Naugard 76
M=530 g/mol

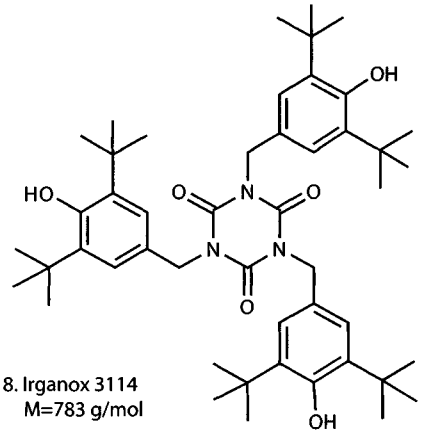


7. Irganox 1098 M=636 g/mol

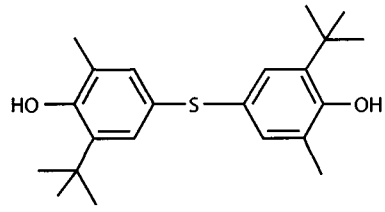


9. Naugard BHT
Ultranox 226 M=220 g/mol

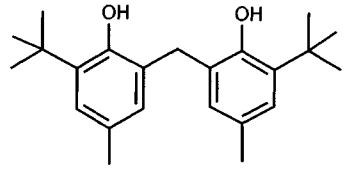
Table 7.24 Continue



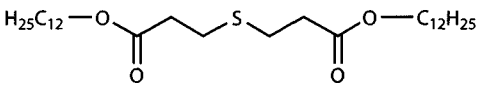
8. Irganox 3114
M=783 g/mol



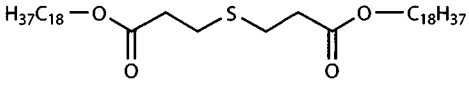
10. Ultranox 236 M=358 g/mol



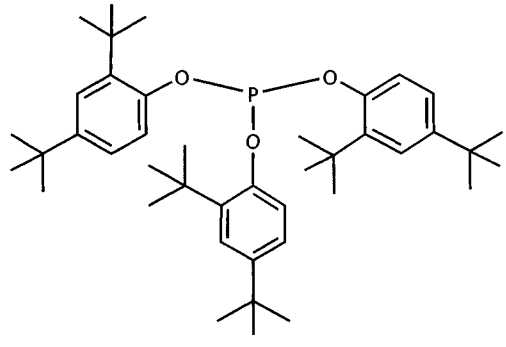
11. Ultranox 246 M=340 g/mol



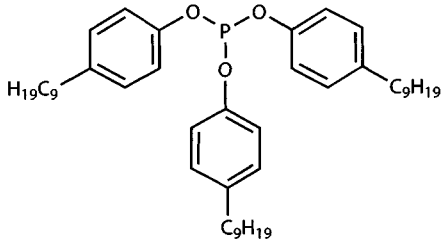
12. Irganox PS 800
Naugard DLTDP M=514 g/mol



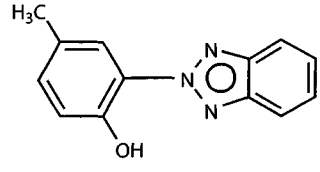
13. Irganox PS 802
Naugard DSTDP M=682 g/mol



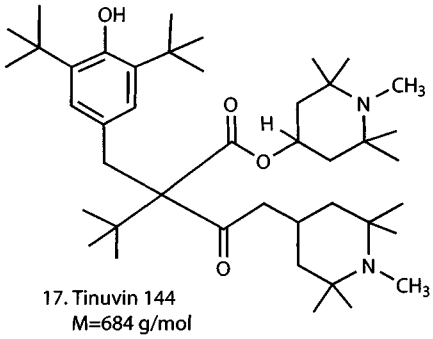
15. Irgafos 168
Naugard 524 M=646 g/mol



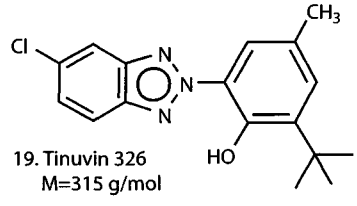
14. Polygard
Weston TNPP M=688 g/mol



16. Tinuvin P
M=225 g/mol

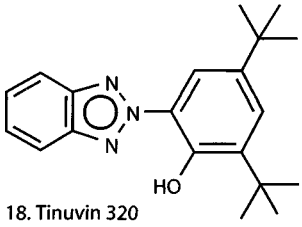


17. Tinuvin 144
M=684 g/mol

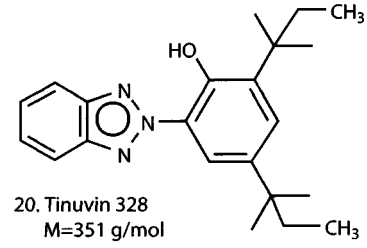


19. Tinuvin 326
M=315 g/mol

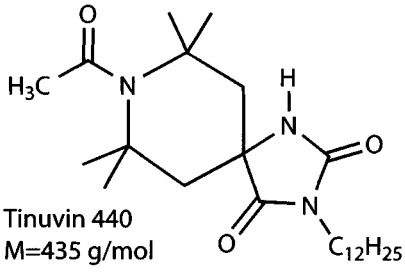
Table 7.24 Continue



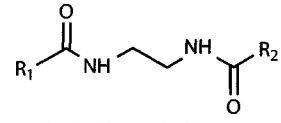
18. Tinuvin 320
M=323 g/mol



20. Tinuvin 328
M=351 g/mol

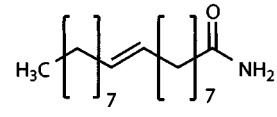


21. Tinuvin 440
M=435 g/mol

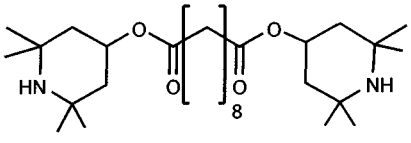


R=$C_{15}H_{31}$ or $C_{17}H_{35}$

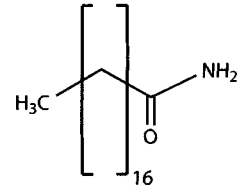
23. Arcawax C
EBS Wax M=592 g/mol



24. Oleamide M=281 g/mol



22. Tinuvin 770
M=480 g/mol



25. Stearamide M=283 g/mol

Table 7.25
LD/FT-ICR mass spectra of additives; numbers (bold) from Table 7.24, intensities in italics (after Asamoto et al., 10.2.1)

Positive ions of phenolic antioxidants											
	$[M+K]^+$	$[M+Na]^+$									
1	*625/75*	*609/30*	*205/100*	*161/45*	*243/40*	*177/35*	*375/30*	*287/20*			
2	*677/100*	*661/40*	*219/20*	*414/15*	*506/10*						
3[a]	*1215/100*	*1199/30*	*219/35*	*921/20*	*785/15*	*495/15*	*840/10*	*693/10*	*551/10*		
4	*591/30*	*575/60*	*219/100*	*329/75*	*237/45*	*385/35*	*203/30*	*441/20*			
5[a]	*681/85*	*665/55*	*331/100*	*379/35*	*252/35*	*219/30*	*193/15*				
6[a]	*569/100*	*553/25*	*290/30*	*320/20*	*258/15*	*607/15*	*531/10*	*219/8*			
6[b]	*569/100*	*553/70*	*113/50*								
7	*675/70*	*659/35*	*525/100*	*469/50*	*321/40*	*582/35*	*413/35*	*219/15*	*377/15*	*613/15*	*637/10*
8[a]	*822/10*	*783/8*	*219/100*	*436/35*	*203/20*	*346/15*	*260/10*				
9	*259/100*	*243/80*	*215/40*								
9[b]	*259/100*	*243/17*	*221/10*	*463/9*	*492/21*						
10[a]	*397/10*	*381/15*	*358/100*	*343/50*							
11	*379/100*	*363/25*	*340/20*	*392/15*	*332/15*	*177/10*					

Table 7.25 Continue

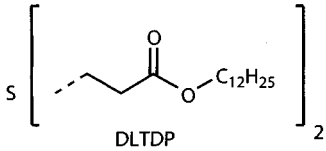
Negative ions of phenolic antioxidants											
	$[M-H]^-$	M^-									
1	585/*30*	586/*10*	367/*100*	189/*65*	163/*20*	235/*15*					
2	637/*100*	638/*45*	377/*30*	419/*25*	231/*15*	277/*10*	205/*10*				
3	1175/*15*	1176/*15*	205/*100*	479/*65*	751/*50*	533/*45*	521/*40*	697/*40*	915/*30*	957/*30*	969/*30*
4	551/*30*	552/*15*	231/*100*	258/*85*	276/*55*	331/*50*	333/*40*	387/*30*			
5[a]	641/30	642/*10*	277/*100*	363/*85*	381/*55*	231/*40*	339/*25*	163/*25*	205/*20*	423/*20*	
6[a]	529/*100*	530/*30*	231/*20*								
7[a]	635/*100*	636/*50*	231/*50*	417/*35*	375/*30*						
8	–	–	564/*100*	346/*45*	230/*30*	194/*25*					
9	219/*100*	220/*15*									
9[b]	219/*100*	220/*15*									
10[a]	357/*100*	358/*25*	219/*15*	194/*10*	153/*5*						
11	339/*100*	340/*25*	163/*40*								
Positive ions of *UV* absorbers											
	$[M+K]^+$	$[M+Na]^+$	$[M+H]^+$								
16	–	–	226/*15*	225/*100*							
17[a]	723/*100*	707/*5*	685/*5*	154/*35*	339/*10*						
18	362/*80*	346/*60*	324/*100*	323/*60*	308/*30*						
19	–	–	316/*95*	300/*100*	315/*40*	272/*15*	260/*15*				
20[a]	390/*10*	374/*25*	350/*100*	322/*80*	351/*50*	378/*10*	282/*10*				
21	–	458/*5*	436/*10*	378/*100*	335/*20*	321/*20*					
22	519/*100*	503/*35*	481/*35*	140/*50*	124/*30*	364/*30*					
Negative ions of *UV* absorbers											
	$[M-H]^-$										
16	224/*100*	225/*15*									
17	–	465/*100*	466/*30*	315/*20*	245/*20*	205/*20*					
18	322/*60*	323/*100*	324/*20*								
19	314/*100*	316/*40*	315/*30*	152/*10*							
20	350/*100*	351/*40*	352/*10*								
21	434/*40*	392/*100*	393/*25*								
22[a]	479/*5*	322/*100*	150/*60*	194/*50*	144/*35*	255/*25*	213/*20*				
Positive ions of miscellaneous additives											
	$[M+K]^+$	$[M+Na]^+$	$[M+H]^+$								
12	553/*100*	537/*35*	–	313/*10*							
13	–	705/*11*	–	413/*100*	233/*75*	325/*54*	407/*45*	485/*14*			
14	727/*17*	711/*100*	–	265/*30*	725/*25*	837/*17*					
14[b]	–	711/*17*	689/*32*	469/*100*	343/*28*	483/*21*					
15	–	–	647/*60*	441/*100*	385/*40*	329/*20*	591/*5*				
24	320/*45*	304/*100*	282/*9*	334/*38*	585/*9*						
25	322/*30*	306/*100*	284/*5*	335/*75*							
23[c]	631/*60*	615/*18*	–	365/*100*							
	603/*67*	587/*16*									
	575/*25*	559/*4*									
23[b,c]	631/*34*	615/*7*									
	603/*100*	587/*30*									
	575/*76*	559/*15*									

Table 7.25 Continue

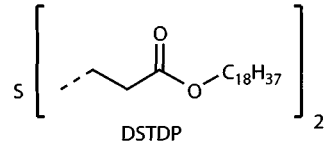
Negative ions of miscellaneous additives											
	$[M-H]^-$	M^-									
12	–	–	254/*100*	135/*82*	169/*80*	242/*64*	194/*55*	232/*36*	359/*21*	332/*18*	387/*15*
13			214/*100*	136/*36*	177/*10*	254/*3*					
14			219/*100*	135/*33*	345/*23*						
14[b]			219/*100*	345/*13*	233/*8*						
15			283/*100*	79/*78*	268/*66*	205/*38*					473/*25*
24	280/*100*	281/*53*	254/*29*								
23[c]	591/*7*	–	283/*100*	255/*23*	325/*18*	297/*12*					
	563/*7*										
	535/*3*										
23[b,c]	591/*9*	–	255/*100*	283/*88*	507/*8*						
	563/*26*										
	535/*25*	536/*7*									

a Defocused condition
b Same composition
c Mixed stearyl/palmityl amides, hence three sets of molecular ions for the possible combinations

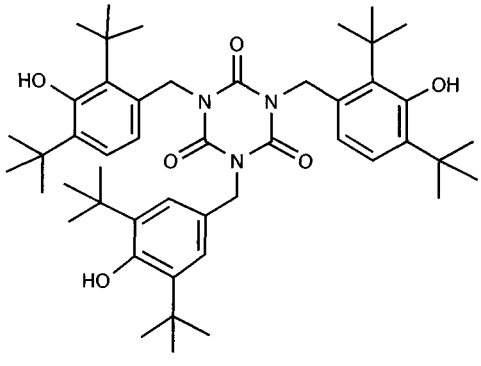
Table 7.26
Trade names, structures and molecular masses of the additives investigated by Johlman et al. (10.2.1)



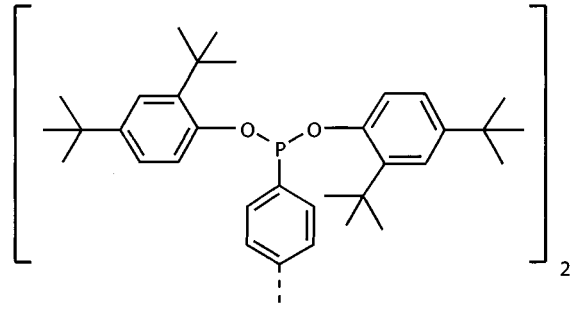
DLTDP
M=514.8 g/mol



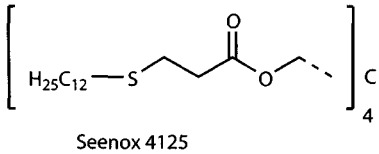
DSTDP
M=683.1 g/mol



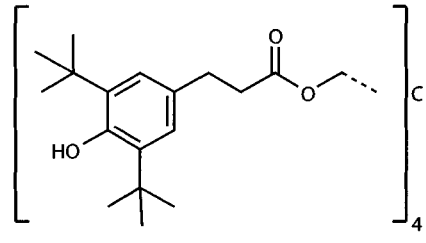
Goodrite
M=784.1 g/mol



Sandostab PEPQ
M=1035 g/mol

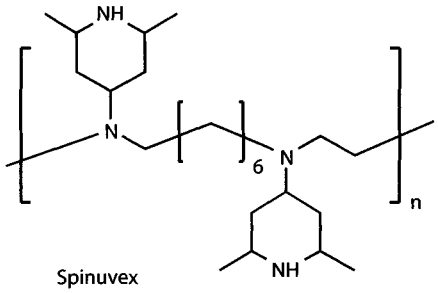


Seenox 4125
M=1162 g/mol

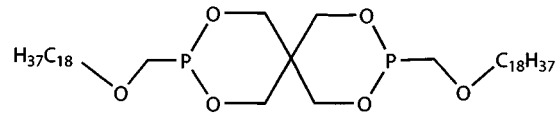


Irganox 1010
M=1177 g/mol

Table 7.26 Continue



Spinuvex
M=378.6 (unit) g/mol



Westin 618
M=761.1 g/mol

Table 7.27
The five polymer additives studied by Jackson et al. (10.2.1) with tandem *MS*

	Trade name	Molecular formula	Molar mass g/mol	Chemical name
1	Tinuvin 327	$C_{20}H_{24}ClN_3O$	357.9	2-(2-Hydroxy-3,5-di-*t*-butylphenyl)-2*H*-5-chlorobenzotriazole
2	Irganox 1076	$C_{35}H_{62}O_3$	530.9	Octadecyl-β-(3,5-di-*t*-butyl-4-hydroxyphenyl)propionate
3	Irganox 3114	$C_{48}H_{69}N_3O_6$	784.1	1,3,5-*tris*(3,5-di-*t*-butyl-4-hydroxybenzyl)isocyanurate
4	Hostanox 03	$C_{50}H_{66}O_8$	795.1	Ethylene-*bis*[(3,3-*bis*(3′-*t*-butyl-4′-hydroxyphenyl-4′-hydroxyphenyl))butyrate]
5	Irganox 1010	$C_{73}H_{108}O_{12}$	1177.7	Pentaerythrityl-*tetrakis*[3-(3,5-di-*t*-butyl-4-hydroxyphenylpropionate

Table 7.28
Parent peaks (*m/z*) observed with *FD* as well as peaks derived from parent peaks and observed with liquid secondary ionisation *MS-MS* (numbers, see Table 7.27)

	M^+(*FD*) *LSI-MS/MS* derived from parent peaks								
1	357	342	126	103	91	77	57	41	39
2	530	515	219	203	57	43			
3	783	768	260	219	203				
4	794	650	325	309					
5	1177	1120	259	219	203				

8
Structure Analysis by *X*-Ray Diffraction

8.1
Fundamentals

The wavelength of *X*-rays is within the same order of magnitude as the distance of atoms or molecules in crystals, i.e. some tenths of a nanometer. In addition, *XR* interfere with electrons, and space in crystals is filled with electrons (and some nuclei). Thus, *XR* traversing crystals suffer diffraction and interference. The interference patterns can be used for crystal structure elucidation; at the same time they are characteristic for the substance the crystals are made of.

Most organic substances are composed of C,H,N,O and have few electrons compared with compounds containing heavy atoms. They are therefore poor scatterers; to obtain *XR* diagrams of CHNO crystals using conventional *XR* sources demands several hours of exposure times. The availability of the intense cyclotron radiation yields good diagrams in reasonably short times.

8.2
Inorganic Pigments and Fillers

All inorganic pigments and fillers contain heavy atoms and are thus good scatterers. This is advantageous if pigmented paints or pigmented amorphous polymers (plastics, rubber) have to be analysed. Several books and publications contain data on *XRD* of pigments. A total of 71 *XRD* patterns (bar graphs) are found in the book of Scholl (l.c.); unfortunately, no spacings and intensities are given in numbers. More data may be found in the powder diffraction file of the International Centre for Diffraction Data (N.N., 10.1). Earlier though valuable sources are the books of König and Kittel (both 10.1). A useful source of reference in *XRD* data on synthetic dyes and pigments is the contribution by Whitaker in the book of Venkataraman (10.1).

8.3
Organic Pigments

The problems with *XRD* of organic pigments can be summed up like this (Curry et al., 10.2.3; with minor changes):

1. Organic pigments are poor scatterers.
2. Many organic OP, due to their intense coloration, are applied in low concentrations. Without separation, their *XRD* are weak and difficult to interpret.
3. The unit cells of OP are generally much larger than those of inorganic pigments. Thus, their diffraction lines are confined to low θ angles. Unfortunately, this region has, in the Debye-Scherrer technique, the highest background and may drown weak diffraction lines.
4. OP in paints may be non-crystalline and will then yield no *XRD* pattern.
5. Many OP may be derived from one parent compound, they belong then to a structurally similar family. Changes in chemical substitutions or inserted metal produce dramatic colour changes yet sometimes only subtle changes in *XRD* patterns.

Despite these problems the authors were able to produce valuable data for the identification of organic pigments in the forensic examination of paints. Debye-Scherrer powder photography was used both for OP and for casework paint flake specimens. Powdered pigments were loaded into 0.3 mm i.d. glass capillary tubes. The camera had 114.6 mm i.d., KODIREX or NO-SCREEN film was used. The samples were exposed for 2 h to iron-filtered Co Kα radiation from 35 kV/34 mA electrons. *d*-Spacings were measured with a film-measuring device; maximal errors were ±10 pm (d>1 nm) or ±1 pm (d<1 nm). The intensities of the lines were determined with a recording microdensitometer and normalised to a scale with maximum 10.

Table 8.1 shows the results of these measurements; intensities are given in italics, the strongest line in bold. Only the spacings of the three most intense diffraction lines of each pigment have been recorded. As far as paint flake analysis is concerned, the minimum size appears to be 0.5×0.5 mm^2, corresponding to an approximate weight of 40 μg.

Table 8.1
Diffraction data (three strongest peaks), CI pigment numbers and colorant class for a selection of organic pigments used in paints (C.J. Curry et al., 10.2.3). The numbers for the strongest interferences (intensity 10) are bold, the intensities on the 1–10 scale are italic. PR=Pigment Red, PY=Pigment Yellow, PV=Pigment Violet, PB=Pigment Blue, PBR=Pigment Brown, PG=Pigment Green, PO=Pigment Orange. The spacings are arranged to suit a Hanawalt-type search (see Powder Diffraction File, N.N., 10.1).

d-spacings/intensities			*CI* number	Class of colorant
19.5	8.16/*3*	3.46/*3*	PR 48:4	Monoazo
19.1	3.40/*2*	4.09/*1*	PR 52	Monoazo
18.8	3.72/*4*	3.42/*3*	PR 48.2	Monoazo
18.6	3.45/*3*	4.92/*2*	PR 48.3	Monoazo
18.4	3.42/*3*	3.25/*2*	PR 57	Monoazo
17.2	6.28/*7*	3.44/*4*	PR 149	Anthraquinone
16.8	**3.29**	3.23/*8*	PR 223	Monoazo
16.0	3.27/*3*	6.32/*2*	PR 122	Indigoid
14.9	**3.36**	6.11/*4*	PR 5	Monoazo
11.3	5.10/*8*	3.29/*7*	PR 58	Monoazo
11.2	3.34/*5*	4.63/*3*	PR 10	Monoazo
10.2	3.25/*8*	20.7/*4*	PR 144	Disazo
9.3	3.32/*5*	3.23/*4*	PR 166	Azo
3.46	12.2/*4*	4.87/*3*	PR 170	Monoazo
3.37	14.7/*6*	6.88/*5*	PR 209	Quinacridone
3.37	10.6/*5*	5.63/*2*	PR 11	Monoazo
3.37	5.92/*5*	7.41/3	PR 112	Monoazo
3.35	7.27/*9*	6.50/*6*	PR 114	Monoazo
3.34	3.51/*4*	4.84/*3*	PR 168	Anthraquinone
3.34	2.78/*4*	3.50/*3*	PR 168	Anthraquinone
3.33	11.4/*7*	6.67/*3*	PR 12	Monoazo
3.31	16.4/*5*	4.95/*4*	PR 146	Monoazo
3.31	3.23/*8*	3.56/*5*	PR 88	Thioindigoid
3.29	8.00/*8*	3.40/*5*	PR 3	Monoazo
13.5	24.4/*3*	3.45/*3*	PY 128	Disazo
13.4	**3.51**	8.76/*7*	PY 83	Disazo
12.6	**9.69**	**8.75**	PY 129	Azomethine
10.3	3.28/*9*	5.69/*2*	PY 1	Monoazo
8.44	**3.50**	3.35/*2*	PY 12	Disazo
8.03	17.1/*4*	3.41/*4*	PY 17	Disazo
3.55	7.18/*7*	4.12/*4*	PY 110	Isoindolinone
3.41	6.66/*4*	4.88/*3*	PY 154	Monoazo
3.40	9.50/*4*	2.84/*4*	PY 109	Isoindolinone
3.35	7.24/*4*	5.31/*4*	PY 156	Azo
3.32	7.46/*9*	3.49/*3*	PY 74	Monoazo
3.32	8.06/*9*	11.7/*6*	PY 13	Disazo
3.31	7.66/*8*	10.5/*4*	PY 14	Disazo
3.31	6.89/*3*	5.13/*2*	PY 3	Monoazo
3.30	8.08/*9*	3.40/*8*	PY 24	Anthraquinone
3.25	5.12/*3*	4.57/*2*	PY 151	Monoazo
3.25	3.52/*8*	17.6/*7*	PY 73	Monoazo
15.5	8.69/*6*	3.45/*6*	PV 23	Dioxazine
15.4	3.29/*9*	5.55/*4*	PV 19	Quinacridone
13.6	6.38/*5*	3.38/*4*	PV 19	Quinacridone
13.5	8.56/*6*	5.01/*4*	PV 37	Dioxazine
3.72	2.63/*3*	2.88/*2*	PV 15	Inorganic
13.1	12.2/*7*	8.97/*2*	PB15:2	Phthalocyanine
13.0	11.9/*7*	5.93/*3*	PB16	Phthalocyanine
12.7	9.71/*5*	3.75/2	PB15:4	Phthalocyanine
12.7	9.67/*7*	3.74/*3*	PB15:3	Phthalocyanine
11.6	5.83/*5*	3.34/*4*	PB64	Anthraquinone
7.82	3.27/*7*	7.12/*5*	PB60	Anthraquinone
3.71	6.44/*4*	2.62/*3*	PB29	Inorganic
11.5	10.0/*8*	21.2/*7*	PBR 25	Monoazo
10.1	6.64/*7*	3.30/*5*	PBR 23	Disazo
9.67	22/*9*	11.9/*9*	PBR 32	Monoazo
15.2	4.53/*3*	3.39/*1*	PG 10	Monoazo
15.1	3.34/*7*	13.0/*4*	PG 7	Phthalocyanine
13.5	**11.5**	8.69/*7*	PG 8	Nitroso
3.40	3.66/*7*	2.92/*5*	PG 36	Phthalocyanine
3.34	14.8/*8*	13.2/*6*	PG 7	Phthalocyanine
3.52	6.97/*9*	11.4/*6*	PO 43	Anthraquinone
3.37	3.46/*6*	11.4/*5*	PO 52	Pyranthrone
3.36	3.30/*6*	3.25/*5*	PO 5	Monoazo
3.24	6.08/*3*	3.92/*2*	PO 36	Monoazo

9
Elemental Analysis

There are numerous spectroscopic techniques for elemental analysis: inductive-coupled plasma atomic spectrometry (*ICP-AES, ICP-MS*), laser ablation (*LA*) mass or atomic emission spectrometry, glow-discharge spectrometry (*GDOES, GDMS*), atomic absorption (*AA*), X-ray fluorescence (*XRF*), X-ray emission and X-ray induced photoelectron (*XP*) spectrometries (I'm sure that some are missing). We can discuss here only three of these techniques.

9.1
Atomic Emission Spectroscopy

AES is a classic, Bunsen and Kirchhoff were its fathers. Compounds, in an electric arc or in a spark discharge, decompose into atomic elements. One outer electron is excited into different energetic (σ) states; when returning to the ground state, the energy used for this transition is emitted as electromagnetic radiation. The lines of the *AES* are (mostly) sharp and characteristic for the elements in the system investigated. Thus, up to about ten different elements can be determined in one measurement. The probabilities for transitions into the different electronic states can vary by several orders of magnitude. This is helpful for quantitative analyses; if an element in a mixture is rare, then its strongest line is used for its determination – and vice versa.

Table 9.1 shows emission lines of elements occurring in additives.

Table 9.1
Emission lines of elements occurring in additives, excitation: arc; strongest line is bold (selected data from H. Moenke, 10.1, and Golloch, Siegmund, 10.2.7)

Symbol	Lines (nm)		
Al	396.15		
As	234.984	228.812	
B	249.773[a]	249.678	
Bi	306.772		
Ba	455.40	233.527	230.424
Br	478.55		

Table 9.1 Continue

Symbol	Lines (nm)				
C	387.10	247.86	229.69[f]		
Ca	393.37				
CaF[d]	529.1				
CaCl[e]	621.1	593.4			
Cd	361.051	326.106	228.802		
Cl	479.45				
Co	412.10	**345.351**			
Cr	428.972	427.480	425.435	360.17	267.70
Cu	327.396	324.754			
H	486.13				
Hg	2536.52[g]				
Li	812.652	**670.784**	610.364	460.286	323.261
Mg	383.80				
Mn	293.30				
Mo	**319.397**	**317.035**	320.883		
Ni	**341.477**	351.51			
P	255.328				
PO	327.05	325.53			
Pb	**405.782**	283.307	220.35[f]		
Sb	259.806				
Se	420				
Si	288.16				
Sn	326.233[b]	317.502	303.41	286.333[b]	283.999
Sr	**460.733**	407.771			
Te	238.576	238.325[c]			
Ti	337.28				
W	**294.698**	289.645			
Zn	**213.856**	334.502			

a Coincides with an SiO band
b May be confused with Ti
c Fe disturbs
d For the determination of F
e For the determination of Cl
f Second order
g Disturbed by Co, 2536.49 nm, and vice versa

In a recent publication, Golloch and Siegmund (10.2.7) described sliding spark spectroscopy as an interesting new method for rapid survey analysis of additives, especially flame retardants, in polymers. The system is portable (16.5 kg) and

allows in-situ analyses (if power supply is available). Basically, it consists of a high-energy (up to 2 kJ per discharge) sliding spark source with generator, an optical fibre ending in a charge-coupled device (*CCD*) spectrometer, computer and screen. Limits of detection of about 0.1% (elements by weight) for chlorine-free polymers were achieved.

The spark generator (Polycon Analytical Systems, Germany) was used for the ablation of the solid material and the excitation of the evaporated atoms. The energy per spark could be varied from 128 J to 2048 J. The spark head (PTFE, home made) is equipped with two thorated tungsten electrodes. The sample is simply placed on the electrodes. A continuous purge-gas flow of 1 dm^3/min through the measuring head prevents pollution of the optics. A multi-mode optical fibre behind a quartz lens collects the emitted radiation from the sample surface with a 10 mm diameter spot. The computer software allows the simultaneous integration and storage of 50 analytical lines.

Figure 9.1 shows as an example the emission spectra of two ABS samples containing Cd and Zn. The background curve is a blank, the line at 229.68 nm (F) is common to both the sample and a metal-free rubber sample; it is caused by carbon.

A remarkable possibility of this high-intensity spark spectroscopy is the direct determination of Cl (479.46 nm) and Br (481.67 nm, in polyurethanes). Figure 9.2 shows the emission lines of PVC (55 wt% Cl), chlorinated polyethylene (PE, 15–20% Cl), ABS rubber with 10% of a flame retardant (ABS-FR) and a chlorine-free ABS sample. The line at 479.46 nm was used for quantitative determinations; the limit of detection was 0.5% Cl.

Using calibration standards, the authors made quantitative determinations of Cd, Cr, Pb, Zn, Sb, Si and Ti in chlorine-free polymers as well as Al, Ba, Ca, Cd, Pb, Sn, Ti and Zn in PVC. Multiple determinations are possible; examples shown were Zn/Si/Mg/Ca/Ti/Ba/Pb in PE and PP as well as Br/P/Cl/Sb/Zn/Al/Mg/B from flame retardants in ABS rubber and PE.

Table 9.2 shows the limits of detection for a number of elements as determined with sliding spark spectroscopy.

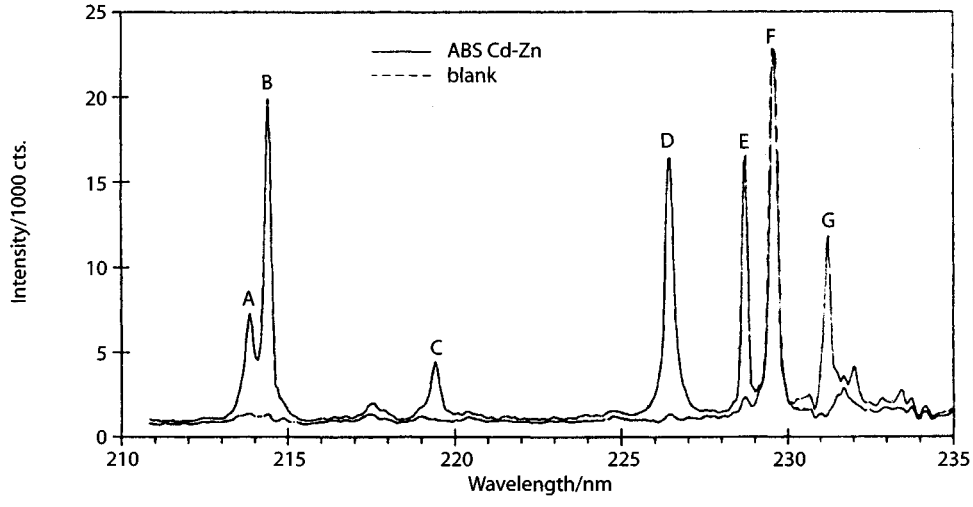


Fig. 9.1
Emission spectra of two samples of ABS rubber in the *UV* region. *Solid line*: rubber containing Cd and Zn. *Dotted (background) line*: metal-free ABS sample. Zn: A (213.86 nm); Cd: B (214.44 nm), C (219.46 nm), D (226.50), E (228.80), G (231.28); C: F (229.68 nm). (Golloch and Siegmund, 10.2.7)

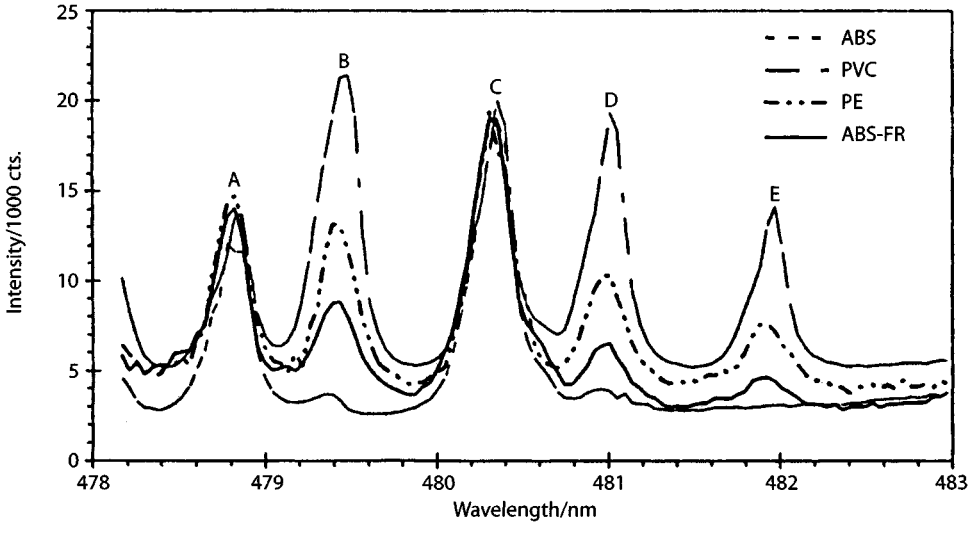


Fig. 9.2
Emission spectra of PVC, chlorinated polyethylene (PE), ABS rubber with flame retardant (ABS-FR) and chlorine-free ABS for the determination of Cl. Cl: B (479.46 nm), D (481.01 nm), E (481.95 nm); N: A (478.81 nm), C (480.32 nm). (Golloch and Siegmund, 10.2.7)

Table 9.2
Limits of detection (LOD) for some elements in different polymers obtained by sliding spark spectrometry and calculated according to DIN 32645 (1994) (Golloch and Siegmund, 10.2.7)

Element	In ABS,PE,PU *LOD* (wt%)	In PVC *LOD* (wt%)	Line(s)/nm
Al		0.065	396.15
Ba		0.09	234.75/493.41
Br	0.29		481.67/493.07
Ca		0.24	373.69
Cd	0.010	0.012	214.44/226.50;219.46/228.80/231.28
Cl	0.90		479.46/481.01/481.95
Cr	0.21		455.87/458.82
Mg		0.21	279.55
Pb	0.56	0.56	405.78;220.35
Sb	0.08		252.90/259.81
Si	0.81		251.61
Sn		0.15	303.41
Ti	0.69	0.06	368.52;350.49/364.12
Zn	0.09	0.13	213.86/250.20/255.80/202.55

9.2 Atomic Absorption Spectroscopy

The law of Kirchhoff says that an atom that emits radiation of a certain wavelength will absorb radiation of the same wavelength. This is the basis of the almost omnipresent flame atomic absorption spectroscopy (*AAS*). Numerous publications describe the different techniques of *AAS*; Table 9.3 shows some of the results which were collected by Knapp and Wegschneider (10.1).

Table 9.3
Analytical wavelengths λ and limits of detection (*LOD*) for elements occurring in additives as determined by flame atomic absorption spectrometry (*AAS*) (selected values from Knapp and Wegscheider, in Kienitz et al., vol. 1, 10.1). Flame: C_2H_2 with air or N_2O

Element	λ/nm	*LOD* absol. g	*LOD* rel./ng cm^{-3} sample vol. 100 mm^3
Al	309.3	2×10^{-12}	0.02
As	193.7	1×10^{-11}	0.1
B	249.7		ca. 2000
Ba	553.6	5×10^{-11}	0.5
Bi	223.1	2×10^{-11}	0.2
Ca	422.7	1×10^{-12}	0.01
Cd	228.8	1×10^{-13}	0.001
Co	240.7	5×10^{-12}	0.05
Cr	357.9	1×10^{-11}	0.1
Cu	324.7	2×10^{-12}	0.02
Fe	248.3	3×10^{-12}	0.03
K	766.5	1×10^{-13}	0.001
Li	670.8	1×10^{-11}	0.1
Mg	285.2	1×10^{-12}	0.01
Mn	280.1	2×10^{-13}	0.002
Mo	313.3	3×10^{-12}	0.03
Na	589.0	5×10^{-13}	0.005
Ni	232.0	1×10^{-11}	0.1
P	213.6	1×10^{-7}	ca. 1000
Pb	283.3	2×10^{-12}	0.02
Sb	217.6	1×10^{-11}	0.1
Se	196.1	5×10^{-11}	0.5
Si	251.6	5×10^{-11}	0.5
Sn	224.6	1×10^{-11}	0.1
Sr	460.7	5×10^{-12}	0.05
Ti	364.3	2×10^{-9}	20
W	400.9		ca. 1000
Zn	213.9	5×10^{-14}	0.0005

9.3 Analysis of Surfaces: *X*-Ray Induced Photoelectron Spectroscopy (*XPS*)

Soft X-rays (in the region of 10^3 eV) are absorbed by matter. At the same time, low-energy (a few 10^2 eV) electrons are emitted (photoelectric effect). The work of separation

(electronic work function, the frequently used term binding energy is misleading) depends on the chemical state of the atom which is hit. Thus, not only the kind of element but also its state of bonding can be determined by *XPS*. The resolution, however, is low: 10^{-1} eV or 10 kJ/mol. The bonding state of, e.g. carbon can be evaluated only if closely superimposed band complexes are separated. Thus, only simple assignments can be made. On the other hand, *XPS* is suitable for the investigation of the chemical nature of surfaces, since soft *X*-rays penetrate only a few nanometers of condensed matter. In this respect it has to compete with *ATR-IRS* and Raman microscopy (molecules) and scanning electron microanalysis (elements). In addition, *XPS* is to some extent able to survey surfaces, and it is a non-destructive technique.

Ström et al. (10.2.3) used *XPS* to study the chemical composition of coated paper surfaces. The white pigment for the coating was a 7:3 mixture of fine $CaCO_3$ with European clay. One hundred parts of pigment were pasted with 17 parts of butadiene-styrene or acrylic latex, 0.5 parts synthetic thickener, 0.3 arts polyvinylalcohol, 0.3 parts optical brightener and 0.7 parts hardener (ammonium zirconium carbonate). *XPS* measurements were performed with a Kratos and an *X*-probe spectrometer (Surface Science Instrument, SSI). The *X*-ray source was Mg Kα 1253.6 eV, the irradiated area was 0.8×0.5 mm^2 or 1 mm^2, respectively. The surface composition was calculated from the survey spectra using sensitivity factors provided by SSI. Peak fitting/separation for high-resolution C1s signals was done with synthetic peaks with a 4:1 Gaussian-Lorenzian shape. It was assumed that the whole carbon complex (280–290 eV) was composed of five bands.

By low-resolution *XPS*, ten elements (including C and O) were found. Figure 9.3 shows the *XPS* (solid lines) and the curve-resolved partial spectra of a coated paper with acrylate latex (above) and the latex itself (below). Carbonate and ester band overlap but can be separated and evaluated quantitatively.

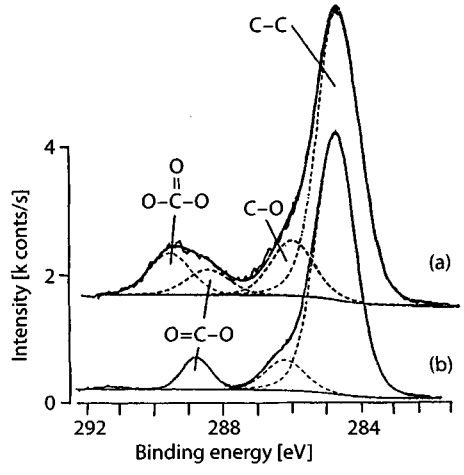


Fig. 9.3
High-resolution and curve-resolved *XPS* spectra of the C1s signal of a coated paper with acrylate binder (**a**) and of the binder itself (**b**) (Ström et al., 10.2.3)

10
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Part B
FTIR Spectral Atlas of Plastics Additives

B

1
Decimal Classification of Additives

1	**Additives with preventive or curative properties**
1.1	**Antioxidants, ageing inhibitors**
1.1.1	amines and salts of amines
1.1.1.1	CHN
1.1.1.1.1	aliphatic
1.1.1.1.1.1	open chain
1.1.1.1.1.2	carbocyclic
1.1.1.1.1.3	heterocyclic
1.1.1.1.2	aliphatic-aromatic
1.1.1.1.2.1	aliphatically bound N
1.1.1.1.2.2	aromatically bound N
1.1.1.1.2.3	aliphatically and aromatically bound N
1.1.1.1.3	aromatic
1.1.1.1.4	polymer
1.1.1.2	CHNO
1.1.1.2.1	aminoalcohols
1.1.1.2.2	aminophenols
1.1.1.2.3	aminoethers
1.1.1.2.4	aminoaldehydes
1.1.1.2.5	aminoketones
1.1.1.2.6	aminoesters
1.1.1.2.7	betaines
1.1.1.2.8	amines with amide functions
1.1.1.2.9	amines with heterocyclic or other CHNO functions
1.1.1.3	CHNS (classification like CHNO; S is treated like C)
1.1.1.4	CHNOS
1.1.1.5	other amines
1.1.2	other N-containing compounds (without amino groups)
1.1.2.1	CHN
1.1.2.1.1	nitriles
1.1.2.1.2	compounds with C=N bonds (carbodiimides)
1.1.2.1.3	compounds with N=N bonds
1.1.2.1.4	aromatic heterocyclics
1.1.2.2	CHNO compounds
1.1.2.3	CHNS compounds
1.1.2.4	CHNOS compounds
1.1.3	phenols
1.1.3.1	CHO
1.1.3.1.1	no substituents besides OH
1.1.3.1.2	substituted with alkyl
1.1.3.1.3	substituted with aralkyl or aryl, multinuclear polyphenols

1.1.3.1.4 having additional CHO functions, phenolethers
1.1.3.2 CHNO
1.1.3.2.1 amino- and hydrazinophenols
1.1.3.2.2 amido- and hydrazidophenols
1.1.3.2.3 phenols with C=N substituents, nitrilophenols
1.1.3.2.4 phenols carrying substituents with other CHN(O) multiple bonds
1.1.3.2.5 heterocyclic-substituted phenols
1.1.3.2.6 other CHNS, CHOS or CHNOS phenols
1.1.3.3 CHNS
1.1.3.4 CHOS
1.1.3.5 CHNOS
1.1.3.6 P-containing phenols, phenolphosphites
1.1.3.7 Si-containing phenols
1.1.3.8 phenols with other hetero-elements
1.1.3.9 other phenolic compounds
1.1.4 non-phenolic, N-free compounds
1.1.4.1 CHO compounds
1.1.4.2 CHS compounds
1.1.4.3 CHOS compounds
1.1.4.4 P-containing compounds
1.1.4.5 compounds containing other heteroelements
1.1.5 other antioxidants and ageing inhibitors

1.2 PVC stabilisers and co-stabilisers, other stabilisers
1.2.1 inorganic (classification like 2.5.1)
1.2.2 metal-free CHO(S) compounds (without P)
1.2.2.1 polyols, ether alcohols
1.2.2.2 phenols and phenolates
1.2.2.3 epoxy compounds
1.2.2.4 esters
1.2.2.5 thiofatty acid esters, other thiocompounds
1.2.3 metal-free CHN(O,S) compounds
1.2.3.1 aminoacid esters (β-aminocrotonic acid esters)
1.2.3.2 urea derivatives
1.2.3.3 thiourea derivatives
1.2.3.4 indole derivatives
1.2.3.5 other metal-free stabilisers
1.2.4 metal-containing organic compounds (without P)
1.2.4.1 metal salts (without Sn) of carboxylic acids
1.2.4.1.1 salts of saturated carboxylic acids
1.2.4.1.2 salts of unsaturated carboxylic acids
1.2.4.1.3 salts of saturated, polybasic, aliphatic carboxylic acids
1.2.4.1.4 salts of unsaturated, polybasic, aliphatic carboxylic acids
1.2.4.1.5 salts of aliphatic-aromatic carboxylic acids
1.2.4.1.6 salts of aromatic carboxylic acids
1.2.4.1.7 metal carboxylates with additional heteroelements
1.2.4.1.8 metal phenolates
1.2.4.2 organo-tin compounds
1.2.4.2.1 S-free tin-stabilisers
1.2.4.2.2 S-containing tin-stabilisers
1.2.4.3 metal-organic compounds with different metals
1.2.4.3.1 ester-free metal-complexes
1.2.4.3.2 ester-containing metal-complexes
1.2.4.4 other metal-containing organic compounds

1.2.5 phosphorus derivatives
1.2.5.1 metal-free alkylphosphites
1.2.5.2 metal-free alkylaryl- and arylphosphites
1.2.5.3 metal-organic phosphites
1.2.5.4 metal-organic phosphates
1.2.5.5 P- and ester-containing metal salts
1.2.5.6 derivatives of thiophosphorous acids
1.2.5.7 other P-containing compounds
1.2.6 silicium derivatives
1.2.7 other stabilisers

1.3 Light stabilisers (*UV* absorbers, radical scavengers)
1.3.1 sterically hindered amines (HALS), acetalamines,triazine derivatives
1.3.2 benzotriazole derivatives
1.3.3 phenols
1.3.4 benzophenone derivatives (ketophenols, ketophenolethers
1.3.5 esters of aromatic acids (benzoates, salicylates)
1.3.6 derivatives of cyanoacrylic and cyanocinnamic acids
1.3.7 oxalic acid anilides
1.3.8 nickel-organic compounds, metal soaps
1.3.9 hydrocarbon waxes, other light stabilisers

1.4 Flame retardants
1.4.1 inorganic compounds
1.4.1.1 metal oxides and hydroxides
1.4.1.2 halogenides
1.4.1.3 B-containing compounds
1.4.1.4 P-containing compounds
1.4.1.5 Sb-containing compounds
1.4.1.6 elements
1.4.2 organic compounds
1.4.2.1 halogen-containing compounds
1.4.2.1.1 chlorinated (cyclo)aliphatic compounds
1.4.2.1.2 brominated (cyclo)aliphatic compounds
1.4.2.1.3 chlorinated (aliphatic-)aromatic compounds
1.4.2.1.4 tetrabromobisphenol A and its derivatives
1.4.2.1.5 tetrabromophthalic acid and its derivatives
1.4.2.1.6 other brominated aromats
1.4.2.1.7 halogenated oligomers and polymers
1.4.2.1.8 other halogenated compounds
1.4.2.2 phosphorus derivatives (classification like 3.6)
1.4.2.3 halogen- and P-containing compounds
1.4.2.4 compounds containing other hetero-elements
1.4.3 metal-organic compounds
1.4.4 other flame retardants

1.5 Metal deactivators
1.5.1 carboxylic acid amides
1.5.1.1 amides of monocarboxylic acids
1.5.1.2 amides of dicarboxylic acids
1.5.1.3 cyclic amides
1.5.2 hydrazones
1.5.2.1 hydrazones of aliphatic aldehydes
1.5.2.2 hydrazones of aromatic aldehydes
1.5.2.3 aliphatic N-acylhydrazones

1.5.2.4 aromatic N-acylhydrazones
1.5.3 hydrazides
1.5.3.1 hydrazides of aliphatic carboxylic acids
1.5.3.2 hydrazides of aliphatic-aromatic carboxylic acids
1.5.3.3 hydrazides of aromatic carboxylic acids
1.5.3.4 hydrazides with CHO functions
1.5.3.5 hydrazides with additional CHN(O,S) functions
1.5.4 heterocyclic compounds
1.5.4.1 *sym*-triazine derivatives (melamine derivatives)
1.5.4.2 (benz)imidazole derivatives
1.5.4.3 (benzo)triazole derivatives
1.5.5 P-containing compounds
1.5.6 other metal deactivators

1.6 Biostabilisers, biocides

1.7 Other additives with preventive and/or curative properties

2 Colouring agents, brightening agents, fillers

2.1 Inorganic pigments (classification like 2.5.1)

2.2 Organic pigments
2.2.1 monoazo pigments
2.2.1.1 acetoacetic acid arylides
2.2.1.2 2-hydroxy-3-naphthoic acid arylides, naphthol-AS derivatives
2.2.1.3 other 2-naphthol derivatives
2.2.1.4 2-hydroxynaphthoic acid arylide (BONS-) lakes (carboxylates and carboxylatesulfonates)
2.2.1.5 benzimidazolone derivatives
2.2.1.6 pyrazolone derivatives
2.2.1.7 diazole derivatives
2.2.1.8 other monoazo pigments
2.2.2 disazo pigments
2.2.2.1 diarylyellow pigments (benzidine derivatives)
2.2.2.2 disazo condensation pigments of the yellow series (*p*-phenylenediamine-*bis*-acetoacetamide derivatives)
2.2.2.3 disazo condensation pigments of the red series(*p*-phenylenediamine-*bis*-naphthamide derivatives)
2.2.2.4 pyrazolone derivatives
2.2.2.5 metal complexes
2.2.2.6 other disazo pigments
2.2.3 polycyclic pigments
2.2.3.1 without heteroelements in the ring system
2.2.3.1.1 anthraquinone derivatives
2.2.3.1.2 perylene derivatives
2.2.3.1.3 anthanthrone derivatives
2.2.3.1.4 (benz-)pyrene derivatives
2.2.3.1.5 pyranthrone derivatives
2.2.3.1.6 violanthrone and isoviolanthrone derivatives
2.2.3.1.7 naphthalene derivatives
2.2.3.1.8 noncondensed polycyclic systems without heteroelement in the ring system (di-, triphenylmethane derivatives)
2.2.3.2 N in the ring system
2.2.3.2.1 benzimidazol- and isoindoline (isoindolinone) derivatives
2.2.3.2.2 acridine (acridone) derivatives
2.2.3.2.3 (anthra-)pyrazole derivatives
2.2.3.2.4 (anthra-)pyrimidine derivatives

2.2.3.2.5 quinoline and phenazine derivatives
2.2.3.2.6 flavanthrone derivatives
2.2.3.2.7 indanthrone derivatives
2.2.3.2.8 phthalocyanine derivatives
2.2.3.2.9 noncondensed polycyclic systems with N in the ring system
2.2.3.3 N and/or O in the ring system (fluorescein-, indigo-, phenoxazine-, anthraoxazole derivatives)
2.2.3.4 S in the ring system (thioindigo and its derivatives)
2.2.3.5 noncondensed polycyclic systems with N and O in the ring system (oxazole derivatives)
2.2.3.6 noncondensed polycyclic systems with N and S in the ring system (thiazole derivatives)
2.2.3.7 metal complexes
2.2.3.8 other polycyclic pigments
2.2.4 other pigments

2.3 Dyes

2.4 Brightening agents
2.4.1 stilbene derivatives
2.4.2 coumarin derivatives
2.4.3 1,3-diphenylpyrazoline derivatives
2.4.4 naphthalimide derivatives
2.4.5 (benz)oxazole derivatives
2.4.6 (benzo)triazole derivatives
2.4.7 triazine derivatives
2.4.8 polyphenylsulfonates
2.4.9 other brightening agents

2.5 Fillers, reinforcing agents
2.5.1 inorganic
2.5.1.1 compounds with molecule-anions
2.5.1.1.1 stick-like and bent anions (cyanides, cyanates, nitrites)
2.5.1.1.2 star-shaped anions (carbonates, nitrates)
2.5.1.1.3 pyramidal anions (sulfites, phosphites)
2.5.1.1.4 tetrahedral anions (sulfates, chromates, orthophosphates, orthosilicates)
2.5.1.1.5 octahedral anions (hexafluorosilicates, hexacyanoferrates)
2.5.1.1.6 anions with lower symmetry (pyrophosphates, dichromates)
2.5.1.1.7 polymeric anions (polysilicates, polyphosphates, metaborates)
2.5.1.2 compounds with molecule-cations (ammonium salts)
2.5.1.3 uncharged inorganic molecules
2.5.1.4 compounds without defined molecules (oxides, hydroxides, sulfides)
2.5.2 organic

2.6 Other colouring agents

3 Plasticisers, Elasticators, Extenders

3.1 Hydrocarbons and halo-hydrocarbons
3.1.1 saturated, noncyclic hydrocarbons (paraffinic mineral oils)
3.1.2 saturated, cyclic hydrocarbons (naphthenic mineral oils)
3.1.3 aliphatic-aromatic hydrocarbons (aromatic mineral oils)
3.1.4 halogen-containing aliphatic hydrocarbons
3.1.5 halogen-containing aliphatic-aromatic hydrocarbons
3.1.6 halogen-containing aromatic hydrocarbons
3.1.7 polyhydrocarbons

3.1.8 halogen-containing polymers (vinylchloride copolymers)

3.2 Alcohols, ethers and etheralcohols, thioethers, ketones
3.2.1 monovalent alcohols (fatty alcohols, resin alcohols)
3.2.2 diols and polyols
3.2.3 ethers
3.2.4 etheralcohols
3.2.5 thioethers
3.2.6 polyethers
3.2.7 other CHO polymers (O singly-bonded)
3.2.8 ketones

3.3 Esters and thioesters of aliphatic carboxylic acids
3.3.1 esters of saturated monocarboxylic acids
3.3.1.1 C_2...C_5-carboxylic acid esters
3.3.1.2 higher carboxylic acid esters (fatty acid esters)
3.3.1.3 esters of (poly-)etheralcohols
3.3.1.4 esters of hydroxycarboxylic acids
3.3.1.5 other monocarboxylic acid esters
3.3.2 esters of saturated dicarboxylic acids
3.3.2.1 unbranched saturated esters
3.3.2.2 branched saturated esters
3.3.2.3 esters of etheralcohols
3.3.2.4 aliphatic polyesters of dicarboxylic acids
3.3.2.5 aliphatic-aromatic esters of saturated dicarboxylic acids
3.3.2.6 esters and polyesters of saturated dicarboxylic acids with (di)phenols
3.3.2.7 other esters of saturated dicarboxylic acids
3.3.3 esters of saturated polycarboxylic acids
3.3.4 esters of unsaturated monocarboxylic acids
3.3.4.1 unbranched esters of unsaturated monocarboxylic acids
3.3.4.2 branched or cyclic esters of unsaturated monocarboxylic acids
3.3.4.3 esters of unsaturated hydroxycarboxylic acids
3.3.4.4 esters of unsaturated monocarboxylic acids with (poly-)etheralcohols
3.3.5 esters of unsaturated dicarboxylic acids
3.3.5.1 maleates
3.3.5.2 fumarates
3.3.5.3 other esters of unsaturated dicarboxylic acids
3.3.6 epoxidized aliphatic carboxylic acid esters (epoxidized biogenic oils)
3.3.7 esters of aliphatic carboxylic acids with aromatically substituted alcohols
3.3.8 thioesters
3.3.9 other esters of aliphatic carboxylic acids

3.4 Esters of aromatic carboxylic acids
3.4.1 esters of aromatic monocarboxylic acids
3.4.2 esters of di- or polybasic aromatic carboxylic acids
3.4.2.1 phthalic acid esters
3.4.2.1.1 from linear aliphatic alcohols
3.4.2.1.2 from branched aliphatic alcohols
3.4.2.1.3 from cycloaliphatic alcohols
3.4.2.1.4 mixed (intra- or intermolecular) aliphatic phthalates
3.4.2.1.5 from aliphatic-aromatic alcohols (equal or mixed substitution)
3.4.2.1.6 from phenols (equal or mixed substitution)
3.4.2.1.7 from etheralcohols
3.4.2.1.8 other phthalic acid esters
3.4.2.2 isophthalic acid esters

3.4.2.3 terephthalic acid esters
3.4.2.4 trimellitic acid esters and -polyesters
3.4.2.5 esters of other di- or polybasic aromatic carboxylic acids
3.4.2.6 polymeric esters of dibasic aromatic carboxylic acids
3.4.3 esters of aromatically substituted aliphatic carboxylic acids
3.4.4 esters of aliphatically substituted aromatic carboxylic acids
3.4.5 other aromatic esters

3.5 Other esters of organic acids

3.6 Phosphorus derivatives
3.6.1 aliphatic phosphates
3.6.2 aliphatic-aromatic phosphates (mixed esters, aliphatically substituted phenol esters)
3.6.3 aromatic phosphates
3.6.4 aliphatic phosphites
3.6.5 aliphatic-aromatic phosphites
3.6.6 aromatic phosphites
3.6.7 phosphonates
3.6.8 other phosphorus derivatives

3.7 Sulfonic acid derivatives
3.7.1 sulfonic acid esters
3.7.2 sulfonamides

3.8 CHN(O) compounds
3.8.1 CHN compounds
3.8.2 amides
3.8.3 urethanes

3.9 Other plasticisers

4 Processing agents, textile auxiliaries

4.1 Lubricating and release agents, antistatics
4.1.1 hydrocarbons and modified hydrocarbons
4.1.1.1 paraffins
4.1.1.2 nonpolar polyethylene wax
4.1.1.3 polar paraffin and polyethylene waxes
4.1.1.3.1 oxidized
4.1.1.3.2 amidized
4.1.1.3.3 others
4.1.1.4 nonpolar polypropylene wax
4.1.1.5 polar polypropylene wax
4.1.1.6 aliphatic-aromatic compounds
4.1.2 fatty alcohols, fatty-alcohol ethers (alkyleneoxide adducts of fatty alcohols)
4.1.3 carboxylic acids, their esters and salts
4.1.3.1 fatty acids, wax acids
4.1.3.2 hydroxy acids
4.1.3.3 fatty and wax acid esters
4.1.3.4 esteralcohols and etheresters of fatty acids
4.1.3.5 fatty acid-alkyleneoxide adducts
4.1.3.6 ethers and esters of fatty alcohols
4.1.3.7 aliphatic-aromatic acids and their esters
4.1.3.8 esters of aromatic acids
4.1.3.9 metal soaps

4.1.4 fatty amines, aminoalcohols and -ethers, quaternary ammonium salts
4.1.5 fatty acid amides, amidized hydrocarbon wax
4.1.6 amidoalcohols, amidoamines
4.1.7 sulfonic acid esters and salts
4.1.8 other lubricating or release agent
4.1.9 other antistatics

4.2 Adhesion agents
4.2.1 silicium derivatives
4.2.1.1 (alkoxy)silanes
4.2.1.2 silicic acid esters
4.2.2 titanium derivatives
4.2.3 zirconium derivatives
4.2.4 chromium derivatives
4.2.5 metal-free organic compounds
4.2.6 other adhesive agents

4.3 PVC processing aids

4.4 Blowing agents
4.4.1 chemical blowing agents
4.4.1.1 azo compounds
4.4.1.2 hydrazine derivatives
4.4.1.3 tetrazoles
4.4.1.4 semicarbazides
4.4.1.5 benzoxazines
4.4.1.6 nitrosamines
4.4.1.7 others
4.4.2 physical blowing agents
4.4.2.1 hydrocarbons
4.4.2.2 halocarbons
4.4.2.3 halohydrocarbons
4.4.2.4 others

4.5 Textile auxiliaries
4.5.1 wetting agents, antistatics, foaming agents, emulsifiers, related substances
4.5.2 dyeing auxiliaries
4.5.3 reviving agents
4.5.4 hydrophobing agents
4.5.5 other textile auxiliaries

4.6 Crosslinking agents, activators
4.6.1 olefinic compounds, other monomers
4.6.2 peroxy compounds
4.6.2.1 inorganic (hydro)peroxides
4.6.2.2 organic (hydro)peroxides
4.6.2.2.1 hydroperoxides
4.6.2.2.2 dialkylperoxides
4.6.2.2.3 aralkylperoxides
4.6.2.2.4 (hydro)peroxyketals
4.6.2.2.5 peresters
4.6.2.2.6 diacylperoxides (peroxyanhydrides)
4.6.2.2.7 peroxy(di)carbonic acid esters
4.6.2.2.8 peroxysulfonic acids and their derivatives
4.6.2.3 siliciumorganic (hydro)peroxides
4.6.3 isocyanates

4.6.4 azo compounds
4.6.5 other crosslinking agents or activators

4.7 Other processing agents

5 Vulcanisation agents and other rubber auxiliaries

5.1 Vulcanisation (crosslinking) agents (see also 4.6)
5.1.1 sulfur donors
5.1.1.1 sulfur
5.1.1.2 disulfurdichloride
5.1.1.3 caprolactam(di)sulfides
5.1.1.4 thiuramtetrasulfides
5.1.1.5 thiosubstituted morpholine derivatives
5.1.1.6 thiosubstituted (benzo)thiazole derivatives
5.1.1.7 other sulfur donors
5.1.2 vulcanisation agents without active sulfur
5.1.2.1 metal oxides
5.1.2.2 compounds with active chlorine
5.1.2.3 polyfunctional amines, blocked amines
5.1.2.4 azo compounds
5.1.2.5 (hydro)peroxides and their derivatives (classification like 4.6.2)
5.1.2.6 quinone derivatives
5.1.2.7 dinitrosobenzene and dinitrobenzene derivatives
5.1.2.8 triallylcyanurate and -isocyanurate
5.1.2.9 other vulcanisation agents

5.2 Vulcanisation accelerators
5.2.1 amines and related compounds
5.2.1.1 aliphatic amines
5.2.1.2 aromatically substituted aliphatic amines
5.2.1.3 aldehyde condensation products of aliphatic amines
5.2.1.4 aldehyde condensation products of aromatically substituted aliphatic amines
5.2.1.5 aniline derivatives
5.2.1.6 toluidine derivatives
5.2.2 guanidine derivatives, derivatives of carbonic and thiocarbonic acids
5.2.2.1 guanidines
5.2.2.2 thiourea and its derivatives
5.2.2.3 dithiocarbamates
5.2.2.3.1 metal dithiocarbamates
5.2.2.3.2 (alkyl)ammonium dithiocarbamates
5.2.2.4 thiuram derivatives
5.2.2.4.1 thiurammonosulfides
5.2.2.4.2 thiuram-di- and poly-sulfides
5.2.2.5 xanthogenates
5.2.3 heterocyclic compounds
5.2.3.1 piperidine derivatives
5.2.3.2 other aliphatic N-heterocyclics
5.2.3.3 pyridine derivatives
5.2.3.4 imidazol(in)e derivatives
5.2.3.5 thiazole derivatives
5.2.3.5.1 (2-mercapto)benzothiazole and its derivatives
5.2.3.5.2 benzothiazolesulfenamides

5.2.3.6 triazine derivatives
5.2.4 derivatives of (di-)thiophosphoric acid
5.2.5 other vulcanisation accelerators

5.3 Vulcanisation activators
5.3.1 inorganic
5.3.1.1 zinc oxide, -hydroxide, -carbonate
5.3.1.2 lead oxide
5.3.1.3 diantimony trioxide
5.3.1.4 silicium dioxide
5.3.2 organic
5.3.2.1 amines
5.3.2.2 glycols, other alcohols
5.3.2.3 fatty acids
5.3.2.4 amides
5.3.2.5 oligofunctional monomers
5.3.2.6 silanes
5.3.3 other vulcanisation activators

5.4 Vulcanisation retarders
5.4.1 organic acids
5.4.2 anhydrides
5.4.3 N-nitroso compounds
5.4.4 sulfonamides
5.4.5 imides
5.4.6 other vulcanisation retarders

5.5 Rubber ageing inhibitors, rubber antioxidants (classification like 1.1)

5.6 Reinforcing agents

5.7 Processing aids (plastificators and peptisers), other rubber chemicals (classification according to the elemental composition)

6 Other additives and auxiliaries

2
FTIR Spectra of Additives

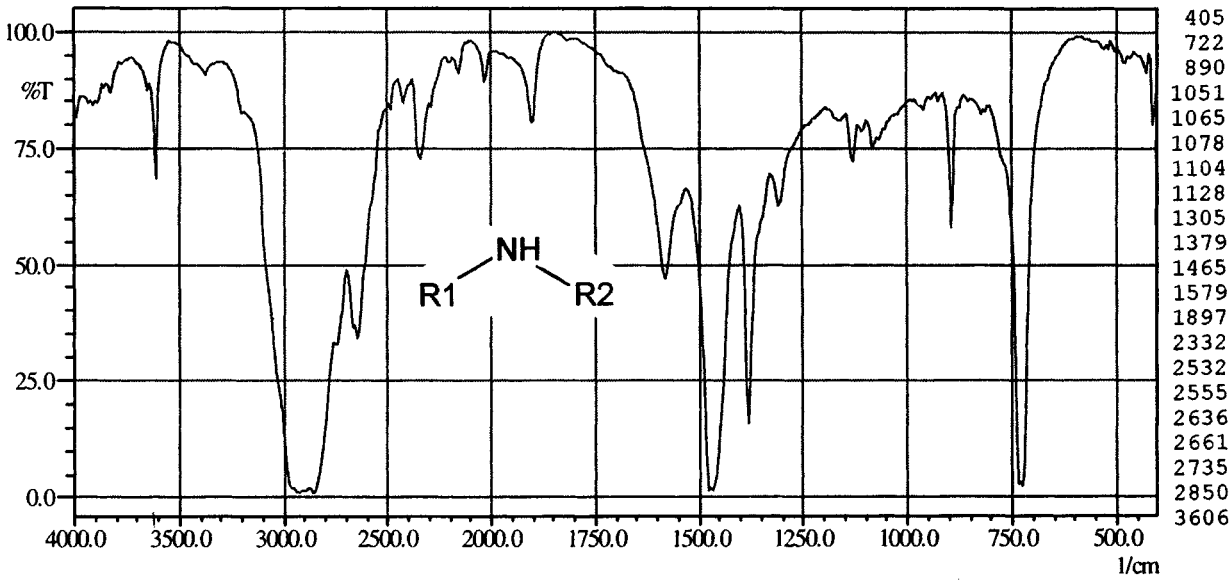
User's Guide

The spectra are arranged in order of their decimal number. You will find this number on the left side above the spectrum. The substance class to which the additives on each page belong is given in the running head of each page. The empirical formula of the structure on which the spectrum is based is also located above the spectrum. The column to the right of each spectrum denotes the strongest peaks in cm^{-1}. The spectrum legend – below the spectrum – shows the following entries:

(1) chemical name
(2) trivial/trade name
(3) source
(4) molar mass in g mol^{-1}
(5) use
(6) appearance
(7) melting point in °C
(8) boiling point in °C
(9) density in g cm^{-3}
(10) refractive index n_D
(11) CIE name
(12) CIE no.
(13) preparation
(14) comment

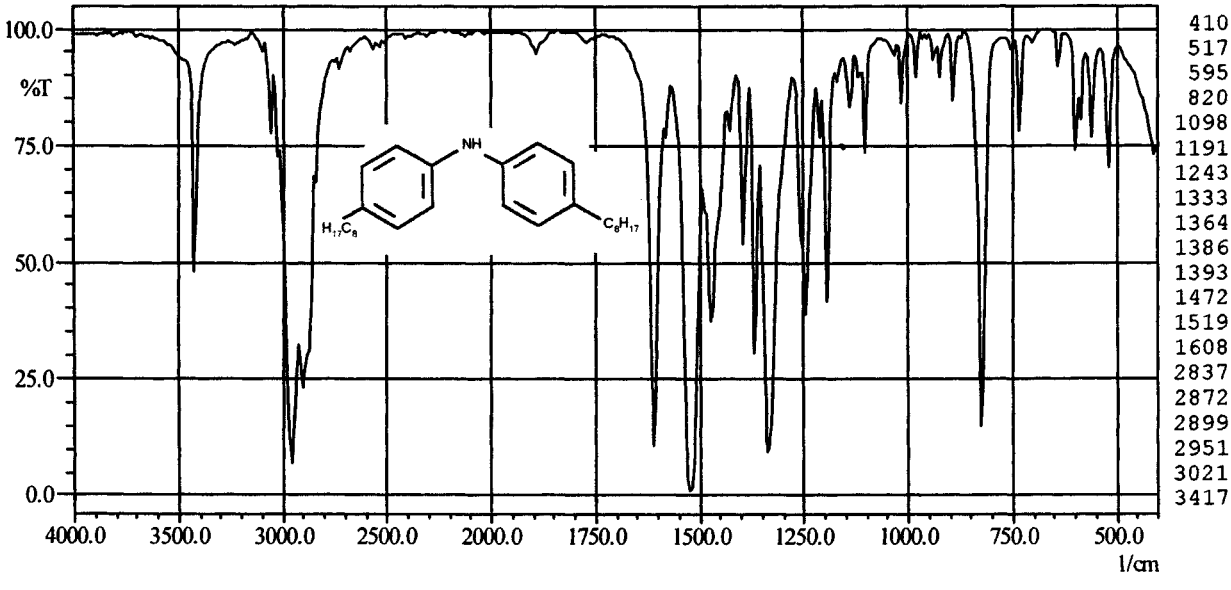
Only those entries are mentioned for each spectrum where the properties are known.

111111



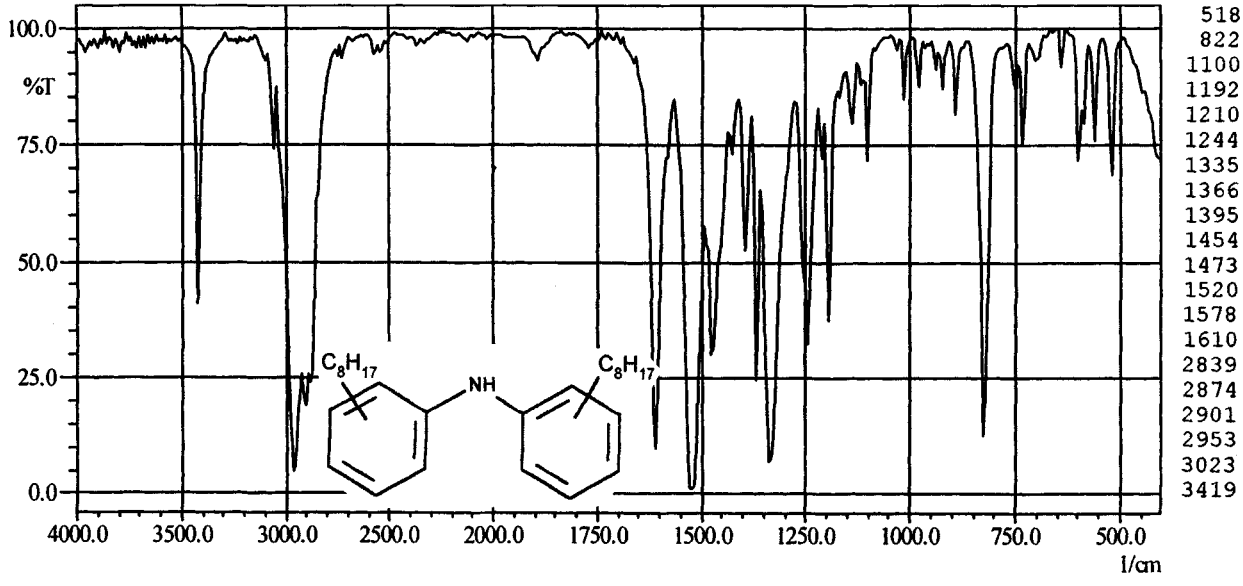
(1) **long-chain aliphatic hindered amine (HALS)**
(2) Antilux 550
(3) Freudenberg (Brunne collection)
(5) light stabiliser
(6) wax-like solid
(13) film from the melt on KBr

111122 $C_{28}H_{43}N$



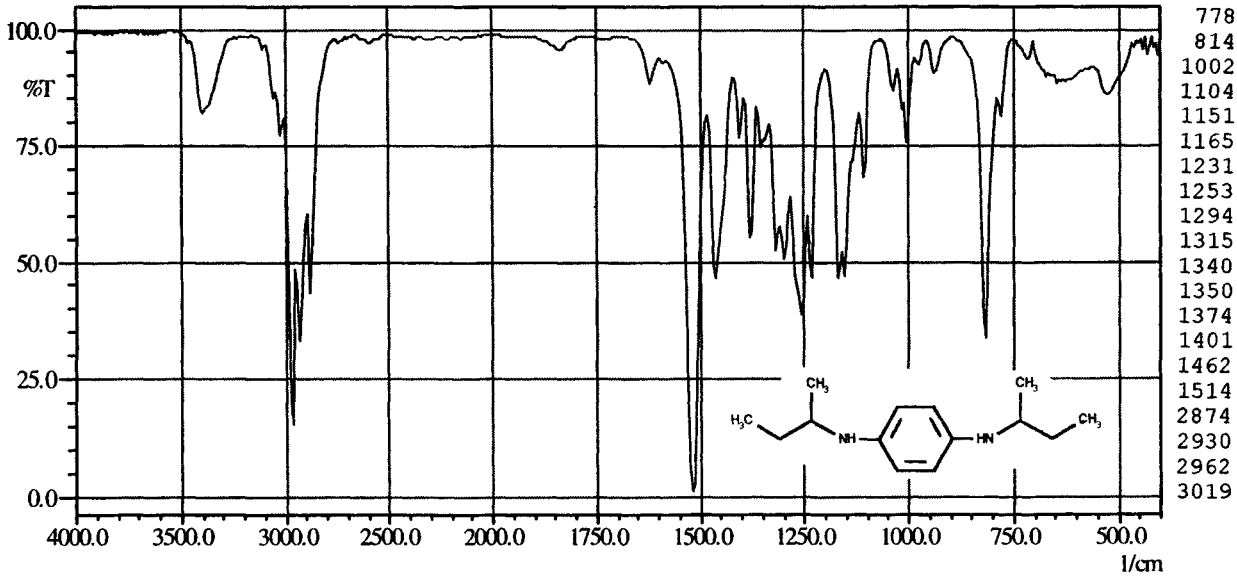
(1) **4,4'-dioctyldiphenylamine**
(2) Vanox 1081
(3) R.T. Vanderbilt
(4) 393.7 g mol^{-1}
(5) antioxidant
(6) colourless solid
(13) KBr pellet

111122 $C_{28}H_{43}N$



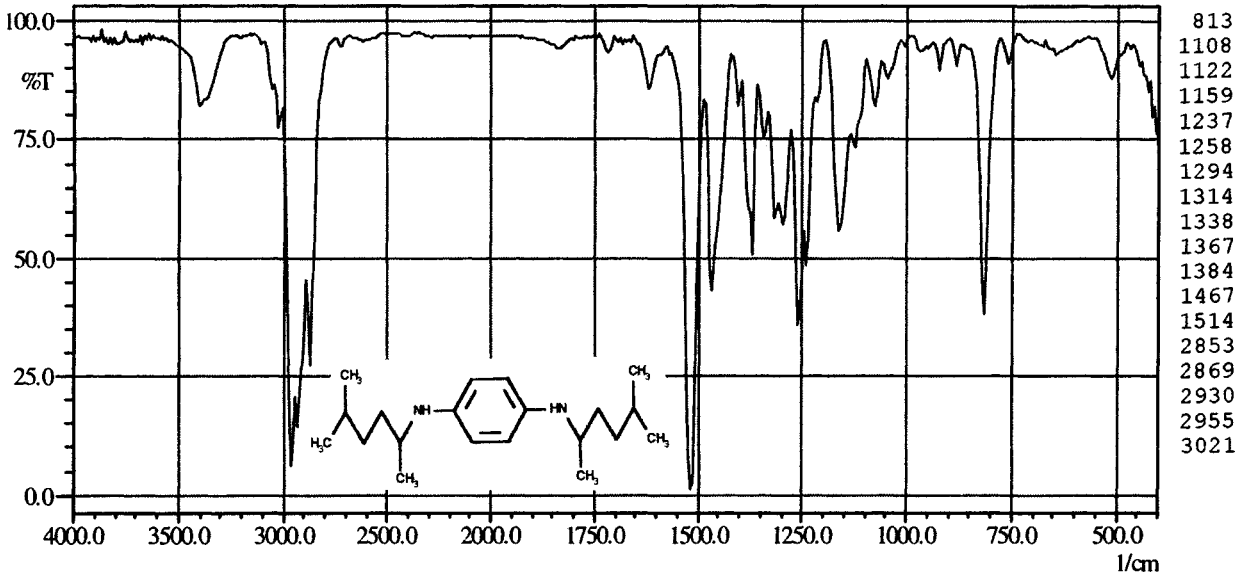
(1) **octylated diphenylamines**
(2) Permanax OD
(3) Akzo Chemicals
(4) 393.7 g mol^{-1}
(5) antioxidant
(6) beige sticks
(13) KBr pellet

111123 $C_{14}H_{24}N_2$



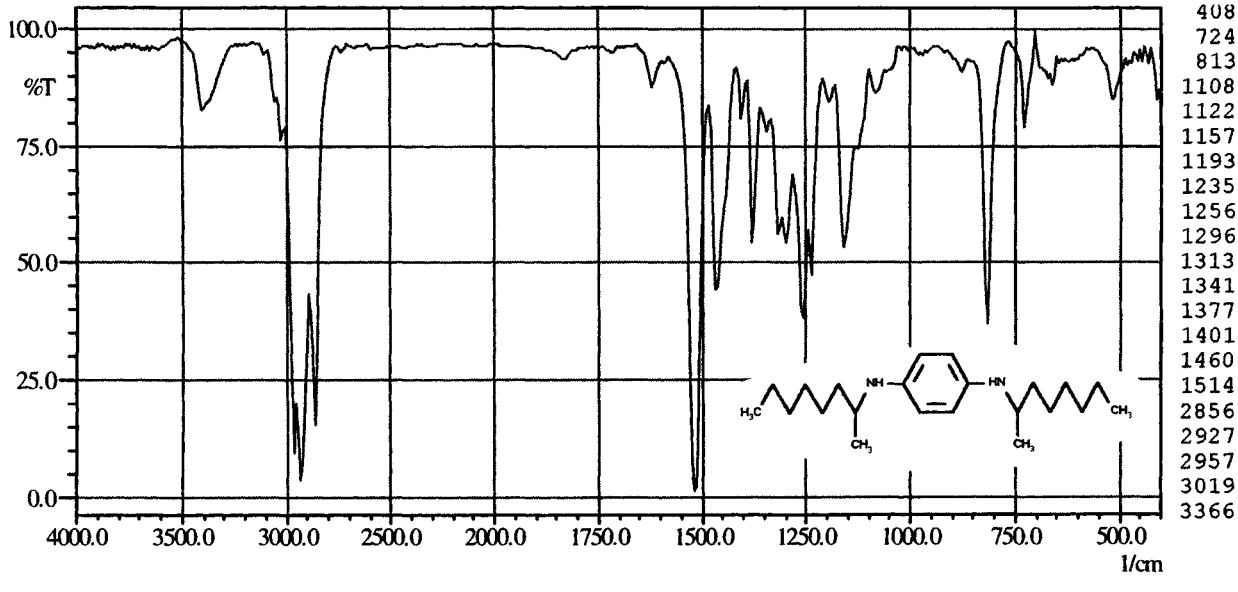
(1) **N,N'-di-*s*-butyl-*p*-phenylenediamine**
(2) HiTEC 4720 (Ethyl Antioxidant PDA)
(3) Ethyl
(4) 220.4 g mol^{-1}
(5) antioxidant
(6) red, clear liquid
(7) 14 °C
(8) 143 °C
(9) 0.94 g cm^{-3}
(13) layer btw KBr

111123 $C_{20}H_{36}N_2$



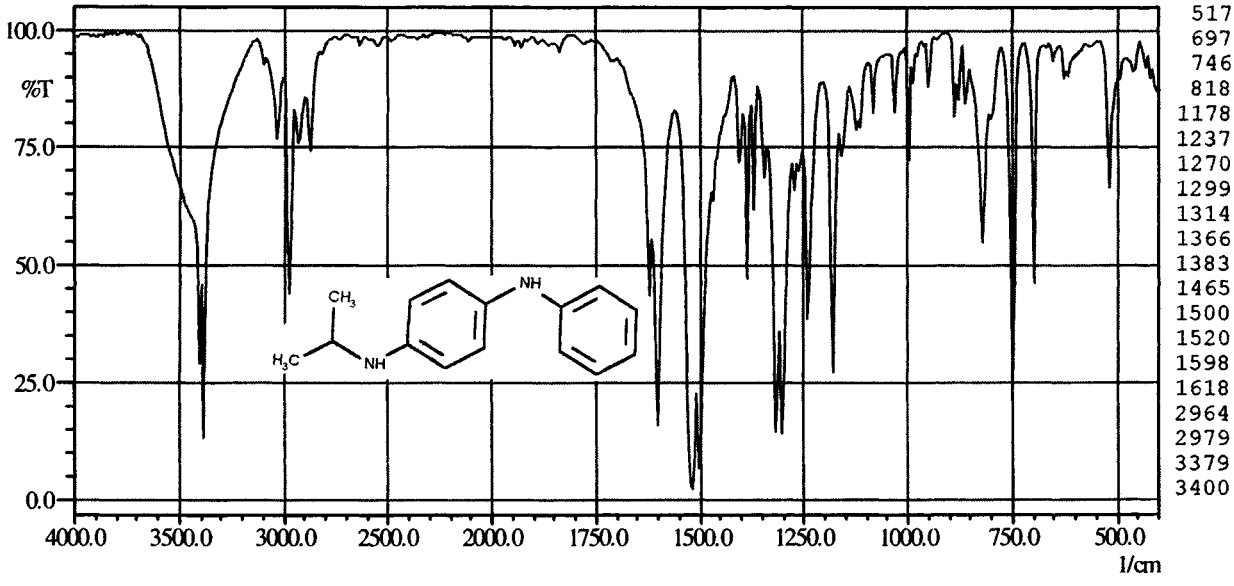
(1) **N,N'-di(1,4-dimethylpentyl)-*p*-phenylenediamine**
(2) Vulkanox 4030
(3) Bayer
(4) 304.5 g mol^{-1}
(5) antioxidant
(6) dark-red, low-viscous liquid
(9) 0.91 g cm^{-3}
(13) layer btw KBr

111123 $C_{22}H_{40}N_2$



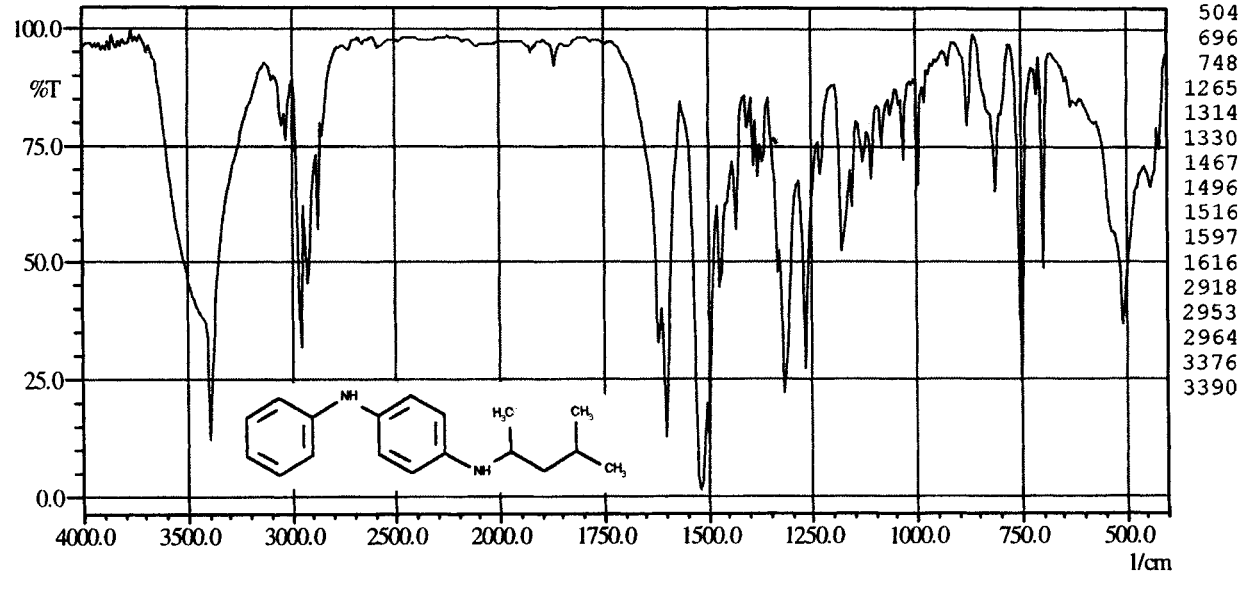
(1) **N,N'-di(*i*-octyl)-*p*-phenylenediamine**
(2) Antozite 1
(3) Vanderbilt
(4) 332.6 g mol^{-1}
(5) antioxidant
(6) liquid
(9) 0.9 g cm^{-3}
(13) layer btw KBr

111123 $C_{15}H_{18}N_2$



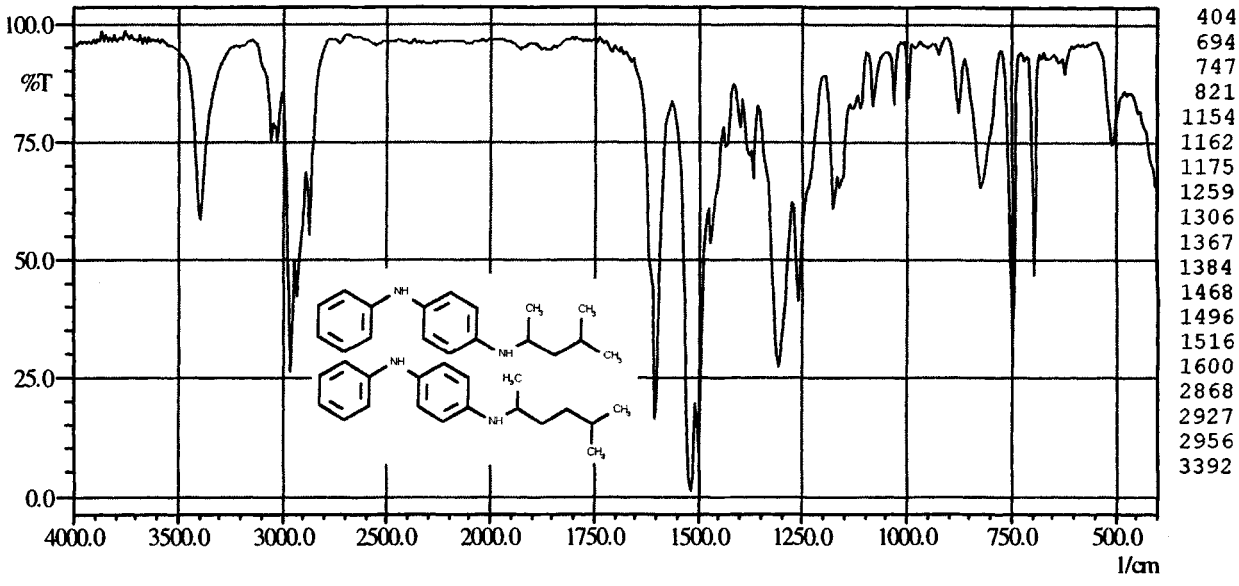
(1) **N-2-propyl-N'-phenyl-*p*-phenylenediamine**
(2) Permanax IPPD
(3) Akzo Chemie
(4) 226.2 g mol^{-1}
(5) antioxidant
(6) brown rods
(13) KBr pellet

111123 $C_{18}H_{24}N_2$



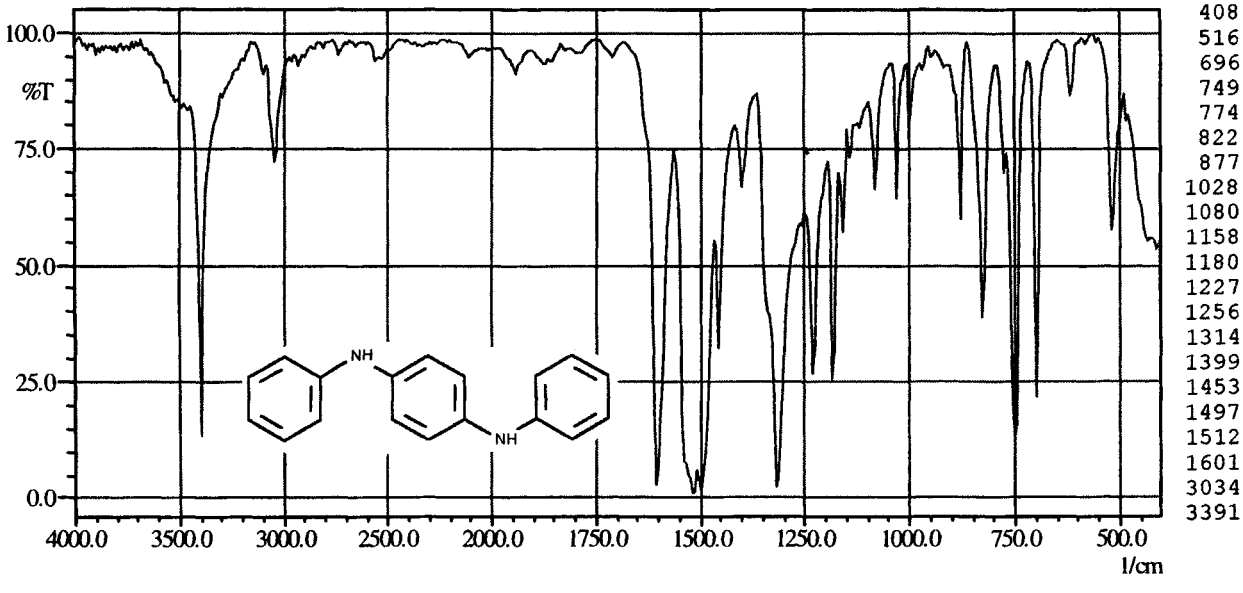
(1) **N-(1,3-dimethylbutyl)-N'-phenyl-*p*-phenylenediamine**
(2) Vulkanox 4020
(3) Bayer
(4) 268.4 g mol^{-1}
(5) antioxidant
(6) brown to violet solid
(7) 45 °C
(9) 1.02 g cm^{-3}
(13) KBr pellet

111123 $C_{18}H_{24}N_2 + C_{20}H_{36}N_2$



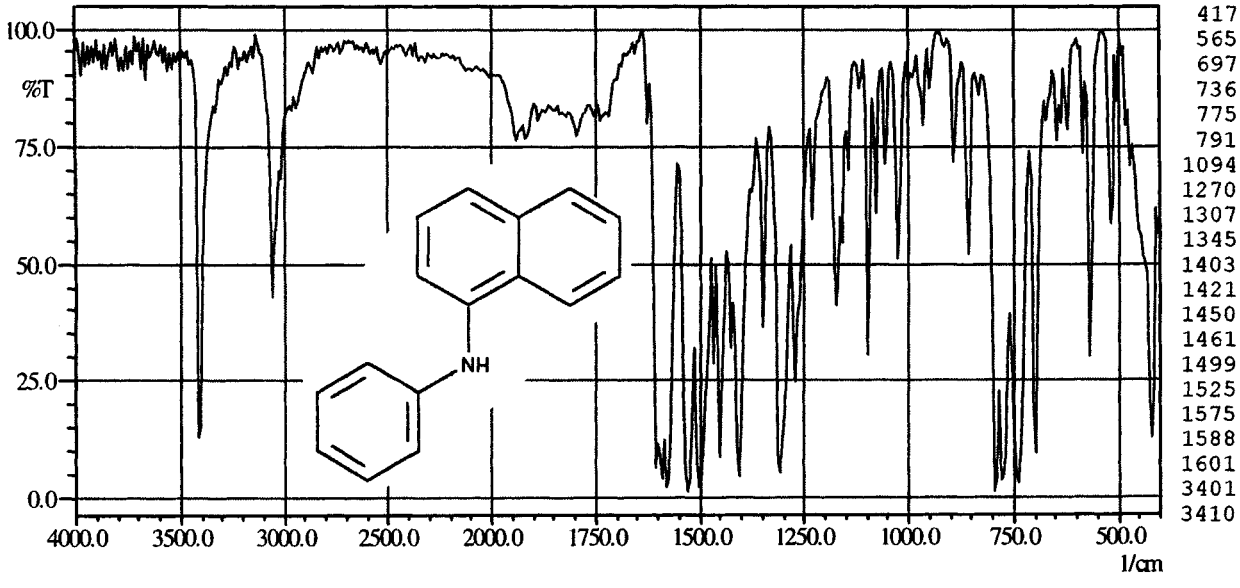
(1) **N-(1,3-dimethylbutyl)- and N-(1,4-dimethylpentyl) -N'-phenyl-*p*-phenylenediamine (1:1)**
(2) Vulkanox 4022
(3) Bayer
(4) 268.4, 304.5 g mol^{-1}
(5) antioxidant
(6) dark-brown, low-viscous liquid
(9) 1.01 g cm^{-3}
(13) layer btw KBr

11113 $C_{18}H_{16}N_2$



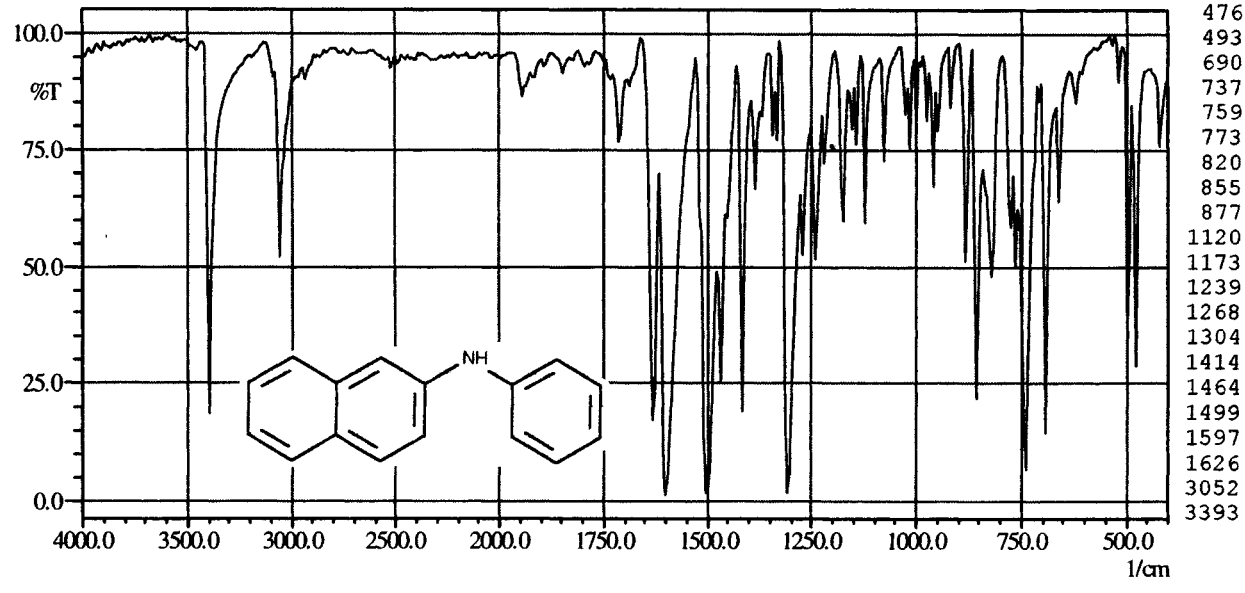
(1) **N,N'-diphenyl-*p*-phenylenediamine**
(2) Permanax DPPD
(3) Akzo Chemicals
(4) 260.3 g mol^{-1}
(5) antioxidant
(6) dark-grey solid
(13) KBr pellet

11113 $C_{16}H_{13}N$



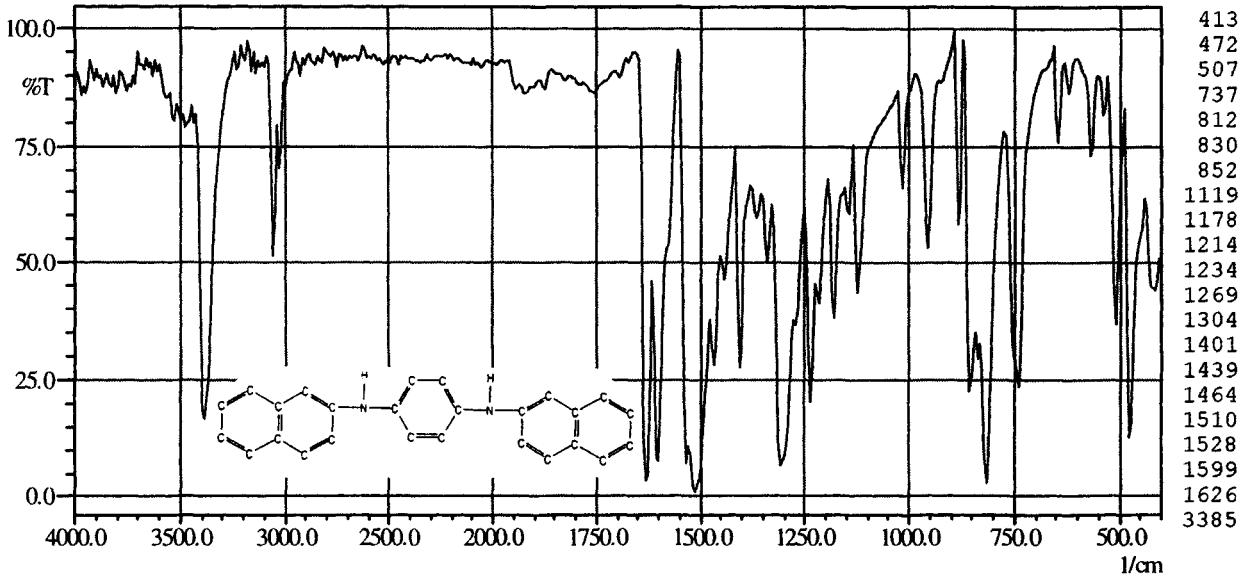
(1) **N-phenyl-N-1-naphthylamine**
(2) Vulkanox P (ASM PAN)
(3) Bayer
(4) 219.2 g mol^{-1}
(5) antioxidant
(6) violet solid
(7) 52 °C
(9) 1.11 g cm^{-3}
(13) KBr pellet

11113 $C_{16}H_{13}N$



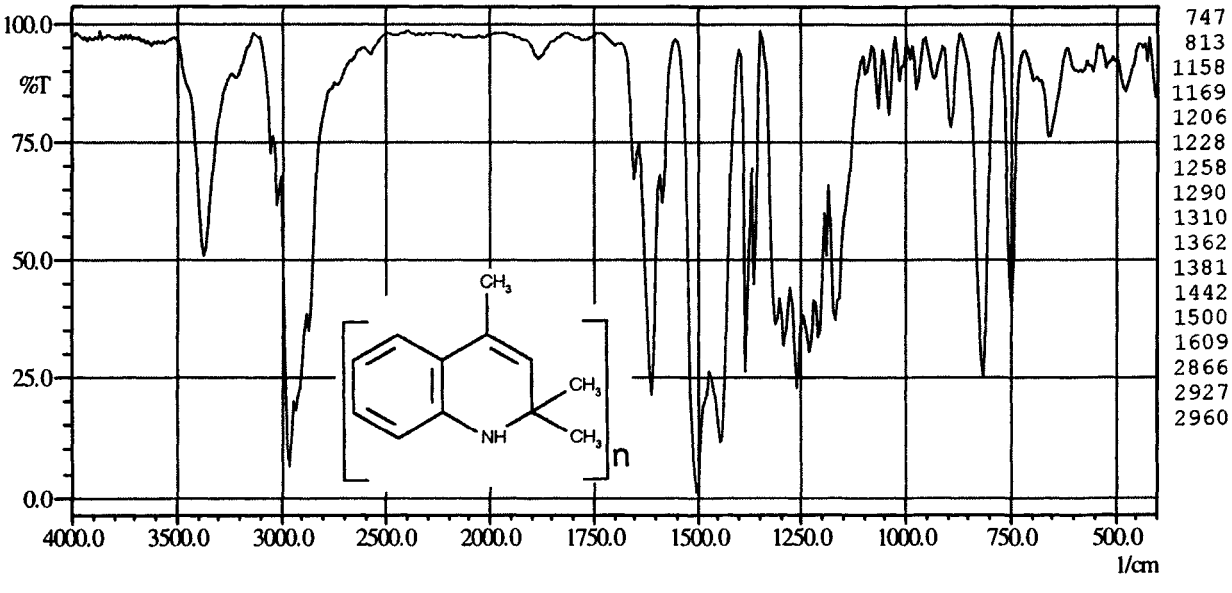
(1) **N-phenyl-2-naphthylamine**
(2) Vulkanox PBN
(3) Bayer
(4) 219.2 g mol^{-1}
(5) antioxidant
(6) violet to brown solid
(7) 105 °C
(9) 1.23 g cm^{-3}
(13) KBr pellet

11113 $C_{26}H_{20}N_2$



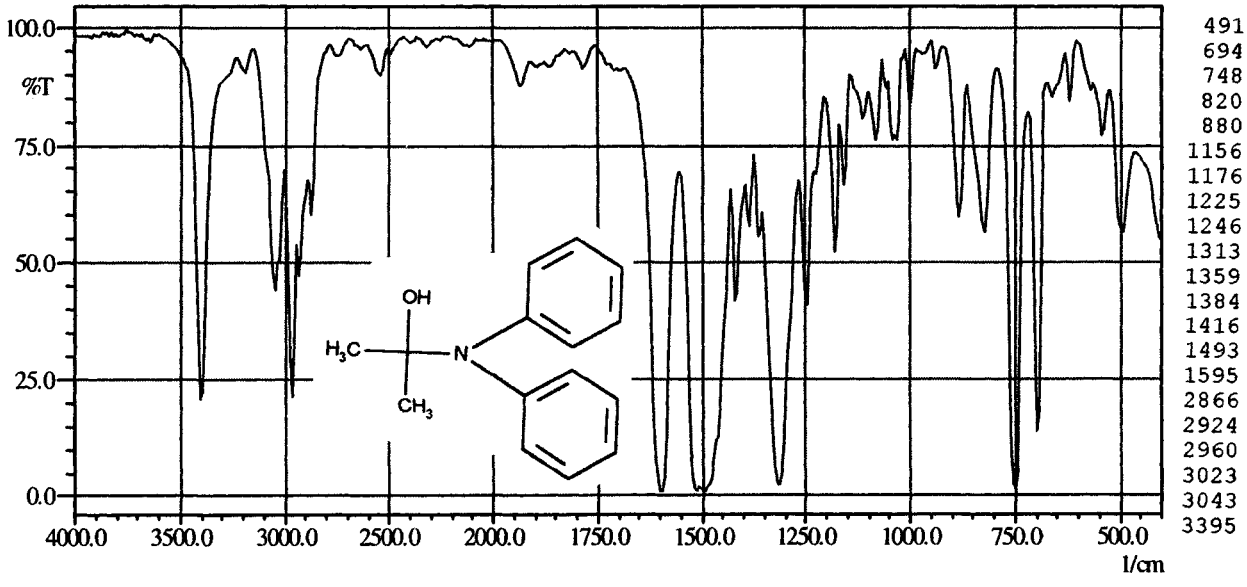
(1) **N,N'-di(2-naphthyl)-*p*-phenylenediamine**
(2) Age Rite White
(3) R.T.Vanderbilt (Brunne collection)
(4) 360.4 g mol^{-1}
(5) antioxidant
(6) colourless solid
(13) KBr pellet (Christiansen effect)

11114



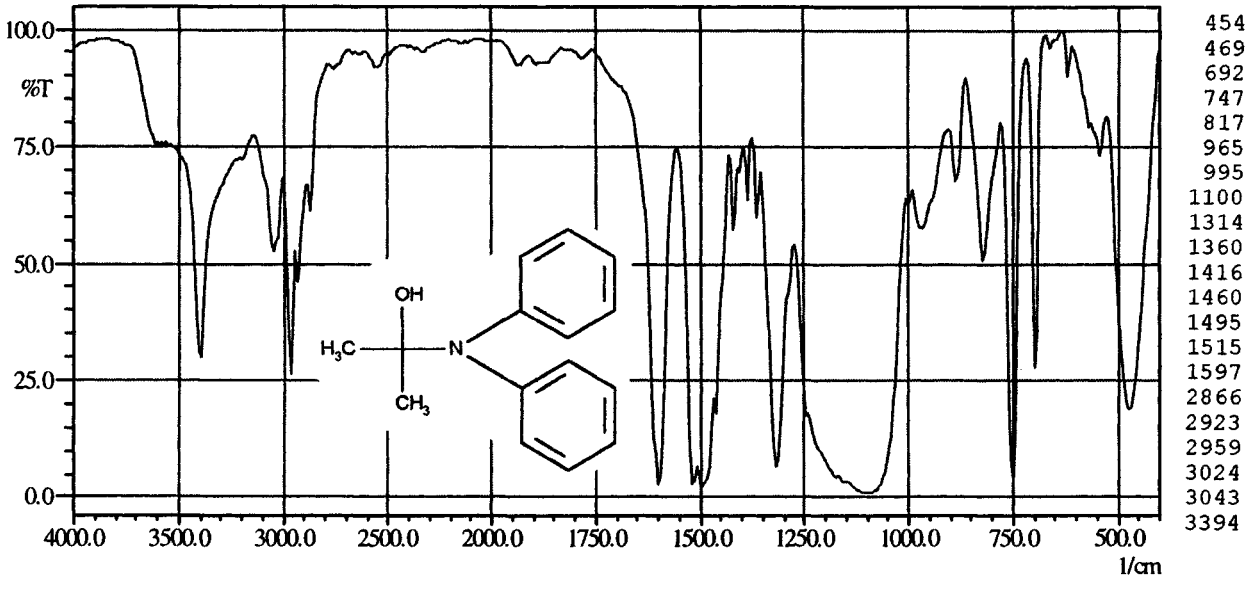
(1) **polymer 2,2,4-trimethyl-1,2-dihydroquinoline**
(2) Vulkanox HS/Pulver
(3) Bayer
(5) antioxidant
(6) yellow to amber-coloured solid
(7) 75 °C
(9) 1.07 g cm^{-3}
(13) KBr pellet
(14) structure shows the monomer unit

11121 $C_{15}H_{17}NO$



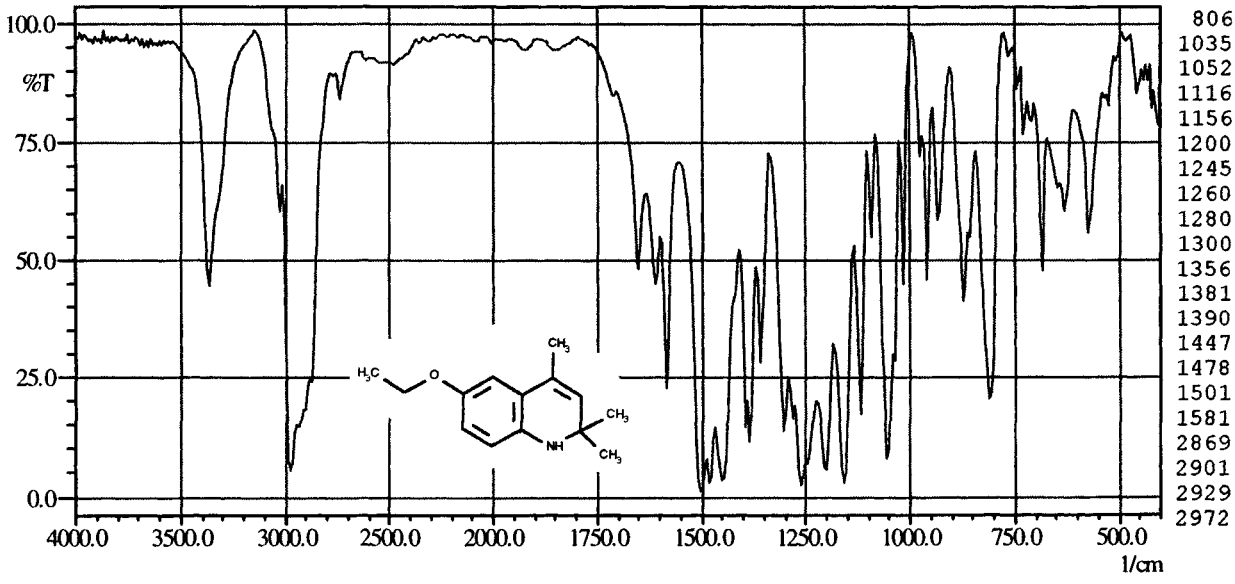
(1) **acetone diphenylamine condensation product**
(2) Permanax BL
(3) Akzo Chemie
(4) 227.3 g mol^{-1}
(5) antioxidant
(6) black, clear, viscous liquid
(13) layer btw KBr

11121 $C_{15}H_{17}NO$



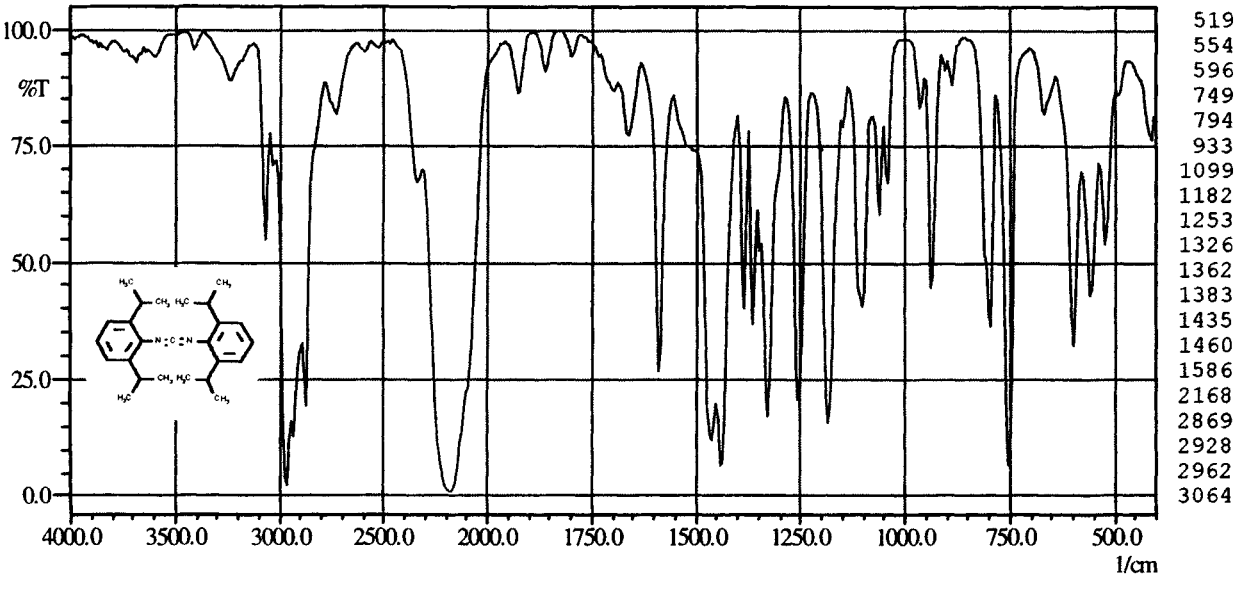
(1) **acetone-diphenylamine condensation product on SiO2**
(2) Permanax BWL
(3) Akzo Chemie
(4) 227.3 g mol^{-1}
(5) antioxidant
(6) black solid
(13) KBr pellet

11123 $C_{14}H_{19}NO$



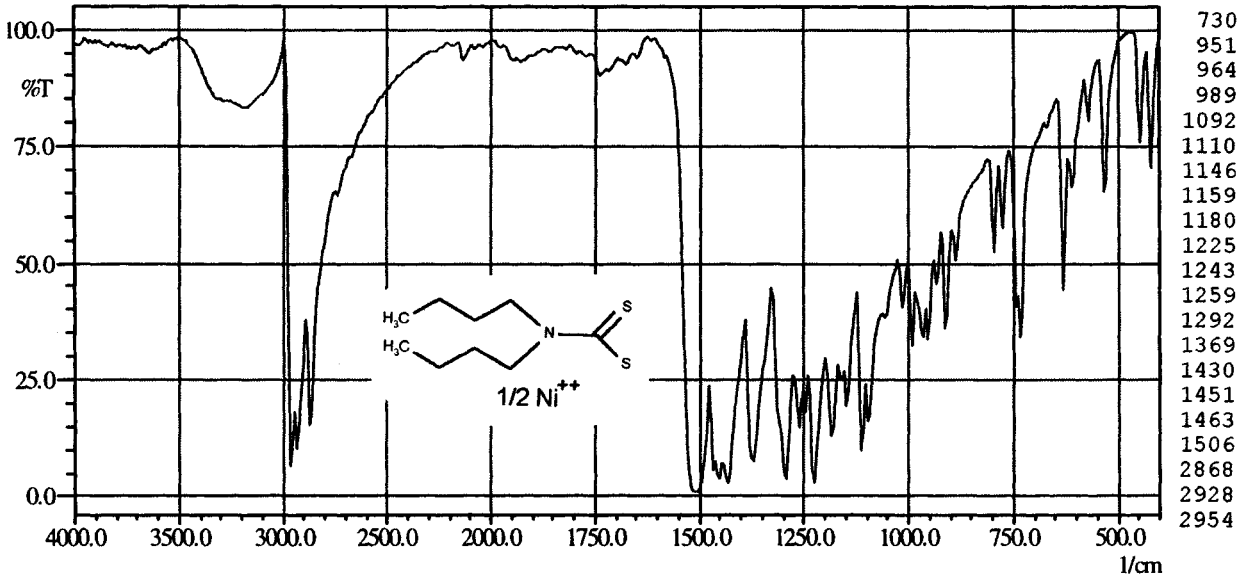
(1) **6-ethoxy-2,2,4-trimethyl-1,2-dihydroquinoline**
(2) Santoflex AW
(3) Monsanto
(4) 217.3 g mol^{-1}
(5) antioxidant
(6) liquid
(13) layer btw KBr

11212 $C_{25}H_{34}N_2$



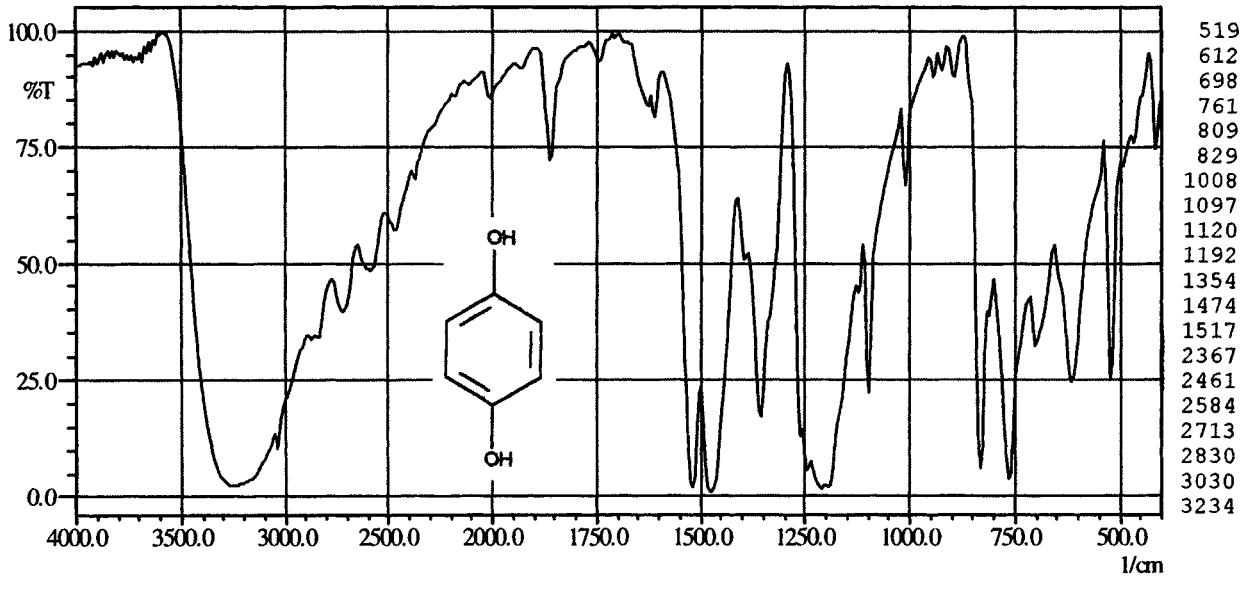
(1) ***bis*(2,6-di-*i*-propylphenyl)carbodiimide**
(2) Stabaxol I
(3) Bayer
(4) 362.5 g mol^{-1}
(5) antioxidant
(6) colourless solid
(13) layer btw KBr

1123 $C_{18}H_{36}N_2S_4Ni$



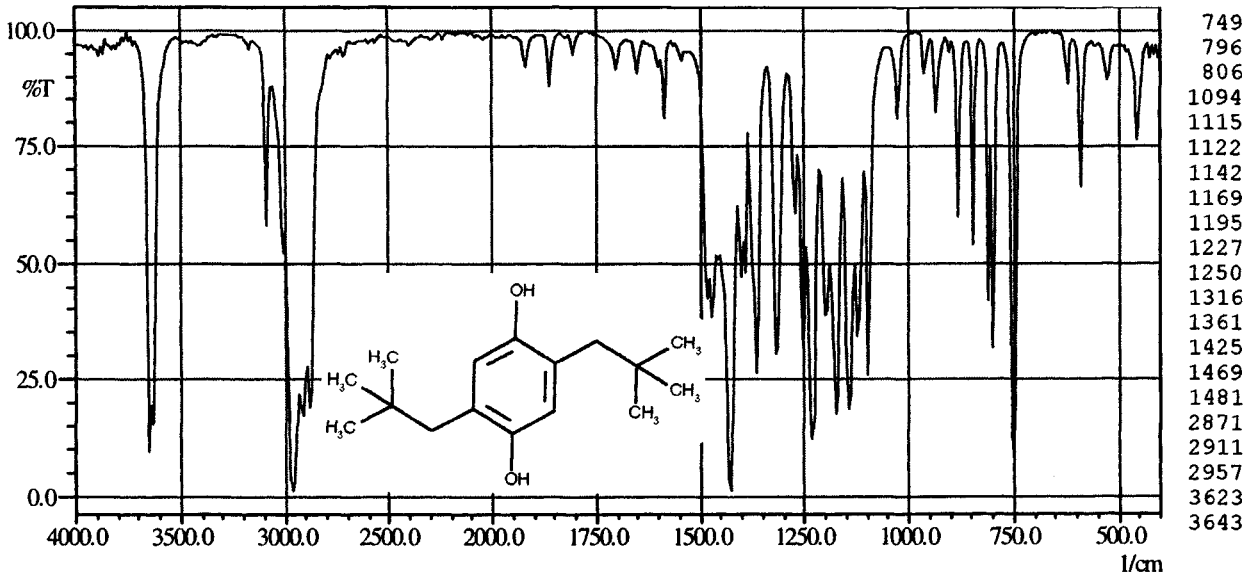
(1) **Ni-dibutyldithiocarbamate**
(2) NBC
(3) DuPont
(4) 467.4 g mol^{-1}
(5) antioxidant
(6) green solid
(13) KBr pellet

11311 $C_6H_6O_2$



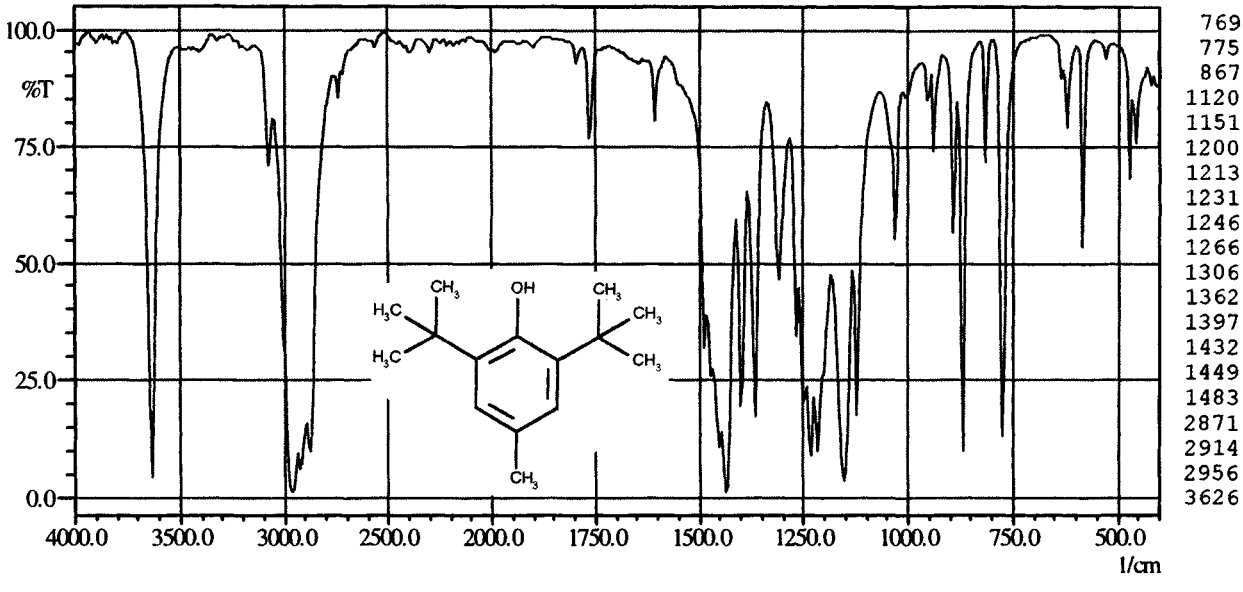
(1) **hydroquinone**
(2) Hydroquinone Inhibitor Grade
(3) Eastman
(4) 110.1 g mol^{-1}
(5) antioxidant
(6) colourless solid
(7) 170 °C
(8) 286 °C
(9) 1.328 g cm^{-3}
(13) KBr pellet

11312 $C_{14}H_{22}O$



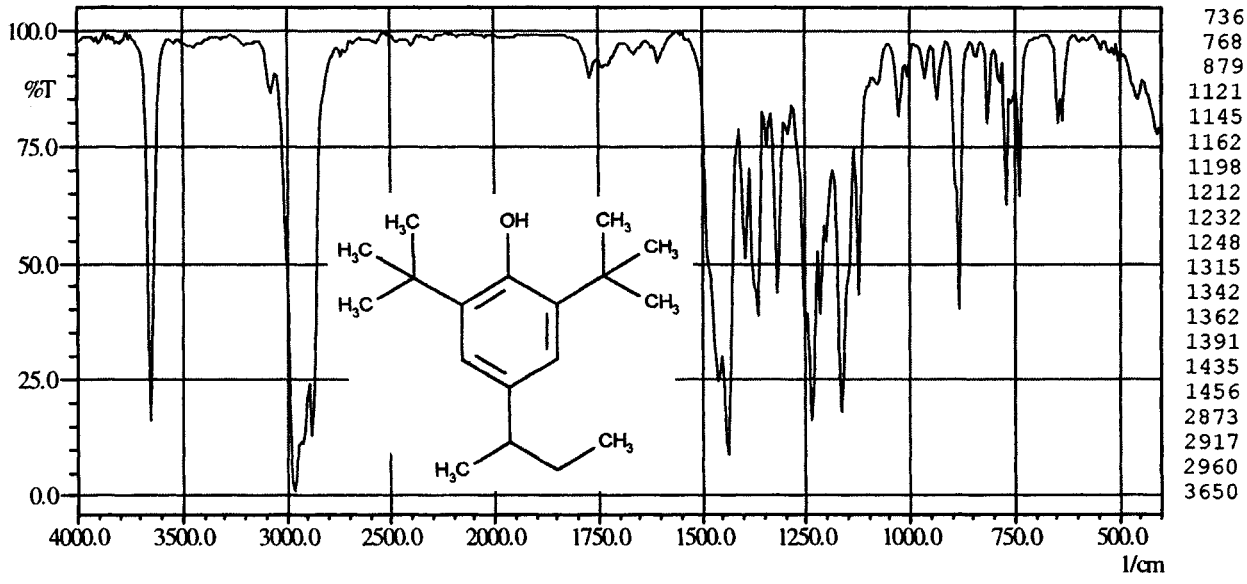
(1) **2,6-di-*t*-butylphenol**
(2) Ethyl 701, HiTEC 4701
(3) Ethyl
(4) 206.3 g mol^{-1}
(5) antioxidant
(6) pale-straw, crystalline solid
(7) 36 °C
(9) 0.914 g cm^{-3}
(13) KBr pellet

11312 $C_{15}H_{24}O$



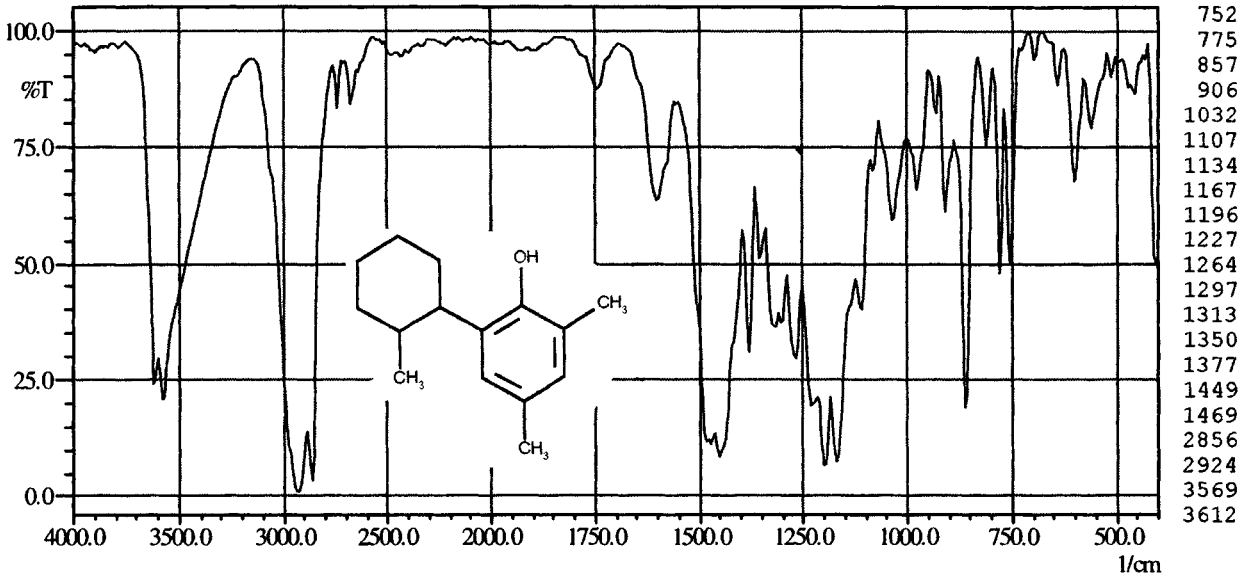
(1) **2,6-di-*t*-butyl-4-methylphenol**
(2) Lowinox BHT
(3) Chemische Werke Lowi
(4) 220.4 g mol^{-1}
(5) antioxidant
(6) colourless solid
(7) 69.2 °C
(13) KBr pellet

11312 $C_{18}H_{30}O$



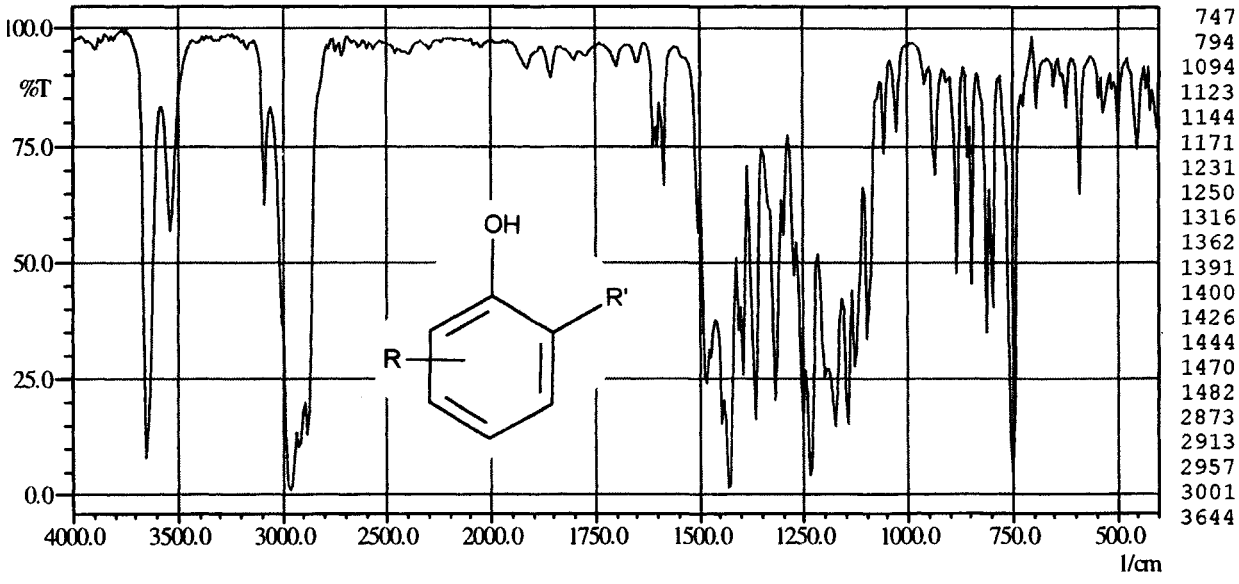
(1) **2,6-di-*t*-butyl-4-*s*-butylphenol**
(2) Vanox 1320
(3) R.T. Vanderbilt
(4) 262.4 g mol^{-1}
(5) antioxidant
(6) straw to light-amber, clear liquid
(9) 0.93 g cm^{-3}
(13) layer btw KBr

11312 $C_{15}H_{22}O$



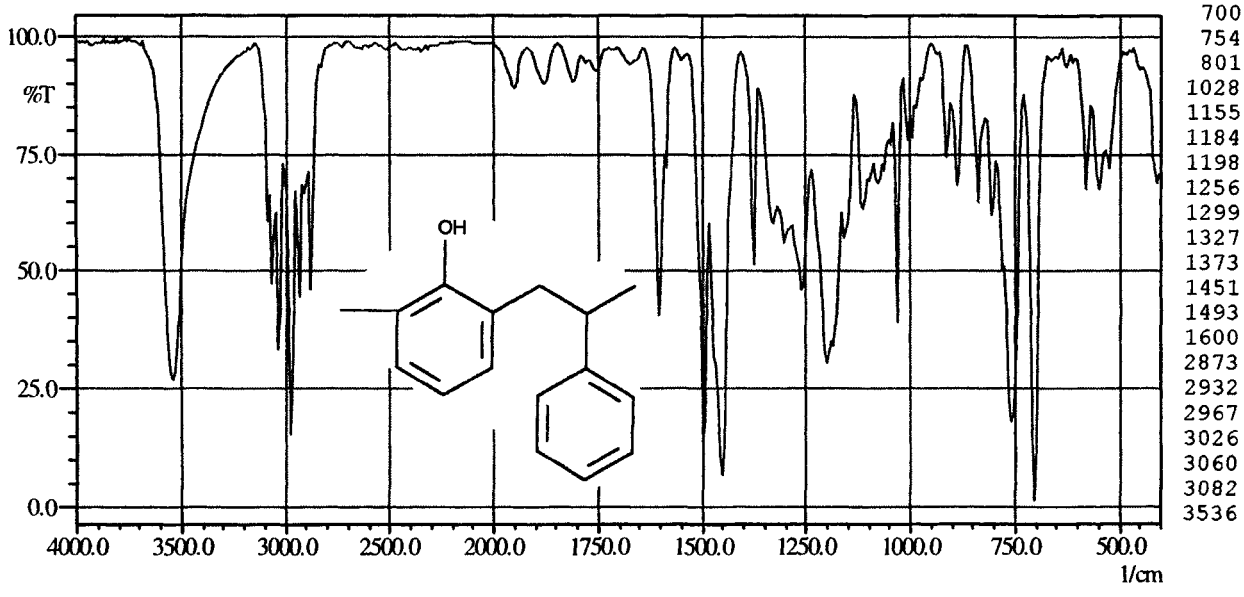
(1) **2,4-dimethyl-6-(*o*-methylcyclohexyl)phenol**
(2) Permanax WSL
(3) Akzo Chemie
(4) 218.3 g mol^{-1}
(5) antioxidant
(6) yellowish, clear liquid
(13) layer btw KBr

11312



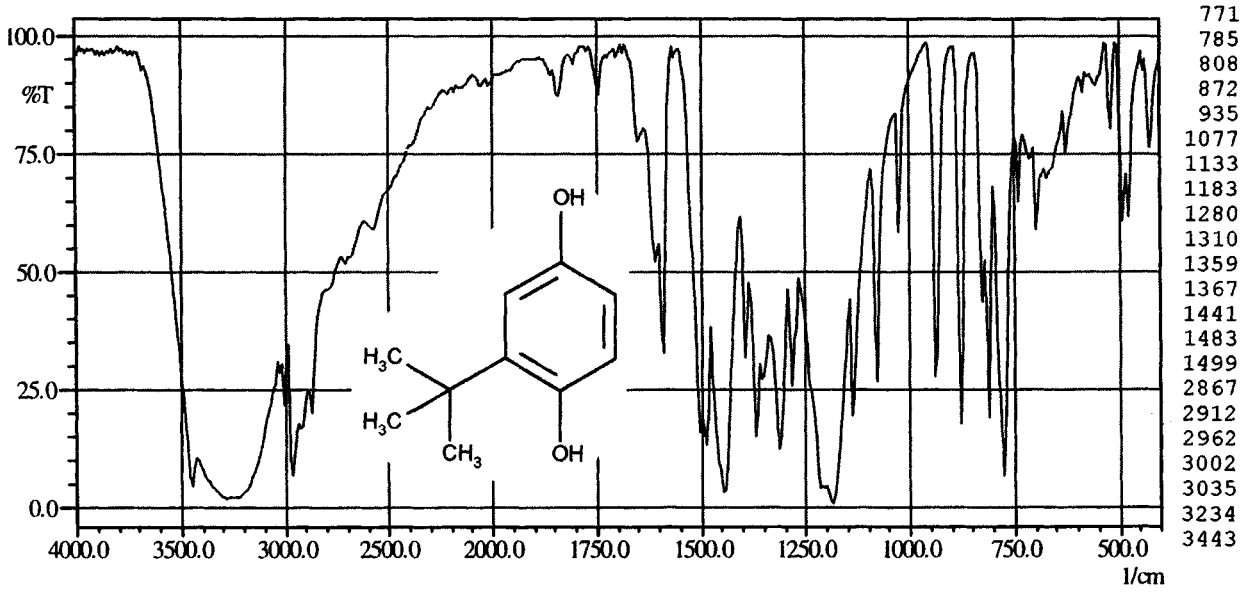
(1) **mixture of alkylated phenols**
(2) HiTEC 4733, Ethanox 733
(3) Ethyl
(5) antioxidant
(6) liquid
(7) 17 °C
(8) 224 °C
(9) 0.94 g cm^{-3}
(13) layer btw KBr

11312



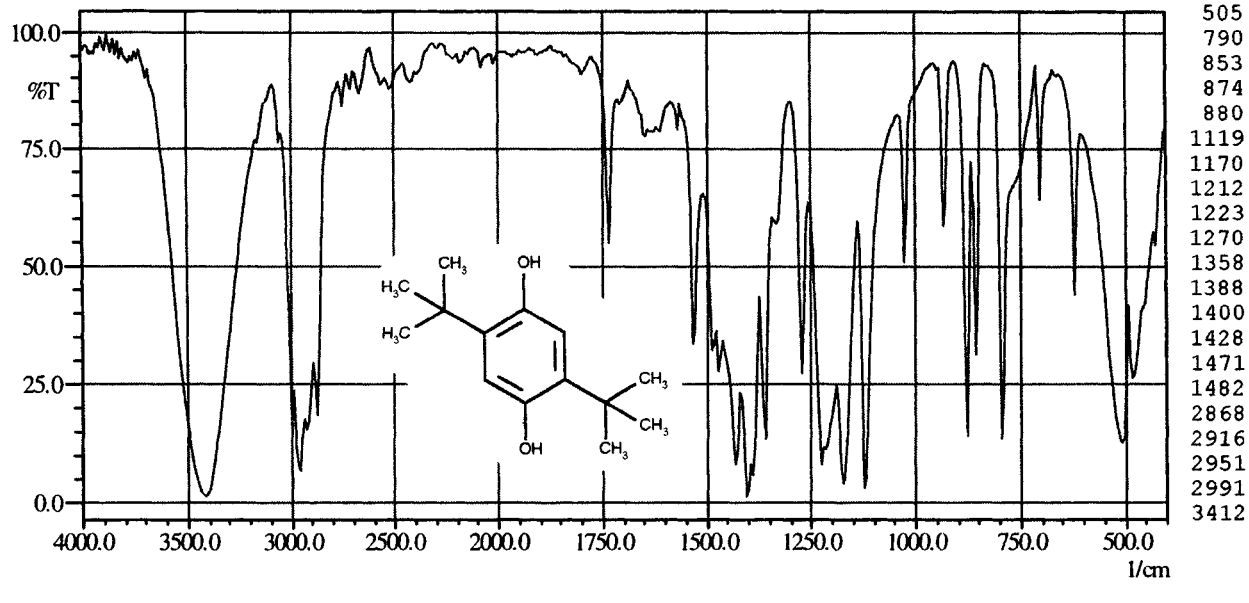
(1) **styrenated phenol**
(2) Montaclere
(3) Monsanto
(5) antioxidant
(6) yellowish to amber-coloured liquid
(9) 1.1 g cm^{-3}
(13) layer btw KBr
(14) structure shows the monomer unit

11312 $C_{10}H_{14}O_2$



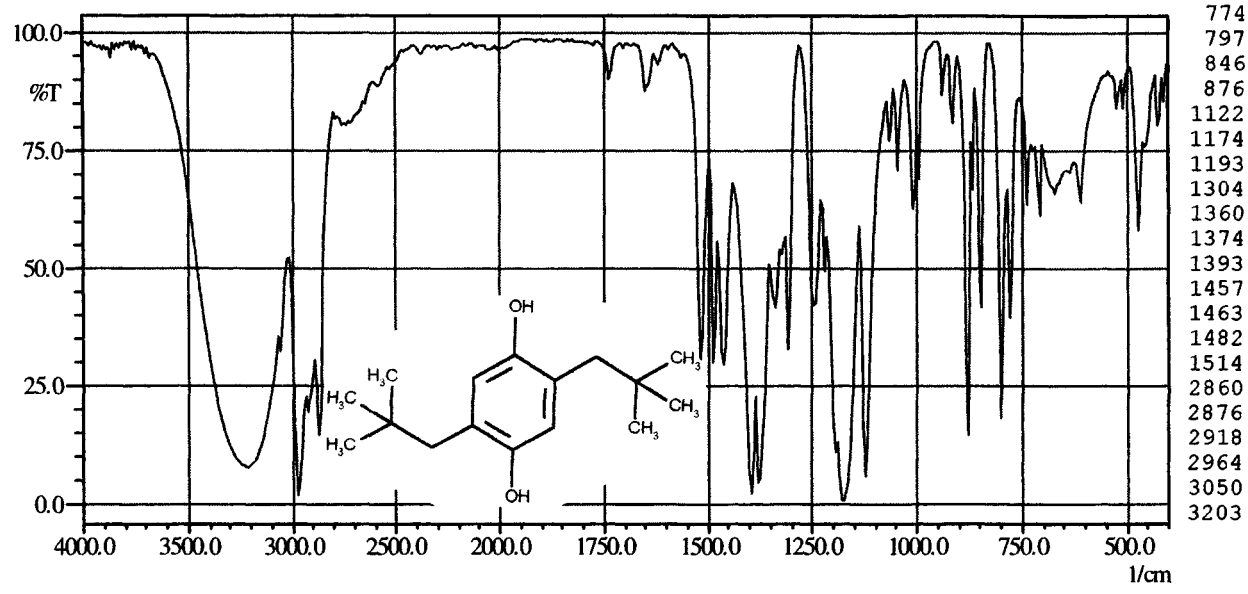
(1) ***t*-butylhydroquinone**
(2) Eastman MTBHQ
(3) Eastman
(4) 166.2 g mol^{-1}
(5) antioxidant
(6) colourless solid
(7) 125 °C
(8) 295 °C
(9) 1.05 g cm^{-3}
(13) KBr pellet

11312 $C_{14}H_{22}O_2$



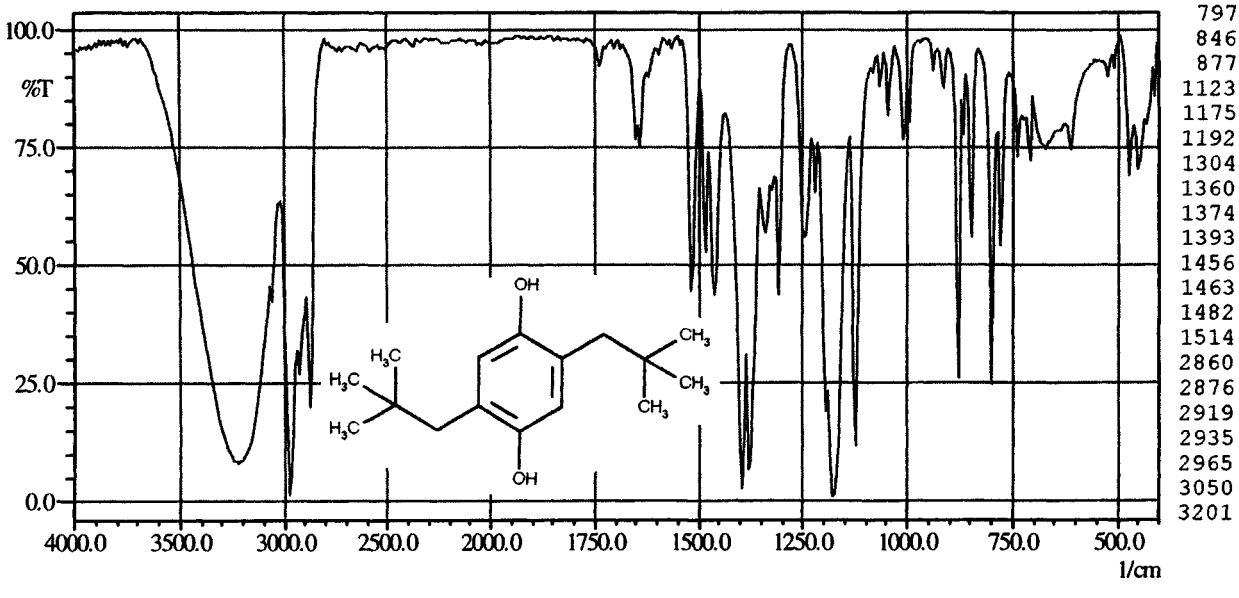
(1) **2,5-di-*t*-butylhydroquinone**
(2) Eastman DTBHQ
(3) Eastman
(4) 222.3 g mol^{-1}
(5) antioxidant
(6) colourless to tan crystals
(7) 210 °C
(8) 321 °C
(9) 1.07 g cm^{-3}
(13) KBr pellet

11312 $C_{16}H_{26}O_2$



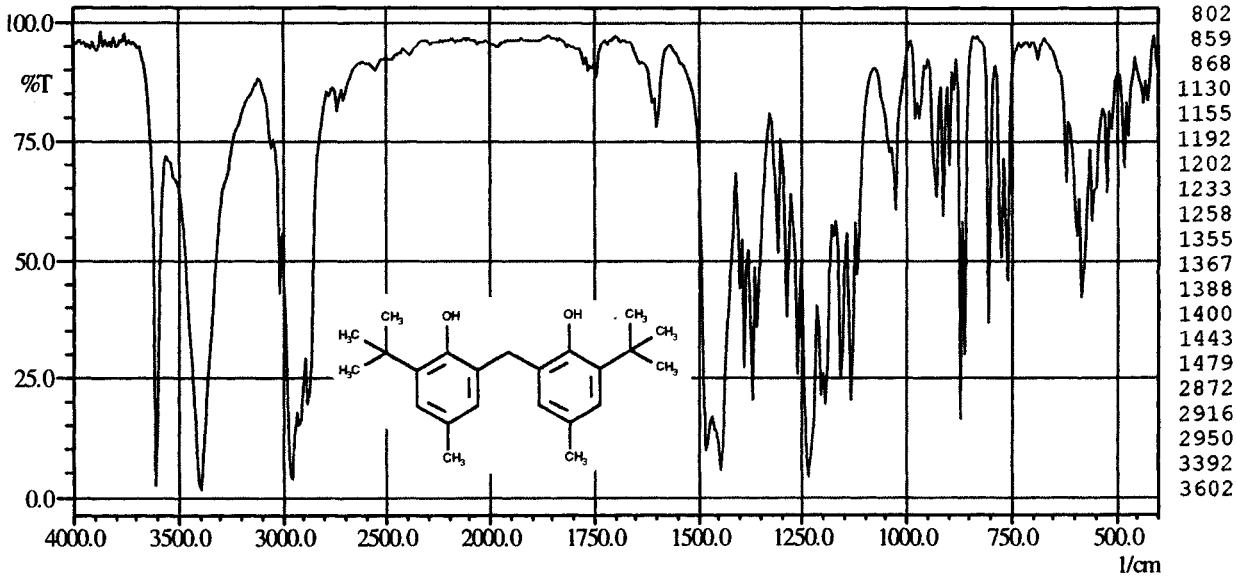
(1) **2,5-di-*t*-pentylhydroquinone**
(2) Santovar A
(3) Monsanto
(4) 250.4 g mol^{-1}
(5) antioxidant
(6) yellowish to grey-white solid
(7) 179 °C
(9) 1.1 g cm^{-3}
(13) KBr pellet

11312 $C_{16}H_{26}O_2$



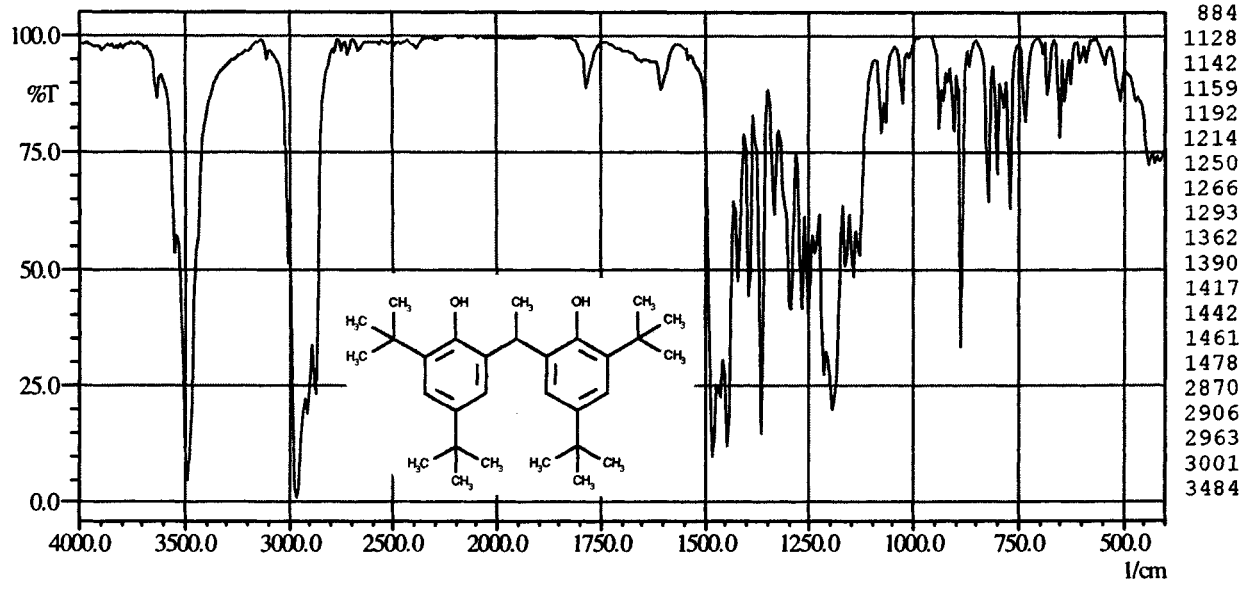
(1) **2,6-di-*t*-pentylhydroquinone**
(2) Lowinox AH 25
(3) Chemische Werke Lowi
(4) 250.4 g mol^{-1}
(5) antioxidant
(6) grey solid
(7) 171 °C
(13) KBr pellet

11313 $C_{23}H_{32}O_2$



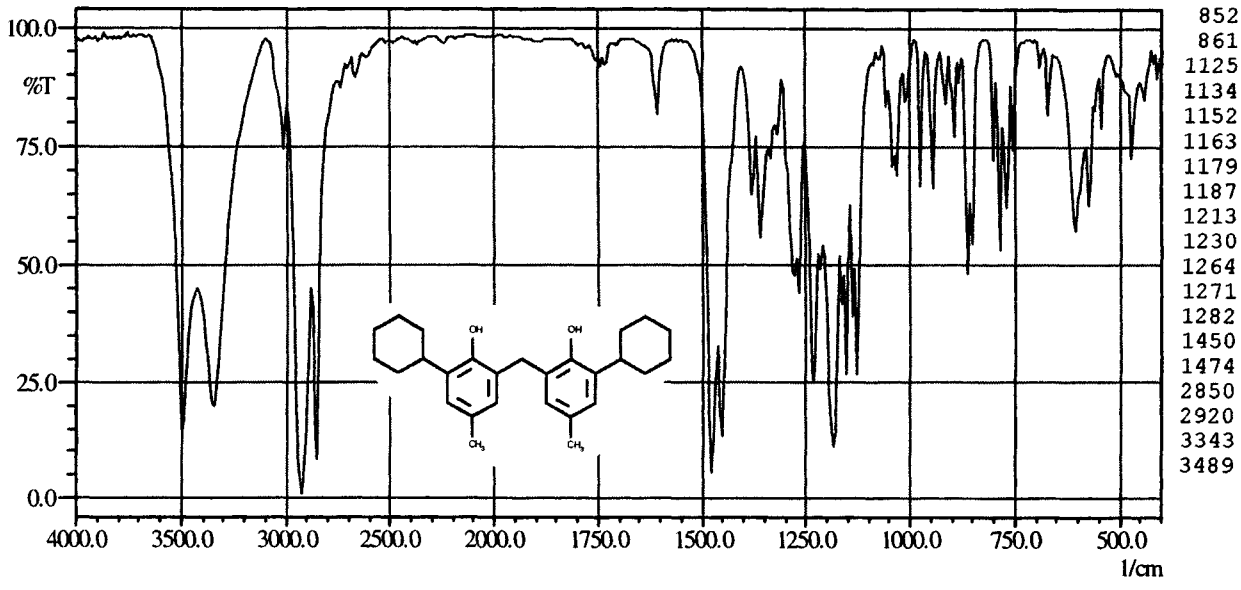
(1) **2,2'-methylene-*bis*(6-*t*-butyl-4-methylphenol)**
(2) Irganox 2246
(3) Ciba-Geigy
(4) 340.5 g mol^{-1}
(5) antioxidant
(6) colourless, crystalline solid
(7) 127 °C
(13) KBr pellet

11313 $C_{30}H_{46}O_2$



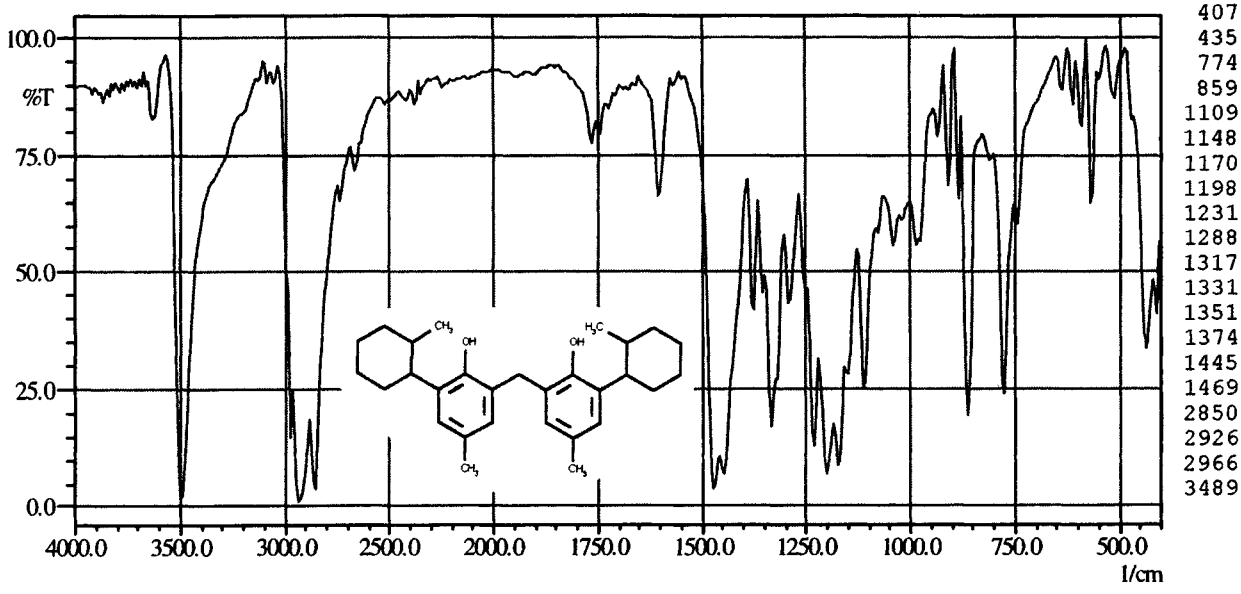
(1) **2,2'-ethylidene-*bis*(4,6-di-*t*-butylphenol)**
(2) Vanox 1290
(3) R.T. Vanderbilt
(4) 438.7 g mol^{-1}
(5) antioxidant
(6) colourless solid
(7) 162.5 °C
(9) 1.01 g cm^{-3}
(13) KBr pellet

11313 $C_{27}H_{36}O_2$



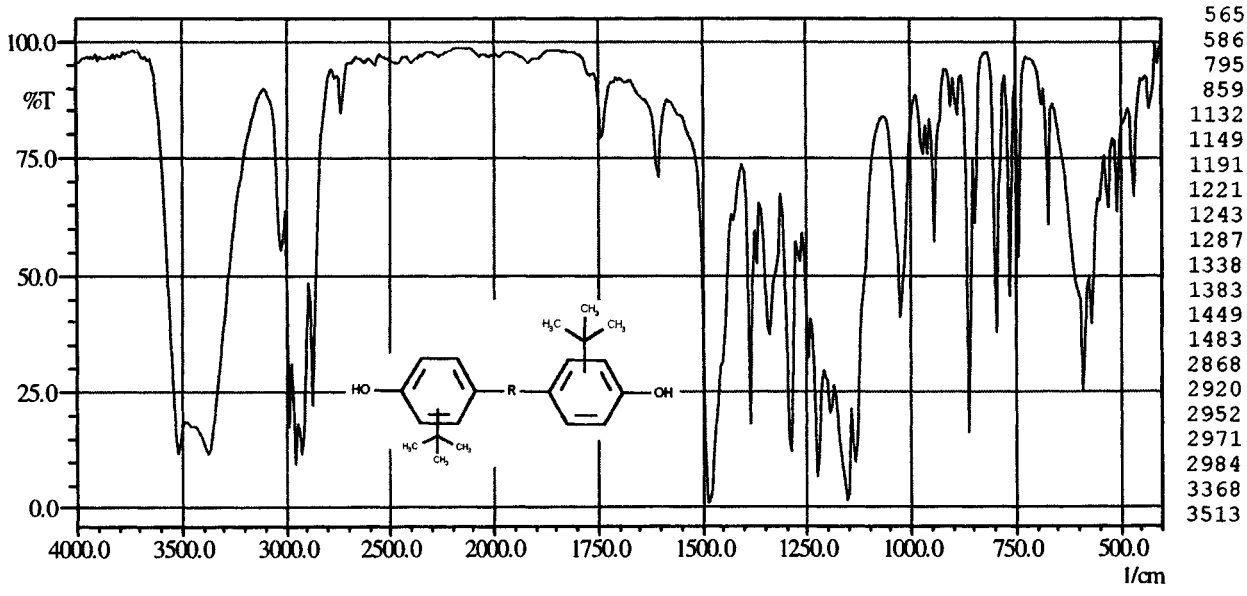
(1) **2,2'-methylene-*bis*(4-methyl-6-cyclohexylphenol)**
(2) Vulkanox ZKF, ASM ZKF
(3) Bayer
(4) 392.4 g mol^{-1}
(5) antioxidant
(6) white solid
(7) 125 °C
(9) 1.8 g cm^{-3}
(13) KBr pellet

11313 $C_{29}H_{40}O_2$



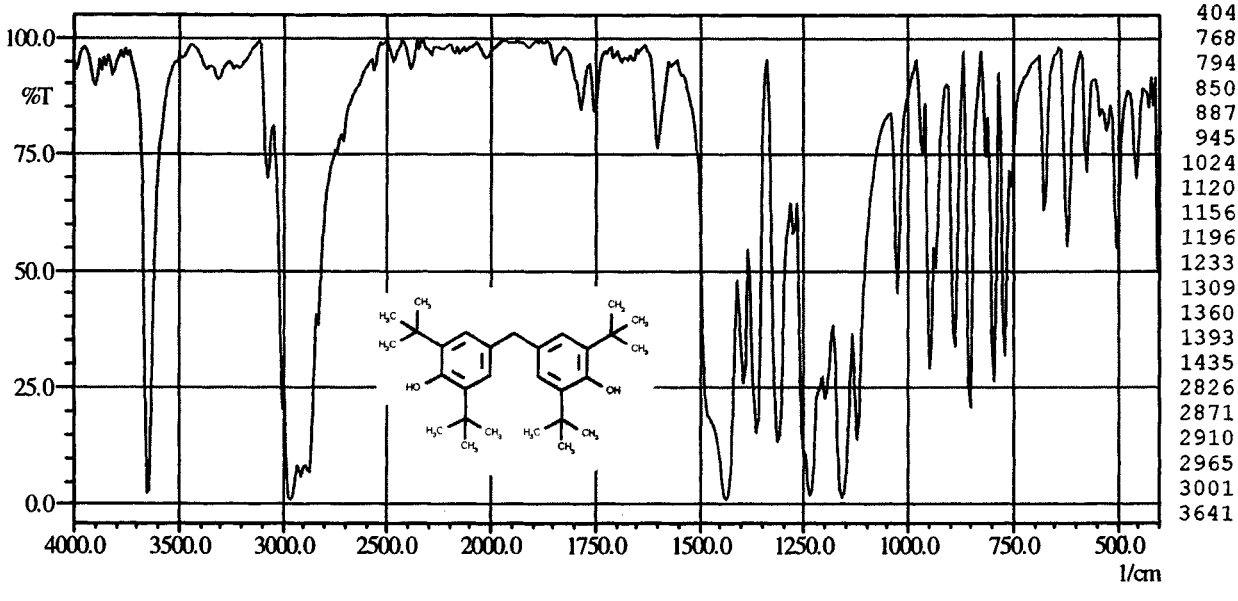
(1) **2,2'-methylene-*bis*(4-methyl-6-(*o*-methylcyclohexyl)phenol)**
(2) Permanax WSP
(3) Akzo Chemie
(4) 420.6 g mol^{-1}
(5) antioxidant
(6) yellowish solid
(13) KBr pellet

11313 $C_{21}H_{28}O_2$



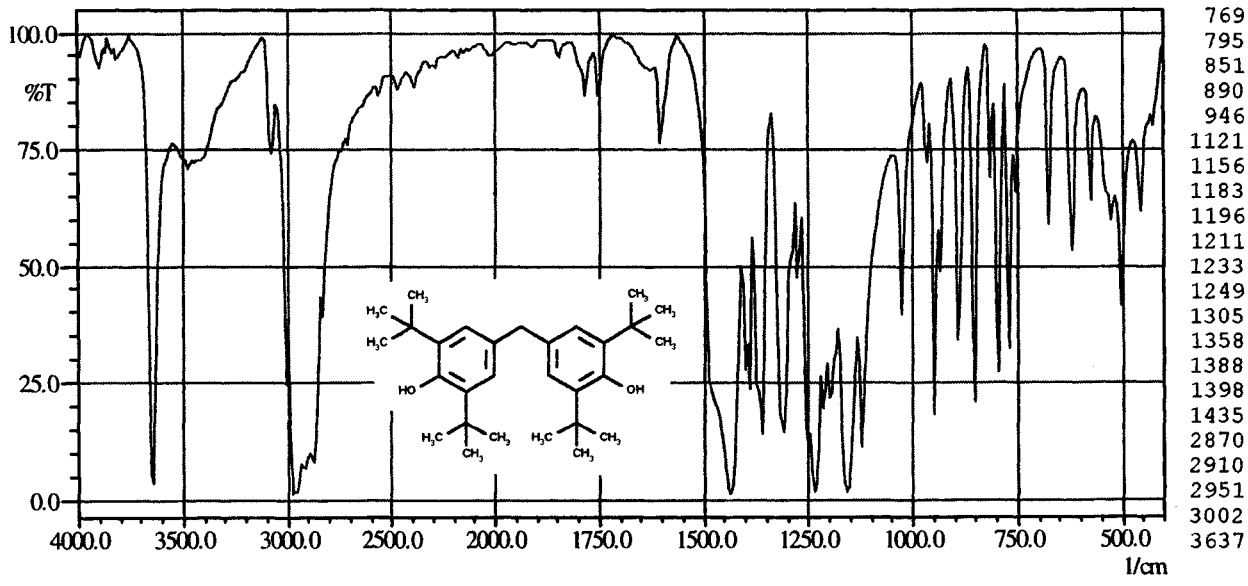
(1) **4,4'-methylene-*bis*(2-*t*-butylphenol)**
(2) Vulkanox NKF
(3) Bayer
(4) 312.4 g mol^{-1}
(5) antioxidant
(6) white solid
(7) 155 °C
(9) 1.12 g cm^{-3}
(13) KBr pellet

11313 $C_{29}H_{44}O_2$



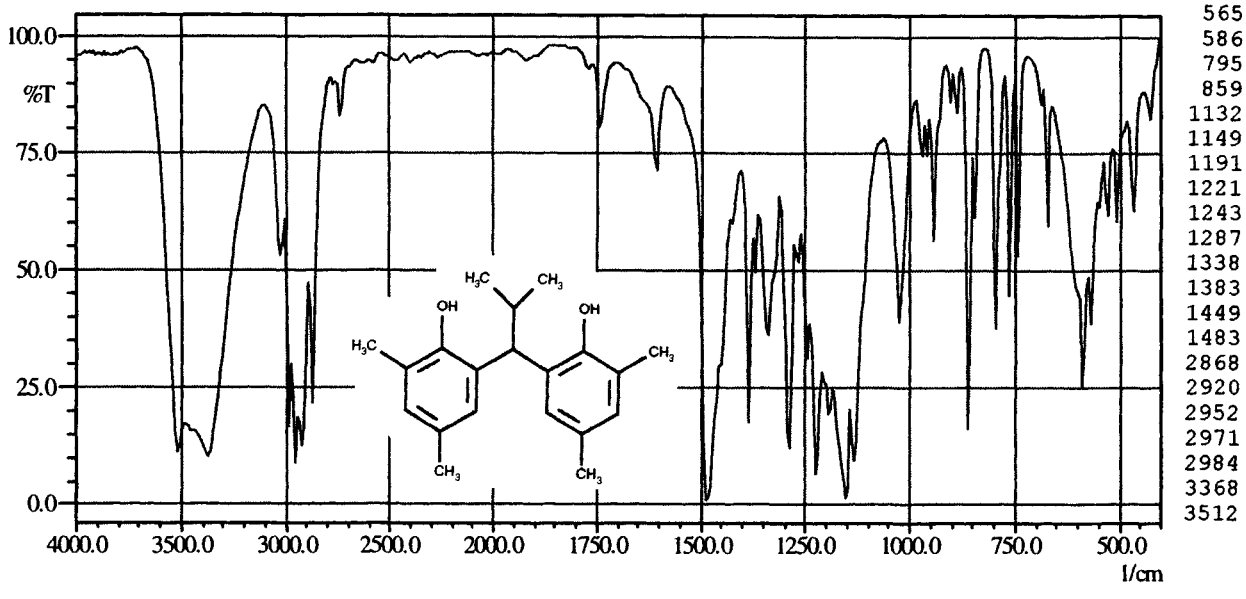
(1) **4,4'-methylene-*bis*(2,6-di-*t*-butylphenol)**
(2) Ethanox 702
(3) Ethyl
(4) 424.7 g mol^{-1}
(5) antioxidant
(6) light-straw, crystalline solid
(7) 154 °C
(9) 0.99 g cm^{-3}
(13) KBr pellet

11313 $C_{29}H_{44}O_2$



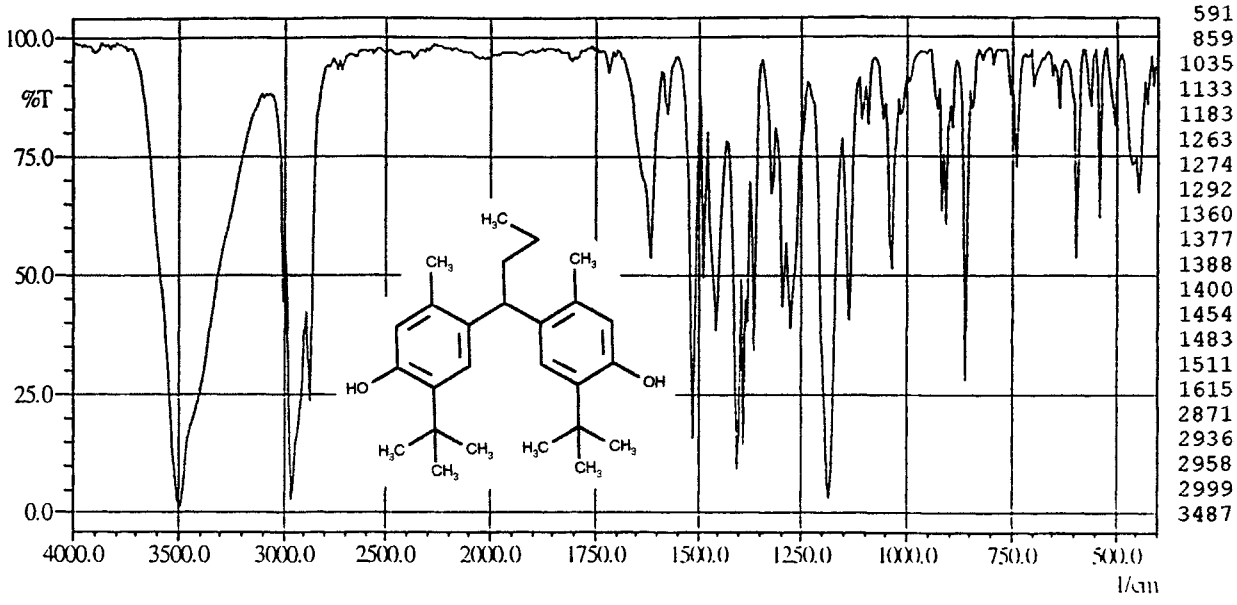
(1) **4,4'-methylene-*bis*(2,6-di-*t*-butylphenol)**
(2) CeMox 02 NP, Antioxidant 702 ND
(3) Chemie-Mineralien
(4) 424.7 g mol^{-1}
(5) antioxidant
(6) yellow solid
(7) 155 °C
(9) 0.99 g cm^{-3}
(13) KBr pellet

11313 $C_{20}H_{26}O_2$



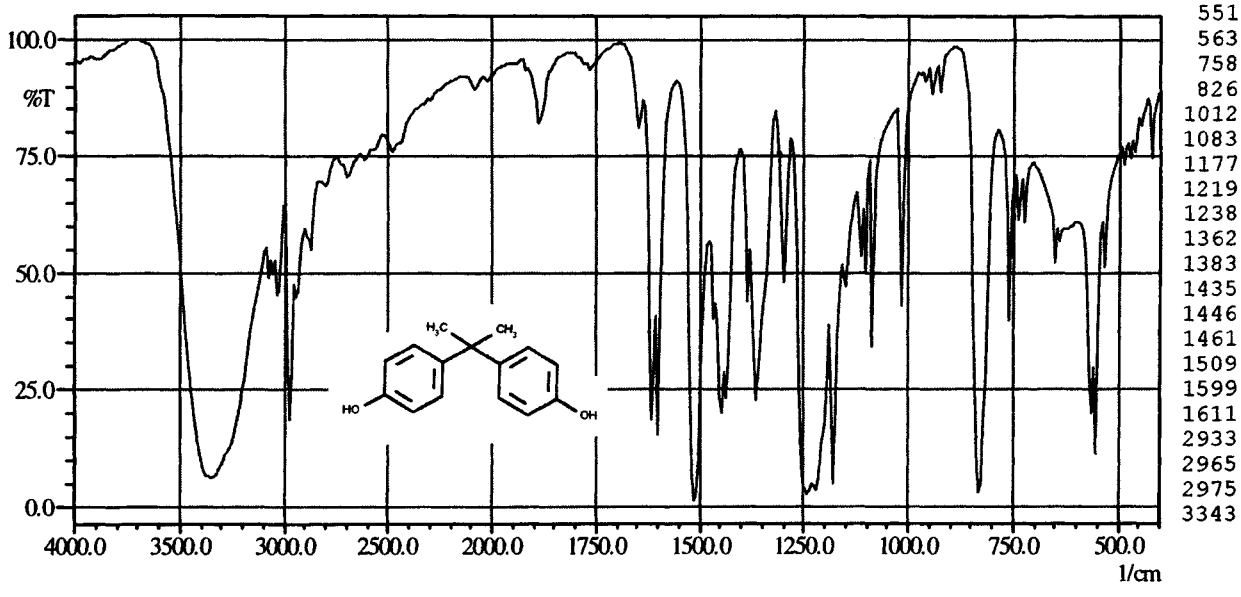
(1) **2,2'-*i*-butylidene-*bis*(4,6-dimethylphenol)**
(2) Lowinox 22 IB 46
(3) Chemische Werke Lowi
(4) 298.4 g mol^{-1}
(5) antioxidant
(6) colourless solid
(7) 155 °C
(13) KBr pellet

11313 $C_{26}H_{38}O_2$



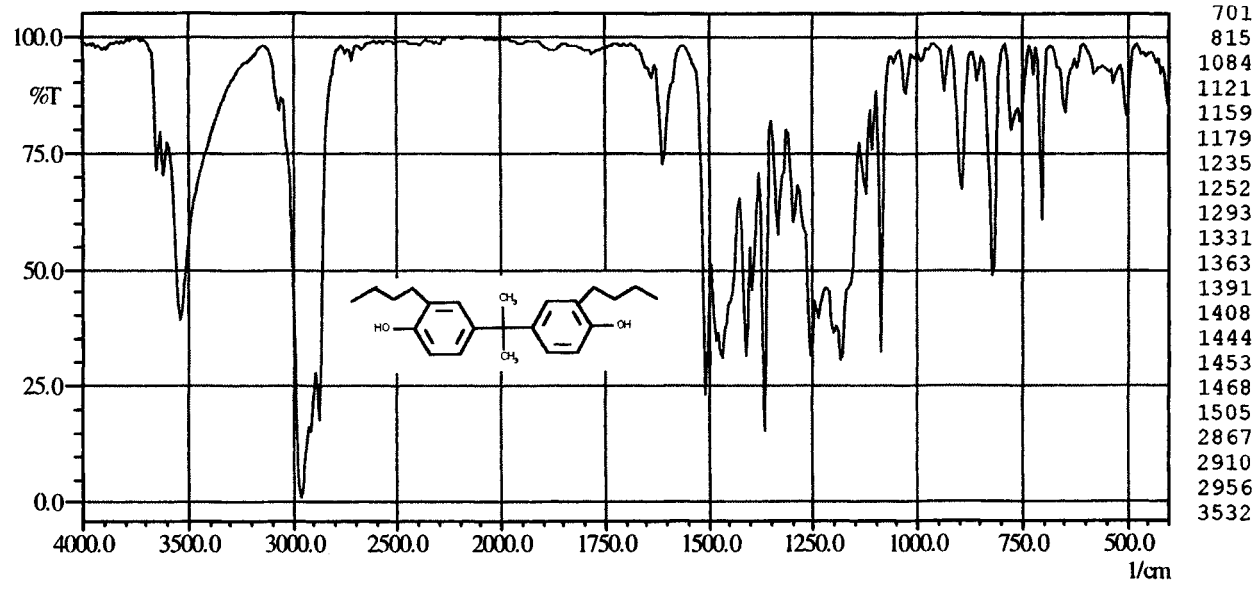
(1) **4,4'-butylidene-*bis*(6-*t*-butyl-3-methylphenol)**
(2) Santowhite Powder
(3) Monsanto
(4) 382.6 g mol^{-1}
(5) antioxidant
(6) colourless solid
(7) 209 °C
(9) 1.03 g cm^{-3}
(13) KBr pellet

11313 $C_{15}H_{16}O_2$



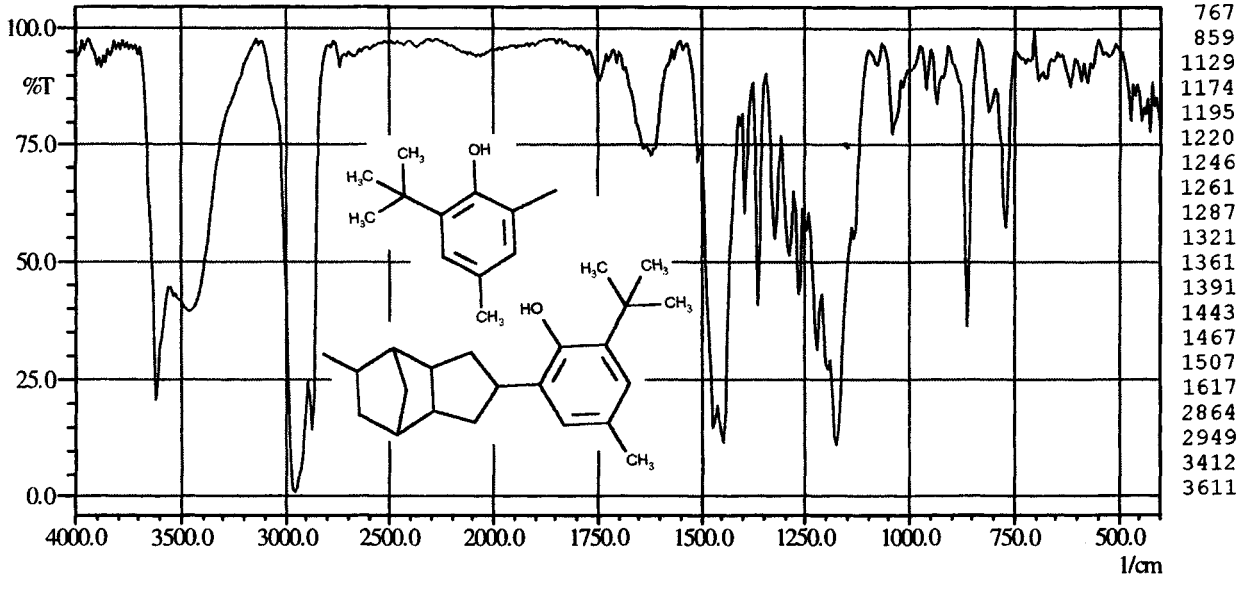
(1) ***bis*(4-hydroxyphenyl)-2-propane**
(2) Bisphenol A
(3) Bayer
(4) 228.3 g mol^{-1}
(5) antioxidant
(6) colourless crystals
(7) 158 °C
(8) 220 °C / 500 Pa

11313 $C_{23}H_{32}O_2$



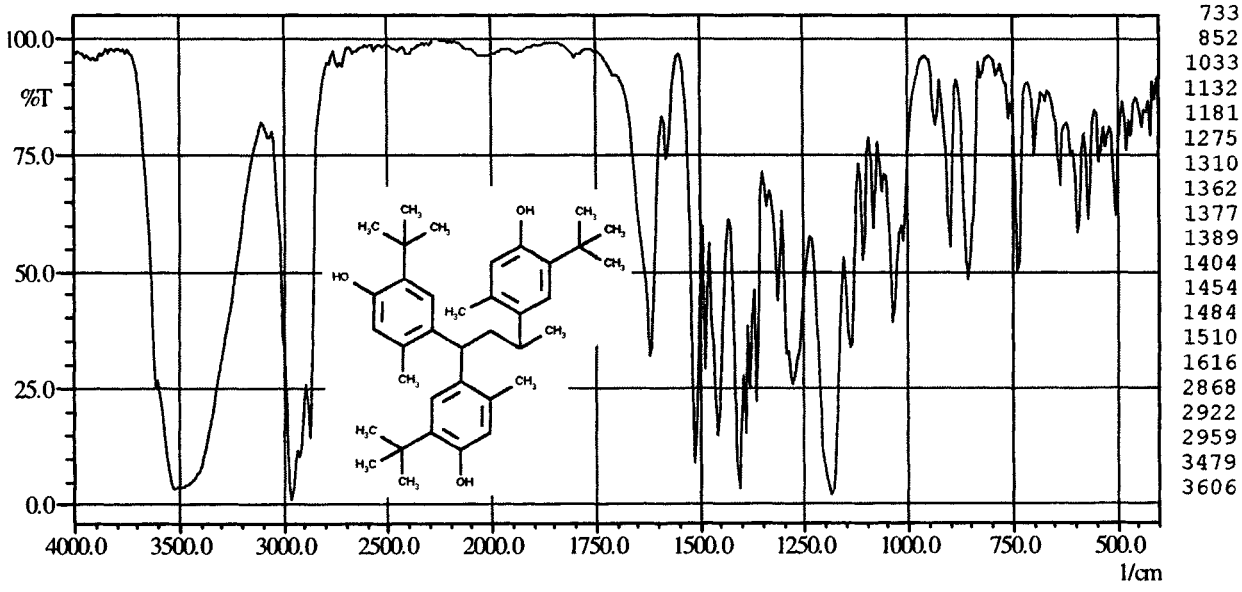
(1) **mixture of polybutylated bisphenol A**
(2) Agerite Superlite
(3) Vanderbilt
(4) 340.5 g mol^{-1}
(5) antioxidant
(6) liquid
(9) 0.95 g cm^{-3}
(13) layer btw KBr
(14) structure is hypothetic

11313 $C_{32}H_{40}O_2$



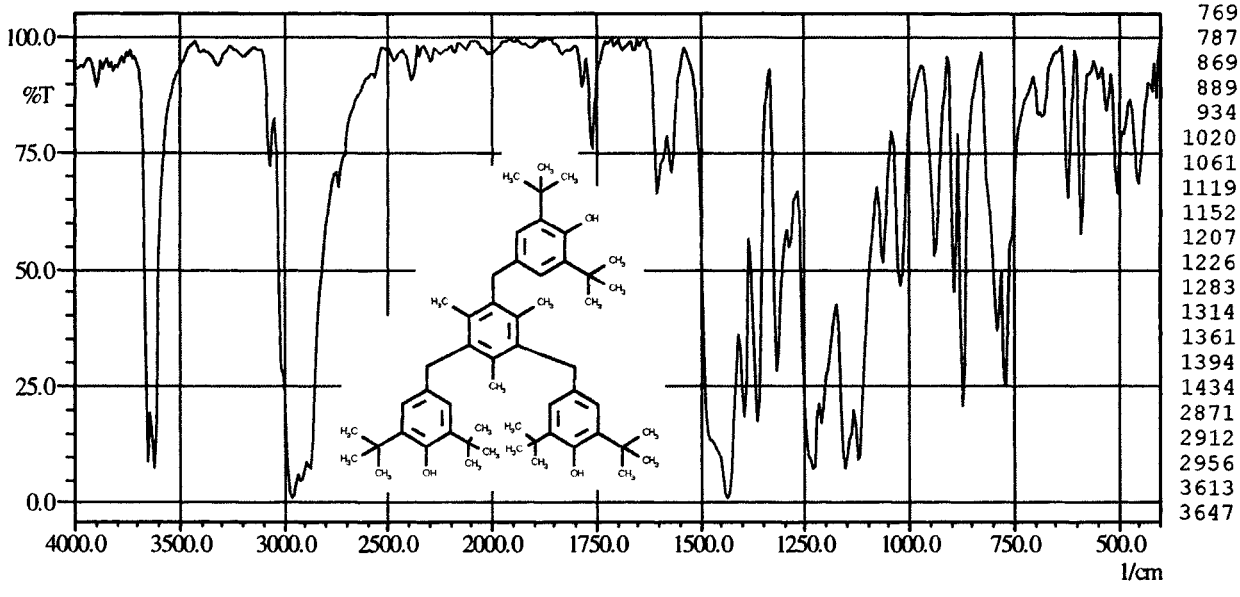
(1) **2,2'-(octahydro-4,7-methano-1H-indenediyl)-*bis*(6-*t*-butyl-4-methylphenol)**
(2) Lowinox CPL
(3) Chemische Werke Lowi
(4) 456.7 g mol^{-1}
(5) antioxidant
(6) colourless solid
(7) 105 °C
(13) KBr pellet

11313 $C_{37}H_{52}O_3$



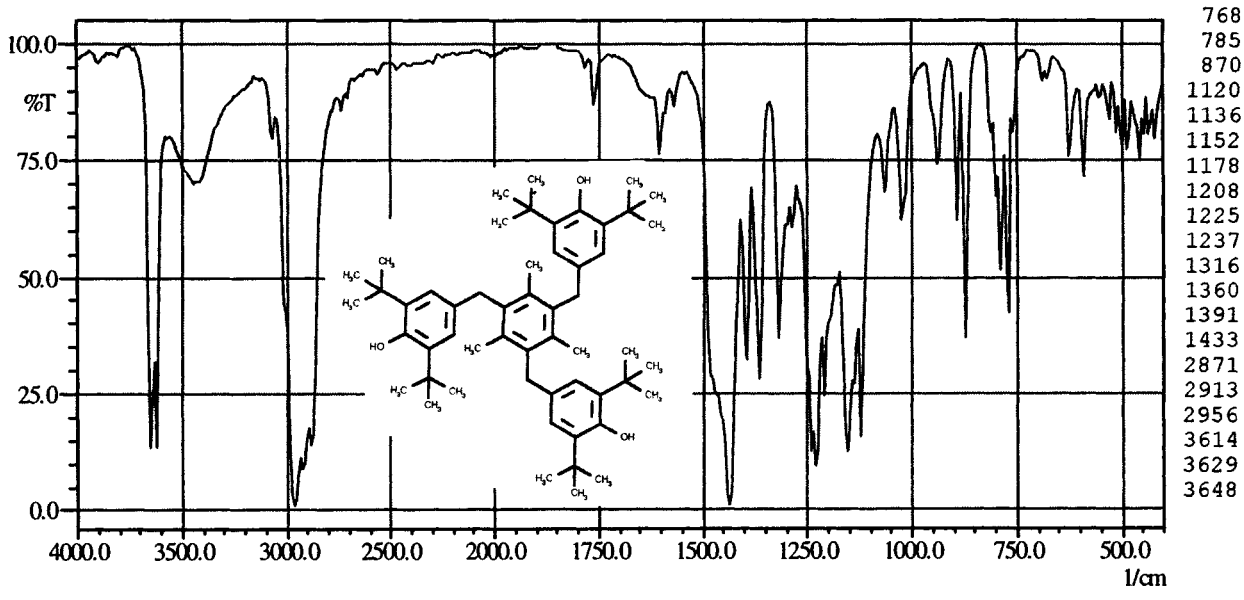
(1) **1,1,3-*tris*(2-methyl-4-hydroxy-5-*t*-butylphenyl)butane**
(2) Topanol CA
(3) ICI
(4) 544.7 g mol^{-1}
(5) antioxidant
(6) colourless solid
(8) 265 °C
(13) KBr pellet

11313 $C_{54}H_{78}O_3$



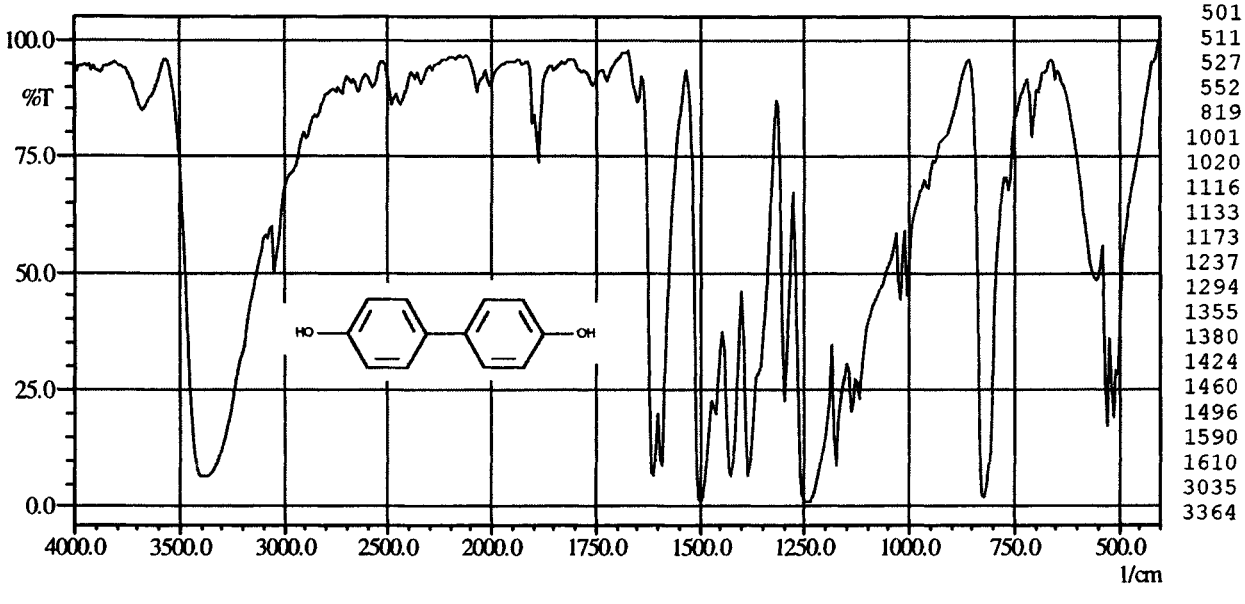
(1) **1,3,5-trimethyl-2,4,6-*tris*(3,5-di-*t*-butyl-4-hydroxybenzyl)benzene**
(2) Ethanox 330
(3) Ethyl
(4) 775.2 g mol^{-1}
(5) antioxidant
(6) colourless, crystalline solid
(8) 244 °C
(13) KBr pellet

11313 $C_{54}H_{78}O_3$



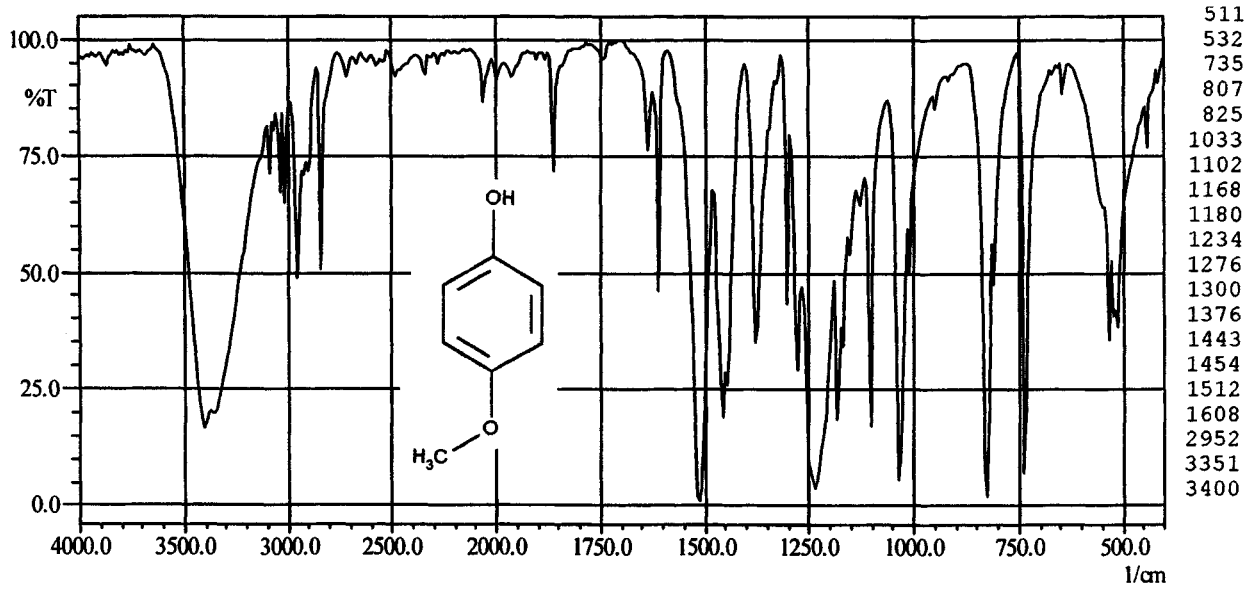
(1) **1,3,5-trimethyl-2,4,6-*tris*(3,5-di-*t*-butyl-4-hydroxybenzyl)benzene**
(2) Irganox 1330
(3) Ciba-Geigy
(4) 775.2 g mol^{-1}
(5) antioxidant
(6) colourless to yellowish, crystalline solid
(7) 240 °C
(13) KBr pellet

11313 $C_{12}H_{10}O_2$



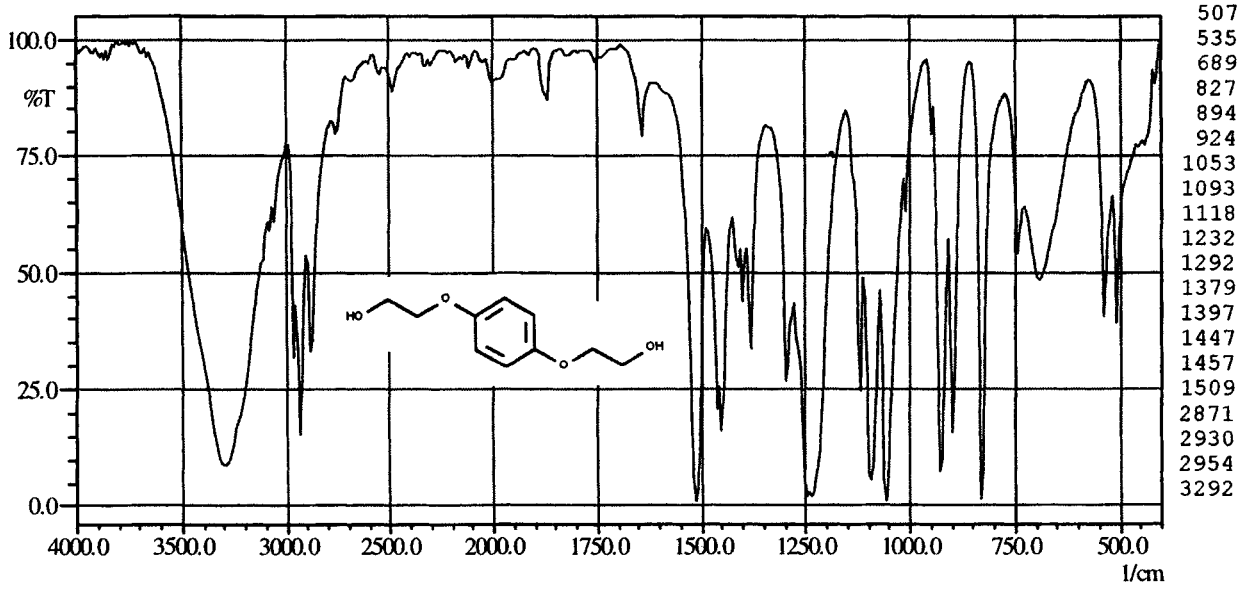
(1) **4,4'-dihydroxybiphenyl, 4,4'-biphenol**
(2) ASM DOD
(3) Bayer
(4) 186.2 g mol^{-1}
(5) antioxidant
(6) colourless solid
(7) 282 °C
(13) KBr pellet

11314 $C_7H_8O_2$



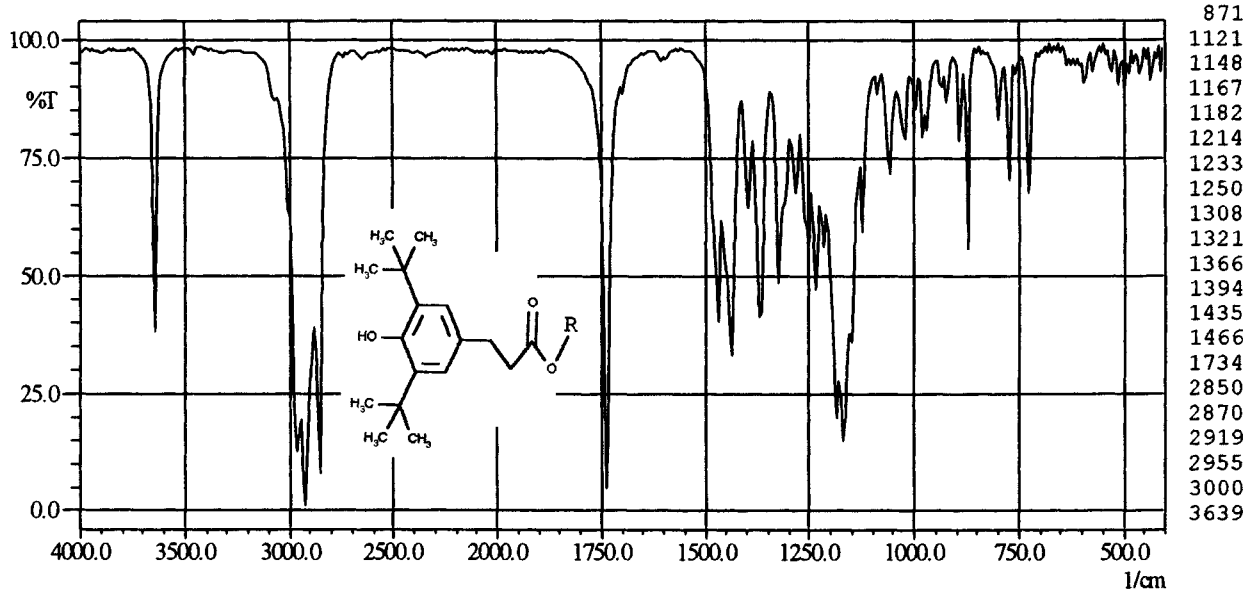
(1) **hydroquinone monomethylether, 4-hydroxyanisole**
(2) Eastman HQMME
(3) Eastman
(4) 124.1 g mol^{-1}
(5) antioxidant
(6) colourless flakes
(7) 54 °C
(8) 246 °C
(13) KBr pellet

11314 $C_{10}H_{14}O_4$



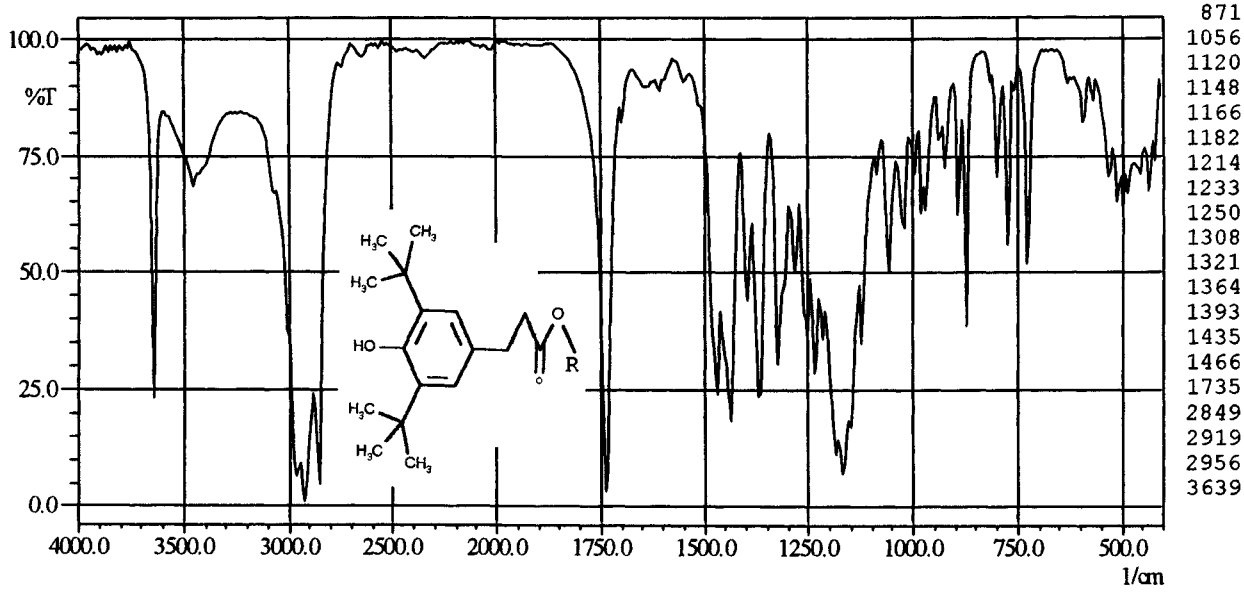
(1) **hydroquinone-*bis*(2-hydroxyethyl)ether**
(2) Eastman HQEE
(3) Eastman
(4) 198.2 g mol^{-1}
(5) antioxidant
(6) colourless flakes
(7) 98 °C
(8) 190 °C / 5300 Pa
(9) 1.15 g cm^{-3}
(13) KBr pellet

11314 $C_{35}H_{62}O_3$



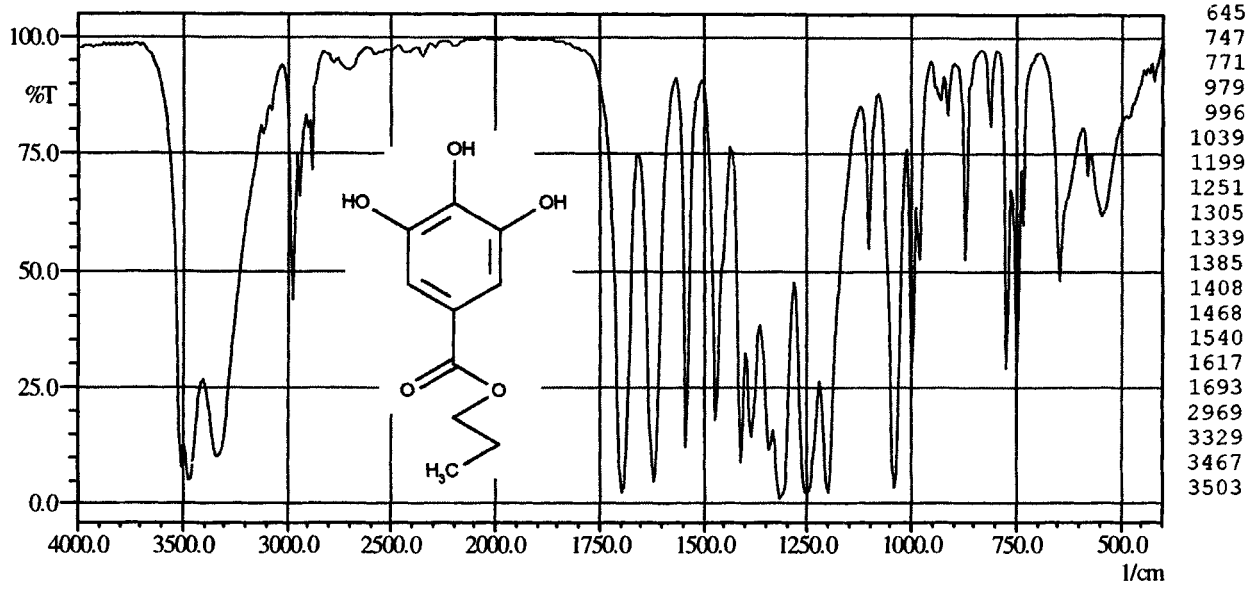
(1) **β-(3,5-di-*t*-butyl-4-hydroxyphenyl)propionic octadecyl ester**
(2) Irganox 1076
(3) Ciba-Geigy
(4) 530,9 g mol^{-1}
(5) antioxidant
(6) colourless solid
(7) 49 °C
(13) KBr pellet

11314 $C_{35}H_{62}O_3$



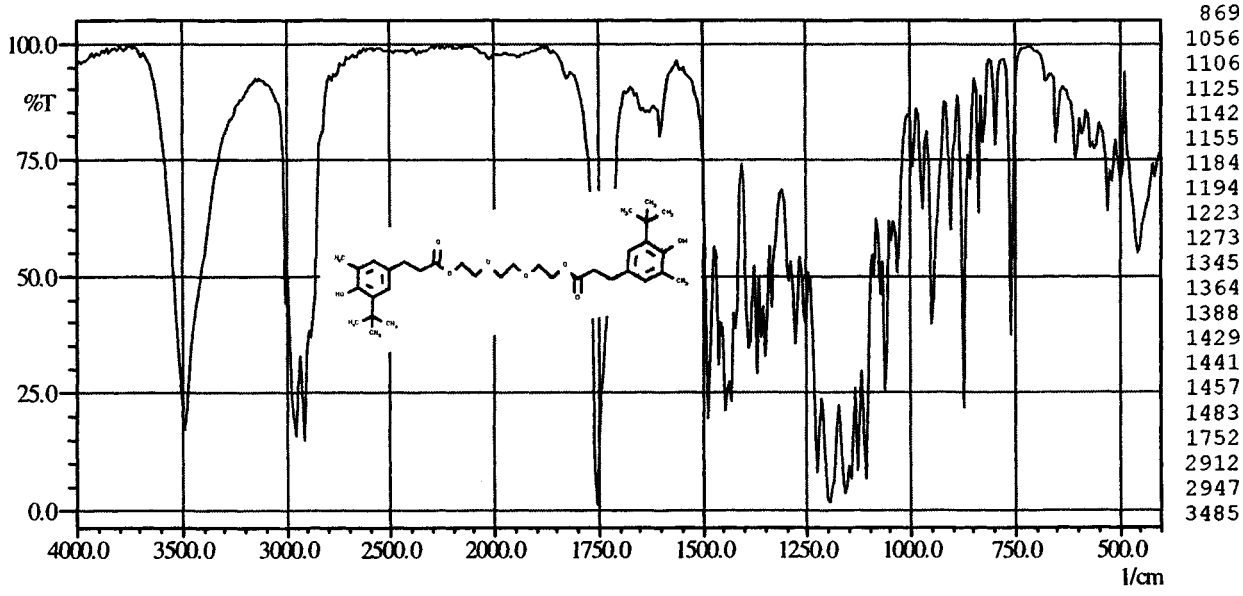
(1) **β-(3,5-di-*t*-butyl-4-hydroxyphenyl)propionic octadecyl ester**
(2) Lowinox PO 35
(3) Chemische Werke Lowi
(4) 530.9 g mol^{-1}
(5) antioxidant
(6) colourless solid
(7) 53 °C
(13) KBr pellet

11314 $C_{10}H_{14}O_5$



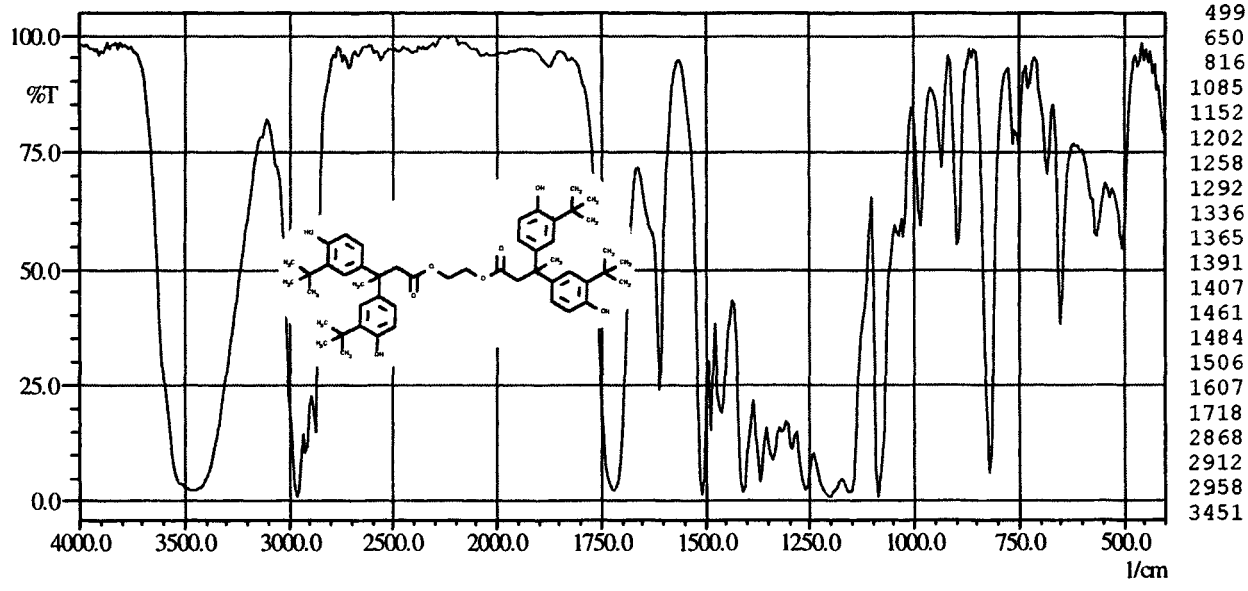
(1) **3,4,5-trihydroxybenzoic acid propyl ester (propyl gallate)**
(2) Tenox PG
(3) Eastman
(4) 212.2 g mol^{-1}
(5) antioxidant
(6) colourless solid
(7) 148 °C
(9) 1.21 g cm^{-3}
(13) KBr pellet

11314 $C_{34}H_{50}O_8$



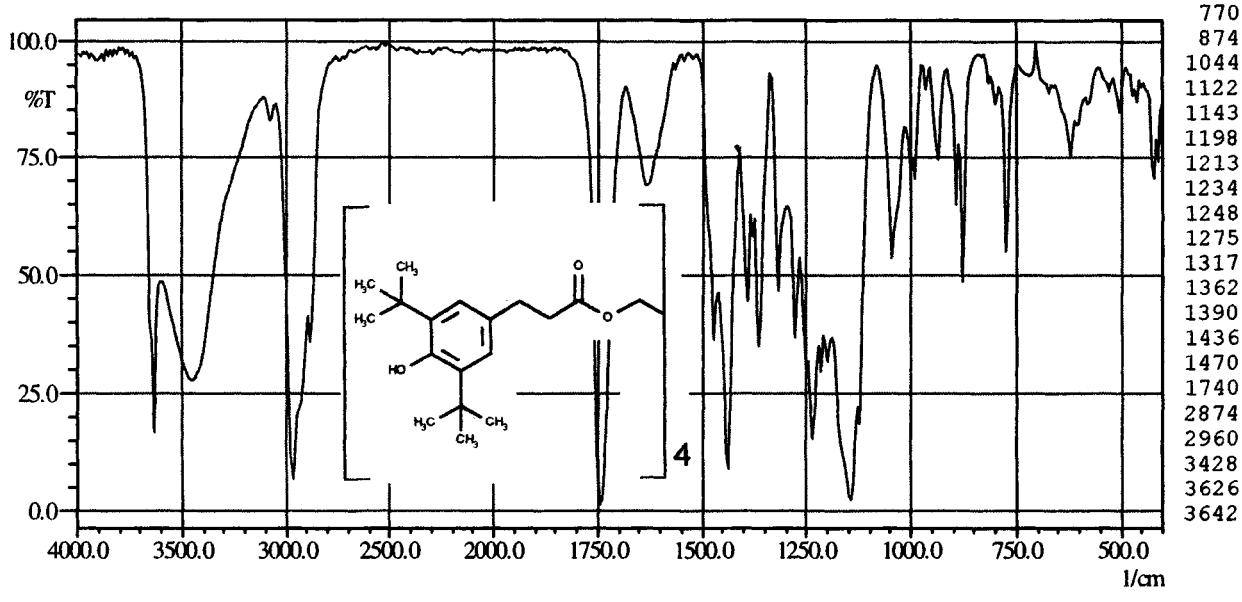
(1) **triethyleneglycol-*bis*-3-(3-*t*-butyl-4-hydroxy-5-methylphenyl)propionate**
(2) Irganox 245
(3) Ciba-Geigy
(4) 586.8 g mol^{-1}
(5) antioxidant
(6) colourless solid
(7) 77.5 °C
(13) KBr pellet

11314 $C_{50}H_{66}O_8$



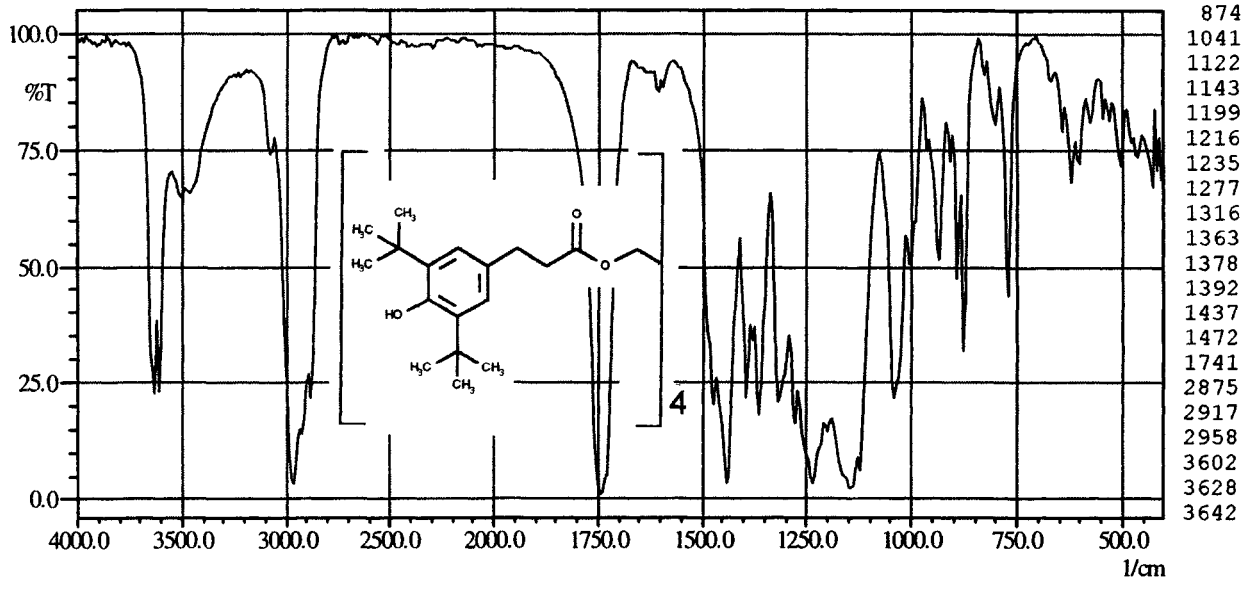
(1) **3,3-*bis*(4-hydroxy-3-*t*-butylphenyl)ethylene butyrate**
(2) Hostanox O 3
(3) Hoechst
(4) 795.1 g mol^{-1}
(5) antioxidant
(6) colourless solid
(7) 170 °C
(9) 1.1 g cm^{-3}
(13) KBr pellet

11314 $C_{73}H_{108}O_{12}$



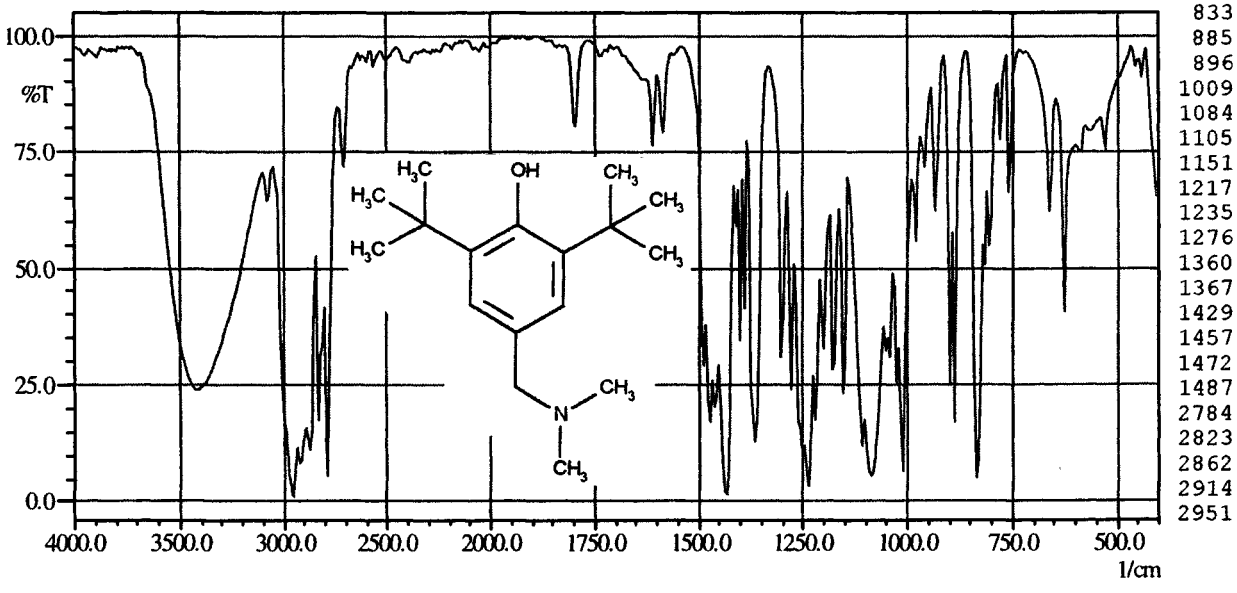
(1) **pentaerythrityl-*tetrakis*(3-(3,5-di-*t*-butyl-4-hydroxyphenyl)propionate)**
(2) Lowinox PP 35
(3) Chemische Werke Lowi
(4) 1178 g mol^{-1}
(5) antioxidant
(6) slightly yellowish solid
(7) 115 °C
(13) KBr pellet

11314 $C_{73}H_{108}O_{12}$



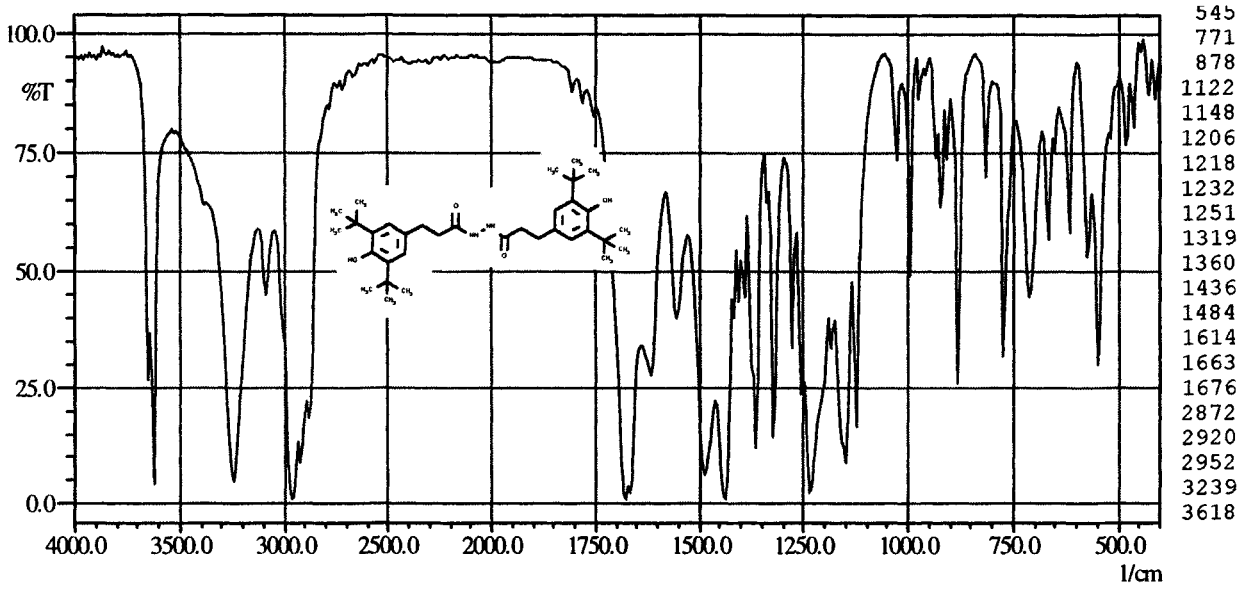
(1) **pentaerythrityl-*tetrakis*(3-(3,5-di-*t*-butyl-4-hydroxyphenyl)propionate)**
(2) Irganox 1010
(3) Ciba-Geigy (Brunne collection)
(4) 1178 g mol^{-1}
(5) antioxidant
(6) colourless solid
(13) KBr pellet

11321 $C_{17}H_{29}NO$



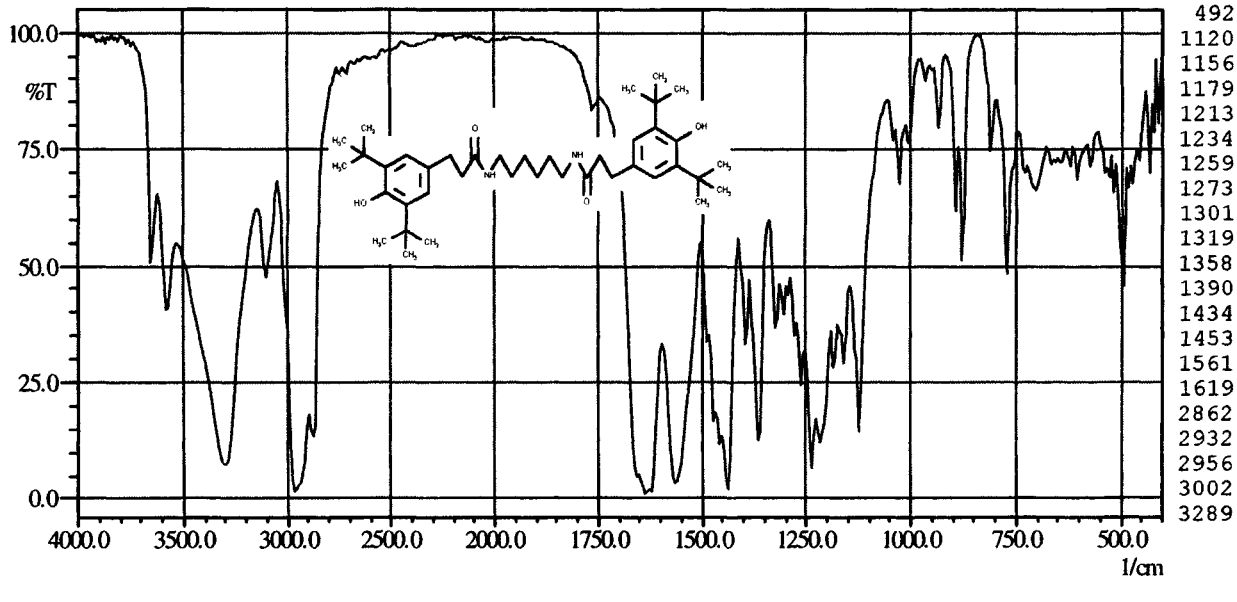
(1) **2,6-di-*t*-butyl-4-dimethylaminomethylphenol**
(2) Ethanox 703
(3) Ethyl
(4) 263.4 g mol^{-1}
(5) antioxidant
(6) pale-yellow, crystalline solid
(7) 94 °C
(8) 179 °C / 5300 Pa
(9) 0.38 g cm^{-3}
(13) KBr pellet

11322 $C_{34}H_{52}N_2O_4$



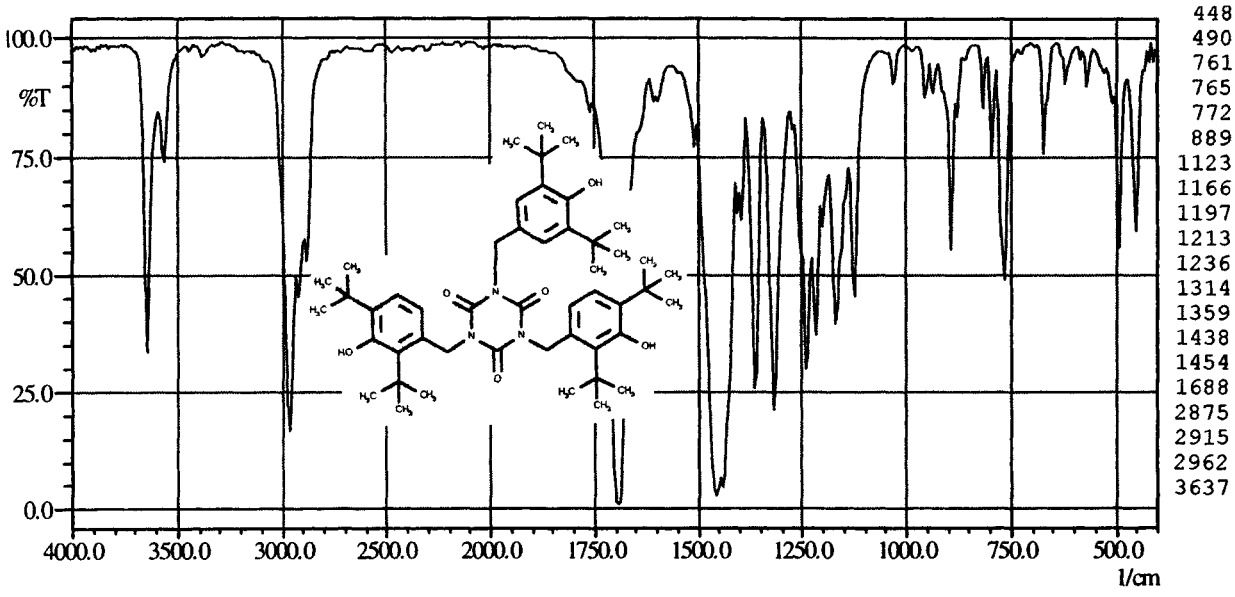
(1) **N,N'-*bis*(3(3',5'-di-*t*-butyl-4'-hydroxyphenyl) propionyl)hydrazine**
(2) Irganox MD 1024
(3) Ciba-Geigy
(4) 552.8 g mol^{-1}
(5) antioxidant
(6) colourless solid
(7) 210 °C
(13) KBr pellet

11322 $C_{36}H_{64}N_2O_4$



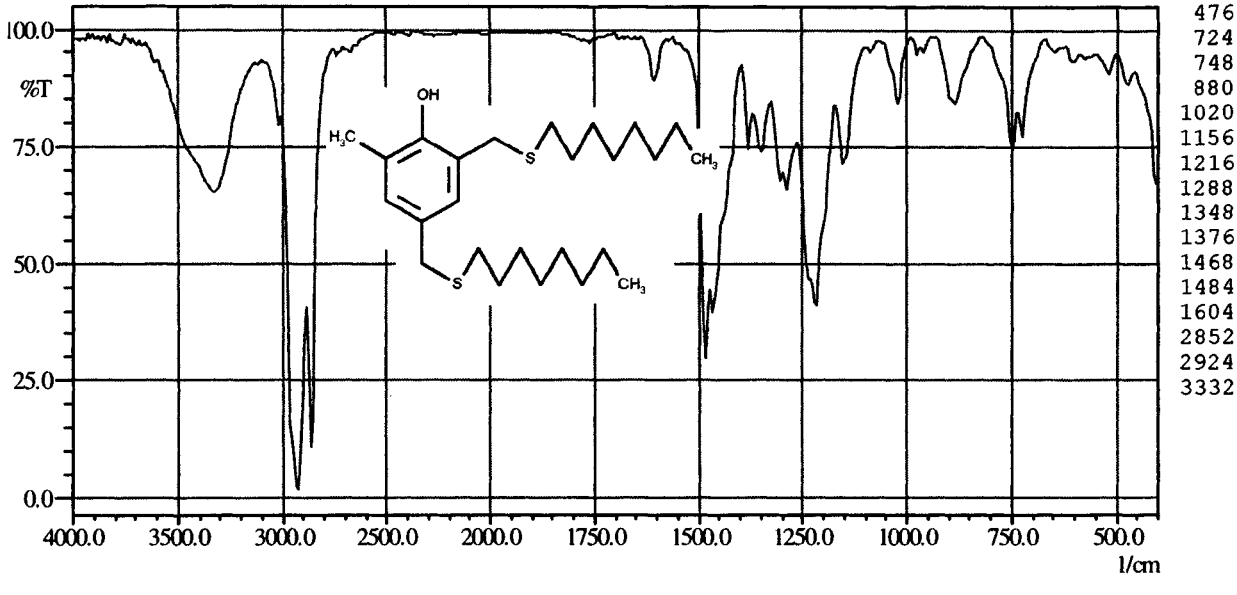
(1) **N,N'-hexamethylene-*bis*(3,5-di-*t*-butyl-4-hydroxyhydrocinnamide)**
(2) Irganox 1098
(3) Ciba-Geigy
(4) 588.9 g mol^{-1}
(5) antioxidant
(6) colourless solid
(7) 156 °C
(9) 1.5 g cm^{-3}
(13) KBr pellet

11325 $C_{48}H_{69}N_3O_6$



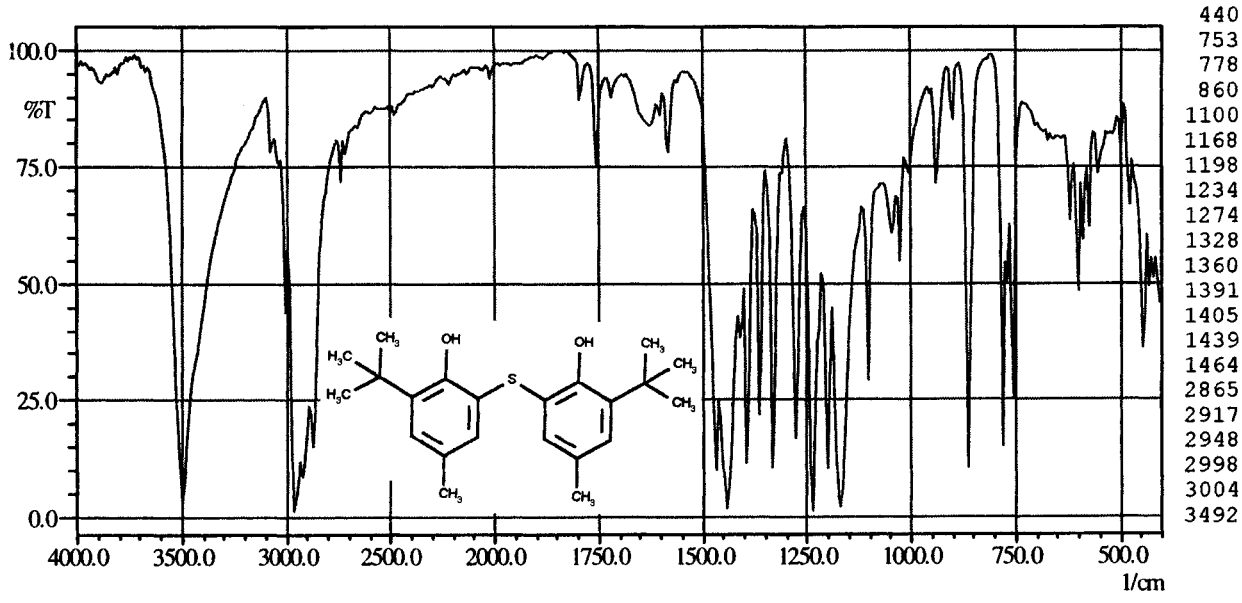
(1) ***tris*(3,5-di-*t*-butyl-4-hydroxybenzyl)isocyanurate**
(2) Irganox 3114
(3) Ciba-Geigy
(4) 784.1 g mol^{-1}
(5) antioxidant
(6) colourless to slightly yellowish solid
(13) KBr pellet

1134 $C_{25}H_{44}OS_2$



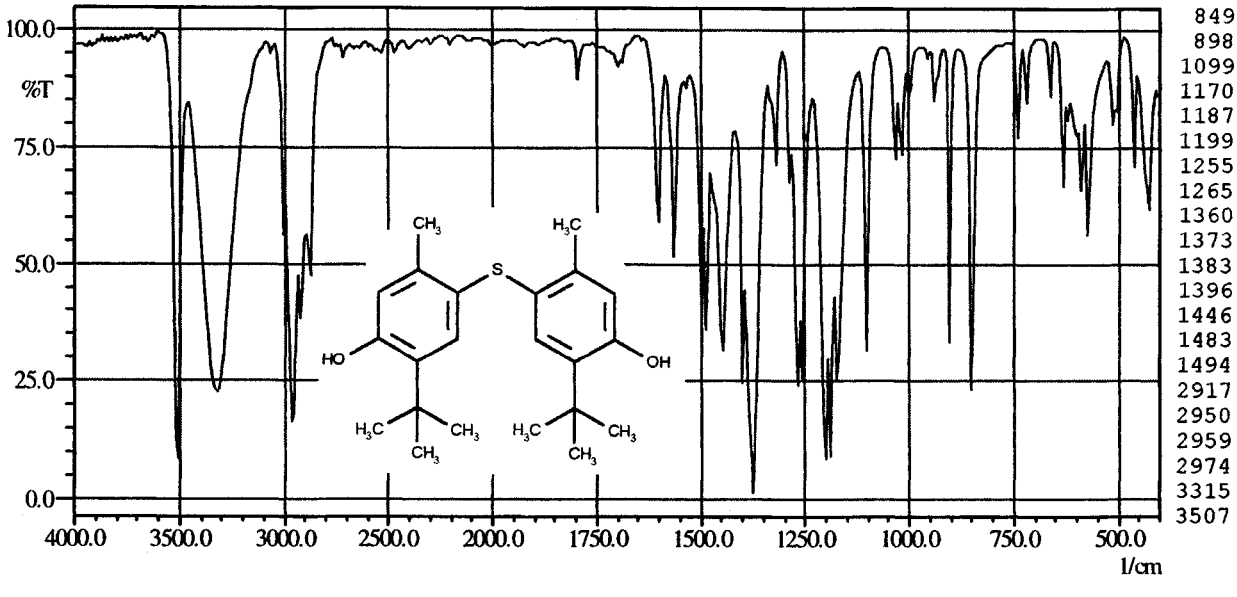
(1) **2-methyl-4,6-*bis*(octylthiomethyl)phenol**
(2) Irganox 1520
(3) Ciba-Geigy
(4) 424.8 g mol^{-1}
(5) antioxidant
(6) pale yellow, low-viscous, free-flowing liquid
(9) 0.98 g cm^{-3}
(13) layer btw KBr

1134 $C_{22}H_{30}O_2S$



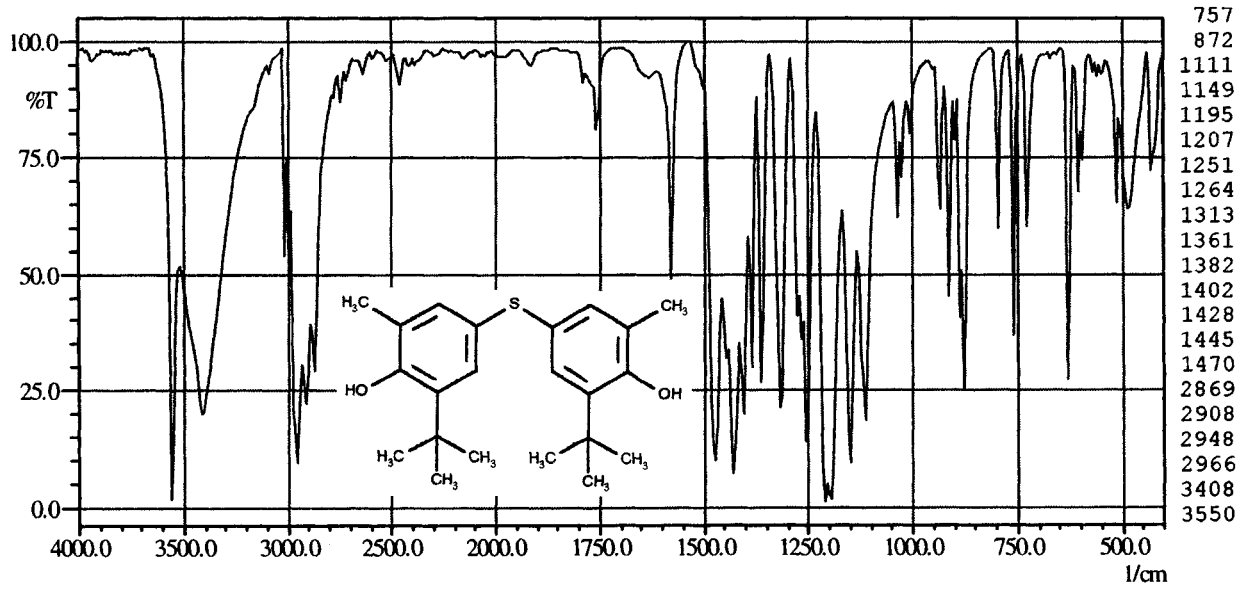
(1) **2,2'-thio-*bis*(6-*t*-butyl-4-methylphenol)**
(2) Irganox 1081
(3) Ciba-Geigy
(4) 358.5 g mol^{-1}
(5) antioxidant
(6) colourless, crystalline solid
(7) 83.5 °C
(13) KBr pellet

1134 $C_{22}H_{30}O_2S$



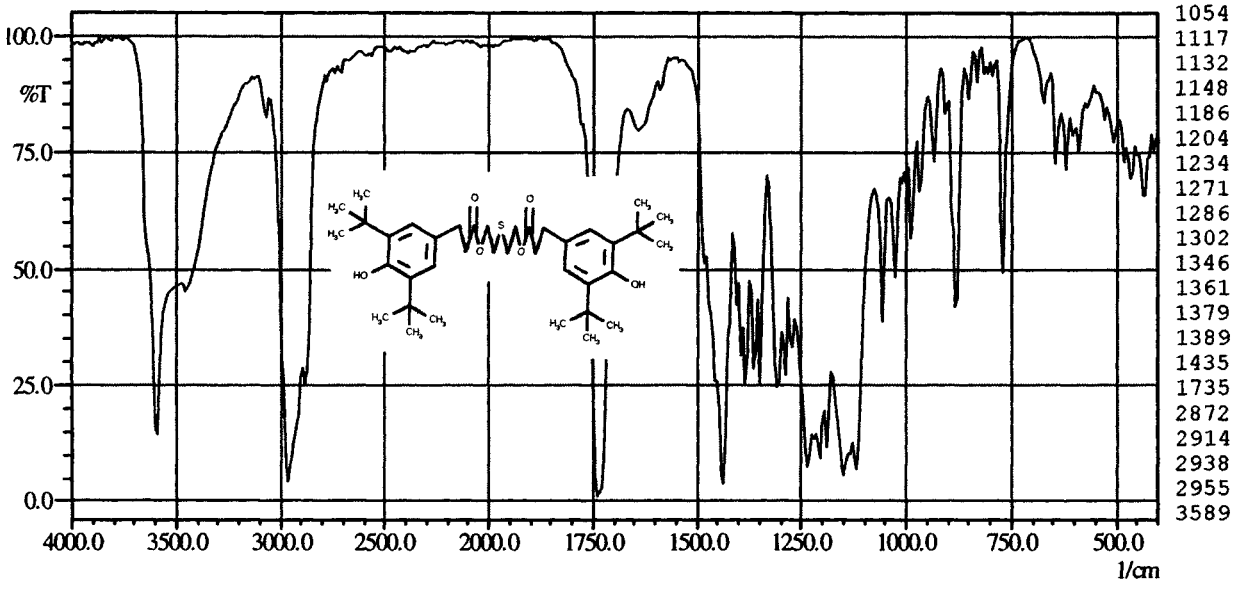
(1) **4,4'-thio-*bis*(2-*t*-butyl-5-methylphenol)**
(2) Irganox 415
(3) Ciba-Geigy
(4) 358.5 g mol^{-1}
(5) antioxidant
(6) colourless solid
(7) 158 °C
(13) KBr pellet

1134 $C_{22}H_{30}O_2S$



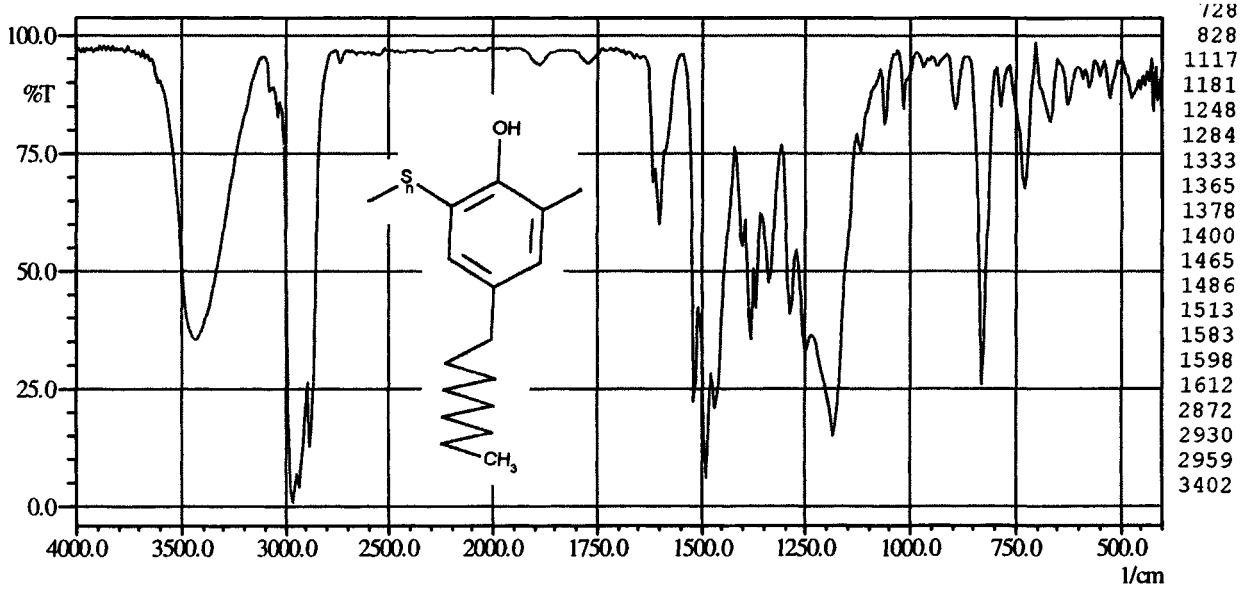
(1) **4,4'-thio-*bis*(6-*t*-butyl-2-methylphenol)**
(2) Ethanox 322 Antioxidant
(3) Ethyl
(4) 358.5 g mol^{-1}
(5) antioxidant
(6) white to yellow-straw, crystalline solid
(7) 124 °C
(8) 312 °C / 5300 Pa
(13) KBr pellet

1134 $C_{38}H_{58}O_6S$



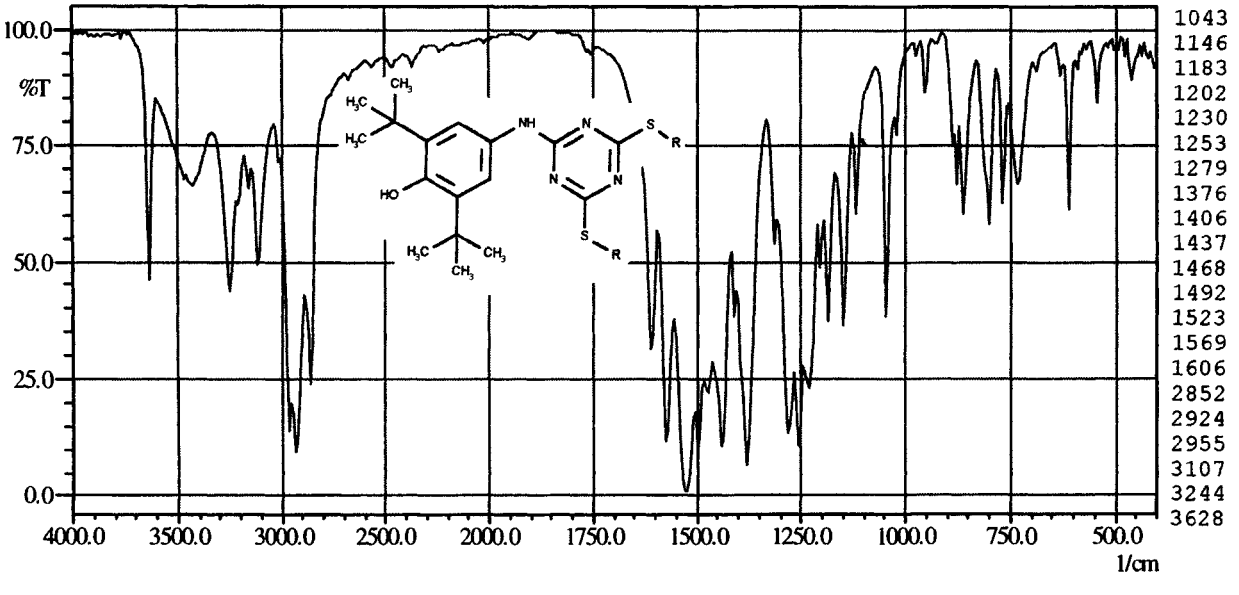
(1) **2,2'-thiodiethyl-*bis*(3-(3,5-di-*t*-butyl-4-hydroxyphenyl)propionate**
(2) Irganox 1035
(3) Ciba-Geigy
(4) 642.9 g mol^{-1}
(5) antioxidant
(6) colourless solid
(7) 63 °C
(13) KBr pellet

1134



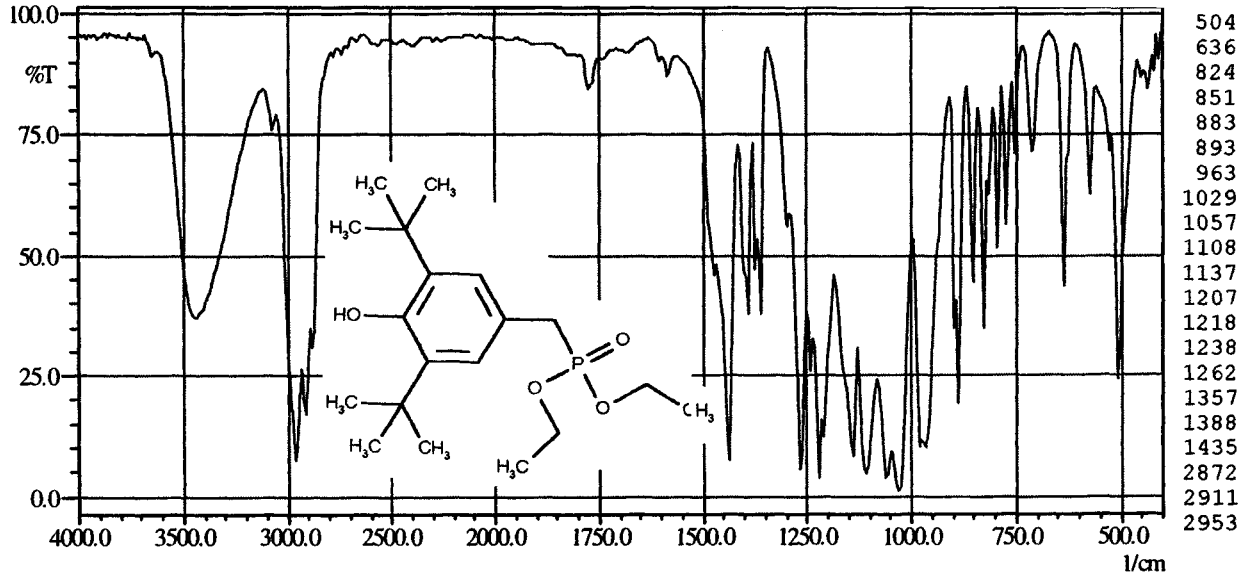
(1) **nonylphenoldisulfide oligomer**
(2) Ethanox 323
(3) Ethyl
(5) antioxidant
(6) liquid
(9) 1.03 g cm^{-3}
(13) layer btw KBr
(14) structure shows only the trimer

1135 $C_{33}H_{56}N_4OS_2$



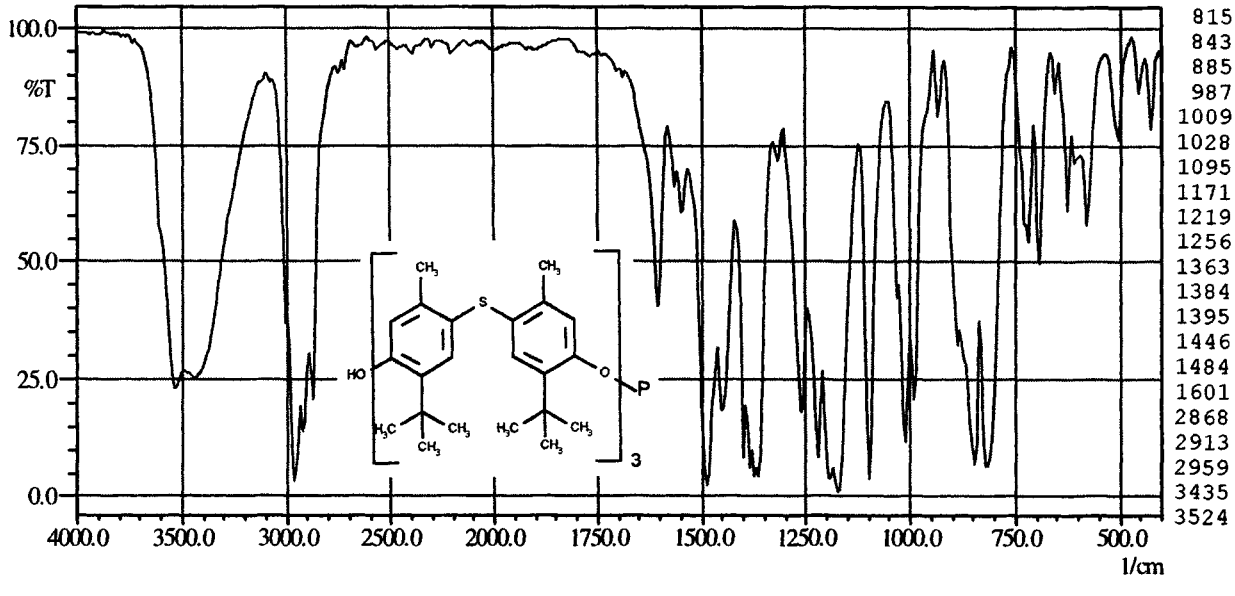
(1) **2,4-*bis*(octylthio)-6-(4-hydroxy-3,5-di-*t*-butylanilino)-1,3,5-triazine**
(2) Irganox 565
(3) Ciba-Geigy
(4) 588.9 g mol^{-1}
(5) antioxidant
(6) colourless solid
(7) 93.5 °C
(13) KBr pellet

1136 $C_{19}H_{33}O_4P$



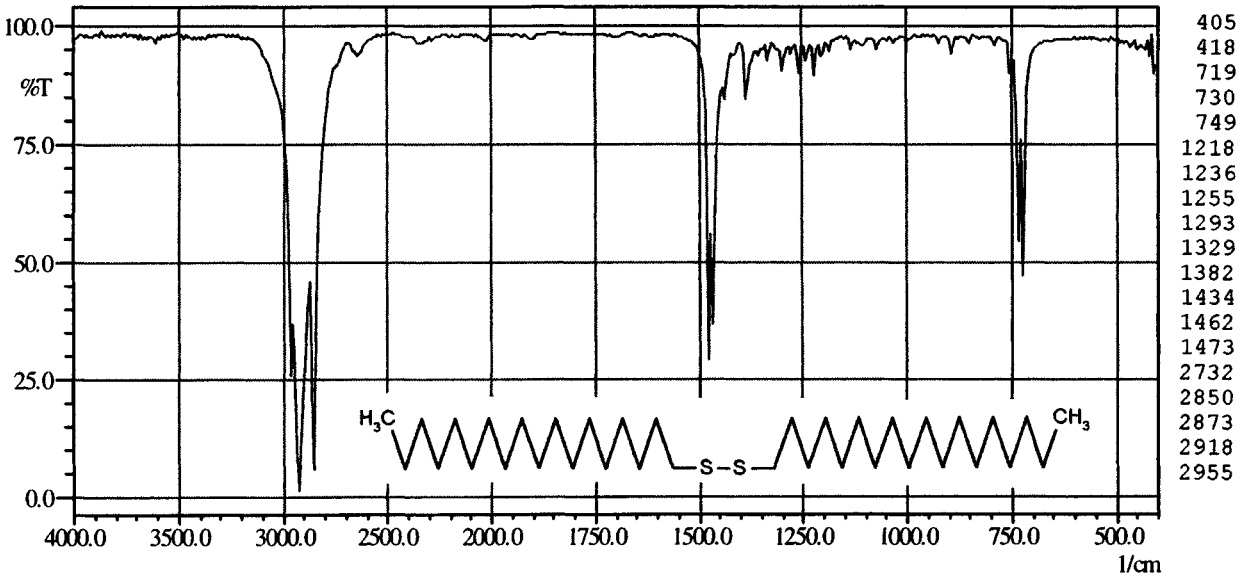
(1) **3,5-di-*t*-butyl-4-hydroxybenzylphosphonic acid diethylester**
(2) Irganox 1222
(3) Ciba-Geigy
(4) 356.4 g mol^{-1}
(5) antioxidant
(6) colourless solid
(7) 119 °C
(13) KBr pellet

1136 $C_{66}H_{87}O_6S_3P$



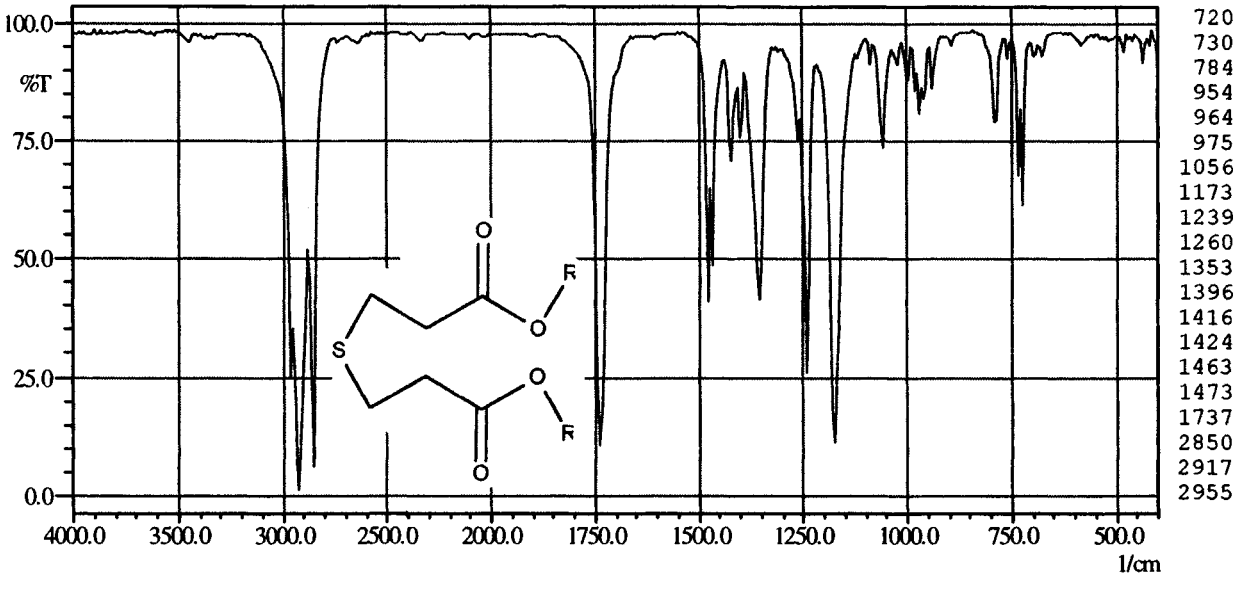
(1) **tris(4,4'-thio-*bis*(2-*t*-butyl-5-methylphenol))phosphite**
(2) Hostanox VP OSP 1
(3) Hoechst
(4) 1105 g mol^{-1}
(5) antioxidant
(6) colourless solid
(7) 110 °C
(13) KBr pellet

1142 $C_{36}H_{74}S_2$



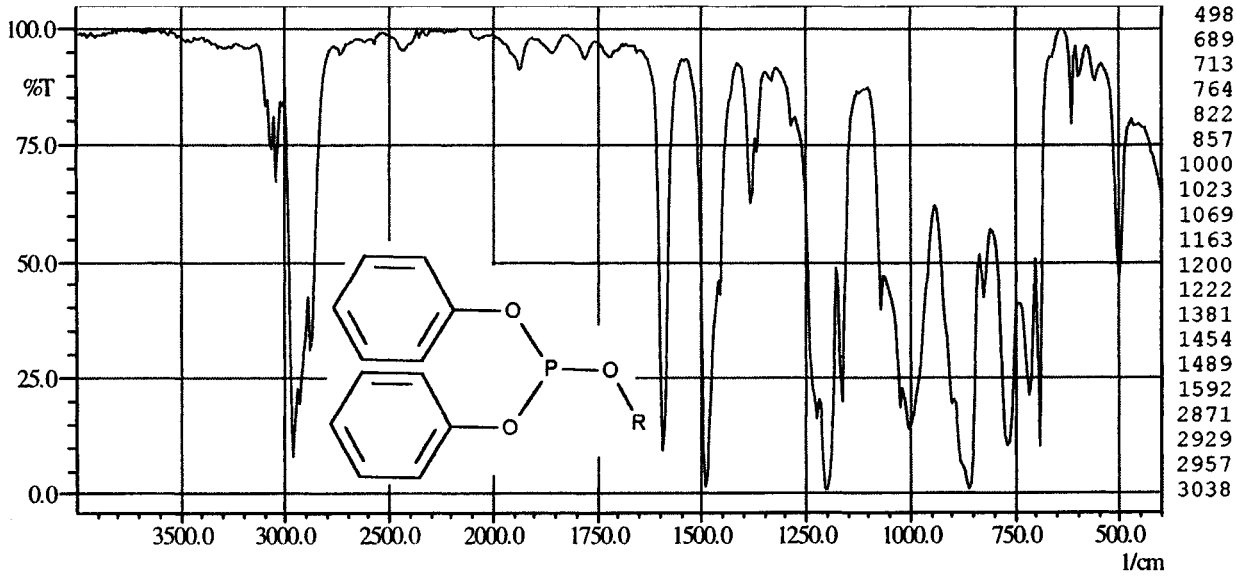
(1) **dioctadecyldisulfide**
(2) Hostanox SE 10
(3) Hoechst
(4) 571.1 g mol^{-1}
(5) antioxidant
(6) colourless solid
(7) 57 °C
(13) KBr pellet

1143 $C_{42}H_{82}O_4S$



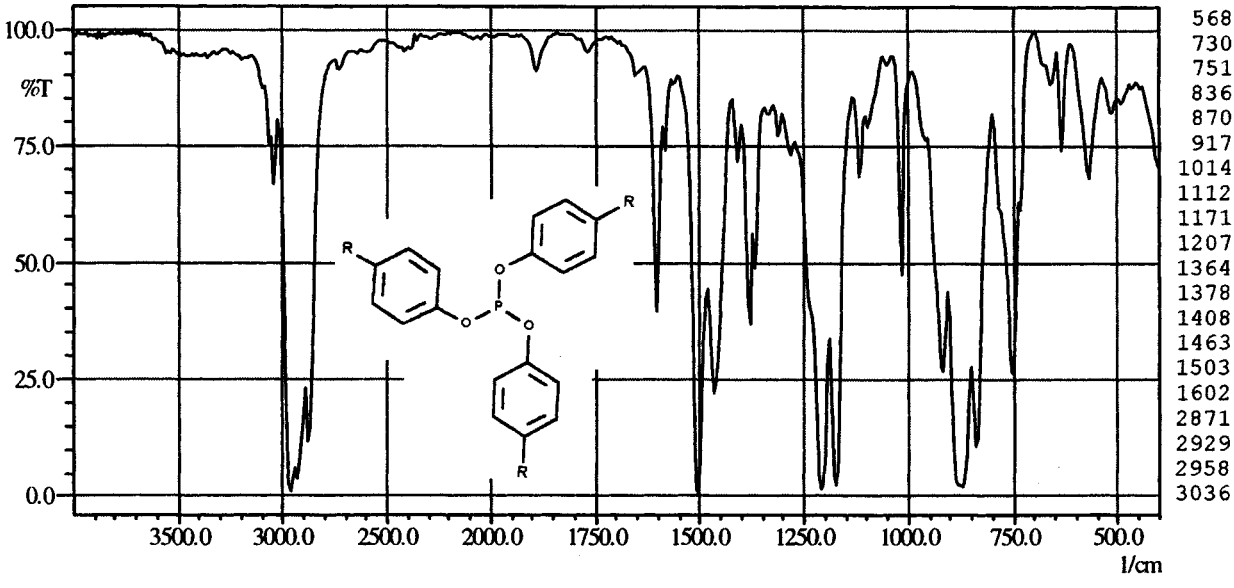
(1) **thiodistearylpropionate**
(2) Hostanox VP SE 2
(3) Hoechst
(4) 683.2 g mol^{-1}
(5) antioxidant
(6) colourless solid
(7) 65 °C
(13) KBr pellet

1144 $C_{20}H_{27}O_3P$



(1) ***i*-octyldiphenylphosphite**
(2) Weston ODPP
(3) Borg-Warner, Parkersburg
(4) 346.4 g mol^{-1}
(5) antioxidant
(6) colourless, clear liquid
(13) layer btw KBr

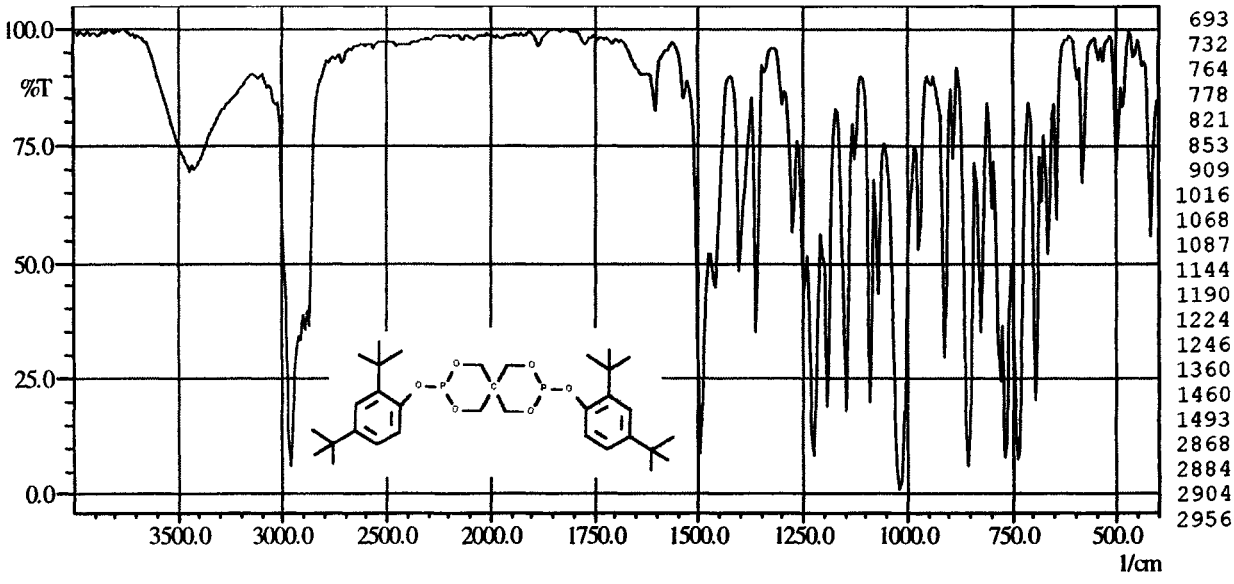
1144 $C_{45}H_{69}O_3P$



(1) ***tris*(nonylphenyl)phosphite**
(2) Weston TNPP
(3) Borg-Warner, Parkersburg
(4) 689.0 g mol^{-1}
(5) antioxidant
(6) yellow, clear liquid
(13) layer btw KBr

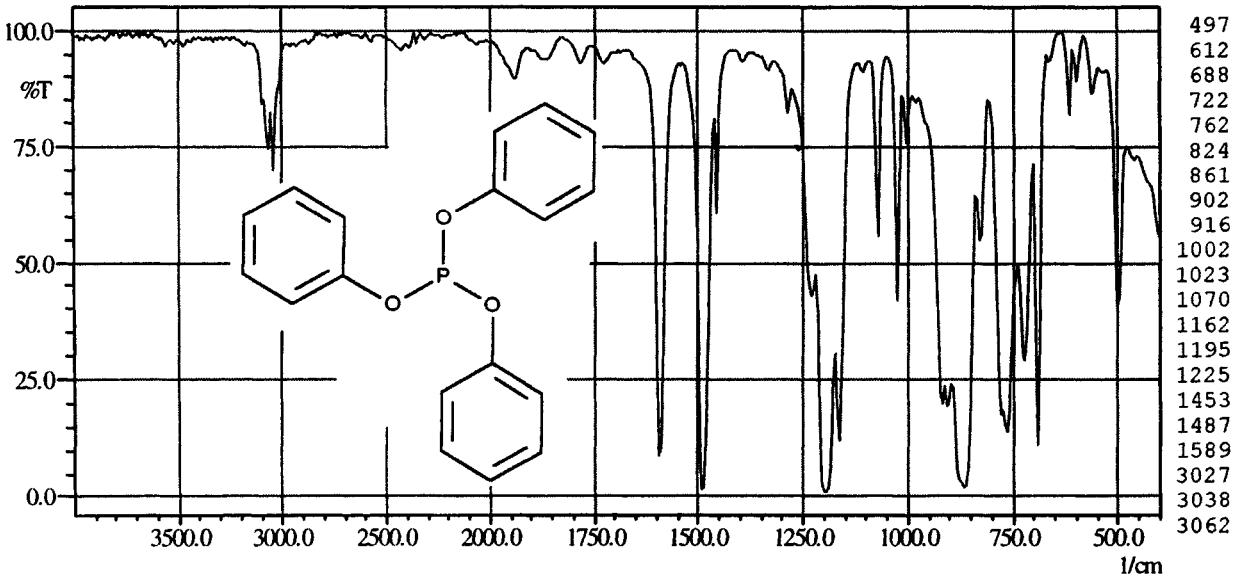
Next Page

1144 $C_{33}H_{50}O_6P_2$



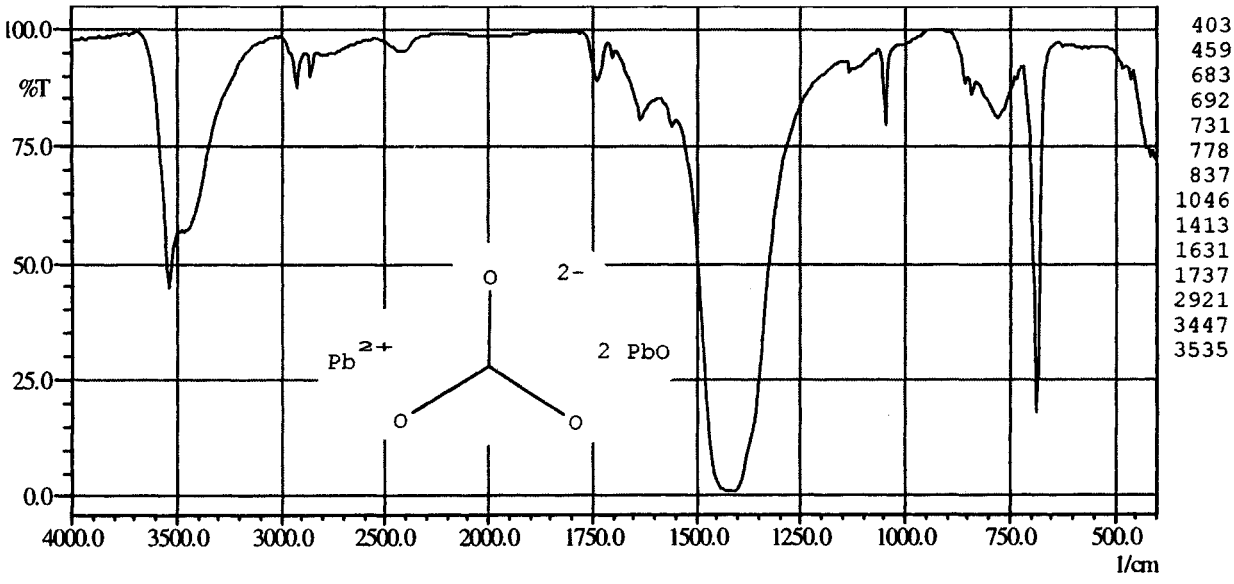
(1) ***bis*(2,4-di-*t*-butylphenyl)pentaerythritoldiphosphite**
(2) Ultranox
(3) Borg-Warner, Parkersburg
(4) 604.7 g mol^{-1}
(5) antioxidant
(6) colourless solid
(13) KBr pellet

1144 $C_{18}H_{15}O_3P$



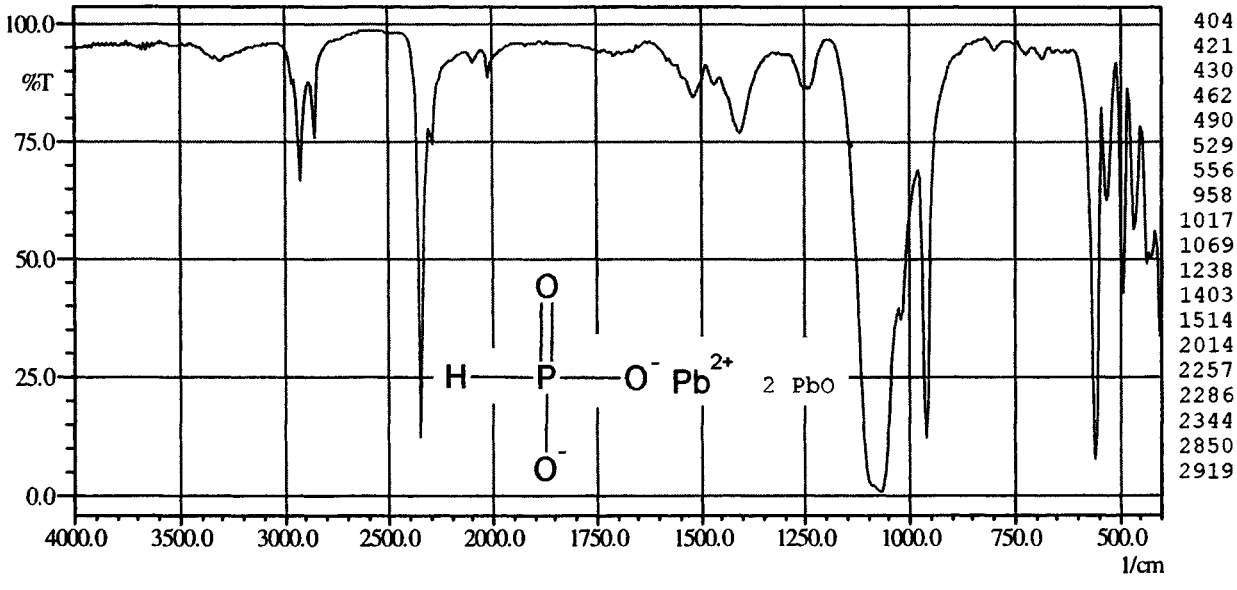
(1) **triphenylphosphite**
(2) Weston TPP
(3) Borg-Warner, Parkersburg
(4) 310.3 g mol^{-1}
(5) antioxidant
(6) colourless, clear liquid
(13) layer btw KBr

12112 $2PbO \cdot PbCO_3$



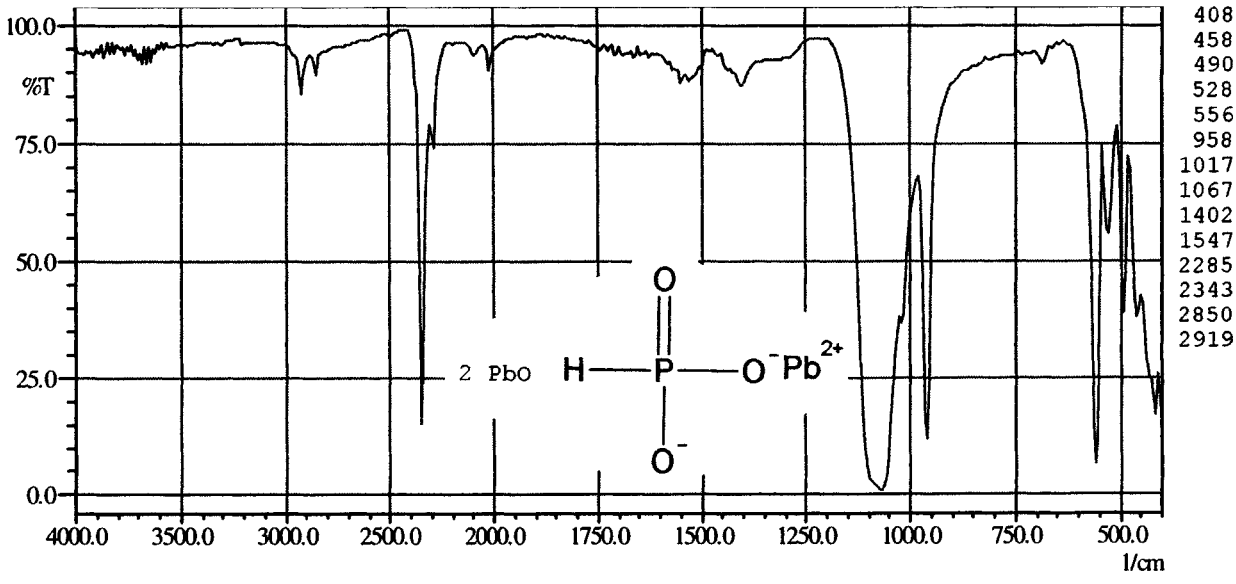
(1) **2-basic Pb carbonate**
(2) 2-bas. Bleicarbonat
(3) Chemson
(5) stabiliser
(6) colourless solid
(13) KBr pellet

12113 $2PbO \cdot PbHPO_3 \cdot 1/2H_2O$



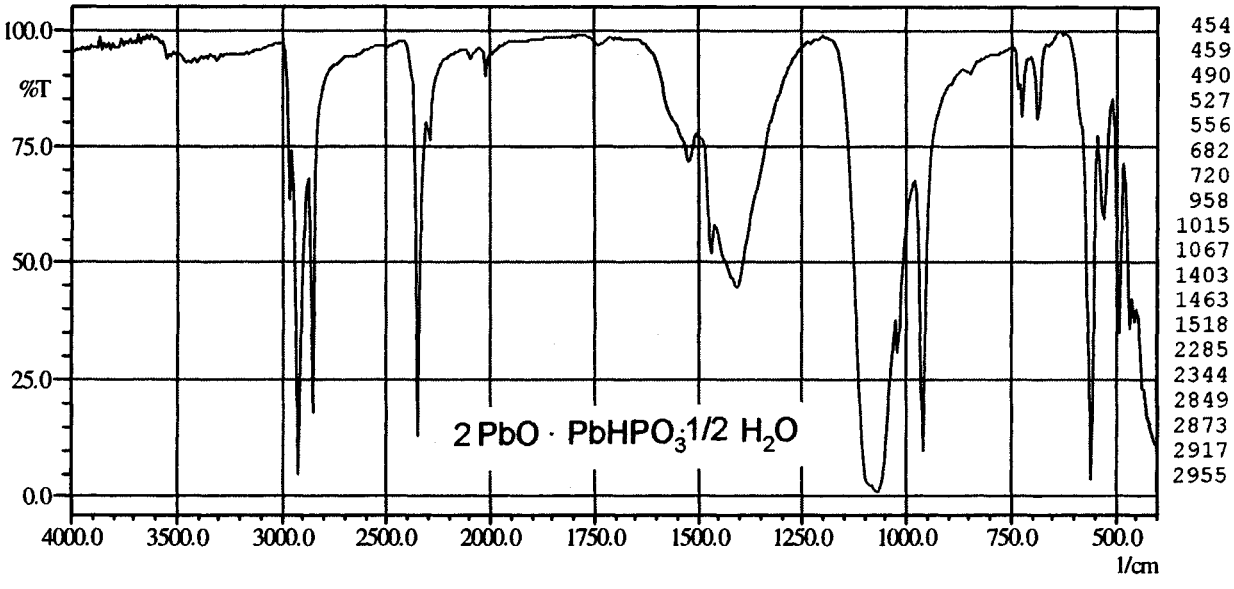
(1) **2-basic Pb phosphite**
(2) Zweibasisches Blei-Phosphit
(3) Reagens
(5) stabiliser
(6) colourless solid
(9) 6.94 g cm^{-3}
(13) KBr pellet

12113 $2PbO \cdot PbHPO_3 \cdot 1/2H_2O$



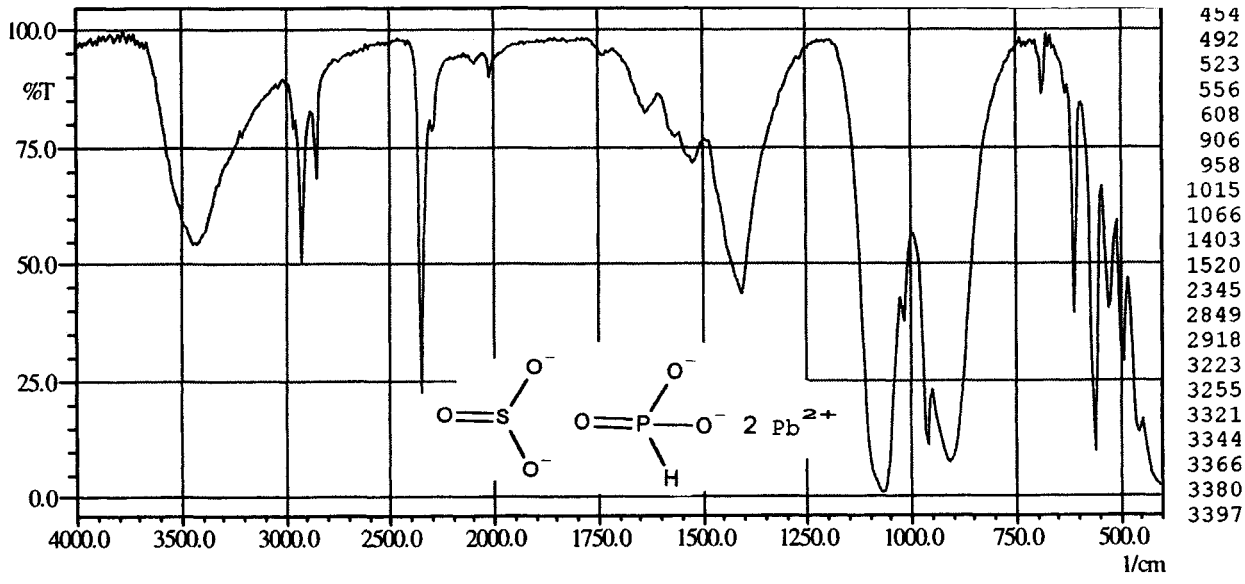
(1) **2-basic Pb phosphite**
(2) Interstab LP 3139
(3) Akzo Chemie
(5) stabiliser
(6) colourless solid
(13) KBr pellet

12113+1241



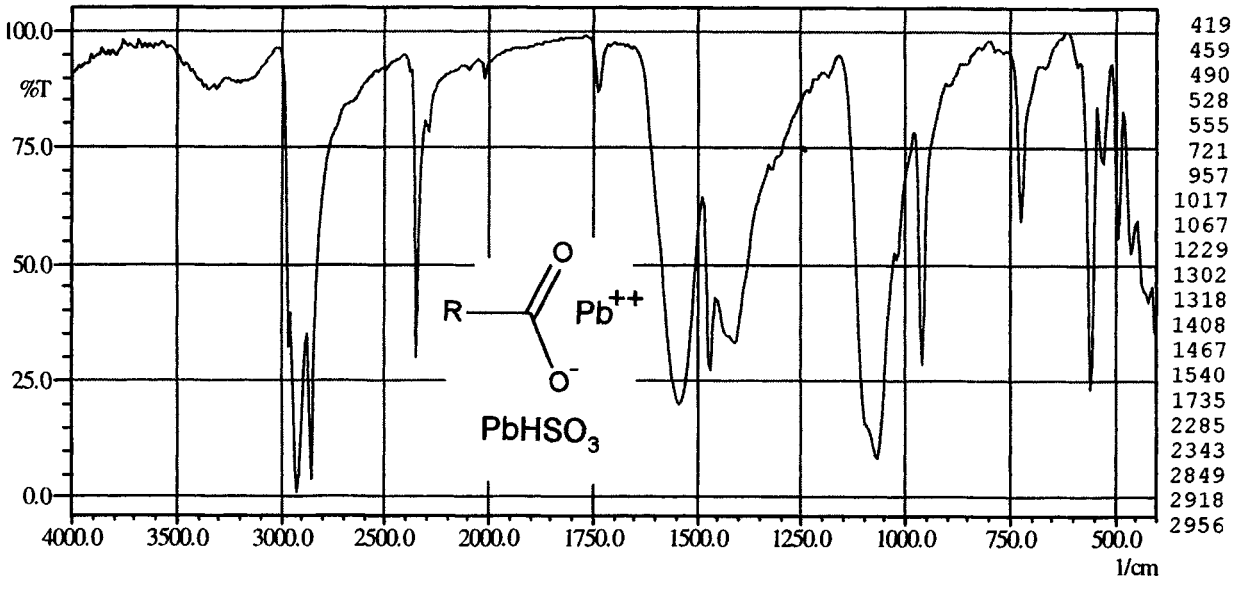
(1) **2-basic Pb phosphite complex**
(2) Baerostab E 502 FP
(3) Baerlocher
(5) stabiliser
(6) colourless granules
(9) 4.5 g cm^{-3}
(13) KBr pellet

12113



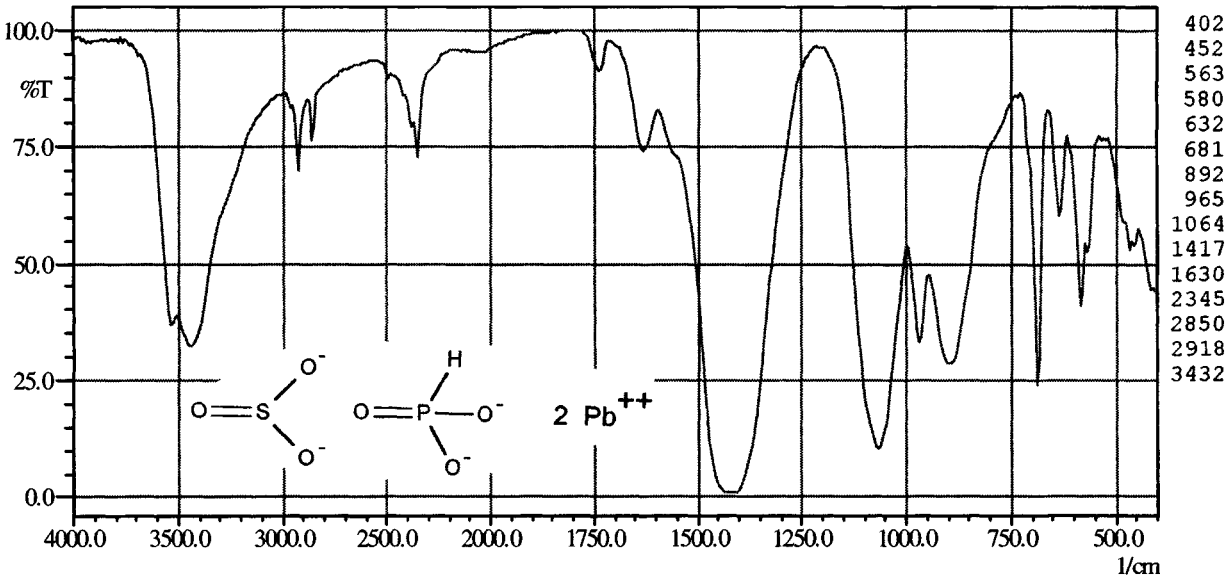
(1) **2-basic Pb phosphite-sulfite complex**
(2) Sulfofos C
(3) Baerlocher
(5) PVC-stabiliser
(6) colourless solid
(9) 6.8 g cm^{-3}
(13) KBr pellet

12113+1241



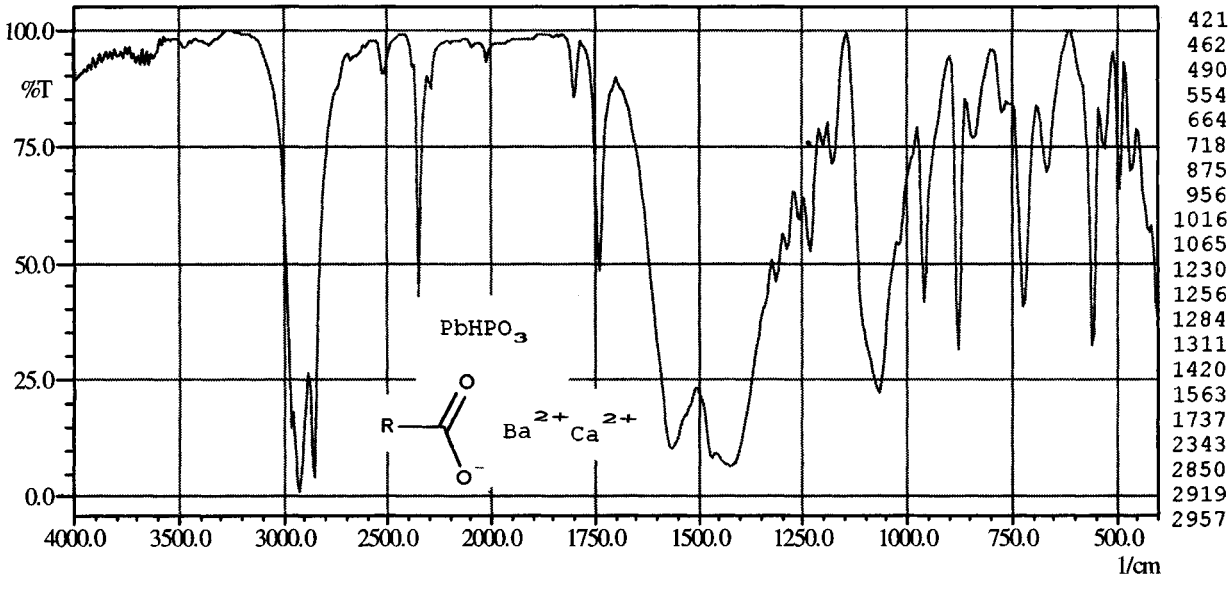
(1) **coprecipitate based on Pb phosphite-carboxylate**
(2) Interstab LF 3638
(3) Akzo Chemie
(5) stabiliser
(6) cream-coloured flakes
(13) KBr pellet

12113



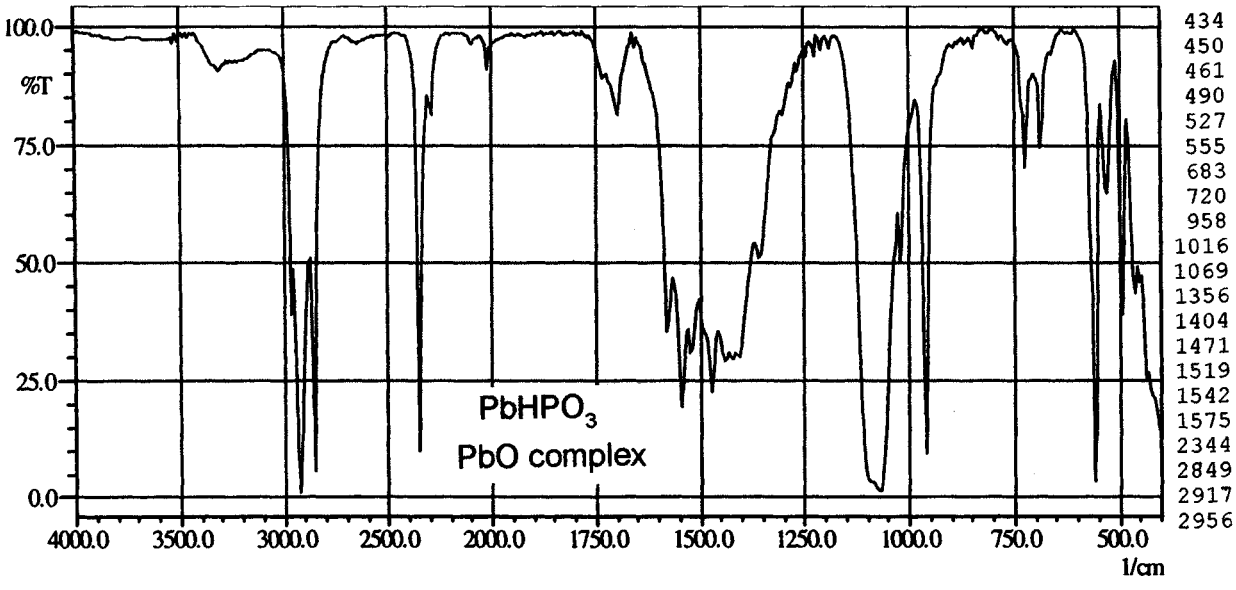
(1) **Pb phosphite-sulfite-carbonate complex**
(2) Naftovin T 82
(3) mg Technologies/Chemson
(5) PVC-stabiliser
(6) colourless solid
(9) 6.7 g cm^{-3}
(13) KBr pellet

12113+1241



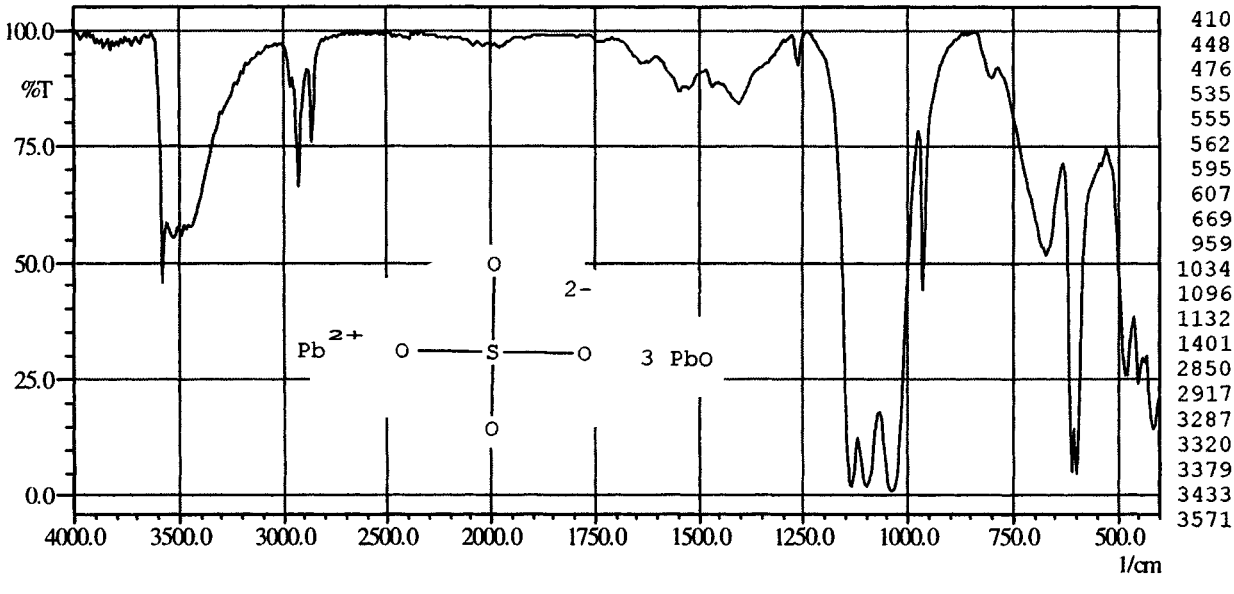
(1) **coprecipitate based on Ba Ca complex and 2-basic lead phosphite (1:1)**
(2) Interstab LT 3631/3
(3) Akzo Chemie
(5) stabiliser
(6) cream-coloured solid
(13) KBr pellet

12113+12411



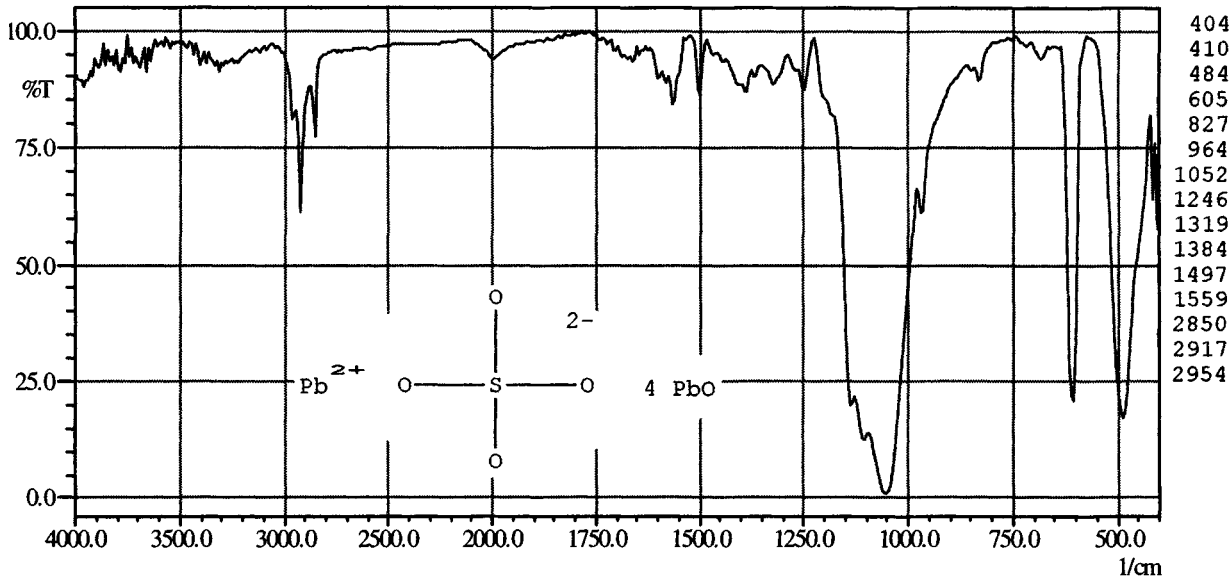
(1) **basic Pb phosphite carboxylate**
(2) Baeropan MC 380 FP
(3) Baerlocher
(5) stabiliser
(6) colourless solid
(13) KBr pellet

12114 **$3PbO \cdot PbSO_4$**



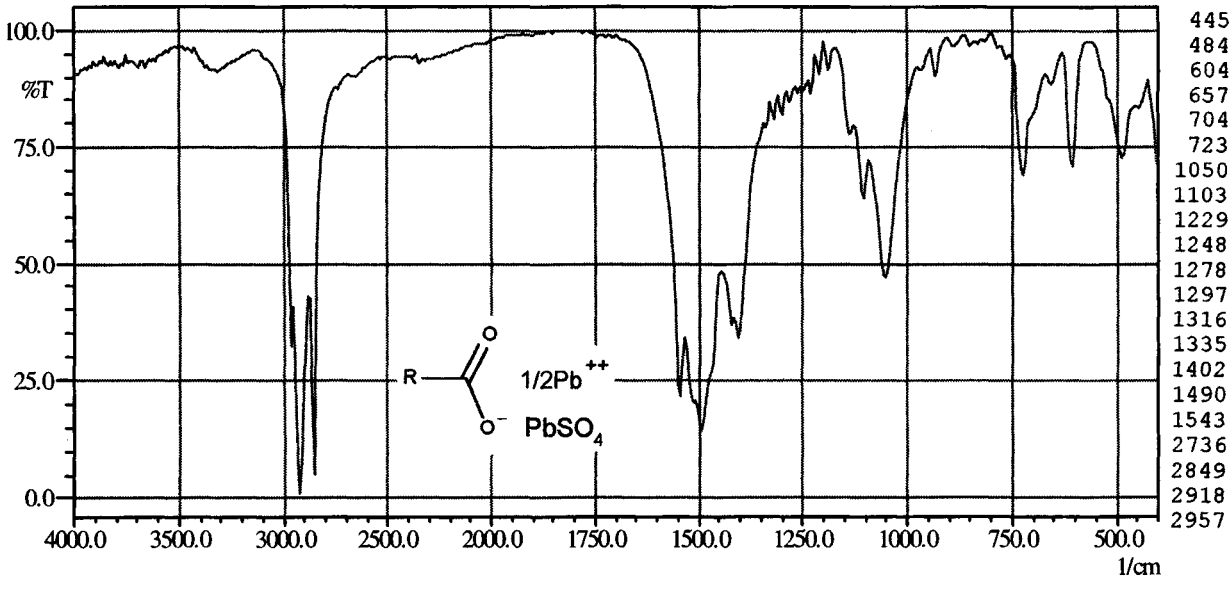
(1) **3-basic Pb sulfate**
(2) Baerostab V 220 MC
(3) Baerlocher
(4) 973.8 g mol^{-1}
(5) stabiliser
(6) colourless solid
(9) 6.6 g cm^{-3}
(13) KBr pellet

12114 **$4PbO \cdot PbSO_4 \cdot H_2O$**



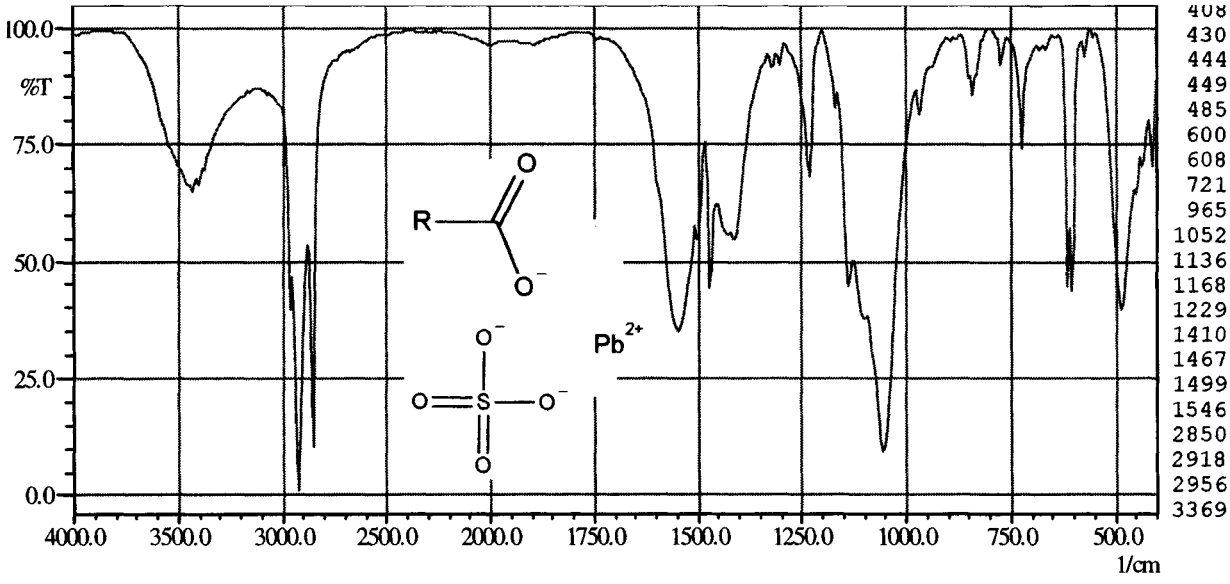
(1) **4-basic Pb sulfate**
(2) Interstab LP 3104
(3) Akzo Chemie
(4) 1214 g mol^{-1}
(5) stabiliser
(6) colourless solid
(13) KBr pellet

12114+1241 **$PbSO_4$**



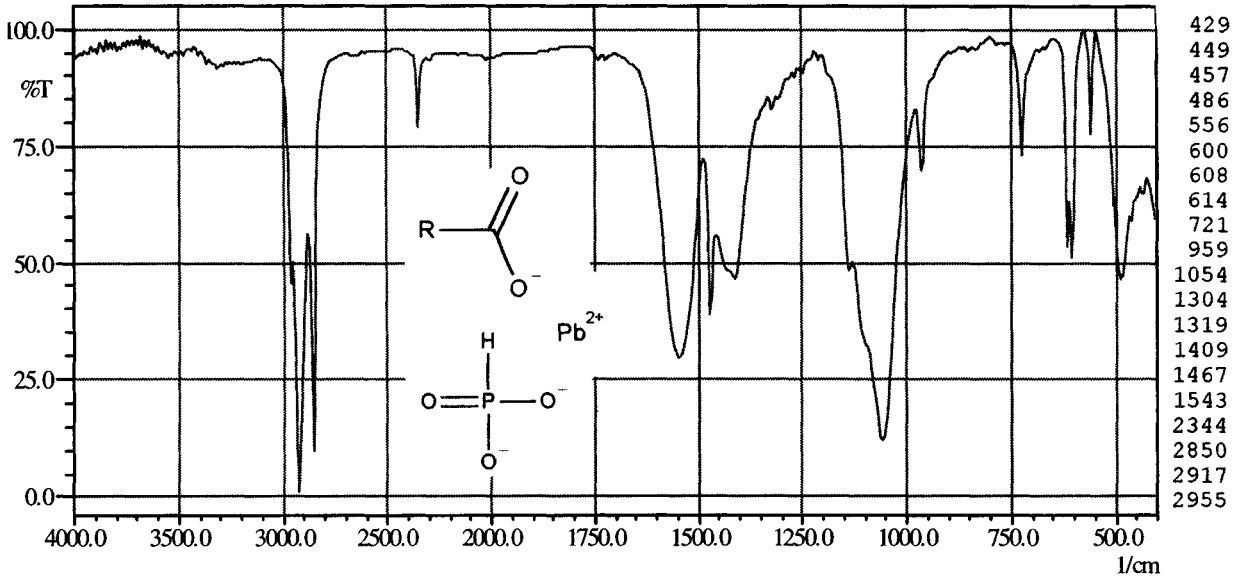
(1) **coprecipitate based on Pb sulfate-carboxylate**
(2) Interstab LP 3636
(3) Akzo Chemie
(5) stabiliser
(6) cream-coloured solid
(13) KBr pellet

12114+1241



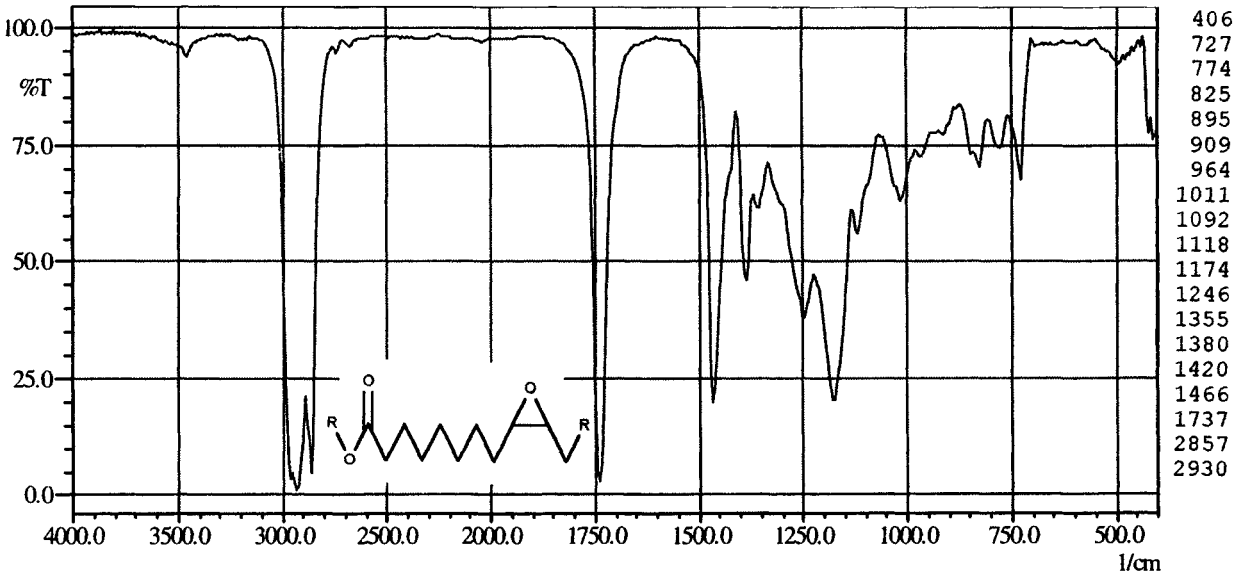
(1) **coprecipitate based on Pb sulfate-carboxylate**
(2) Interstab LT 3679
(3) Akzo Chemie
(5) stabiliser
(6) cream-coloured solid
(13) KBr pellet

12114+12113+1241



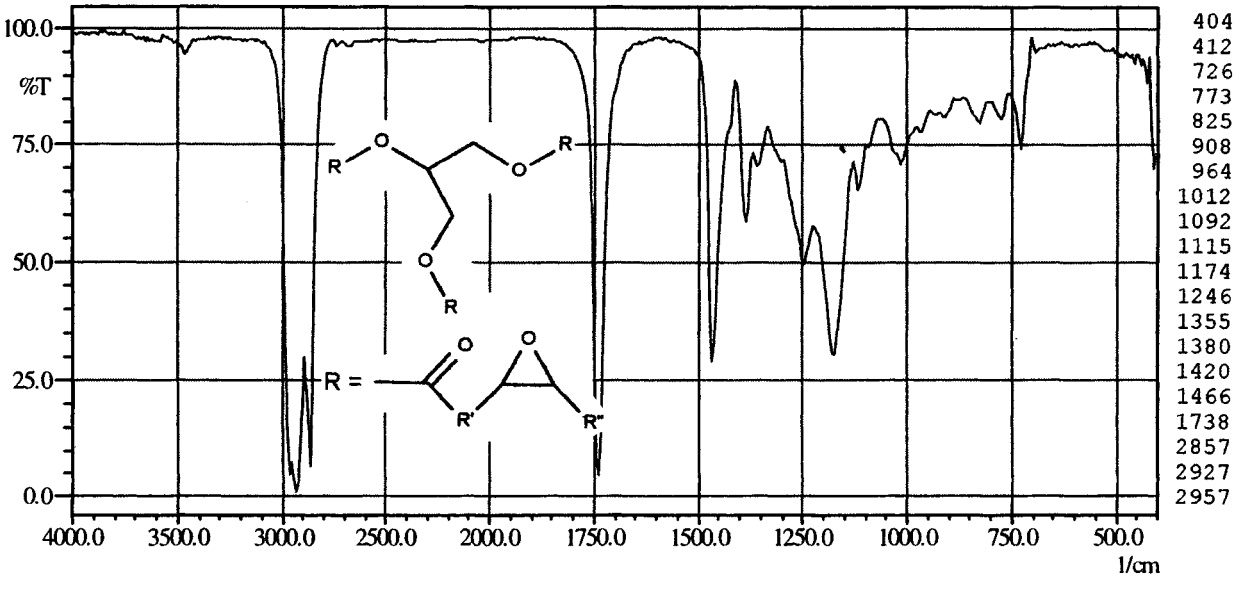
(1) **coprecipitate based on Pb sulfate-phosphite-carboxylate**
(2) Interstab LF 3734
(3) Akzo Chemie
(5) stabiliser
(6) cream-coloured granules
(13) KBr pellet

1223



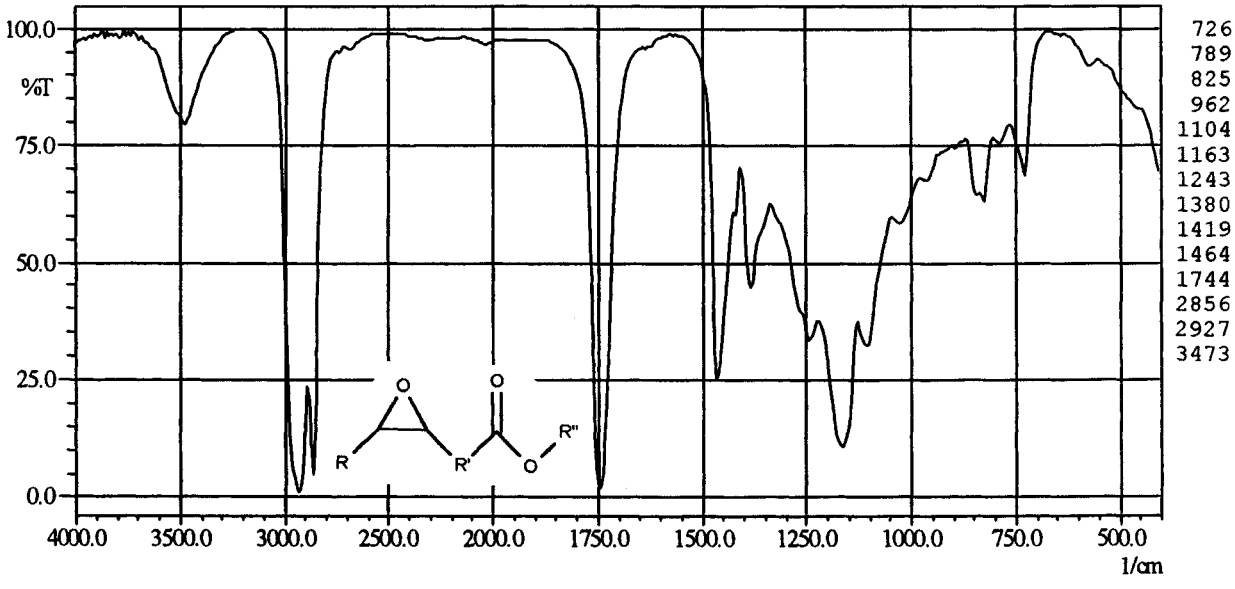
(1) **epoxidized octanoic ester**
(2) Plastepon 451
(3) L'air Liquide
(5) stabiliser
(6) light-yellow, clear liquid
(9) 0.9 g cm^{-3}
(10) 1.46
(13) layer btw KBr

1223



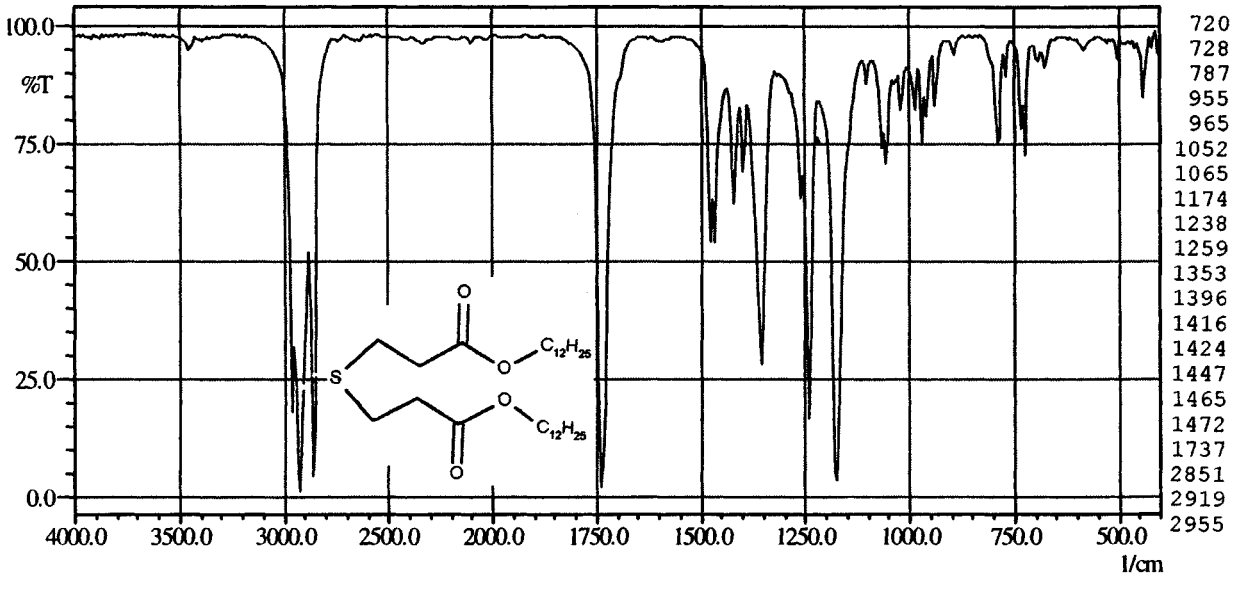
(1) **epoxidized soybean oil**
(2) Baerostab LSU
(3) Baerlocher
(5) PVC-costabiliser
(6) colourless, clear liquid
(9) 1 g cm^{-3}
(13) layer btw KBr

1223



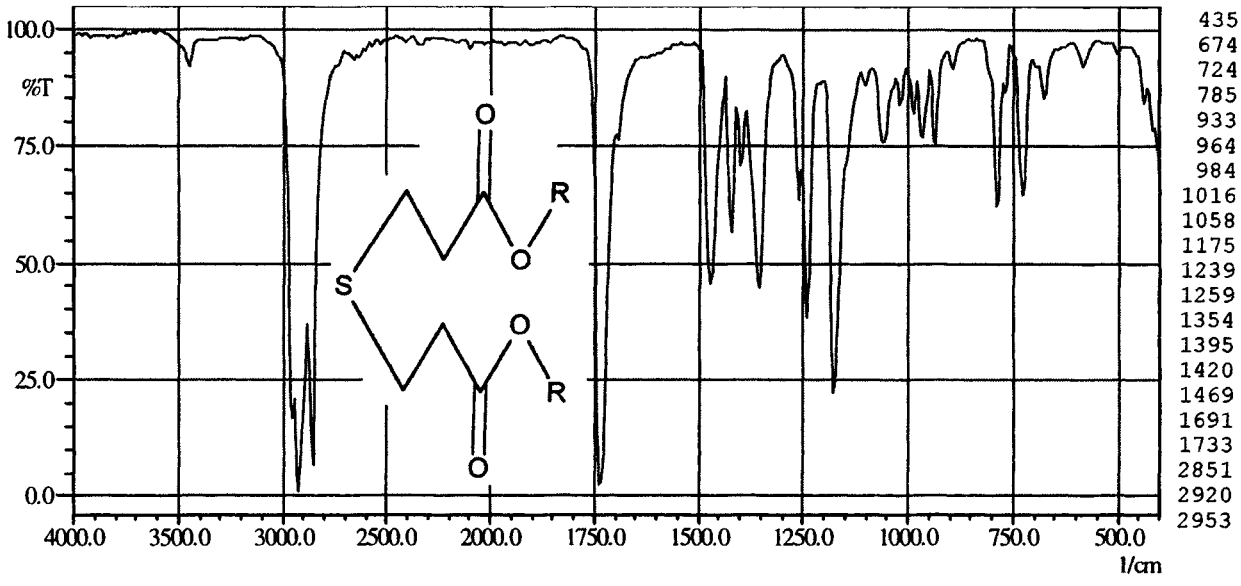
(1) **epoxidized soybean oil**
(2) Reoplast 39
(3) Ciba-Geigy
(5) co-stabiliser
(6) yellowish, clear liquid
(9) 0,99 g cm^{-3}
(10) 1,473
(13) layer btw KBr

1225 $C_{30}H_{58}O_4S$



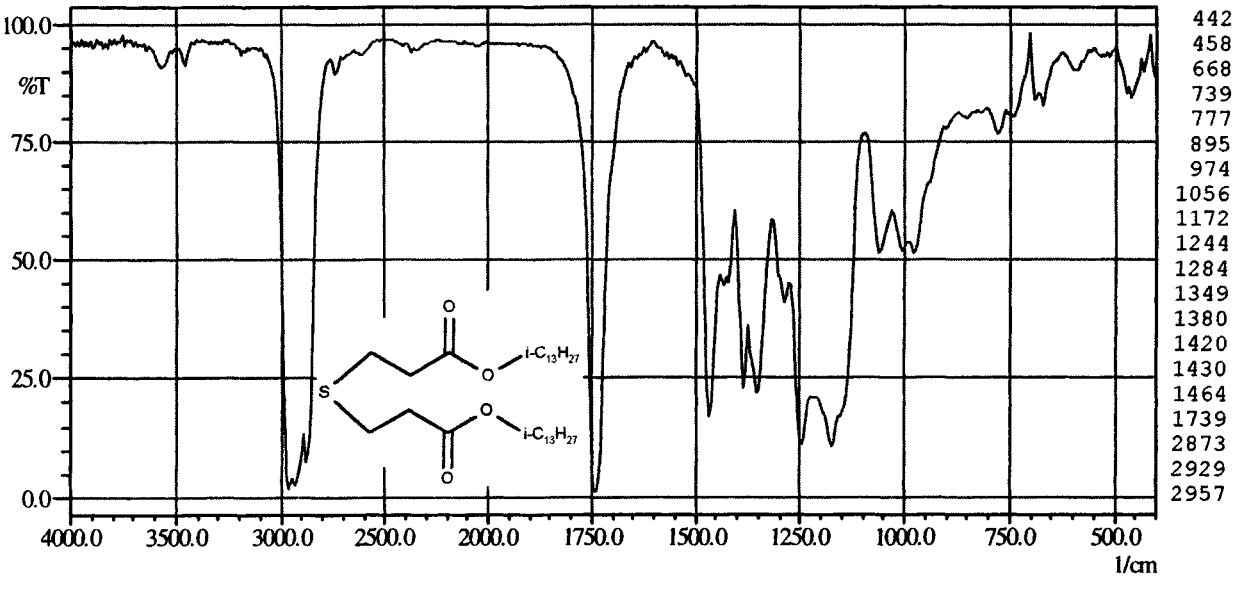
(1) **β,β'-thiodilaurylpropionate**
(2) Hostanox Se 1
(3) Hoechst
(4) 514.9 g mol^{-1}
(5) antioxidant
(6) colourless solid
(13) KBr pellet

1225 $C_{30}H_{58}O_4S$



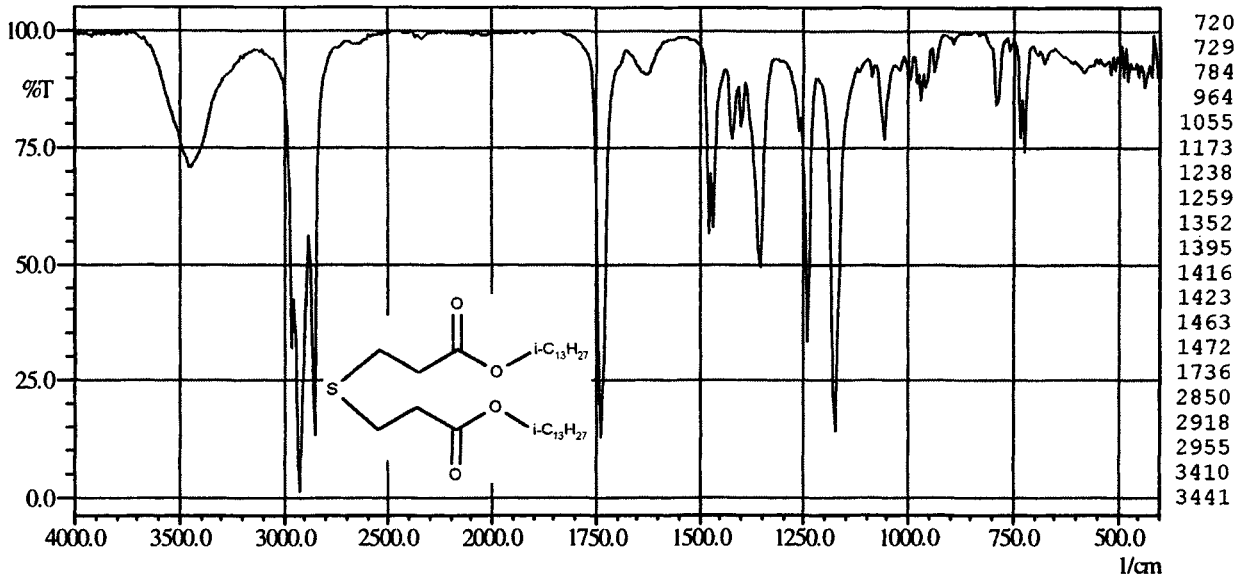
(1) **dilaurylthiodipropionate**
(2) Dilaurylthiodipropionat
(3) Reagens
(4) 514.9 g mol^{-1}
(5) stabiliser
(6) colourless solid
(7) 39.5 °C
(13) layer btw KBr

1225 $C_{32}H_{62}O_4S$



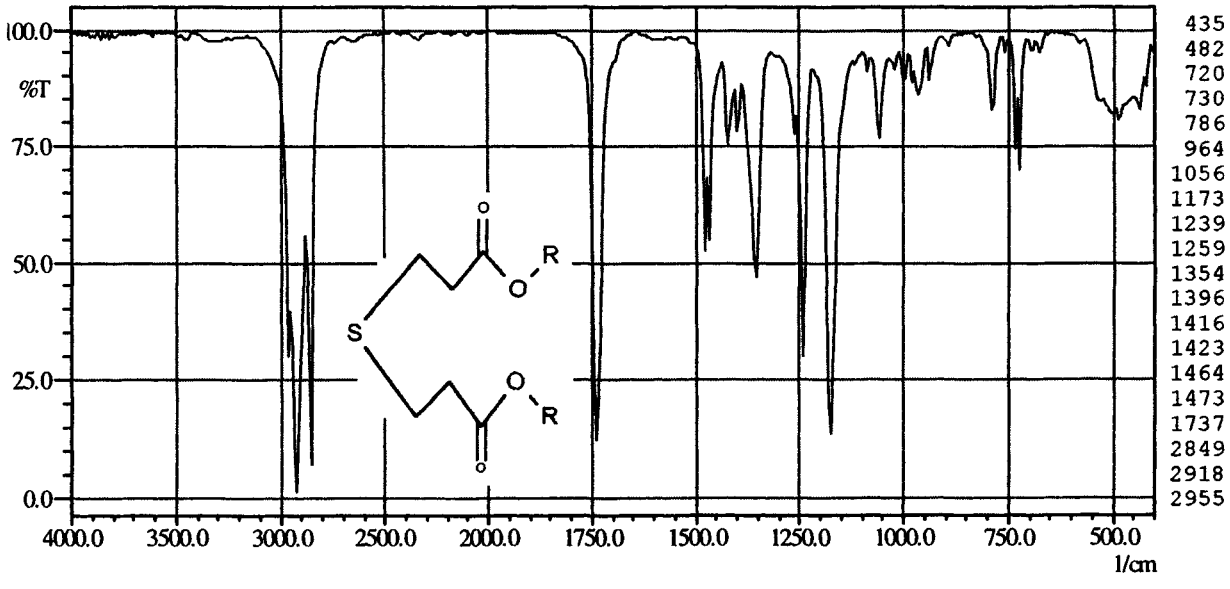
(1) **di(tridecyl)thiopropionate**
(2) Ditridecylthiopropionat
(3) Reagens
(4) 542.9 g mol^{-1}
(5) stabiliser
(6) colourless, clear liquid
(9) 0.936 g cm^{-3}
(10) 1.468
(13) layer btw KBr

1225 $C_{34}H_{66}O_4S$



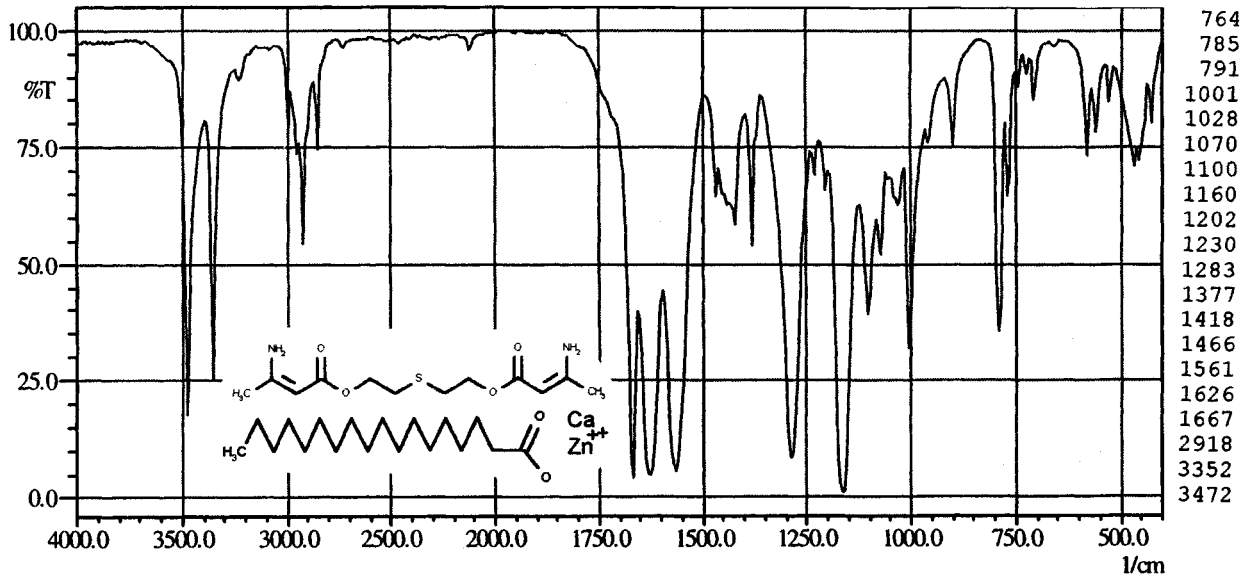
(1) **dimyristyl-3,3'-thiodipropionate**
(2) Irganox PS 801
(3) Ciba-Geigy
(4) 571.0 g mol^{-1}
(5) antioxidant
(6) colourless crystals
(7) 50 °C
(13) KBr pellet

1225 $C_{42}H_{82}O_4S$



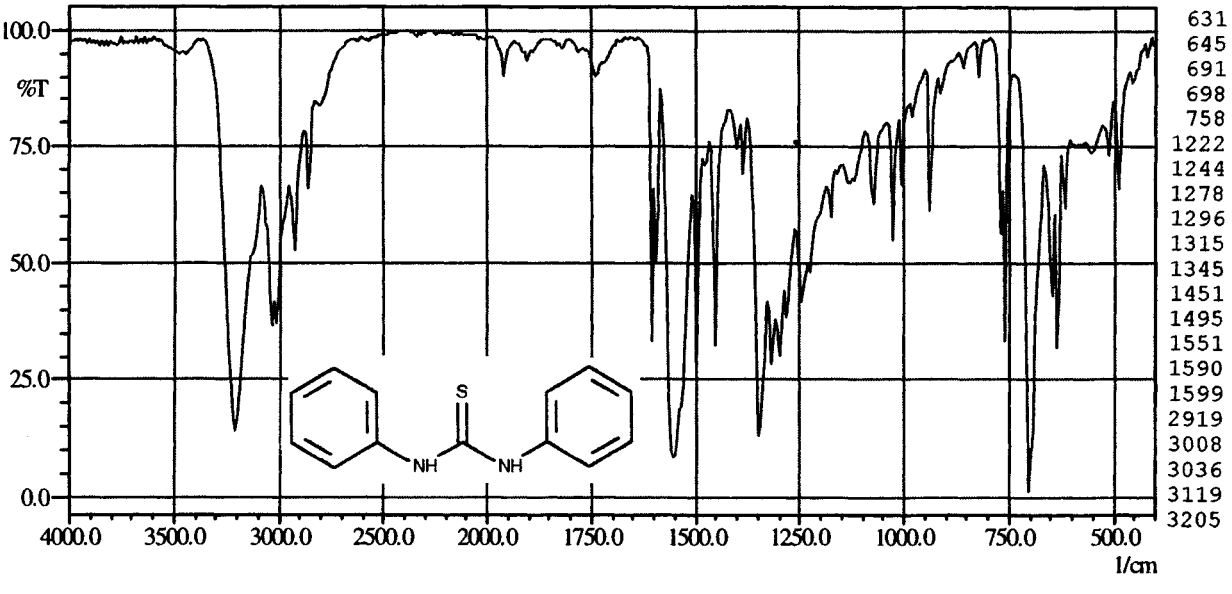
(1) **3,3'-thio-*bis*(stearyldipropionate)**
(2) Lowinox DSTDP
(3) Chemische Werke Lowi
(4) 683.2 g mol^{-1}
(5) antioxidant
(6) colourless flakes
(7) 63 °C
(13) KBr pellet

1231



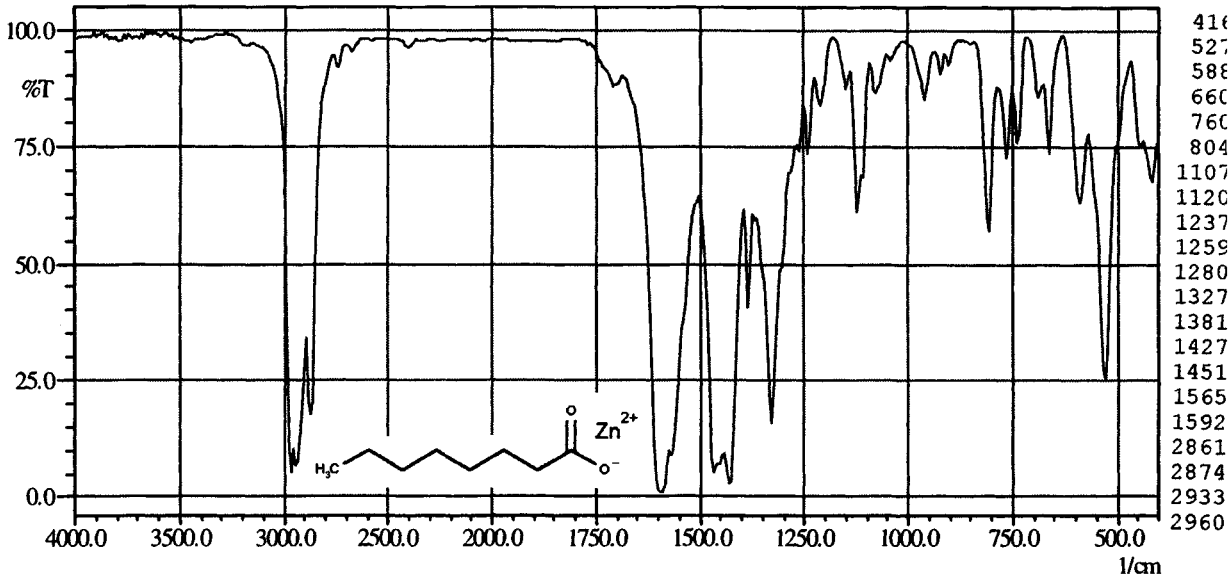
(1) **thiodiethyleneglycol-β-aminocrotonic acid ester with Ca and Zn stearate**
(2) Irgastab A 80
(3) Ciba-Geigy
(5) PVC-stabiliser
(6) yellowish solid
(13) KBr pellet

1233 $C_{13}H_{12}N_2S$



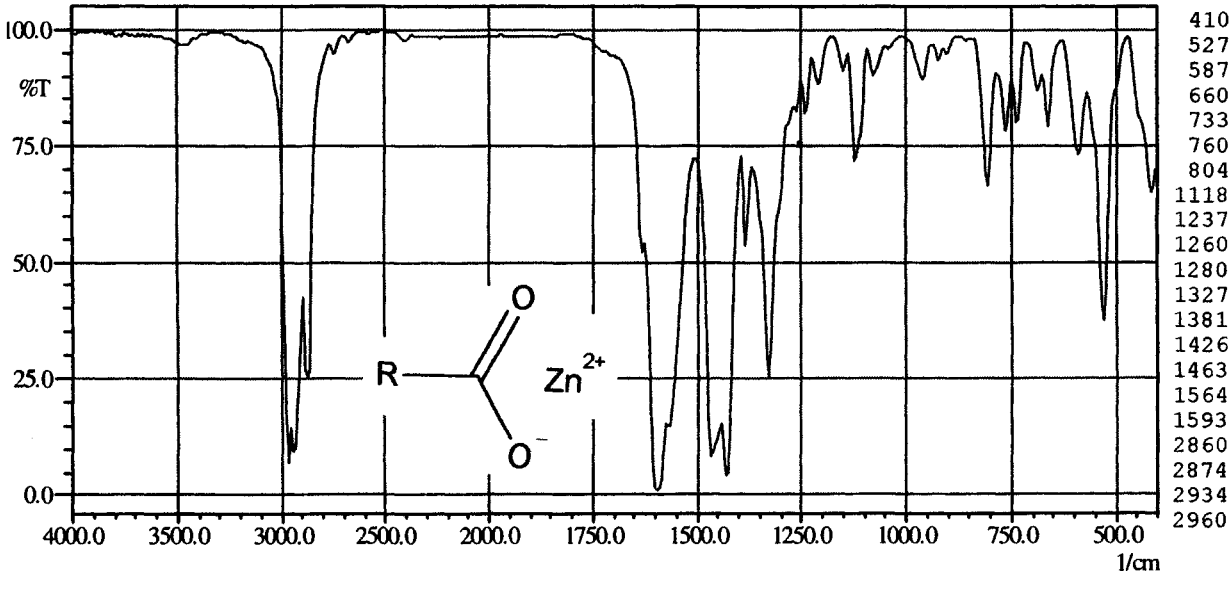
(1) **N,N'-diphenylthiourea**
(2) Diphenylthioharnstoff
(3) commercial
(4) 228.3 g mol^{-1}
(5) PVC stabiliser
(6) colourless solid
(7) 155 °C
(9) 1.32 g cm^{-3}
(13) KBr pellet

12411 $C_{16}H_{30}O_4Zn$



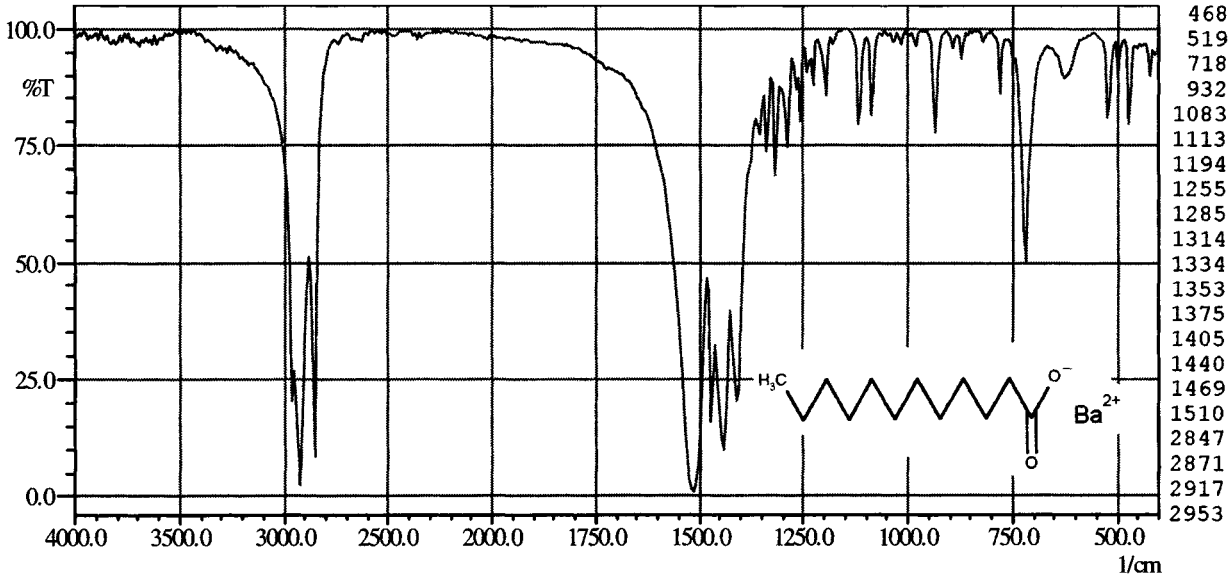
(1) **Zn octoate**
(2) Baerostab L 230
(3) Baerlocher
(4) 351.8 g mol^{-1}
(5) stabiliser
(6) slightly yellowish, clear liquid
(9) 1.19 g cm^{-3}
(13) layer btw KBr

12411



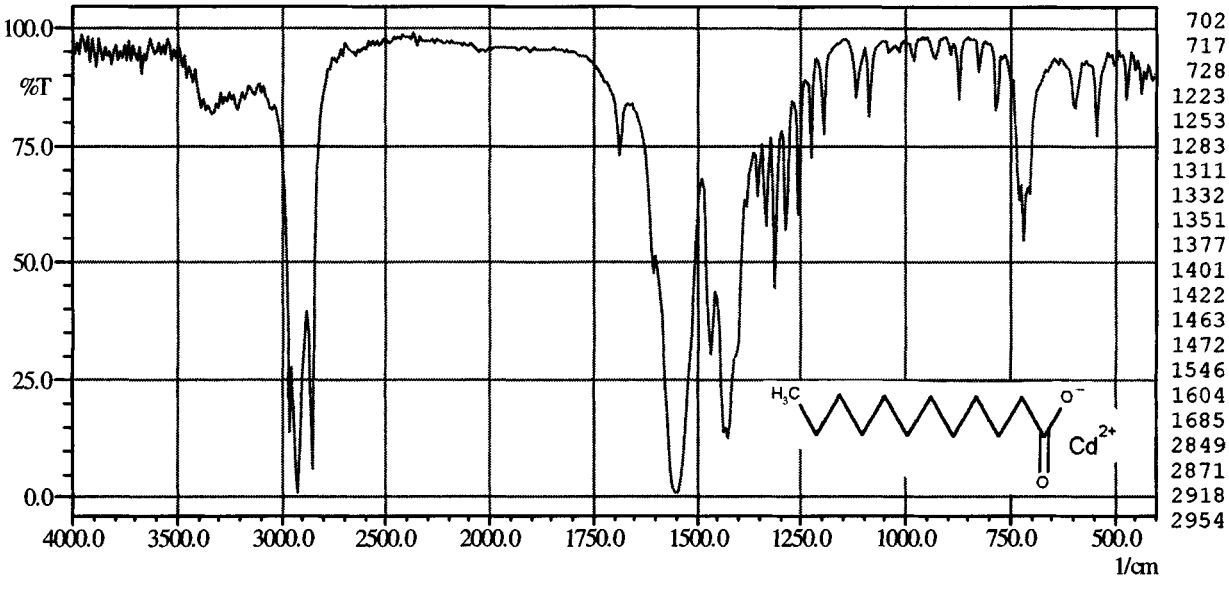
(1) **Zn complex**
(2) Interstab M 823
(3) Akzo Chemie
(5) stabiliser
(6) pale-yellowish, clear, viscosus liquid
(13) layer btw KBr

12411 $C_{24}H_{46}O_4Ba$



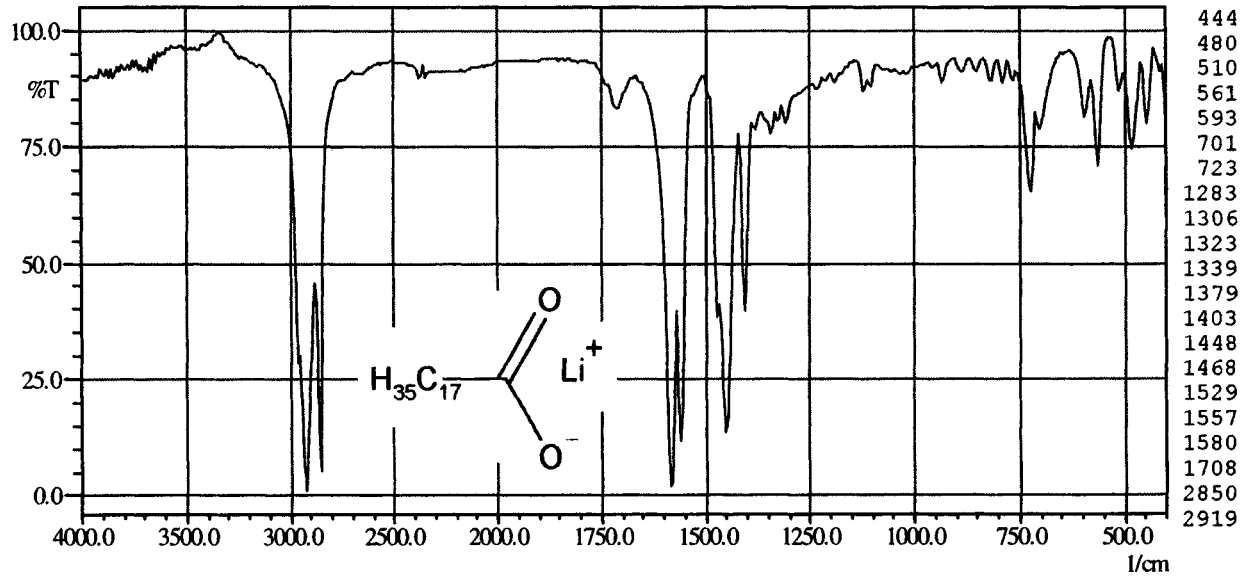
(1) **Ba laurate**
(2) Barium-Laurat
(3) Reagens
(4) 536.0+E154 g mol^{-1}
(5) PVC-costabiliser
(6) colourless solid
(7) 200 °C
(13) KBr pellet

12411 $C_{24}H_{46}O_4Cd$



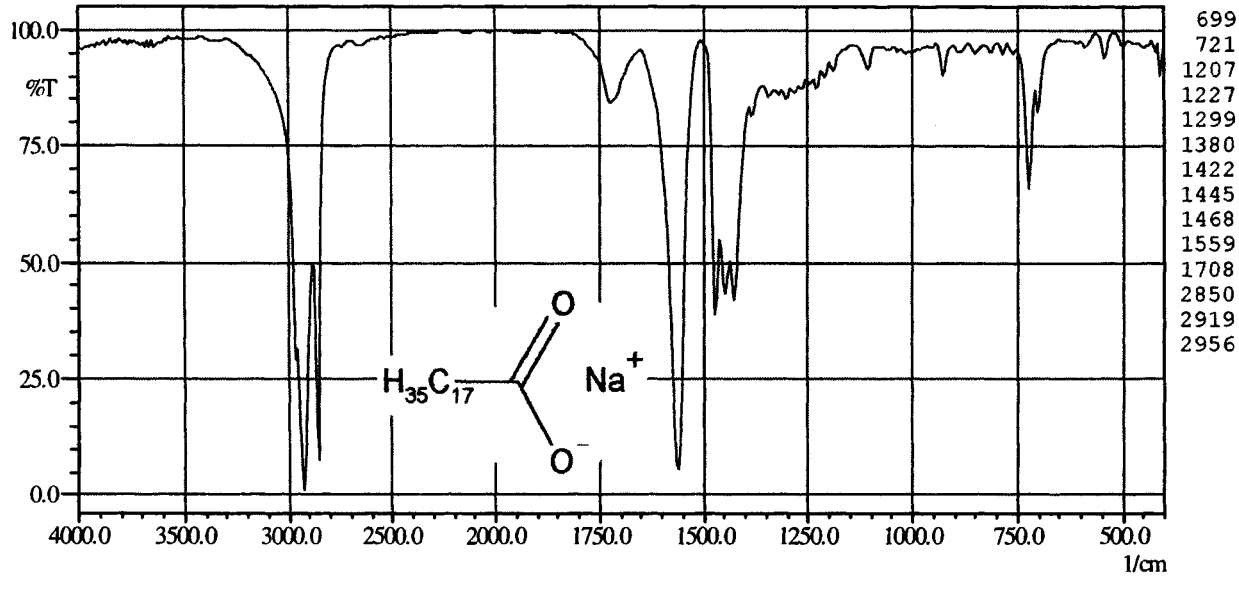
(1) **Cd laurate**
(2) Cadmium-Laurat
(3) Reagens
(4) 511.0 g mol^{-1}
(5) PVC-costabiliser
(6) colourless solid
(7) 100 °C
(13) KBr pellet

12411 $C_{18}H_{36}O_2Li$



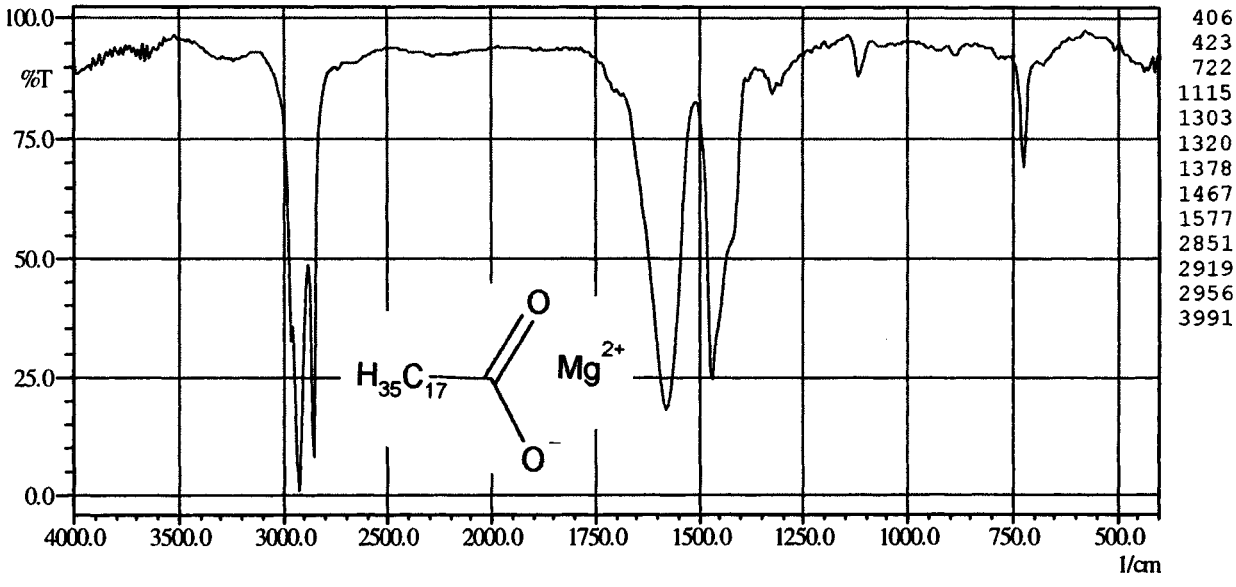
(1) **Li stearate**
(2) Lithium-Stearat
(3) Reagens
(4) 291.4 g mol^{-1}
(5) stabiliser
(6) colourless solid
(13) KBr pellet

12411 $C_{18}H_{36}O_2Na$



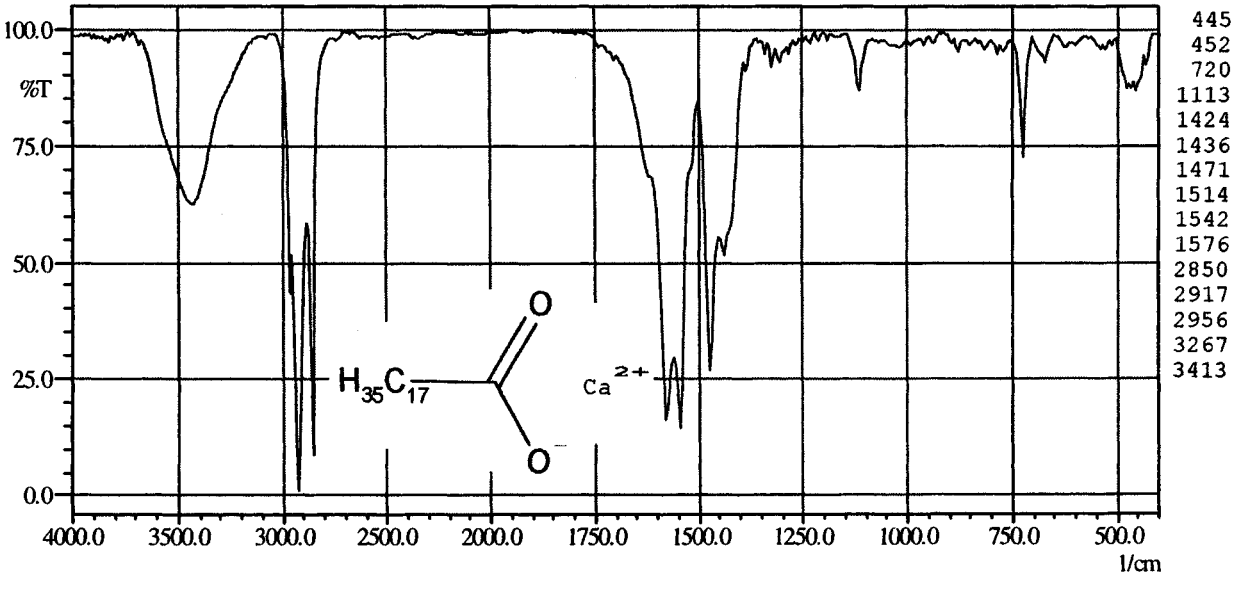
(1) **Na stearate**
(2) Natrium-Stearat
(3) Reagens
(4) 307.5 g mol^{-1}
(5) stabiliser
(6) colourless solid
(13) KBr pellet

12411 $C_{36}H_{70}O_4Mg$



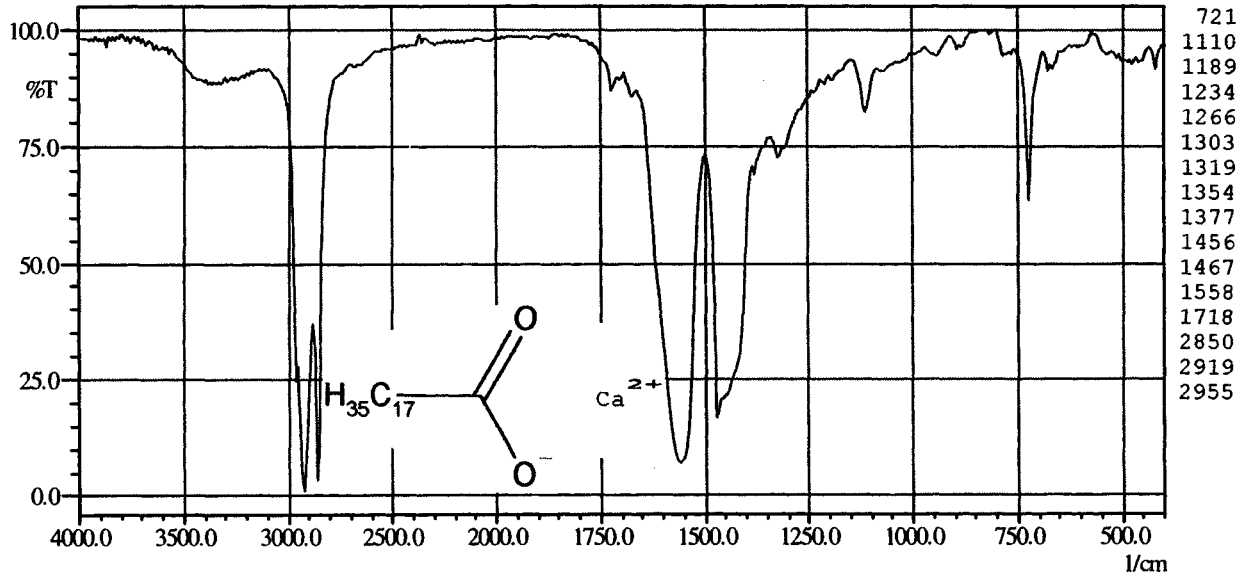
(1) **Mg stearate**
(2) Magnesium-Stearat
(3) Reagens
(4) 591.3 g mol^{-1}
(5) stabiliser
(6) colourless solid
(13) KBr pellet

12411 $C_{36}H_{70}O_4Ca$



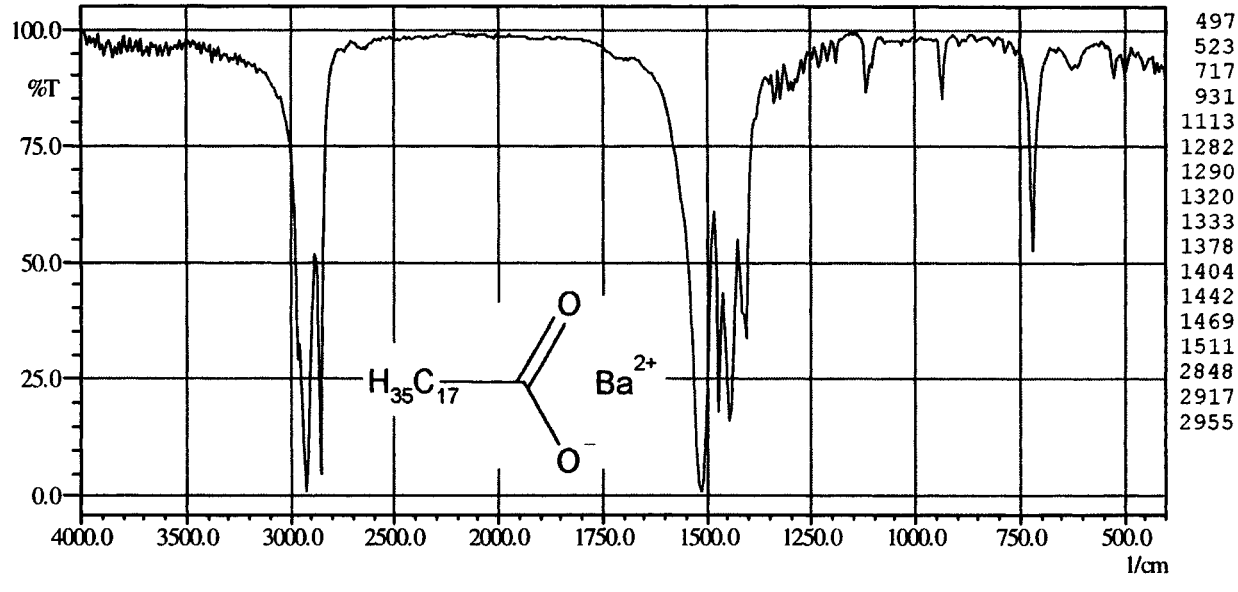
(1) **Ca stearate**
(2) Calcium Stearate IT
(3) Swedstab
(4) 607.0 g mol^{-1}
(5) PVC-stabiliser
(6) colourless solid
(13) KBr pellet

12411 $C_{36}H_{70}O_4Ca$



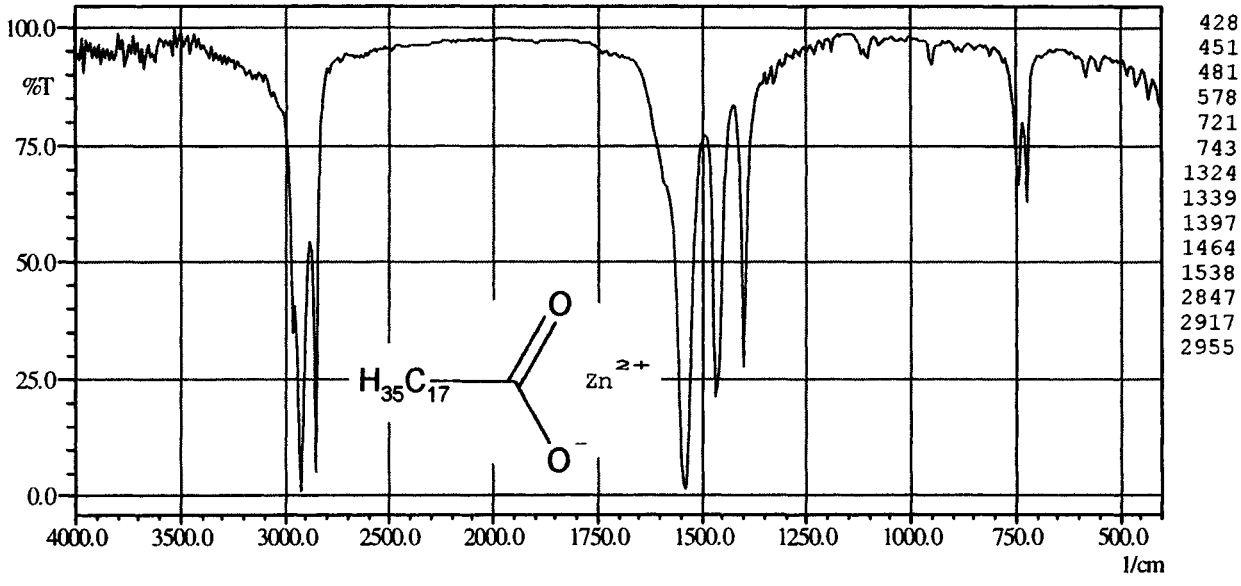
(1) **Ca stearate**
(2) Listab Ca
(3) mg Technologies/Chemson
(4) 607.0 g mol^{-1}
(5) PVC-stabiliser
(6) colourless solid
(13) solidified melt btw KBr

12411 $C_{36}H_{70}O_4Ba$



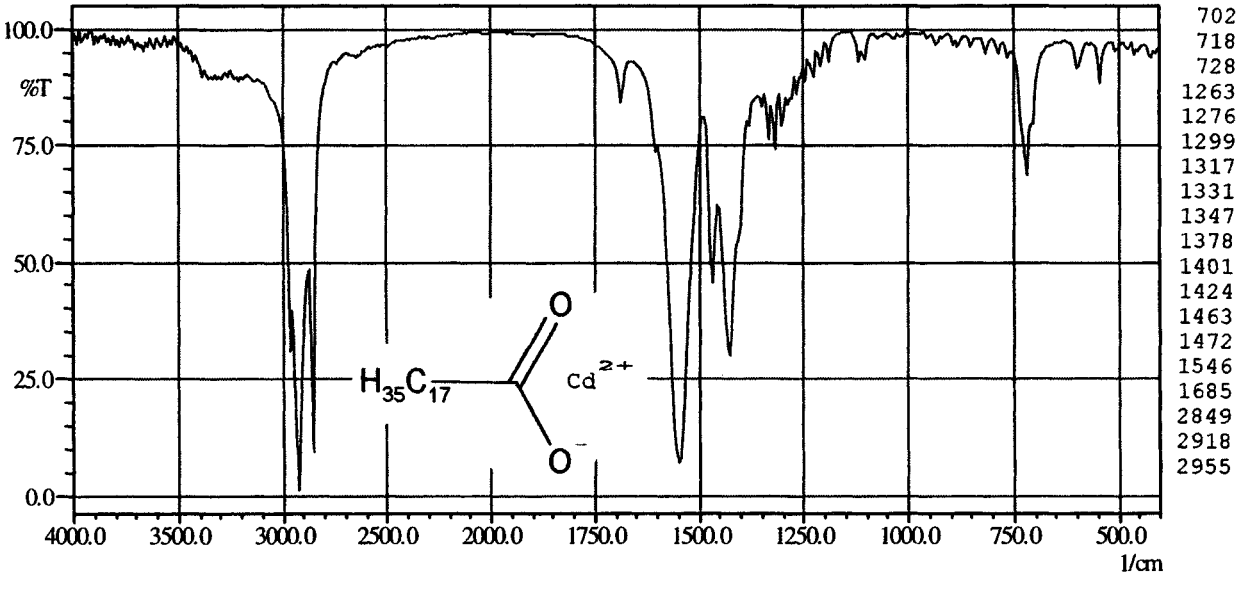
(1) **Ba stearate**
(2) Barium-Stearat
(3) Reagens
(4) 704.2 g mol^{-1}
(5) PVC-costabiliser, lubricant
(6) colourless solid
(13) KBr pellet

12411 $C_{36}H_{70}O_4Zn$



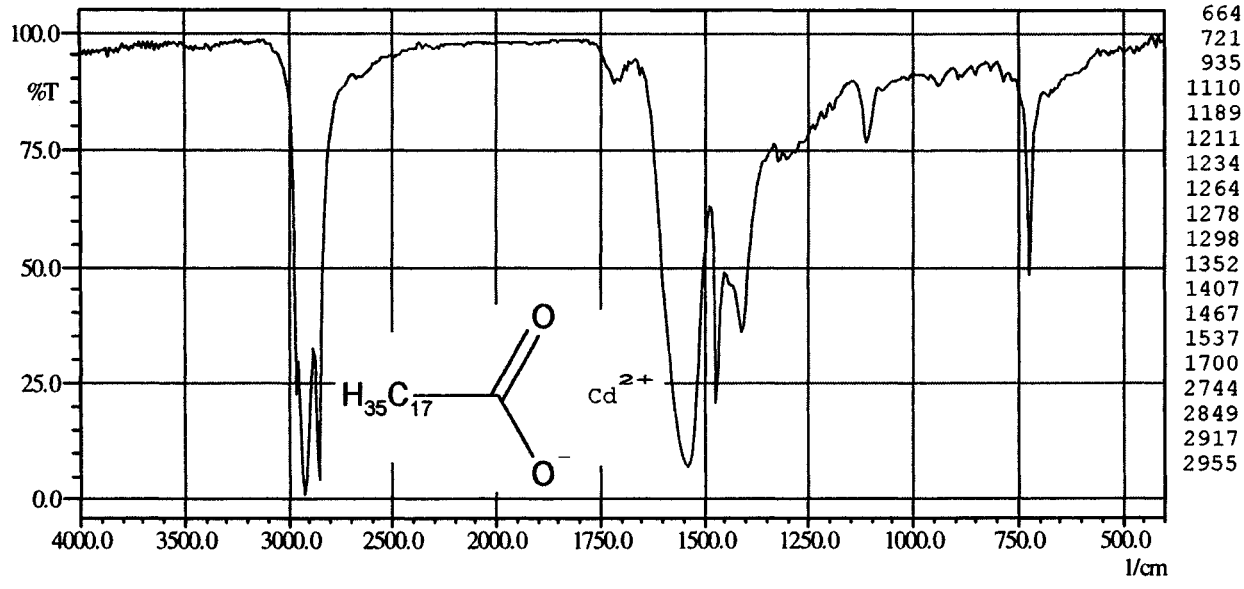
(1) **Zn stearate**
(2) Zink-Stabilisator LF
(3) Reagens
(4) 632.3 g mol^{-1}
(5) PVC-costabiliser
(6) colourless solid
(7) 121 °C
(13) KBr pellet

12411 $C_{36}H_{70}O_4Cd$



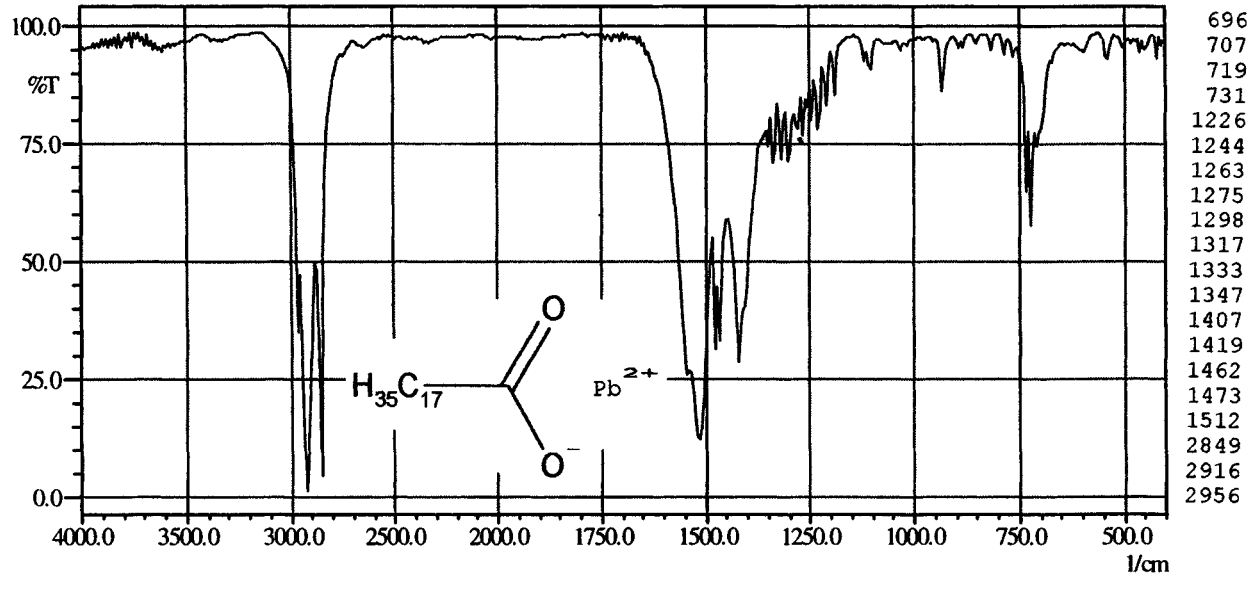
(1) **Cd stearate**
(2) Cadmium-Stearat
(3) Reagens
(4) 679.4 g mol^{-1}
(5) PVC-costabiliser
(6) colourless solid
(7) 105 °C
(13) KBr pellet

12411 $C_{36}H_{70}O_4Cd$



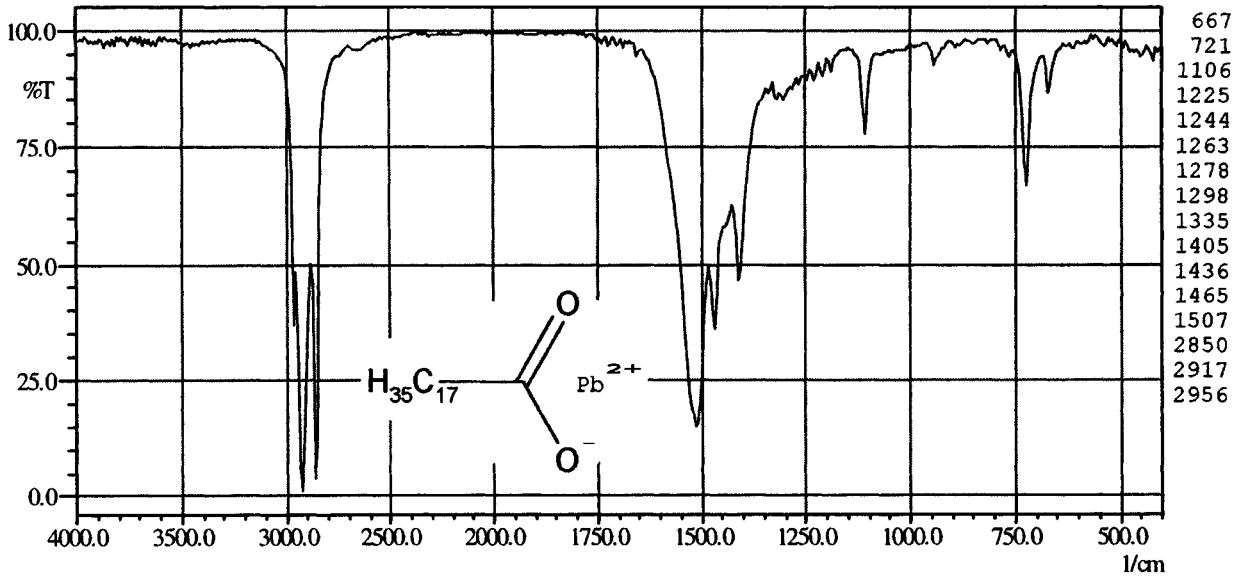
(1) **Cd stearate**
(2) Naftovin BM 16
(3) mg Technologies/Chemson
(4) 679.4 g mol^{-1}
(5) PVC-stabiliser
(6) colourless solid
(13) solidified melt btw KBr

12411 $C_{36}H_{70}O_4Pb$



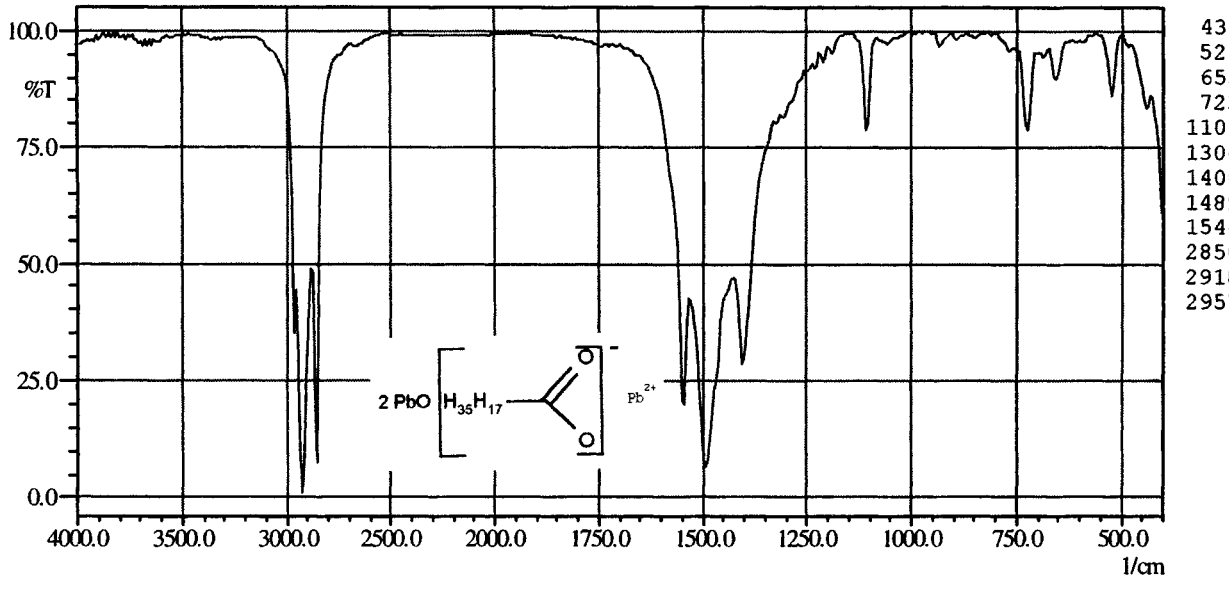
(1) **Pb stearate**
(2) Interstab LP 3155
(3) Akzo Chemie
(4) 774.2 g mol^{-1}
(5) stabiliser
(6) cream-coloured solid
(13) KBr pellet

12411 $C_{36}H_{70}O_4Pb$



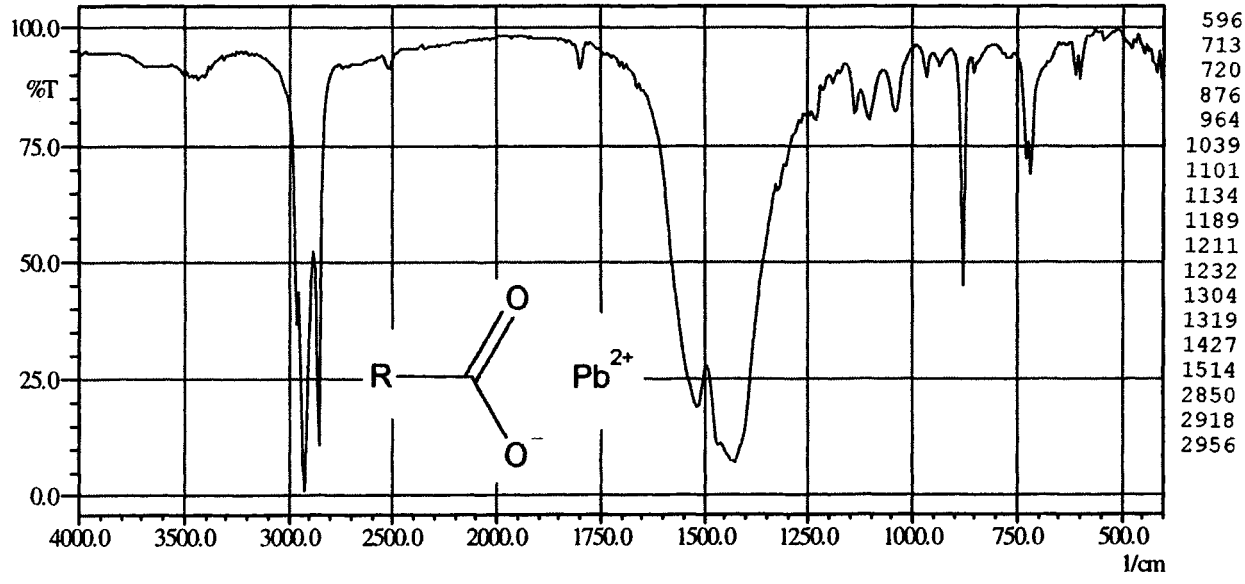
(1) **Pb stearate**
(2) Listab 28 ND
(3) mg Technologies/Chemson
(4) 774.2 g mol^{-1}
(5) PVC-stabiliser
(6) colourless solid
(9) 1.4 g cm^{-3}
(13) KBr pellet

12411 $_2PbO\ C_{36}H_{70}O_4Pb$



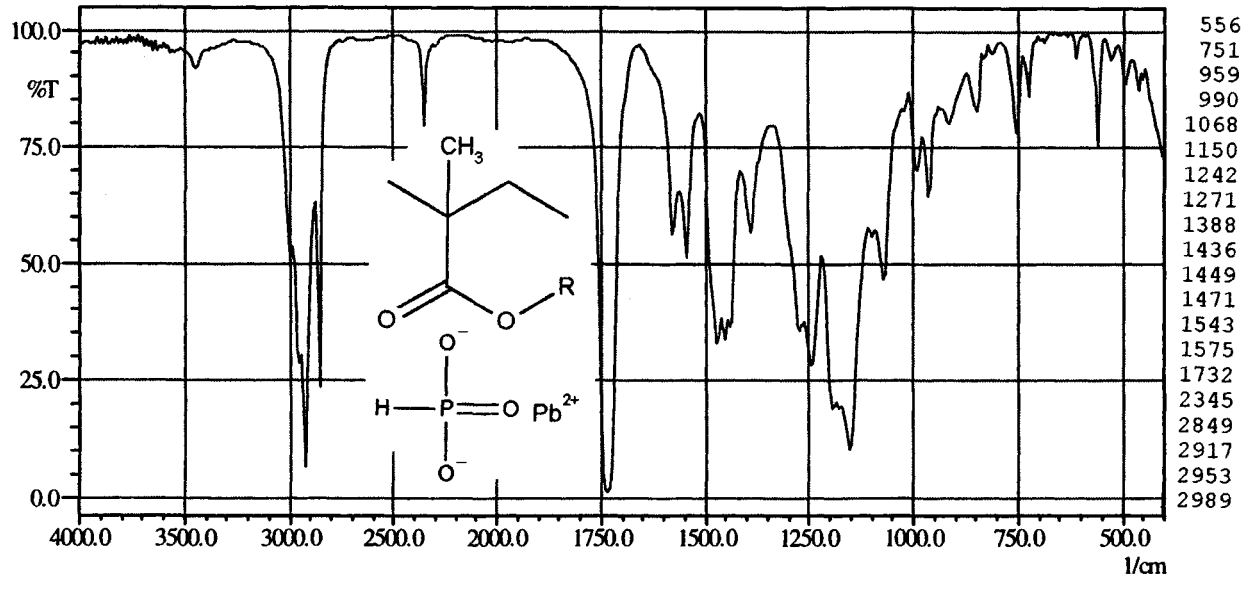
(1) **2-basic Pb stearate**
(2) Zweibasisches Blei-Stearat
(3) Reagens
(4) 1221 g mol^{-1}
(5) stabiliser
(6) colourless solid
(9) 2.02 g cm^{-3}
(13) KBr pellet

12411



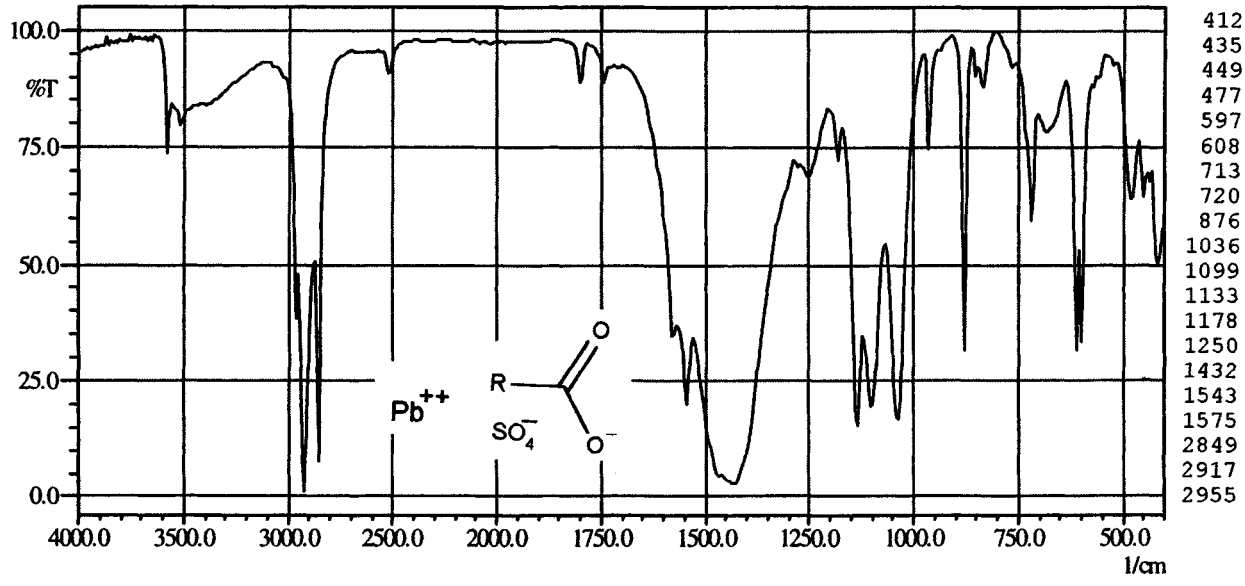
(1) **basic Pb carboxylate + $CaCO_3$**
(2) Baeropan SMS 314
(3) Baerlocher
(5) PVC stabiliser
(6) light-brown flakes
(9) 1.8 g cm^{-3}
(13) KBr pellet

12411+11213



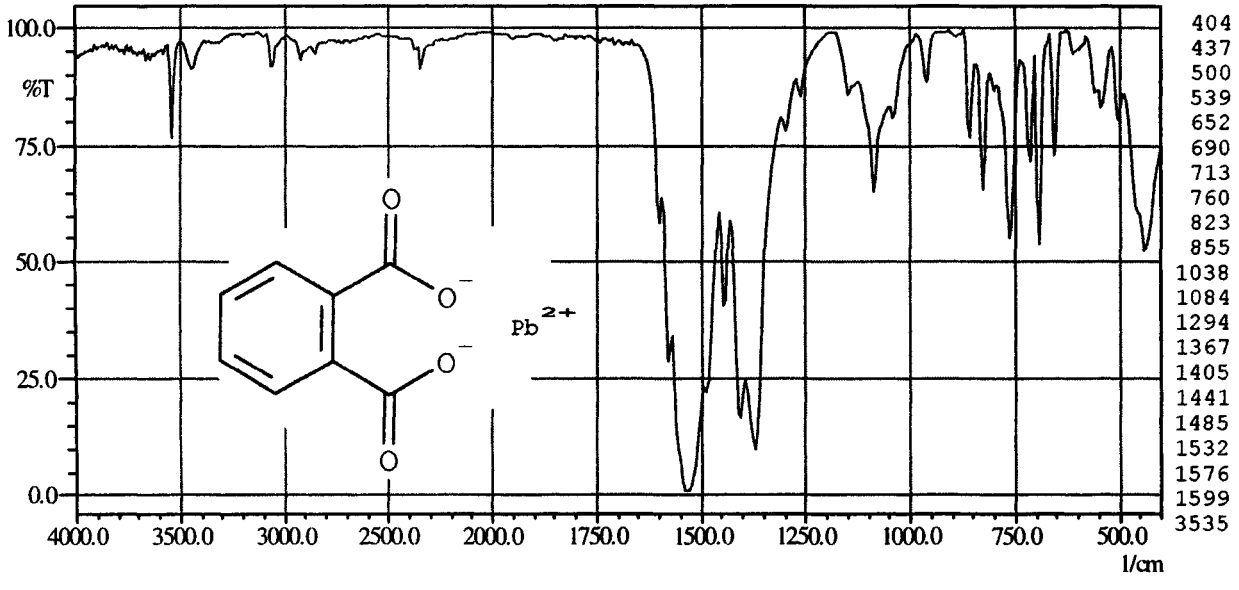
(1) **basic Pb complex with ester, carboxylate and phosphite groups**
(2) Baeropan MC 2567 SL
(3) Baerlocher
(5) stabiliser
(6) colourless solid
(9) 1.3 g cm^{-3}
(13) KBr pellet

12411+12114



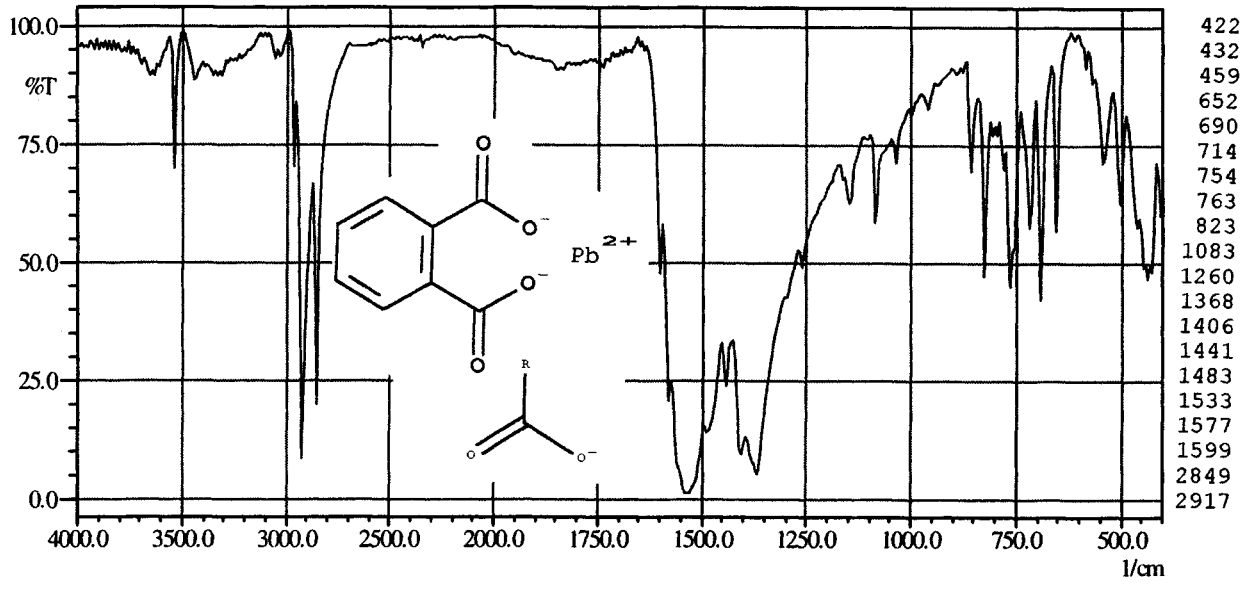
(1) **coprecipitate Pb-carboxylate + $PbSO_4$+$CaCO_3$**
(2) Baeropan 2028 SP
(3) Baerlocher
(5) PVC stabiliser
(6) colourless solid
(13) KBr pellet

12416 **$2PbO \cdot C_8H_4O_4Pb$**



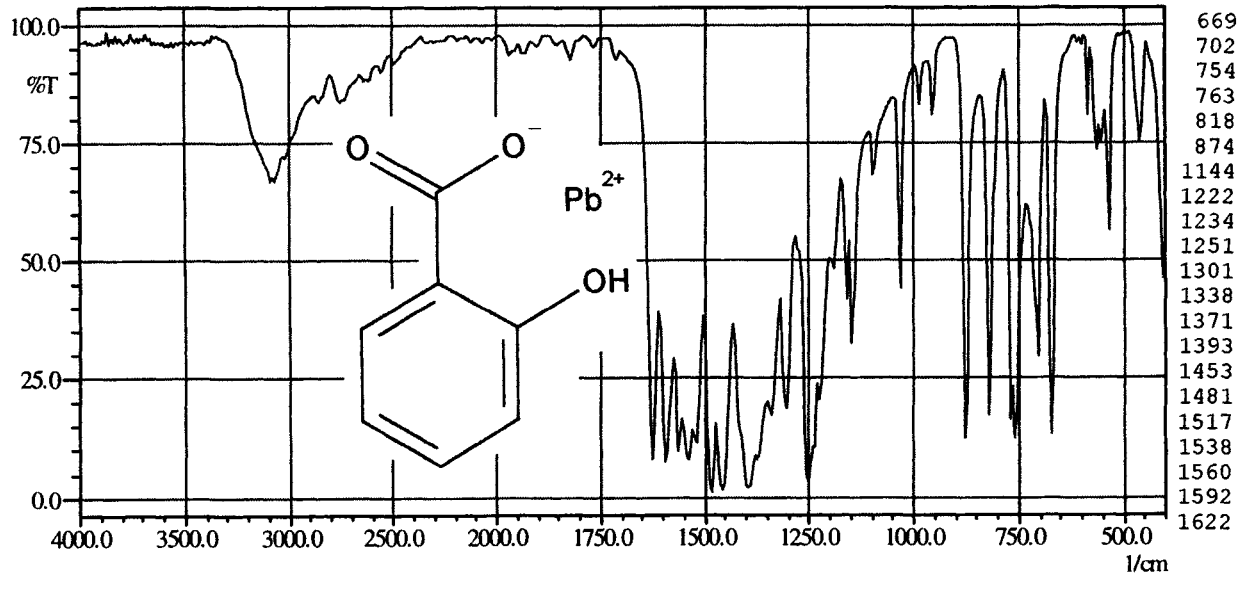
(1) **2-basic Pb phthalate**
(2) Interstab PDP-E
(3) Akzo Chemie
(4) 817.8 g mol^{-1}
(5) stabiliser
(6) colourless solid
(13) KBr pellet

12416 $2PbO \cdot C_8H_4O_4Pb$



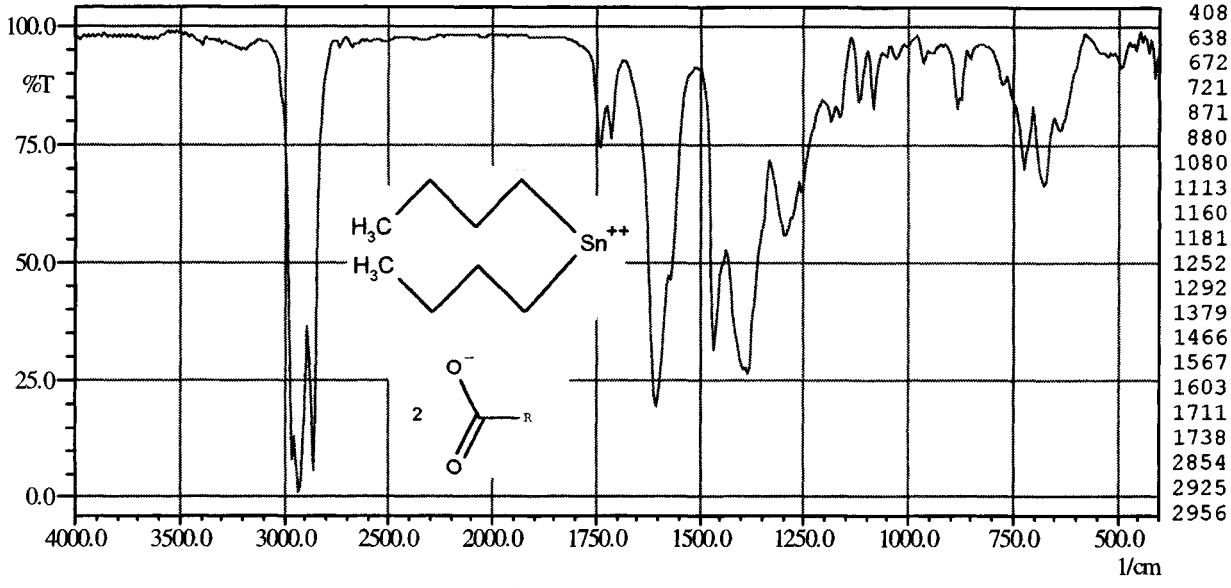
(1) **2-basic Pb phthalate with fatty acid carboxylate**
(2) Baerostab E 503
(3) Baerlocher
(4) 817.8 g mol^{-1}
(5) stabiliser
(6) colourless granules
(9) 3 g cm^{-3}
(13) KBr pellet

12418 $C_7H_4O_3Pb$



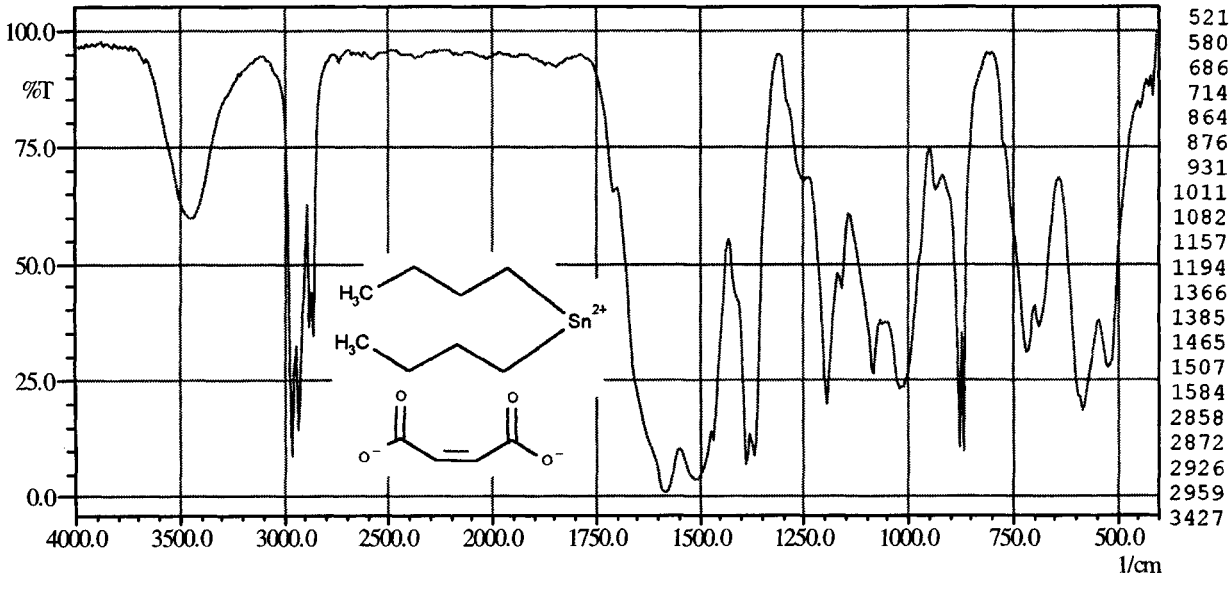
(1) **Pb salicylate**
(2) Naftovin T 50
(3) mg Technologies/Chemson
(4) 343.3 g mol^{-1}
(5) PVC-stabiliser
(6) colourless, fine-crystalline solid
(9) 2.4 g cm^{-3}
(13) KBr pellet

12421 $C_{32}H_{64}O_4Sn$



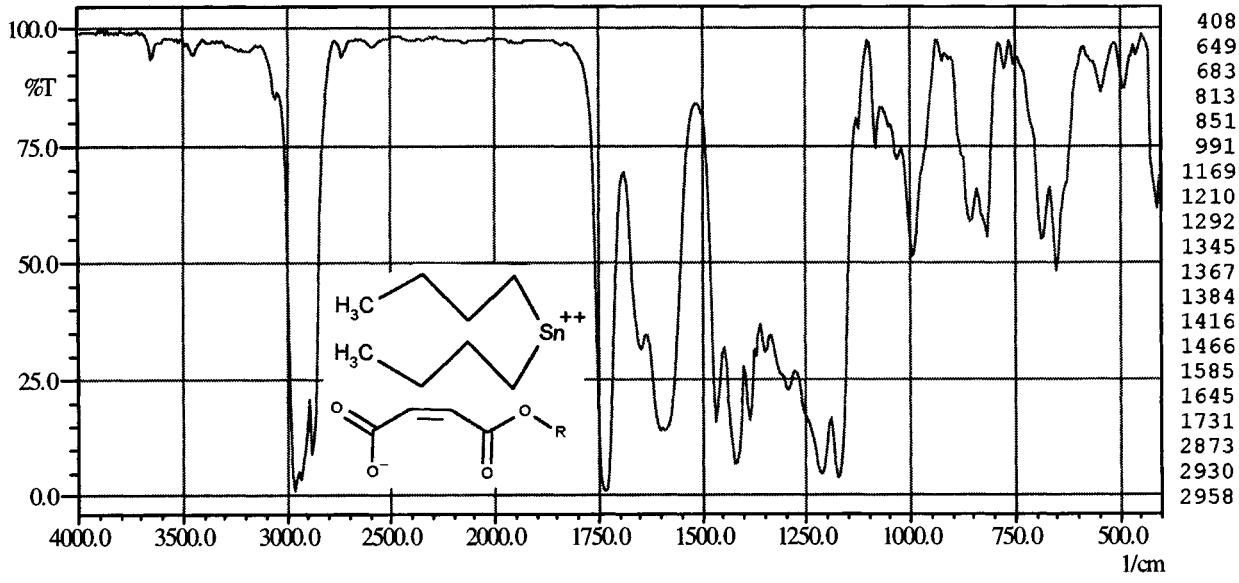
(1) **dibutyltin dilaurate**
(2) Meister Z 4101
(3) Meister
(4) 631.6 g mol^{-1}
(5) stabiliser
(6) slightly yellowish, clear liquid
(13) layer btw KBr

12421 $C_{12}H_{20}O_4Sn$



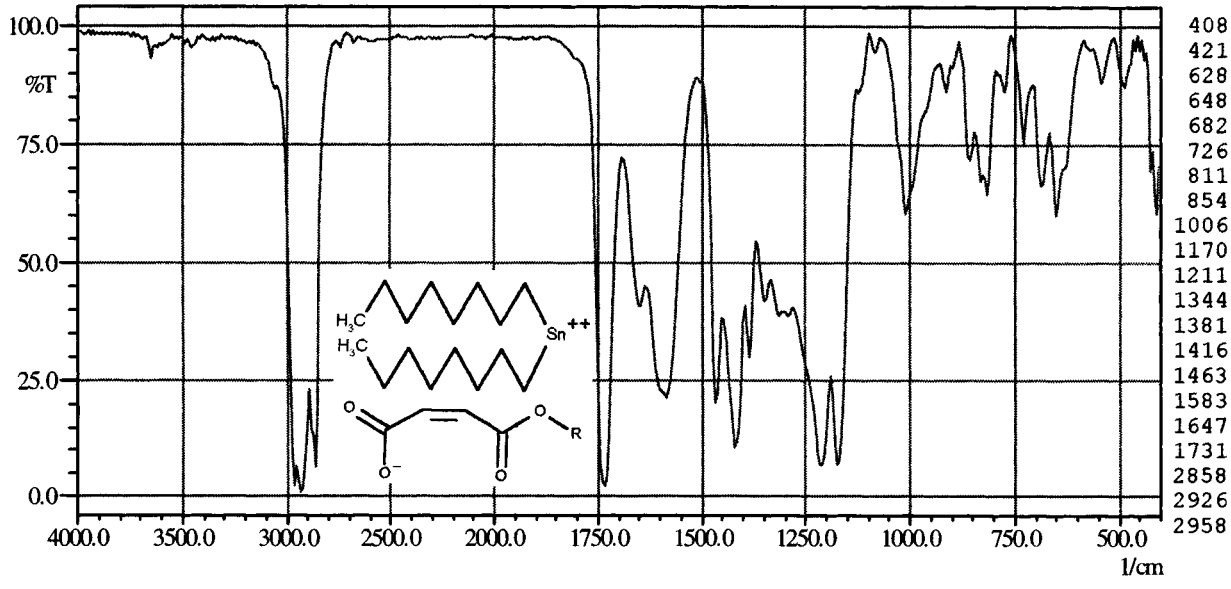
(1) **dibutyltin maleate**
(2) Meister DBTM
(3) Meister
(4) 347.0 g mol^{-1}
(5) PVC-costabiliser
(6) colourless solid
(13) KBr pellet

12421



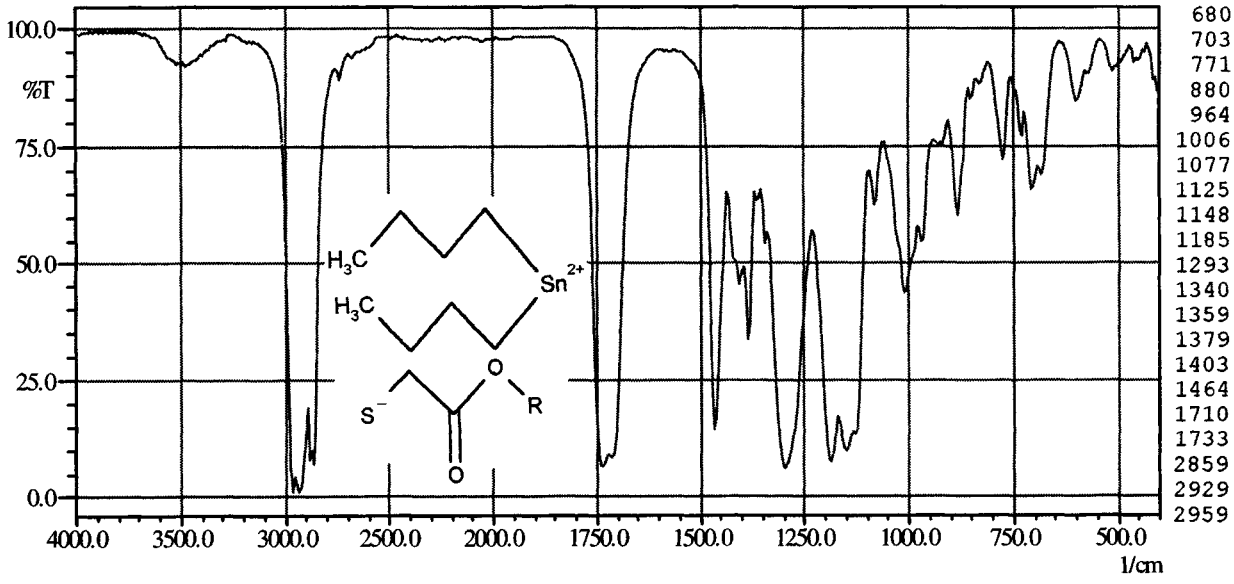
(1) **dibutyltin maleicester carboxylate**
(2) Stanclere T 85
(3) Akzo Chemicals
(5) stabiliser
(6) colourless, clear liquid
(13) layer btw KBr

12421



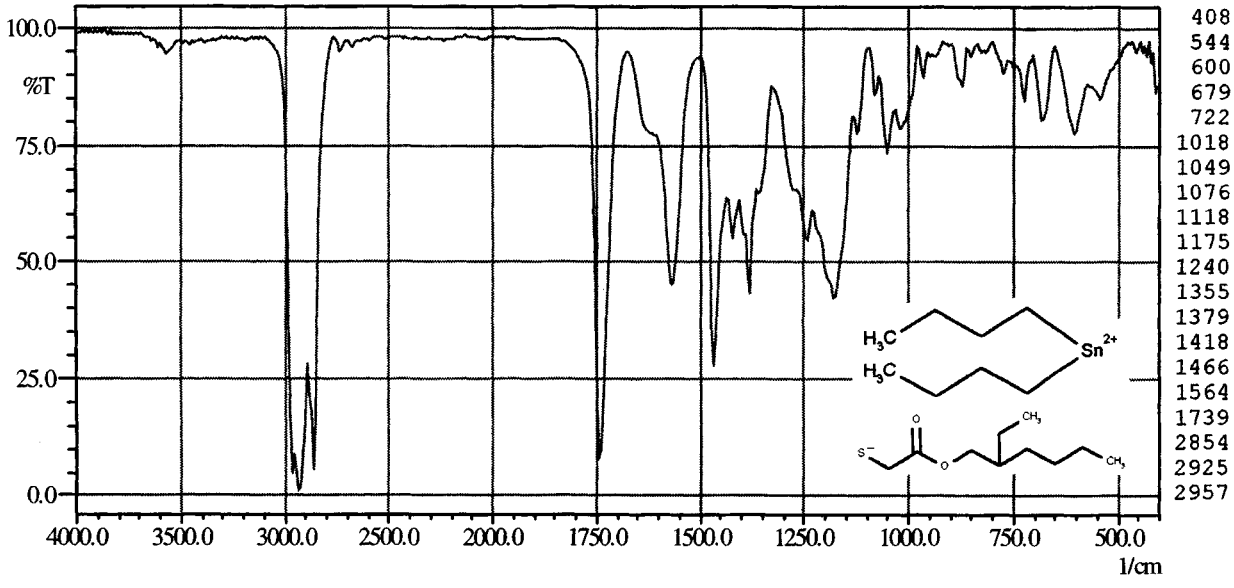
(1) **dioctyltin maleicester carboxylate**
(2) Stanclere T 80
(3) Akzo Chemicals
(5) stabiliser
(6) colourless, clear liquid
(13) layer btw KBr

12422



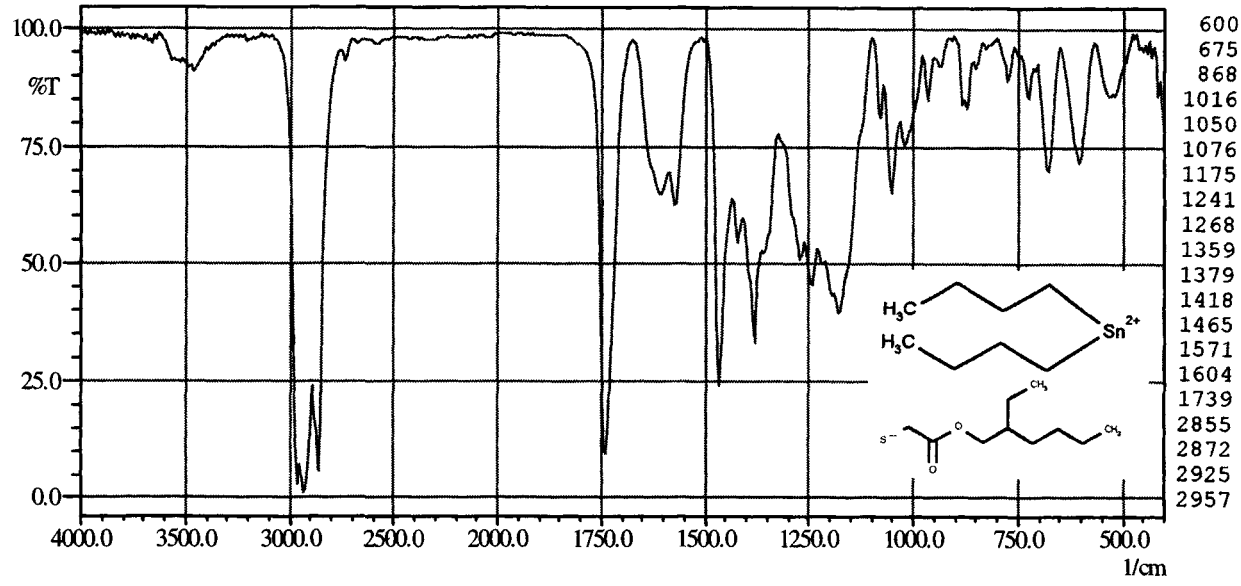
(1) **dibutyltin thioglycolate**
(2) Hostastab Sn S 61
(3) Hoechst
(5) PVC-stabiliser
(6) colourless, clear liquid
(7) -50 °C
(9) 1.1 g cm^{-3}
(10) 1.499
(13) layer btw KBr

12422 $C_{28}H_{56}O_4SSn$



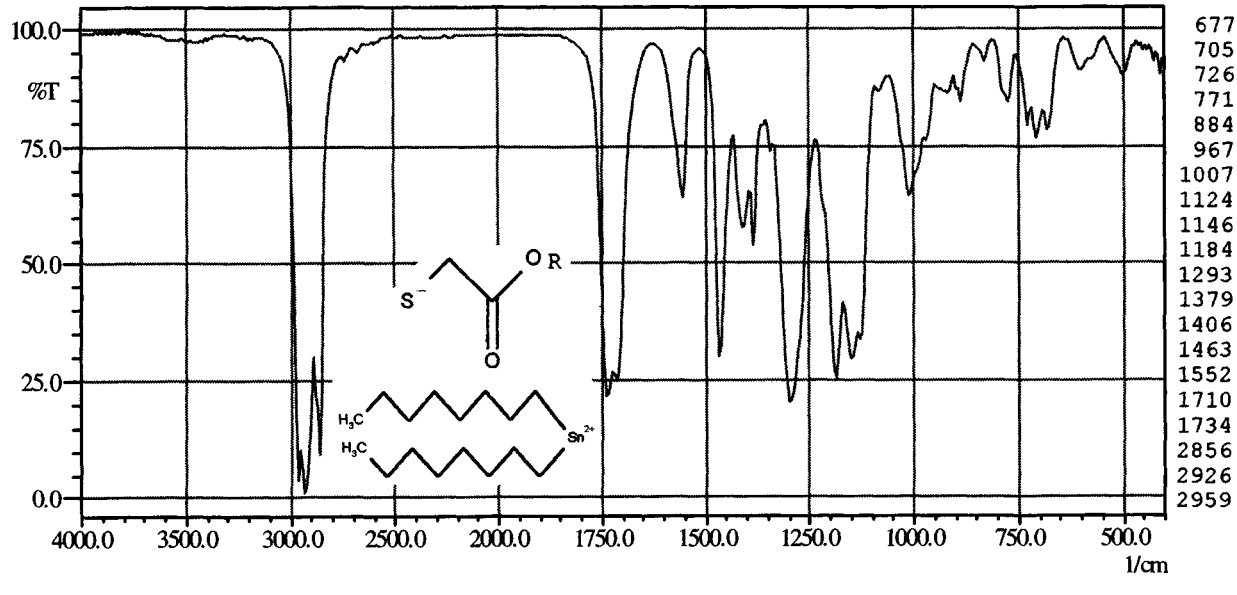
(1) **dibutyltin thioglycolic acid 2-ethylhexylester mercaptide**
(2) Stanclere T 160
(3) Akzo Chemicals
(4) 607.5 g mol^{-1}
(5) stabiliser
(6) colourless, clear liquid
(13) layer btw KBr

12422 $C_{28}H_{56}O_4SSn$



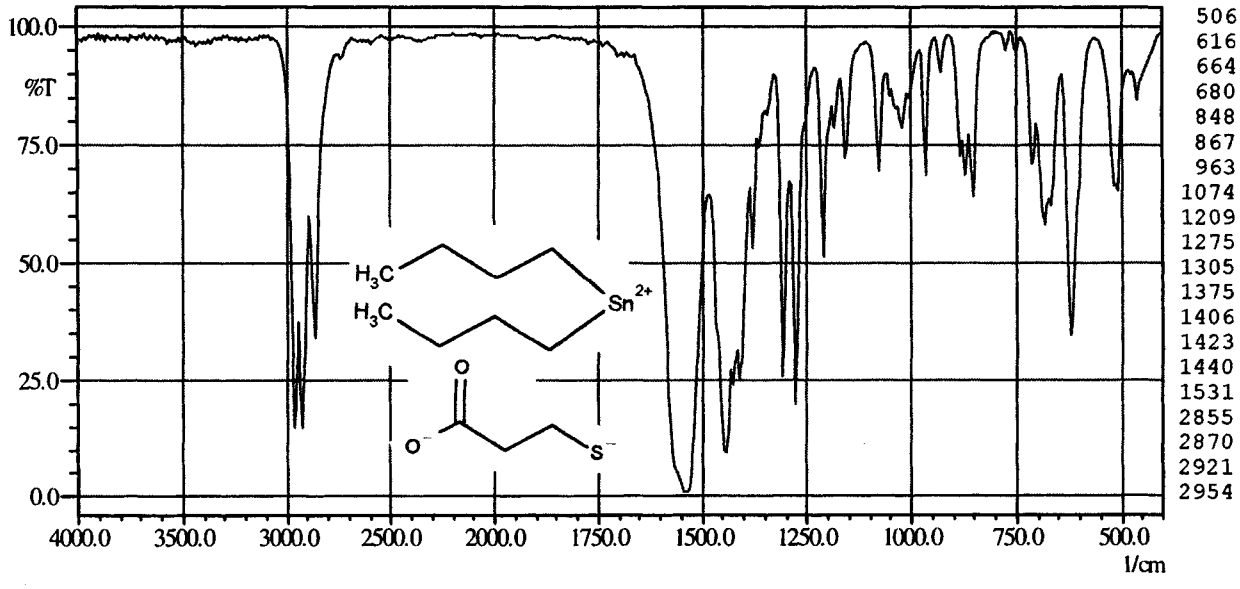
(1) **dibutyltin thioglycolic acid 2-ethylhexylester mercaptide**
(2) Stanclere T 161
(3) Akzo Chemicals
(4) 607.5 g mol^{-1}
(5) stabiliser
(6) colourless, clear liquid
(13) layer btw KBr

12422



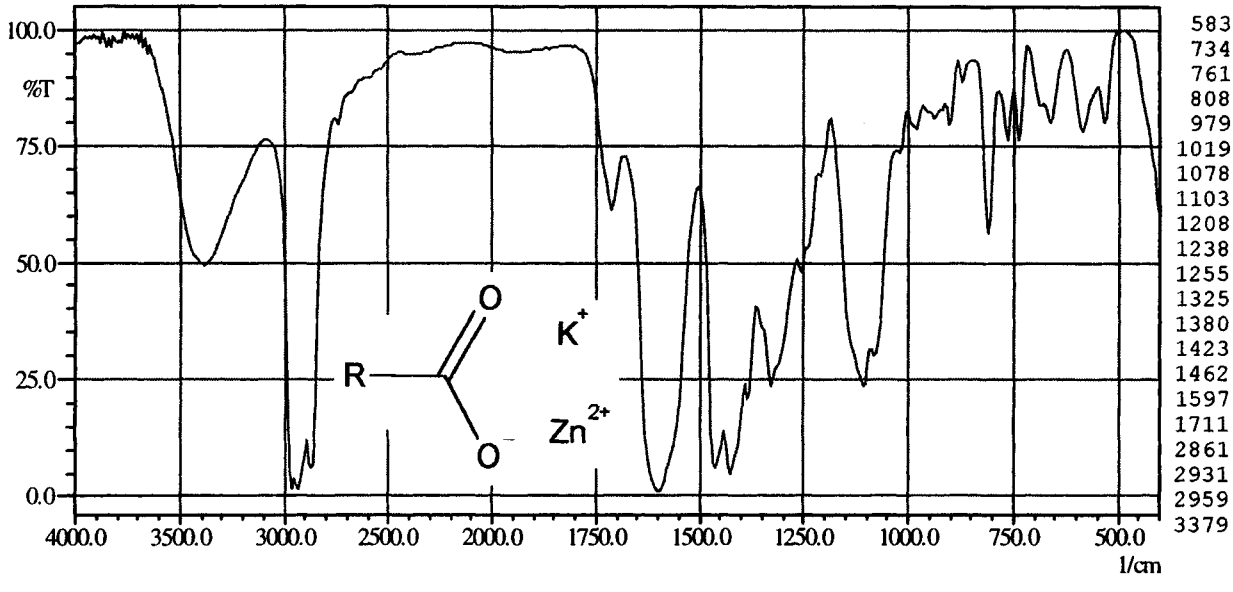
(1) **dioctyltin thioglycolic alkylester mercaptide**
(2) Hostastab Sn S 15
(3) Hoechst
(5) PVC-stabiliser
(6) colourless, clear liquid
(7) −50 °C
(9) 1.08 g cm^{-3}
(10) 1.499
(13) layer btw KBr

12422 $C_{11}H_{22}O_2SSn$



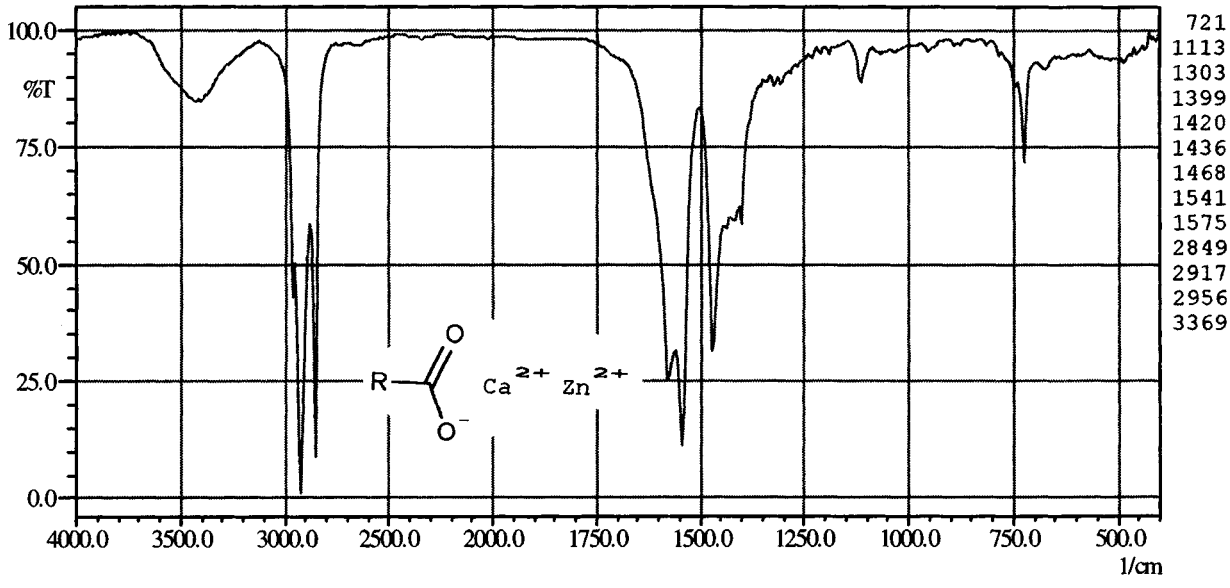
(1) **dibutyltin mercaptopropionate**
(2) Stanclere T 186
(3) Akzo Chemicals
(4) 337.1 g mol^{-1}
(5) stabiliser
(6) colourless solid
(13) KBr pellet

12431



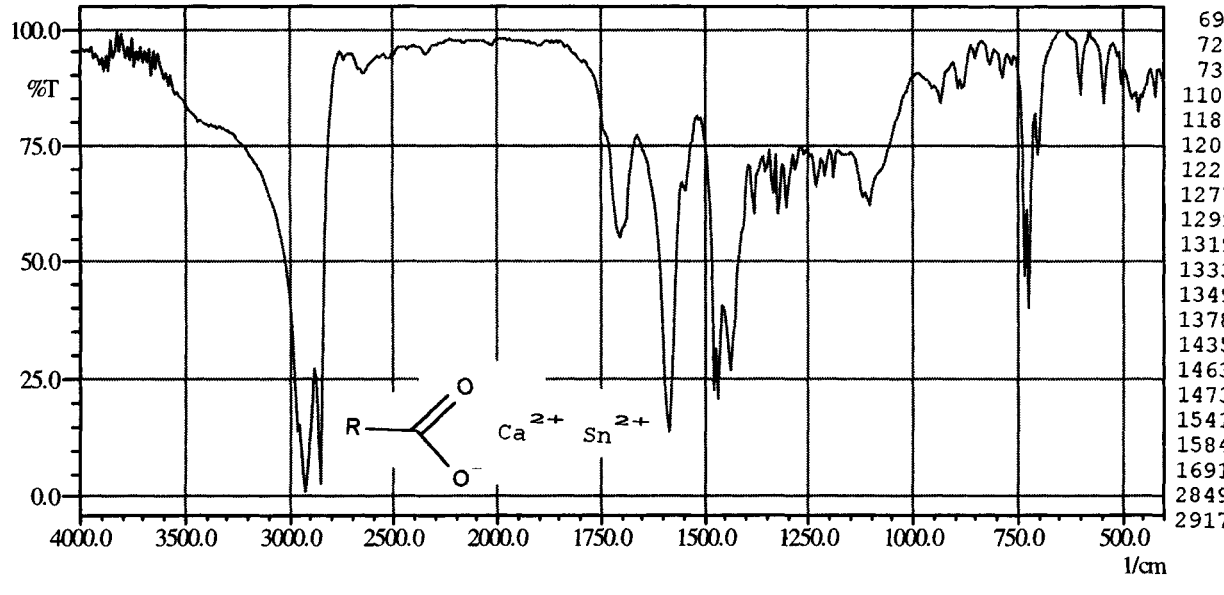
(1) **K Zn complex**
(2) Interstab M 731
(3) Akzo Chemie
(5) stabiliser
(6) amber-coloured, clear liquid
(13) layer btw KBr

12431



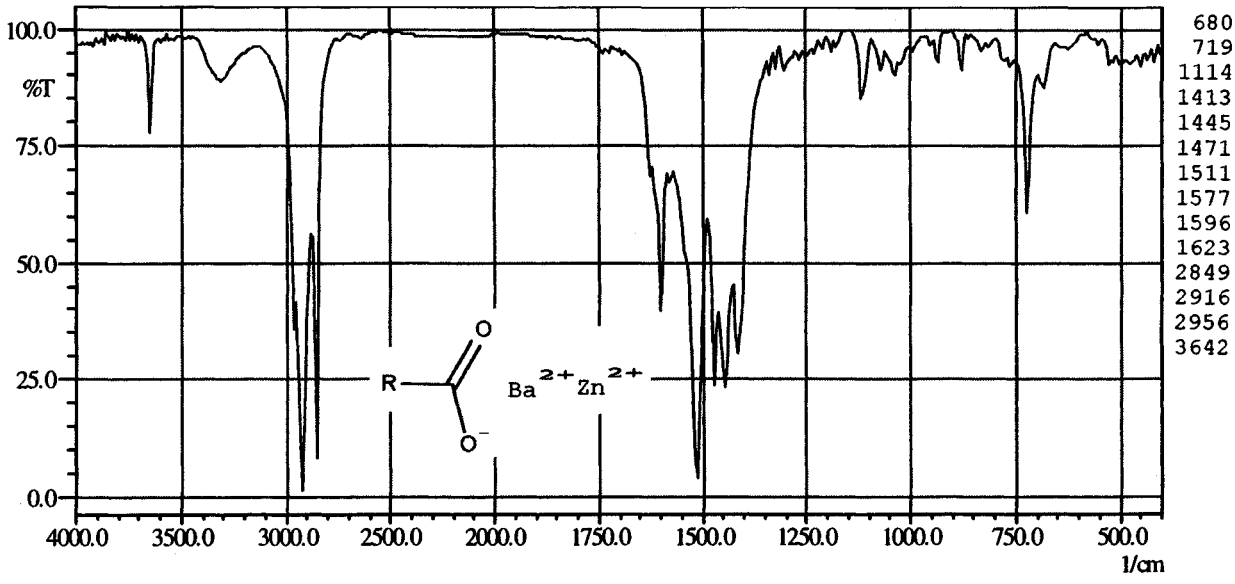
(1) **Ca Zn complex**
(2) Baerostab NT 1 S
(3) Baerlocher
(5) stabiliser
(6) colourless solid
(13) KBr pellet

12431



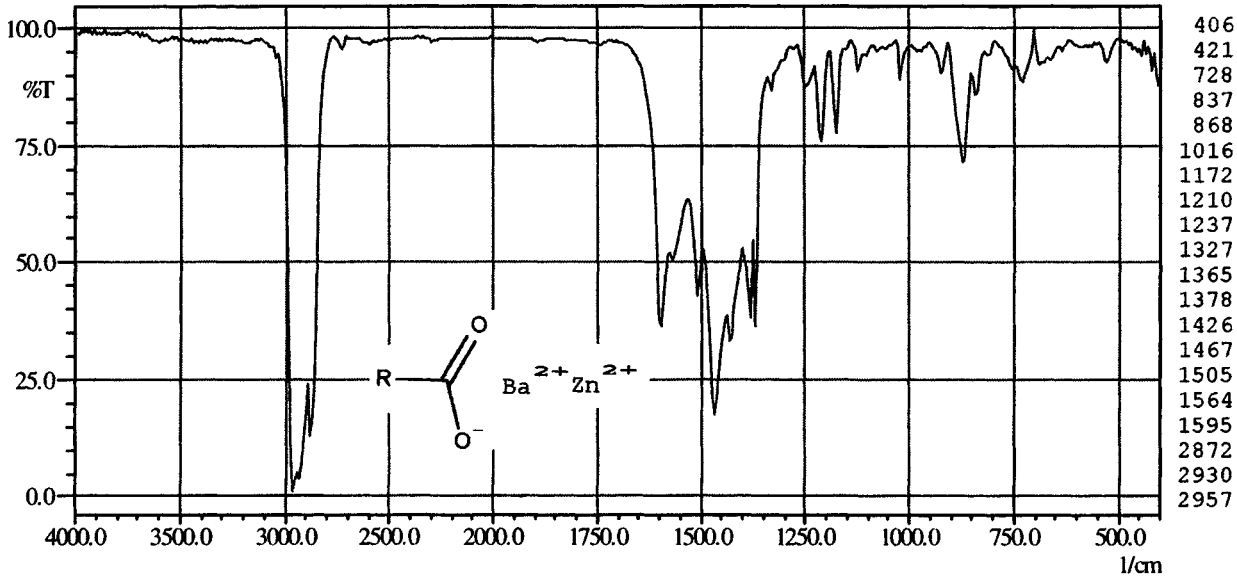
(1) **Ca Sn complex**
(2) Baeropan SN 200
(3) Baerlocher
(5) stabiliser-lubricant
(6) colourless solid
(9) 1 g cm^{-3}
(13) KBr pellet

12431



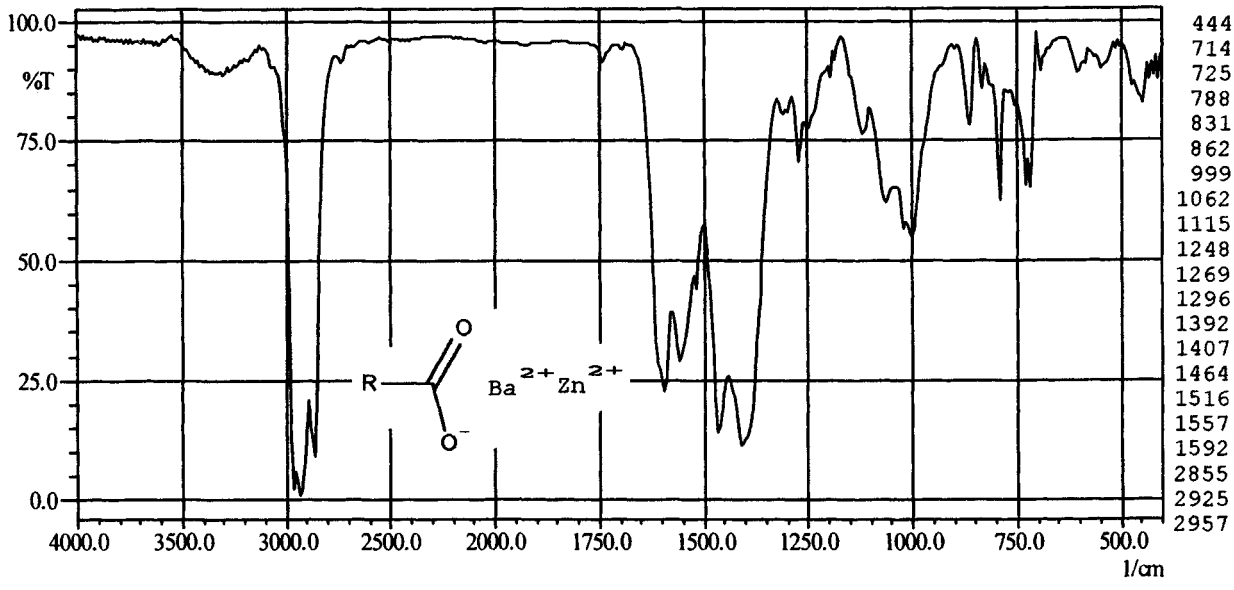
(1) **Ba Zn complex**
(2) Baerostab OE 666
(3) Baerlocher
(5) stabiliser
(6) colourless solid
(13) KBr pellet

12431



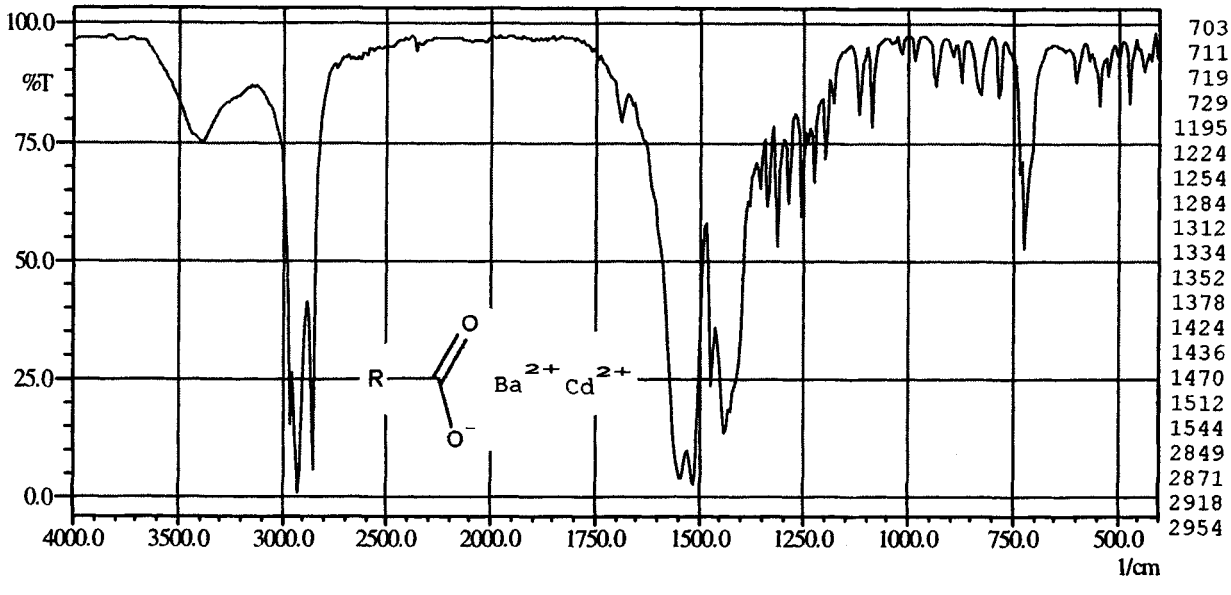
(1) **Ba Zn complex**
(2) Swedstab 504
(3) Swedstab
(5) PVC-stabiliser
(6) colourless, clear liquid
(9) 0.902 g cm^{-3}
(10) 1.448
(13) layer btw KBr

12431



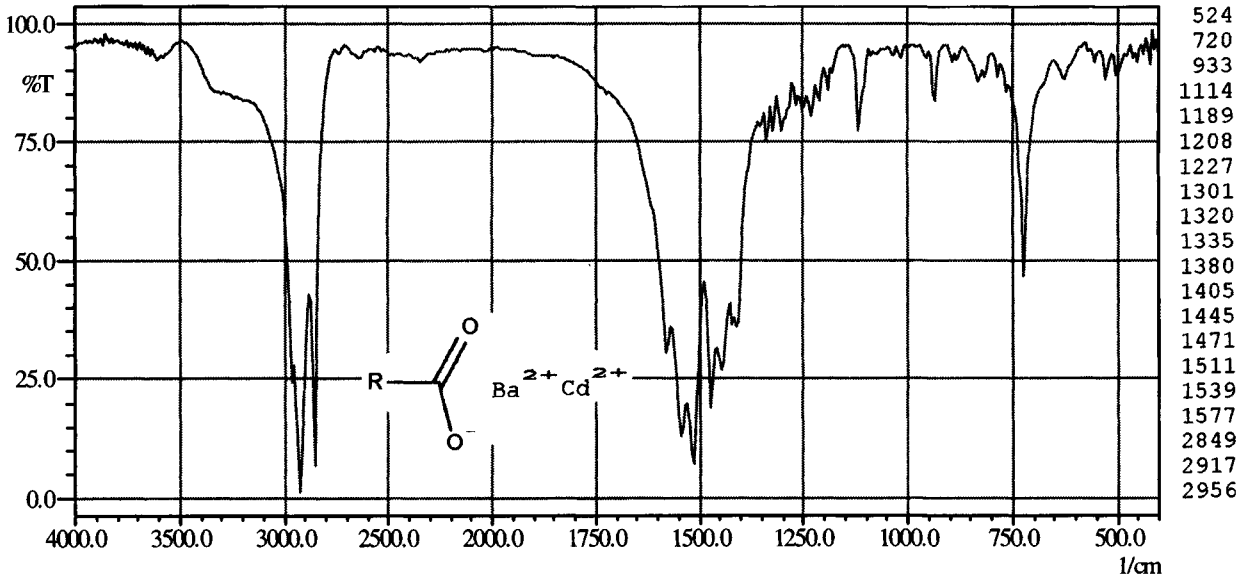
(1) **Ba Zn complex**
(2) Naftovin BZ 580
(3) mg Technologies/Chemson
(5) PVC-stabiliser
(6) yellow, clear liquid
(9) 1.08 g cm^{-3}
(10) 1.489
(13) layer btw KBr

12431



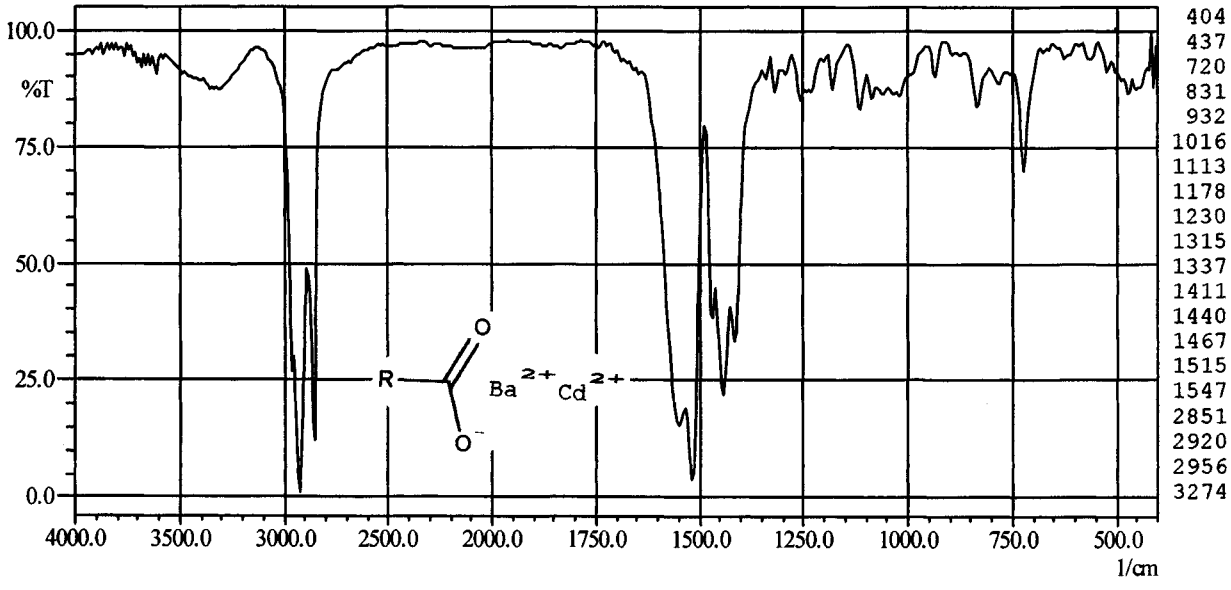
(1) **Ba Cd complex**
(2) Baerostab ZPS-F
(3) Baerlocher
(5) stabiliser
(6) colourless solid
(7) 90 °C
(13) KBr pellet

12431



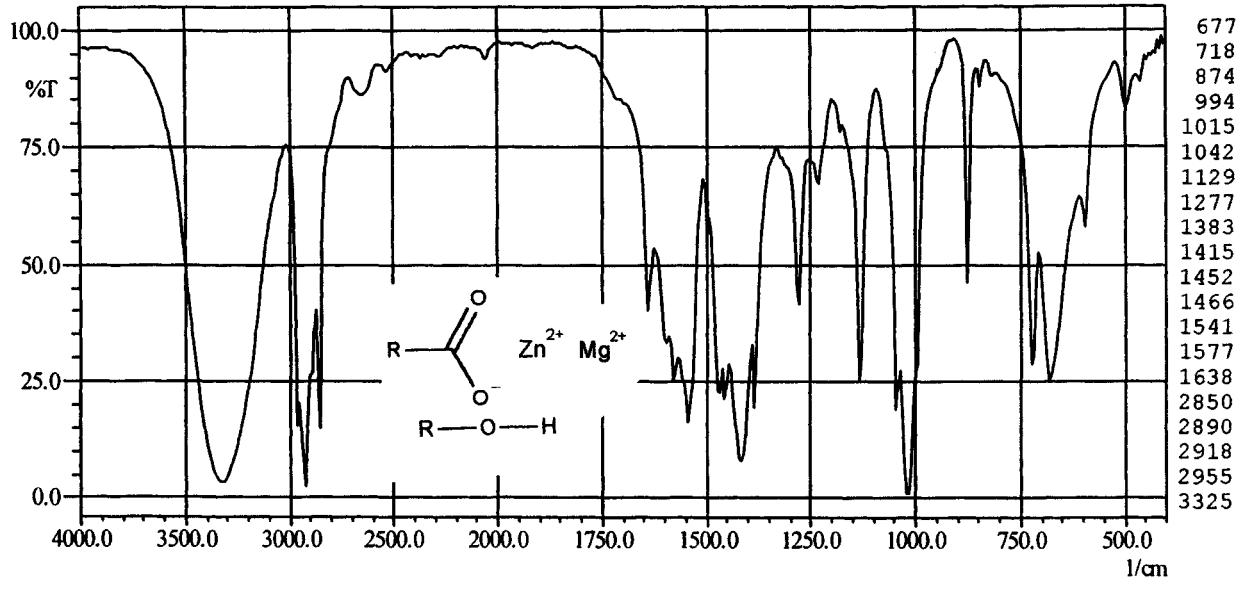
(1) **Ba Cd complex**
(2) Baerostab PC 52
(3) Baerlocher
(5) stabiliser
(6) colourless solid
(7) 90 °C
(13) KBr pellet

12431



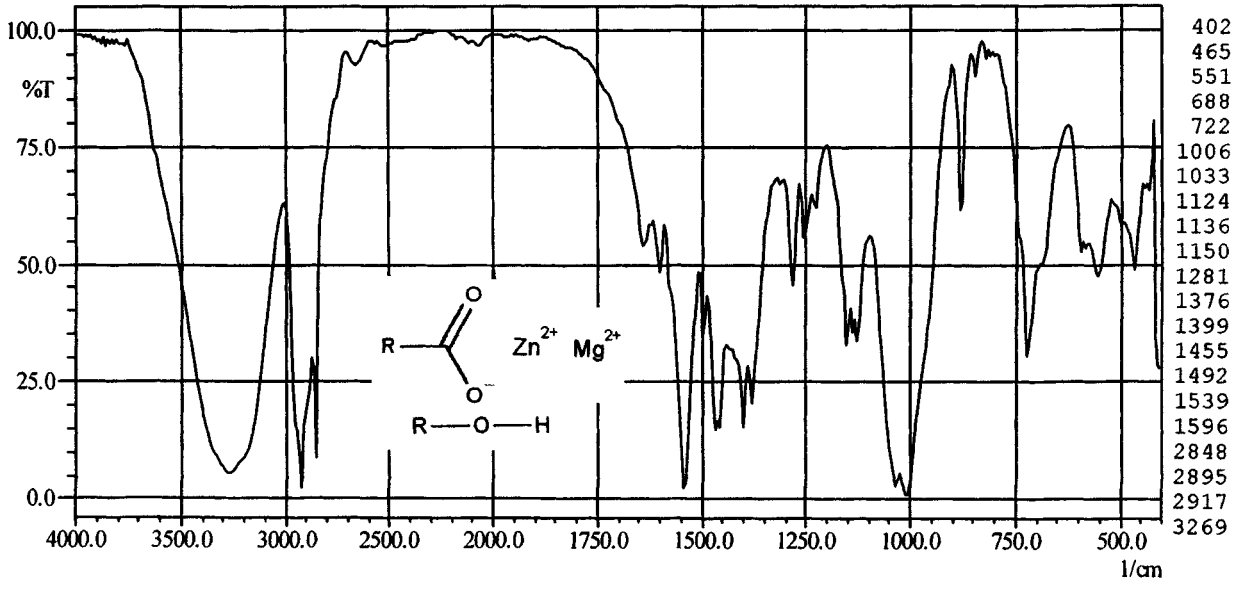
(1) **Ba Cd complex**
(2) Reagens FF/49
(3) Reagens
(5) stabiliser
(6) colourless solid
(13) KBr pellet

12431



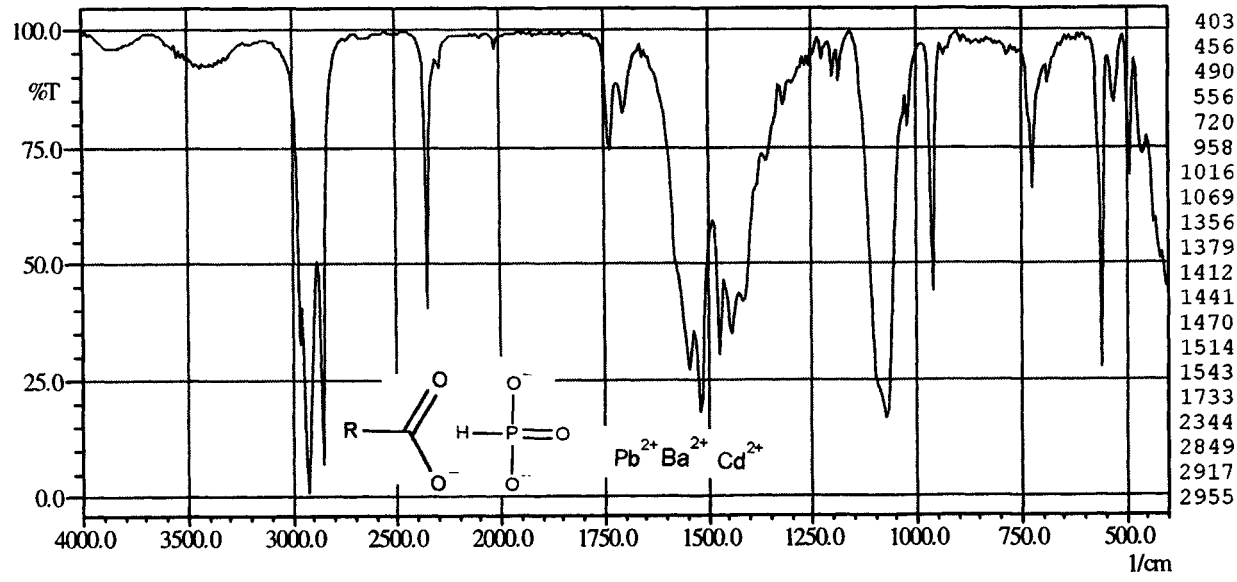
(1) **Zn Mg complex**
(2) Naftovin CKP 90030
(3) mg Technologies/Chemson
(5) PVC-stabiliser
(6) colourless solid
(9) 1.3 g cm^{-3}
(13) KBr pellet

12431



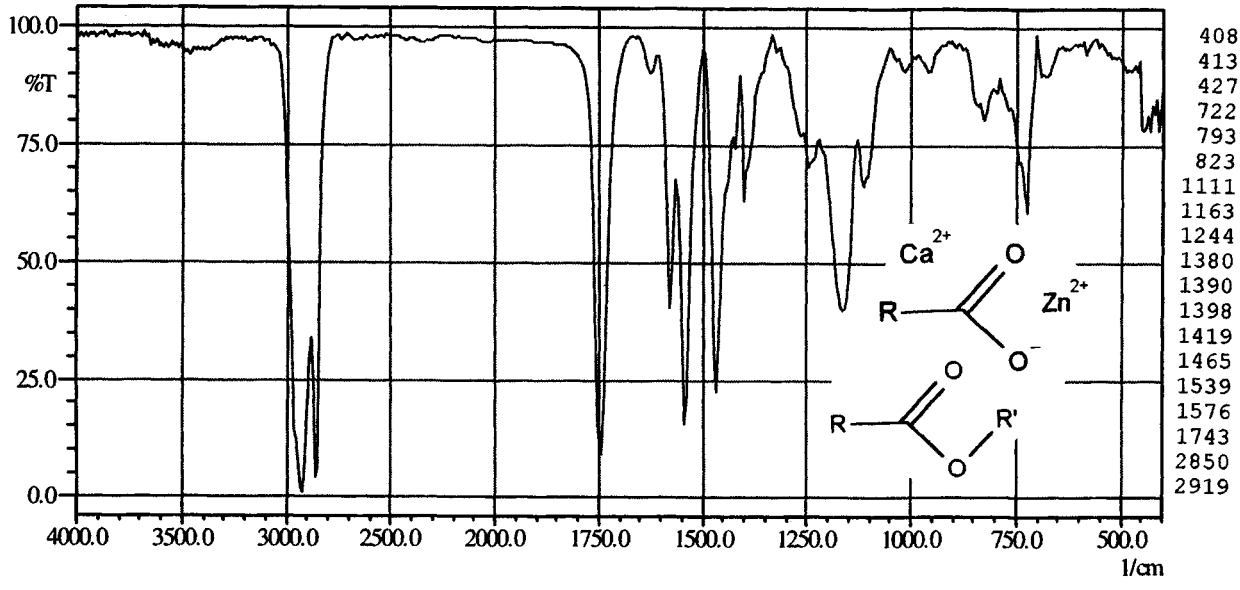
(1) **Zn Mg complex**
(2) Naftovin CKP 90172
(3) mg Technologies/Chemson
(5) PVC-stabiliser
(6) colourless solid
(9) 1.5 g cm^{-3}
(13) KBr pellet

12431



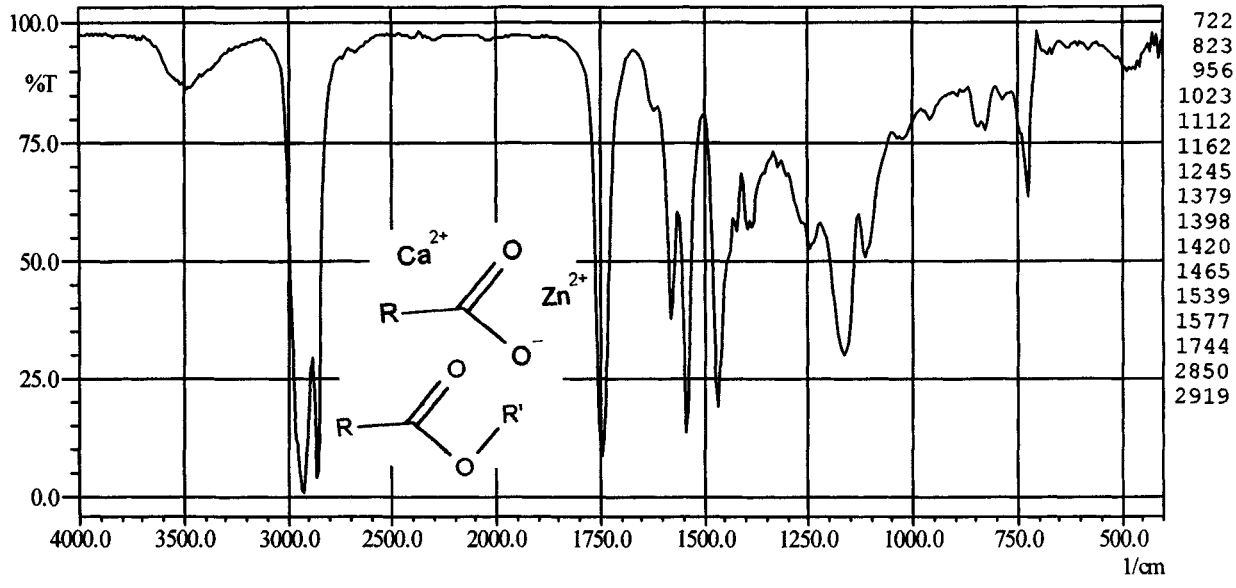
(1) **Pb Ba Cd-phosphite carboxylate**
(2) Baeropan 16435 FP
(3) Baerlocher
(5) stabiliser-lubricant
(6) colourless solid
(9) 2.1 g cm^{-3}
(13) KBr pellet

12432



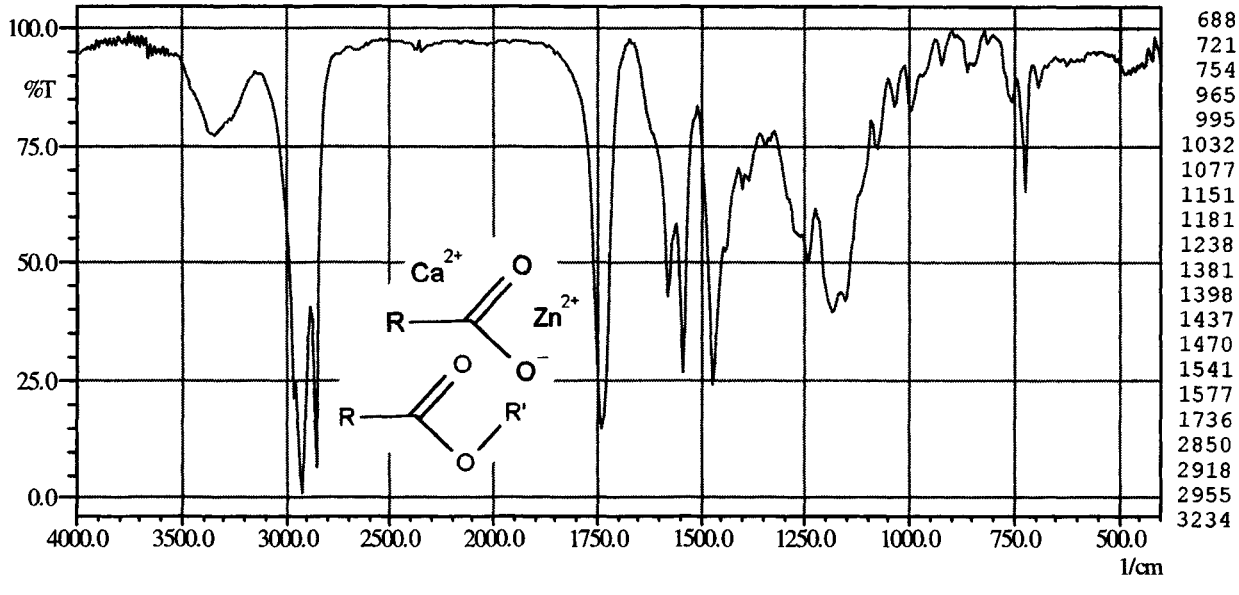
(1) **Ca Zn ester carboxylate**
(2) Irgastab CZ 110
(3) Ciba-Geigy
(5) PVC-stabiliser
(6) yellowish-white, high-viscous paste
(13) layer btw KBr

12432



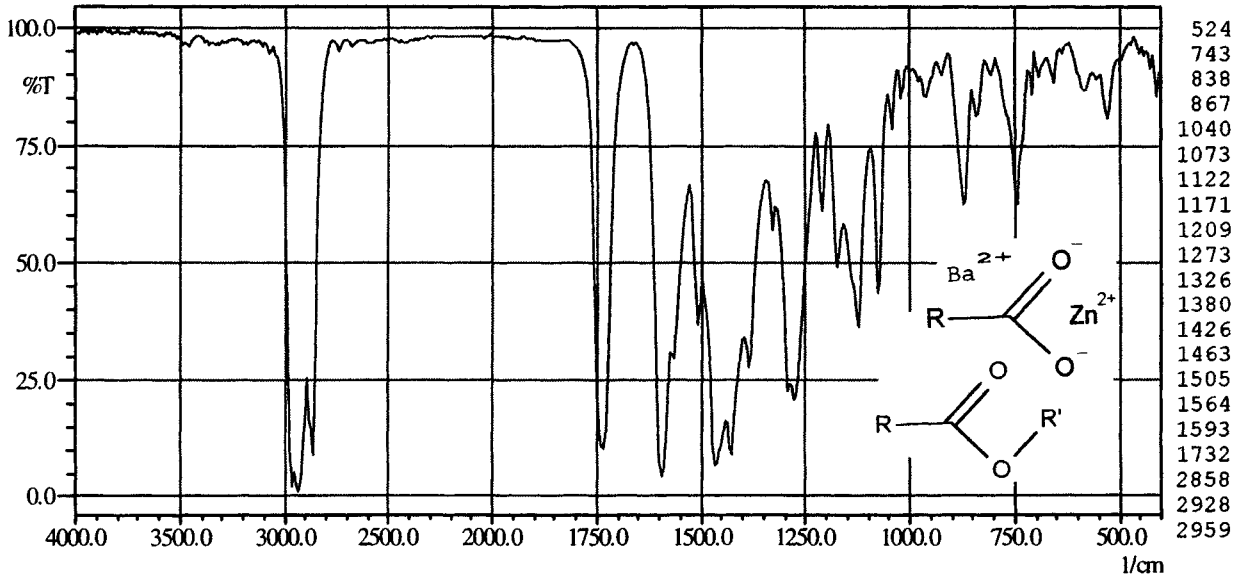
(1) **Ca Zn ester carboxylate**
(2) Stabiol VCZ 1616
(3) Henkel
(5) PVC-stabiliser
(6) colourless solid
(13) layer btw KBr

12432



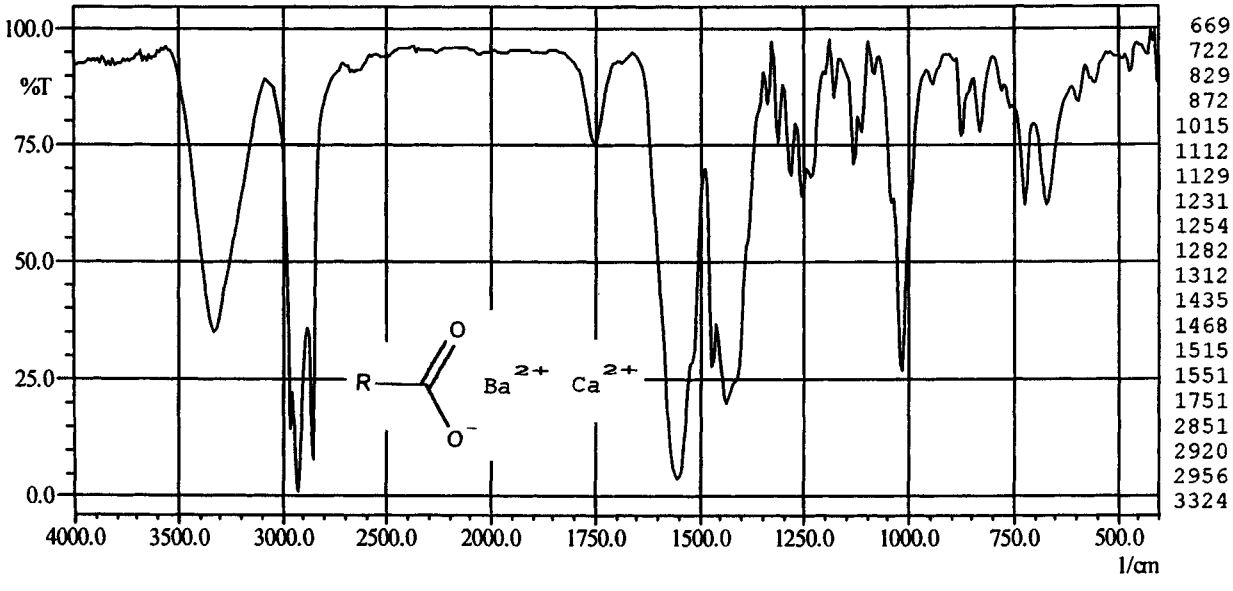
(1) **Ca Zn ester carboxylate**
(2) Baeropan NT 328 FLA
(3) Baerlocher
(5) stabiliser-lubricant
(6) colourless solid
(13) KBr pellet

12432



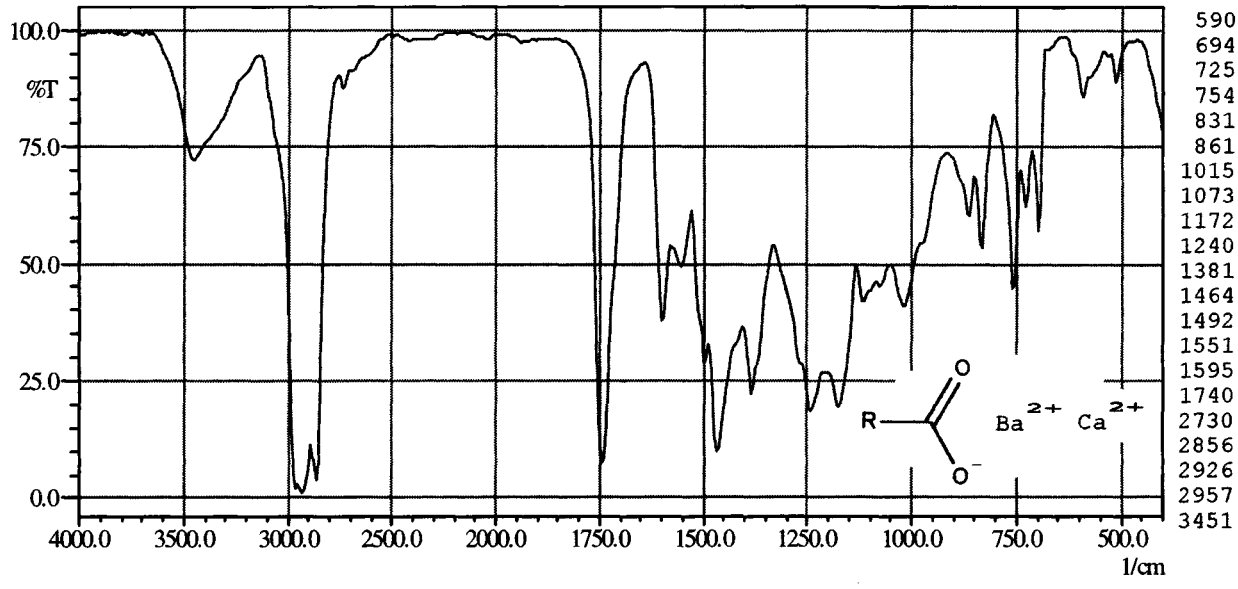
(1) **Ba Zn ester carboxylate**
(2) Swedstab 502
(3) Swedstab
(5) PVC-stabiliser
(6) colourless, clear liquid
(9) 1.1 g cm^{-3}
(13) layer btw KBr

12432



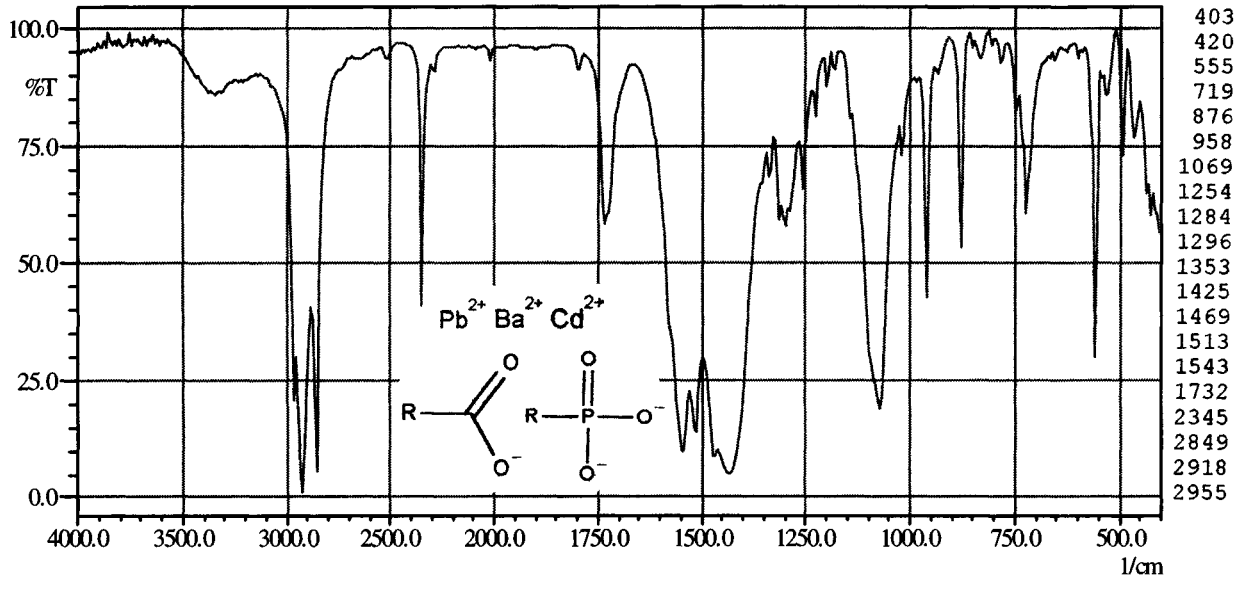
(1) **Ba Ca soap complex**
(2) Reagens F/95
(3) Reagens
(5) stabiliser
(6) colourless solid
(13) KBr pellet

12432



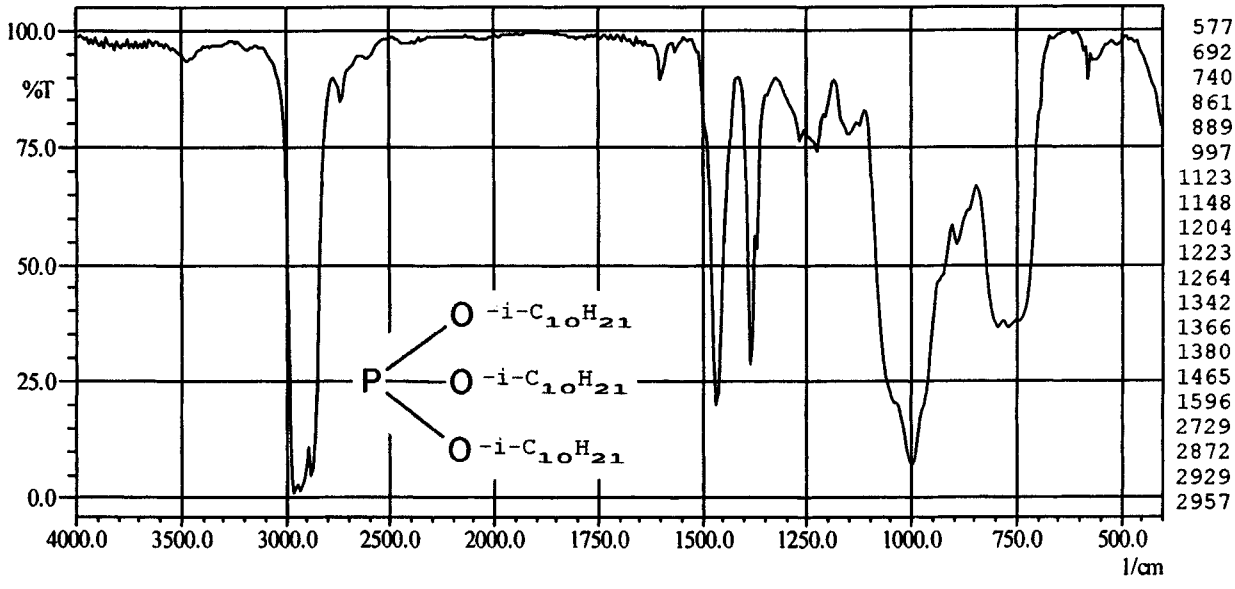
(1) **Ba Cd soap complex with epoxester**
(2) Reagens Gl/52
(3) Reagens
(5) stabiliser, lubricant
(6) brown, clear liquid
(9) 0.98 g cm^{-3}
(10) 1.48
(13) layer btw KBr

12432



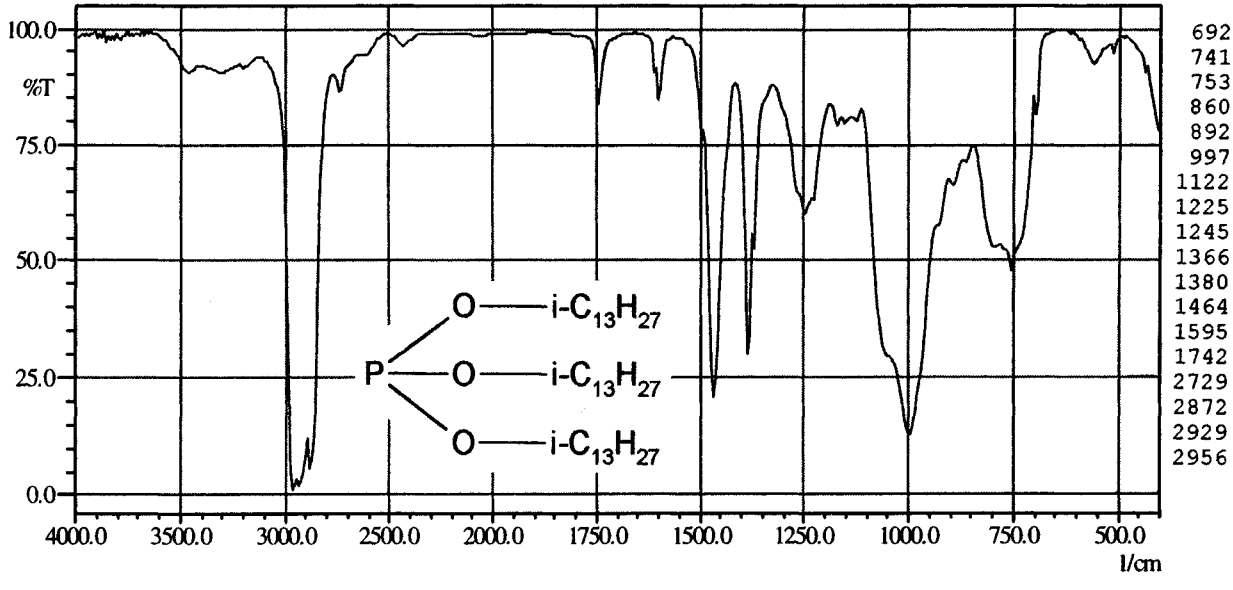
(1) **Pb Ba Cd compound with phosphite and carboxylate groups**
(2) Baeropan 16511 FP
(3) Baerlocher
(5) stabiliser-lubricant
(6) colourless solid
(9) 1.6 g cm^{-3}
(13) KBr pellet

1251 $C_{30}H_{63}O_3P$



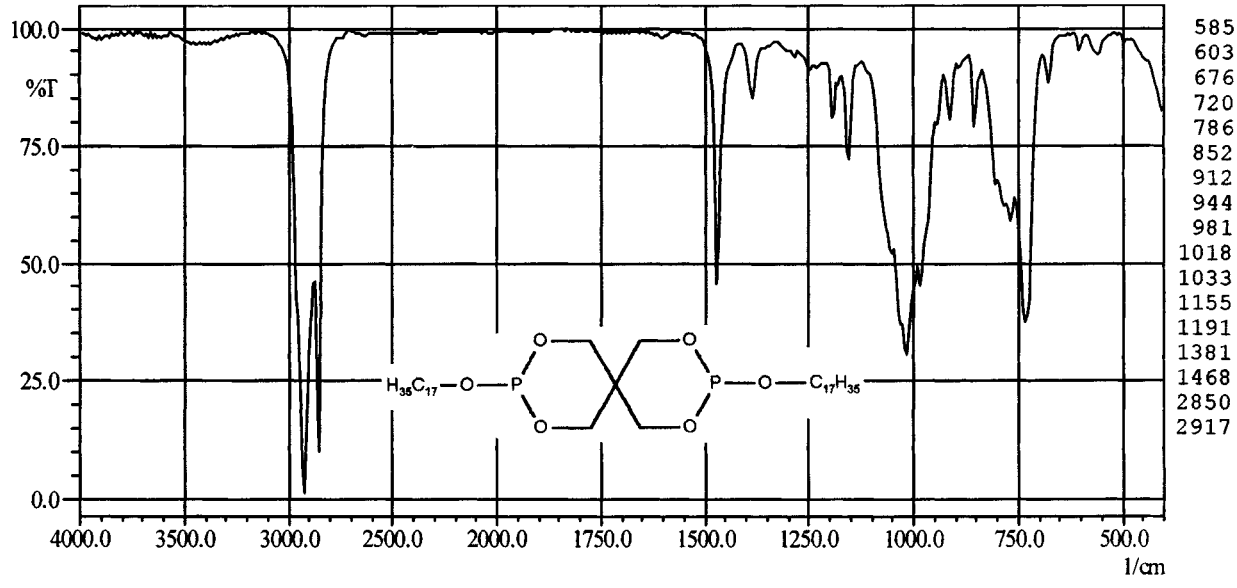
(1) **tri-*i*-decylphosphite**
(2) Weston TDP
(3) General Electric Chemicals
(4) 502.8 g mol^{-1}
(5) stabiliser
(6) colourless, clear liquid
(9) 0.89 g cm^{-3}
(10) 1.49
(13) layer btw KBr
(14) structure of *i*-decyl is undefined

1251 $C_{39}H_{81}O_3P$



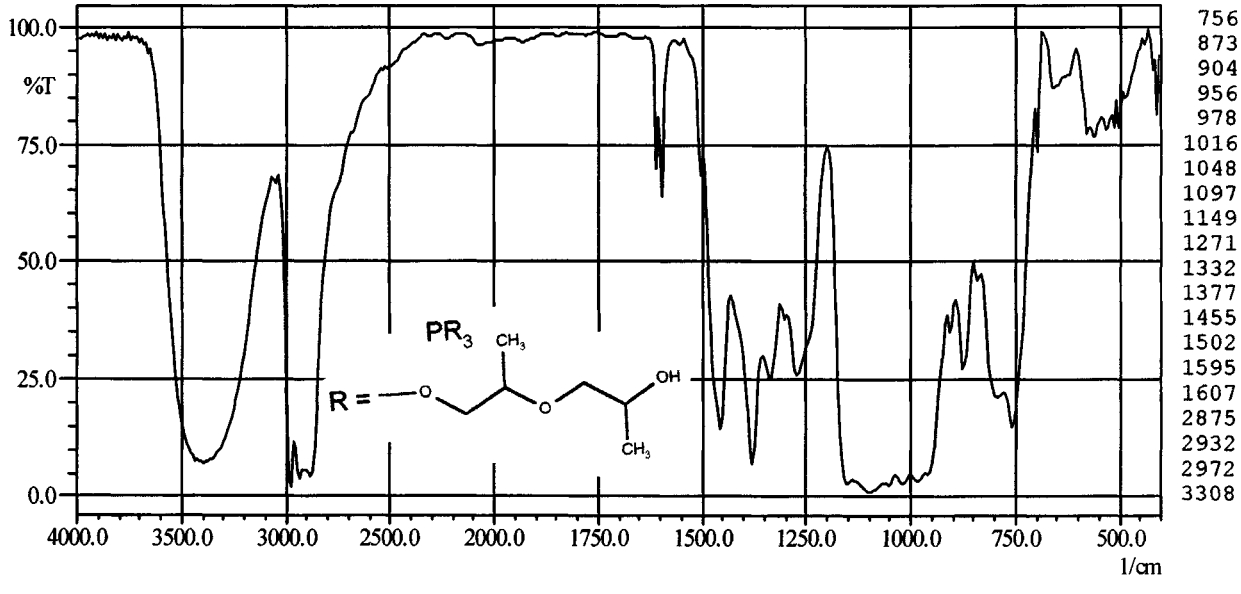
(1) **tri(tridecyl)phosphite**
(2) Tritridecylphosphit
(3) Reagens
(4) 629.0 g mol^{-1}
(5) stabiliser, antioxidant
(6) colourless, clear liquid
(9) 0.885 g cm^{-3}
(10) 1.463
(13) layer btw KBr

1251 $C_{41}H_{82}O_6P_2$



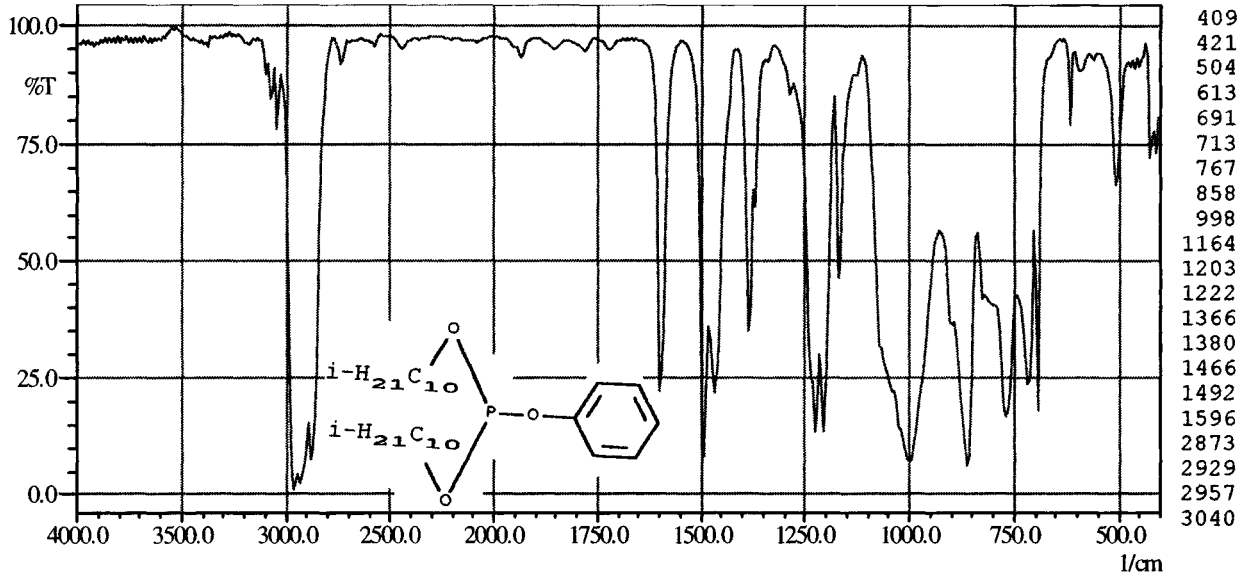
(1) **distearylpentaerythrityldiphosphite**
(2) Weston 619 F
(3) General Electric Chemicals
(4) 733.1 g mol^{-1}
(5) stabiliser
(6) colourless solid
(13) film from melt

1251 $C_{18}H_{37}O_7P$



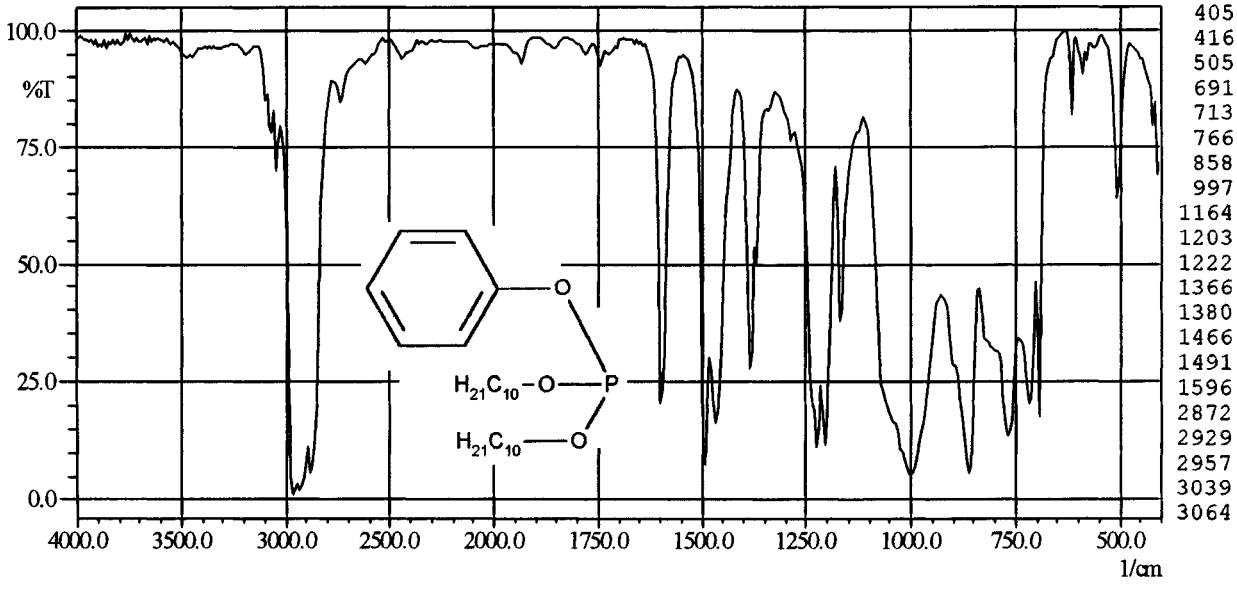
(1) **tri(dipropyleneglycol)phosphite**
(2) Weston 430
(3) General Electric Chemicals
(4) 396.5 g mol^{-1}
(5) stabiliser
(6) colourless, clear liquid
(13) layer btw KBr

1252 $C_{26}H_{47}O_3P$



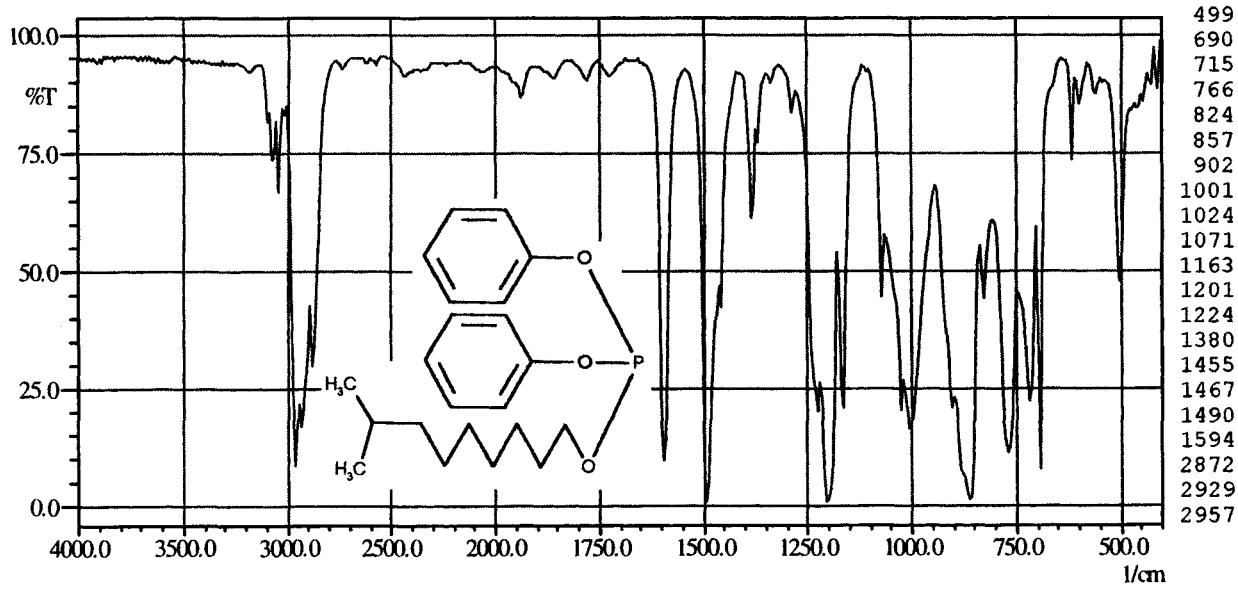
(1) **di-*i*-decylphenyl phosphite**
(2) Irgastab CH 300
(3) Ciba-Geigy
(4) 438.6 g mol^{-1}
(5) PVC-stabiliser
(6) colourless, clear liquid
(13) layer btw KBr
(14) structure of *i*-decyl is undefined

1252 $C_{26}H_{47}O_3P$



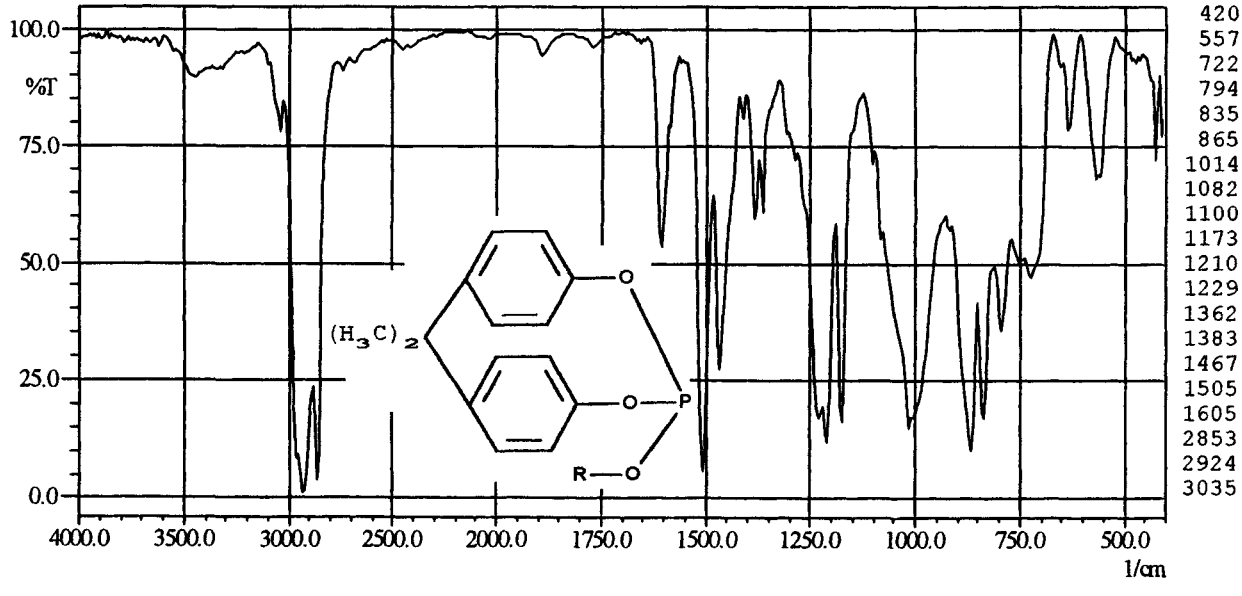
(1) **phenyldidecylphosphite**
(2) Weston PDDP
(3) General Electric Chemicals
(4) 438.6 g mol^{-1}
(5) stabiliser
(6) colourless, clear liquid
(13) layer btw KBr

1252 $C_{22}H_{31}O_3P$



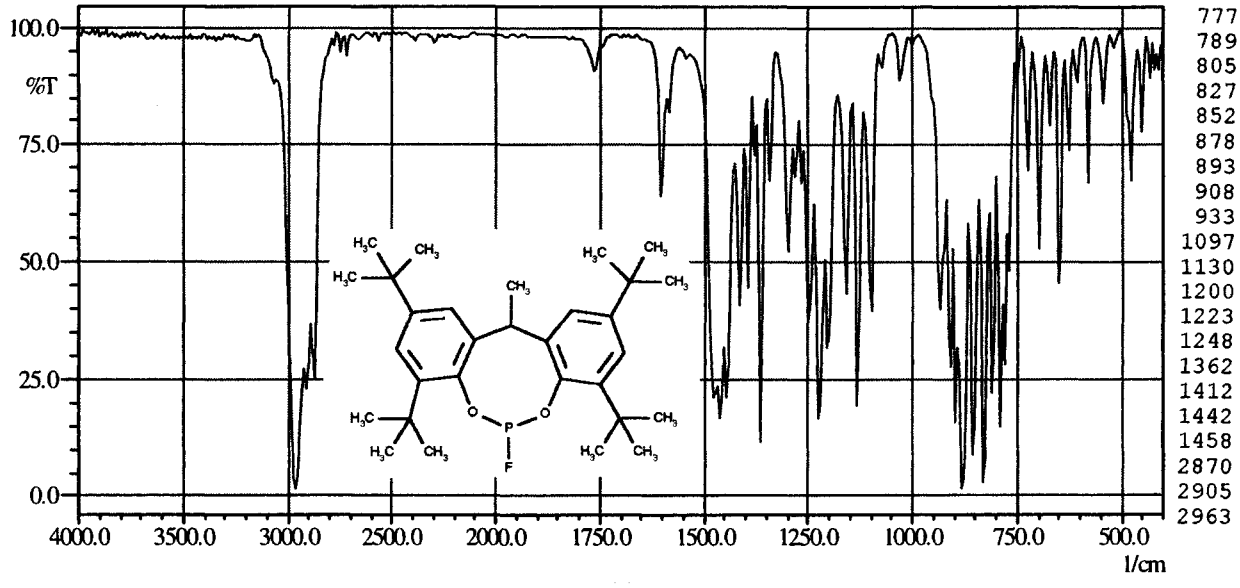
(1) ***i*-decyldiphenyl phosphite**
(2) Irgastab CH 301
(3) Ciba-Geigy
(4) 374.5 g mol^{-1}
(5) PVC-stabiliser
(6) colourless, clear liquid
(13) layer btw KBr
(14) structure of *i*-decyl is undefined

1252



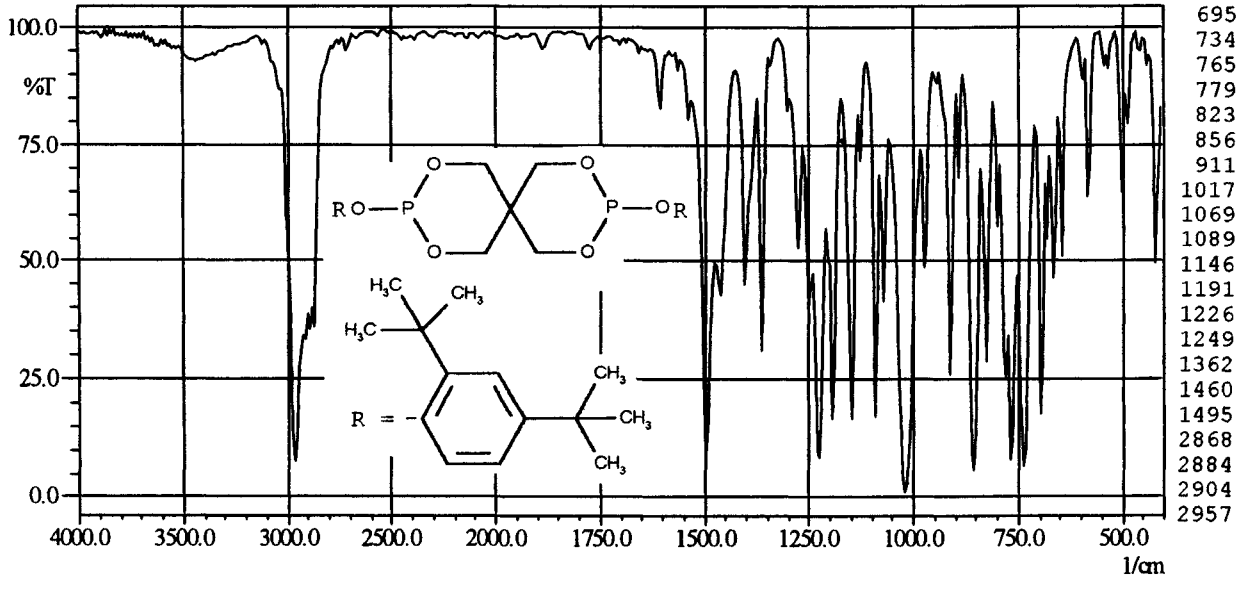
(1) **4,4'-*i*-propylidenediphenol-alkylphosphite**
(2) Weston 439
(3) General Electric Chemicals
(5) stabiliser
(6) colourless, clear liquid
(13) layer btw KBr

1252 $C_{30}H_{44}FO_2P$



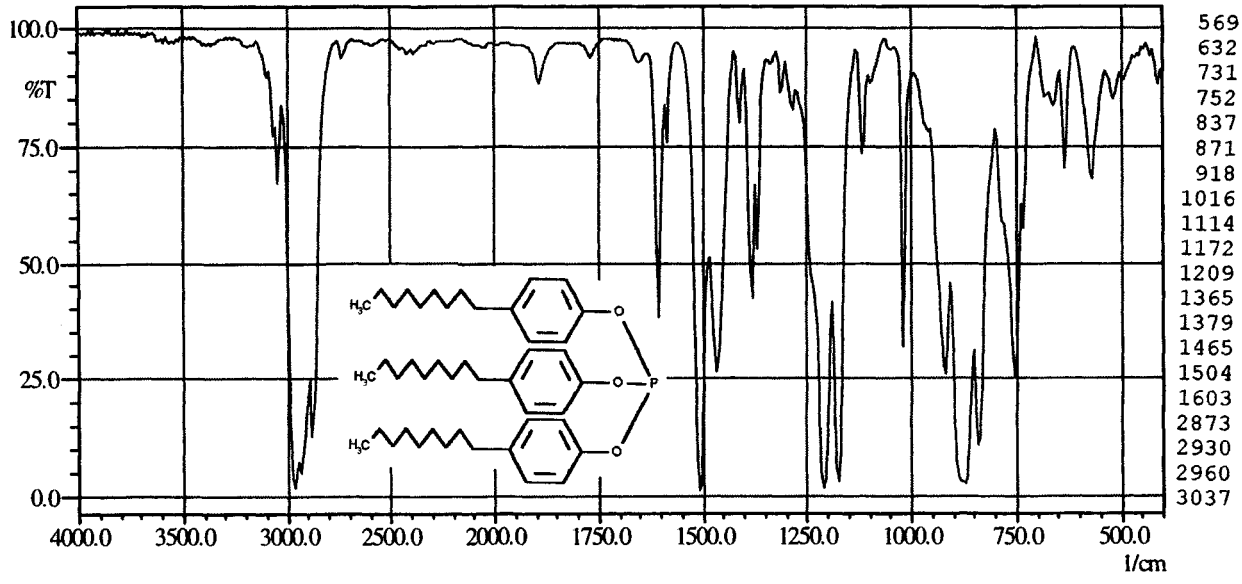
(1) **2,2'-ethylene-*bis*(4,6-di-*t*-butylphenyl)fluorophosphite**
(2) Ethanox 398
(3) Ethyl
(4) 486.7 g mol^{-1}
(5) stabiliser, antioxidant
(6) white, crystalline solid
(7) 200 °C
(13) KBr pellet

1252 $C_{33}H_{50}O_6P_2$



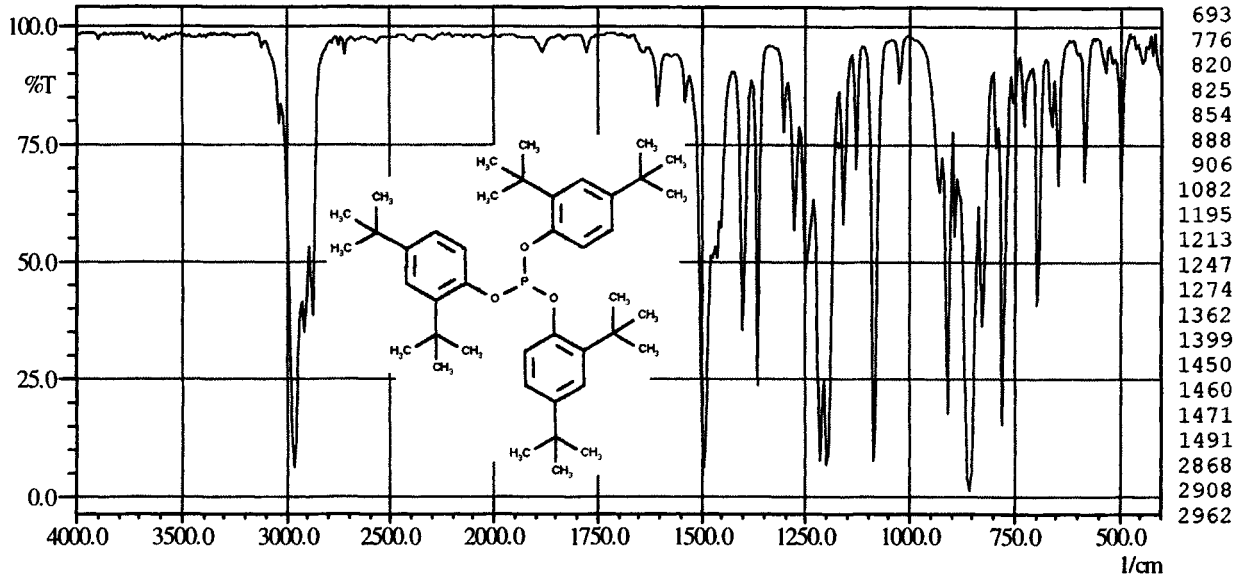
(1) ***bis*(2,4-di-*t*-butylphenyl)pentaerythrityldiphosphite**
(2) Ultranox 626
(3) General Electric Chemicals
(4) 604.7 g mol^{-1}
(5) stabiliser
(6) colourless solid
(13) KBr pellet

1252 $C_{45}H_{69}O_3P$



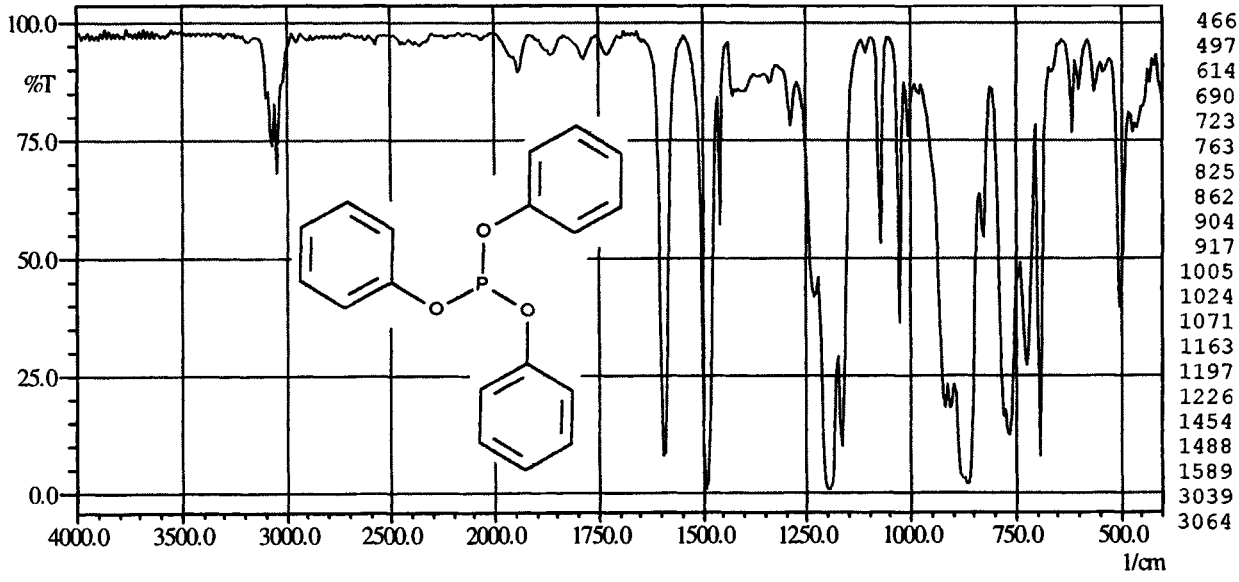
(1) ***tris*(nonylphenyl)phosphite**
(2) Baerostab CWM 35
(3) Baerlocher
(4) 689.0 g mol^{-1}
(5) stabiliser
(6) colourless, clear liquid
(9) 0.99 g cm^{-3}
(13) layer btw KBr

1252 $C_{42}H_{63}O_3P$



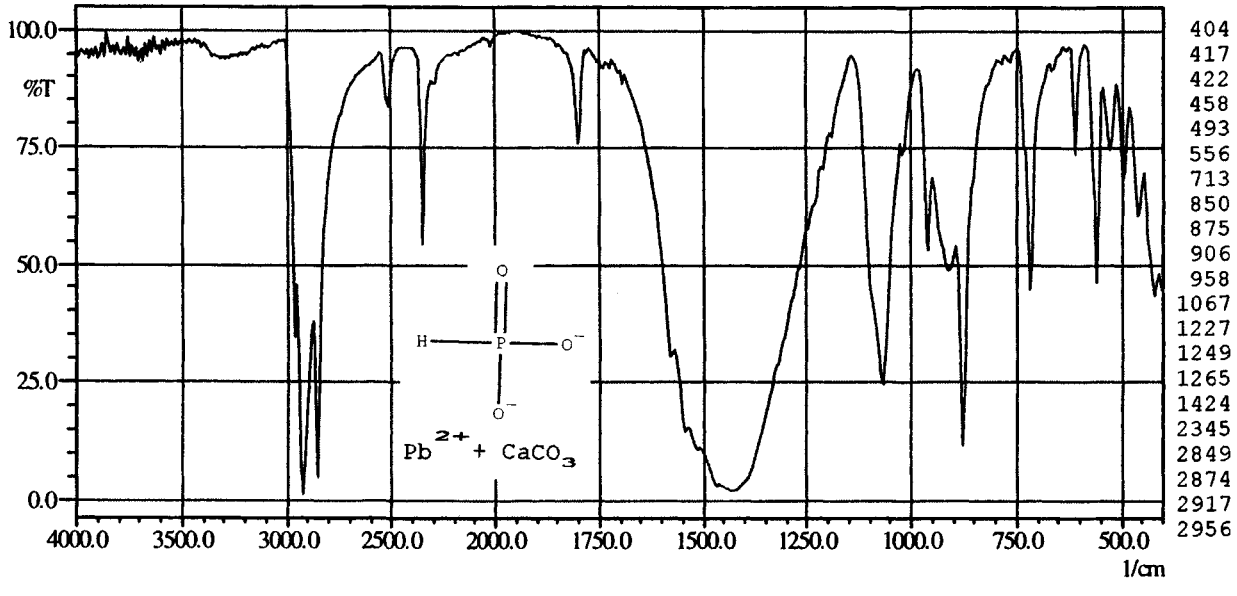
(1) ***tris*(2,4-di-*t*-butylphenol)phosphite**
(2) Hostanox PAR 24
(3) Hoechst
(4) 646.9 g mol^{-1}
(5) antioxidant (co-stabiliser)
(6) colourless solid
(7) 185 °C
(13) KBr pellet

1252 $C_{18}H_{15}O_3P$



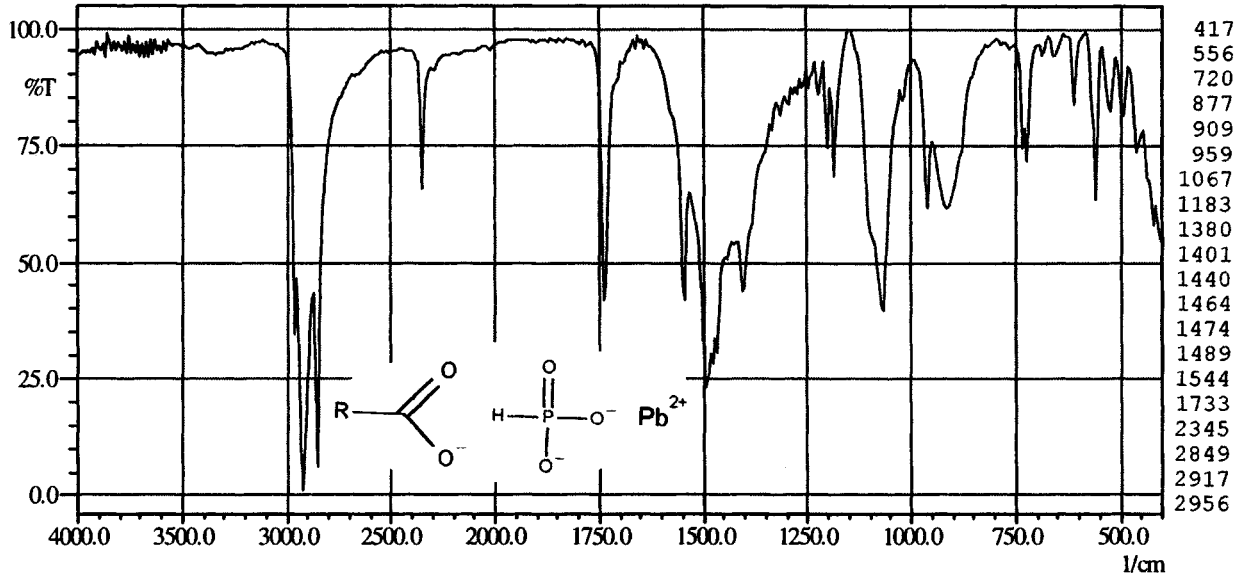
(1) **triphenylphosphite**
(2) Irgastab CH 55
(3) Ciba-Geigy
(4) 310.3 g mol^{-1}
(5) PVC-stabiliser
(6) colourless, clear liquid
(13) layer btw KBr

1253+12411



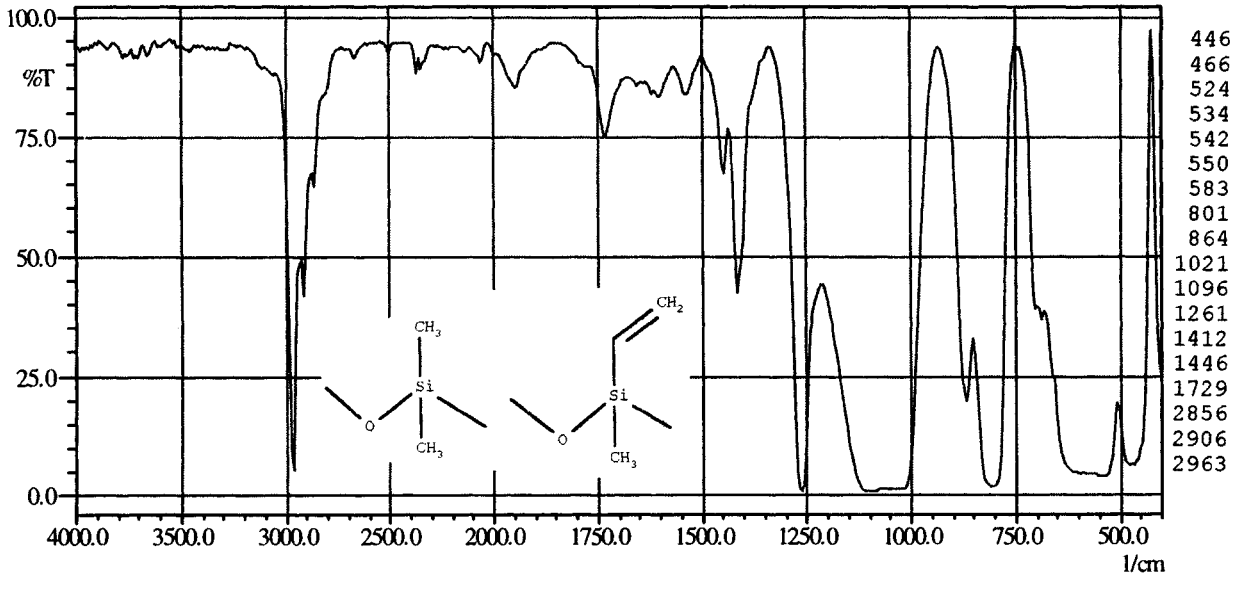
(1) **Pb phosphite-carboxylate on $CaCO_3$**
(2) Baeropan E-RL 25
(3) Baerlocher
(5) stabiliser-lubricant
(6) colourless granules
(9) 2 g cm^{-3}
(13) KBr pellet

1255



(1) **Pb phosphite-carboxylate with aliphatic ester**
(2) Baeropan E-RL 15
(3) Baerlocher
(5) stabiliser-lubricant
(6) colourless granules
(9) 2.1 g cm^{-3}
(13) KBr pellet

126 SiC_2H_6O M



(1) **vinyl-functional poly(dimethylsiloxane) with filler**
(2) Hitzestabilisator H1 Rot
(3) Wacker (Brunne collection)
(5) heat stabiliser
(6) red-brown paste
(13) layer on KBr

Previous Page

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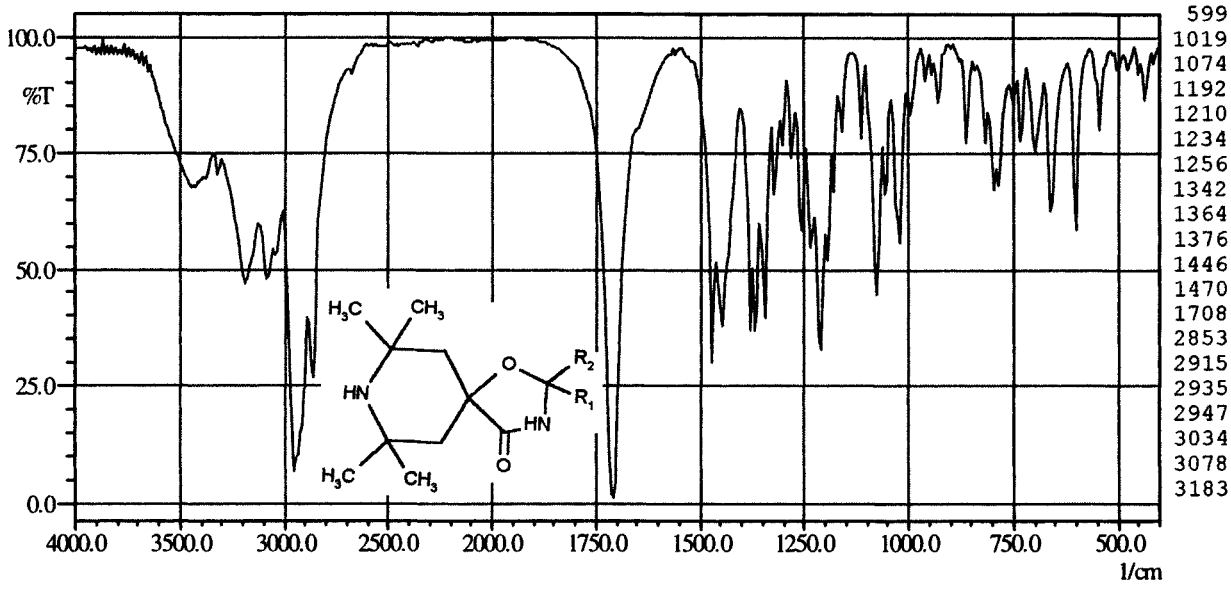
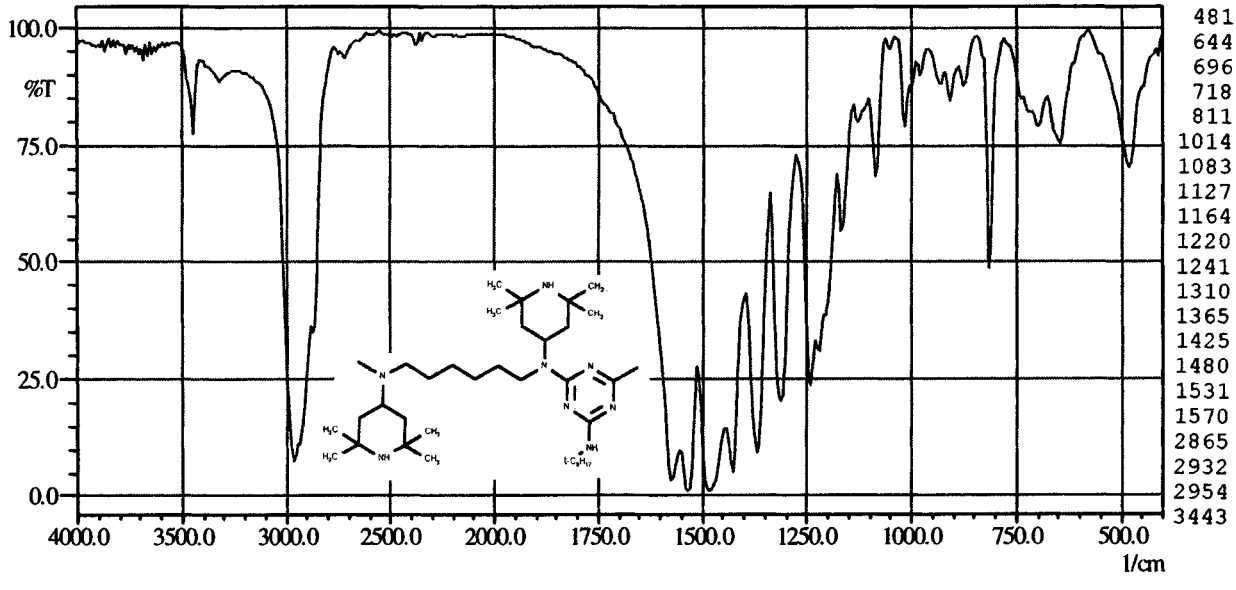


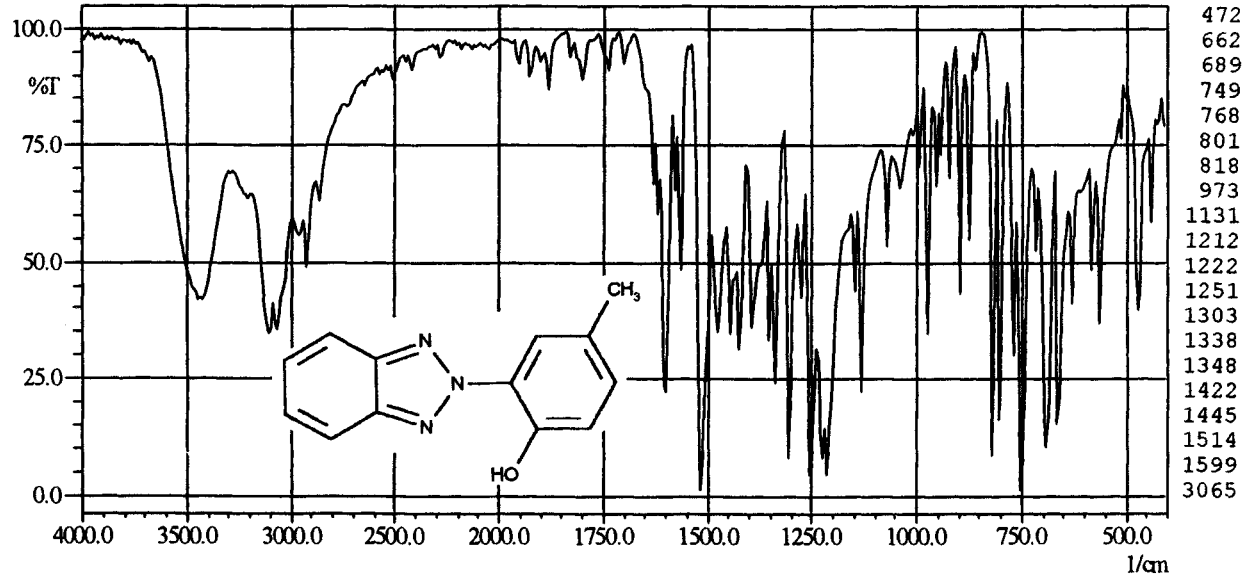
(1) **sterically hindered amine, HALS**
(2) Hostavin N 20
(3) Hoechst
(5) light stabiliser
(6) colourless solid
(9) 1.06 g cm^{-3}
(13) KBr pellet

131



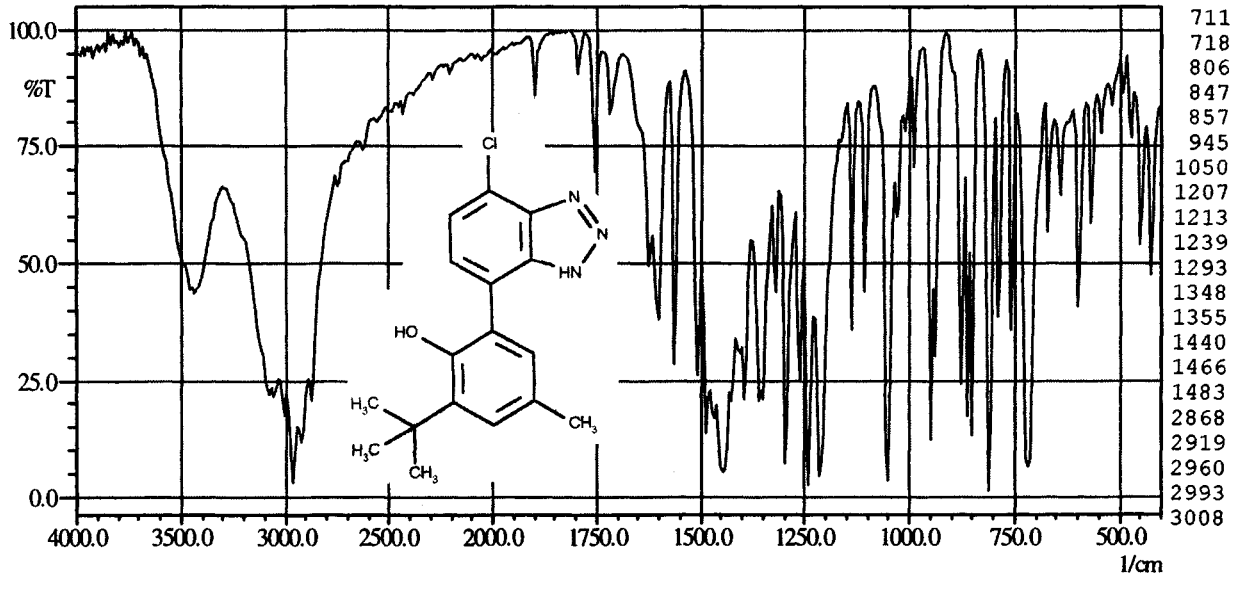
(1) **poly(*bis*(2,2,6,6-tetramethyl-4-piperidinylimino)-1,6-hexanediyl-*alt*-4-*t*-octylamino-1,3,5-triazine-2,4-diyl)**
(2) Chimassorb 944 FL
(3) Ciba-Geigy
(5) *UV*-stabiliser
(6) light-yellow granules, low dusting
(8) 117.5 °C
(9) 0.98 g cm^{-3}
(13) KBr pellet
(14) sterically hindered amine, HALS

132 $C_{13}H_{11}N_3O$



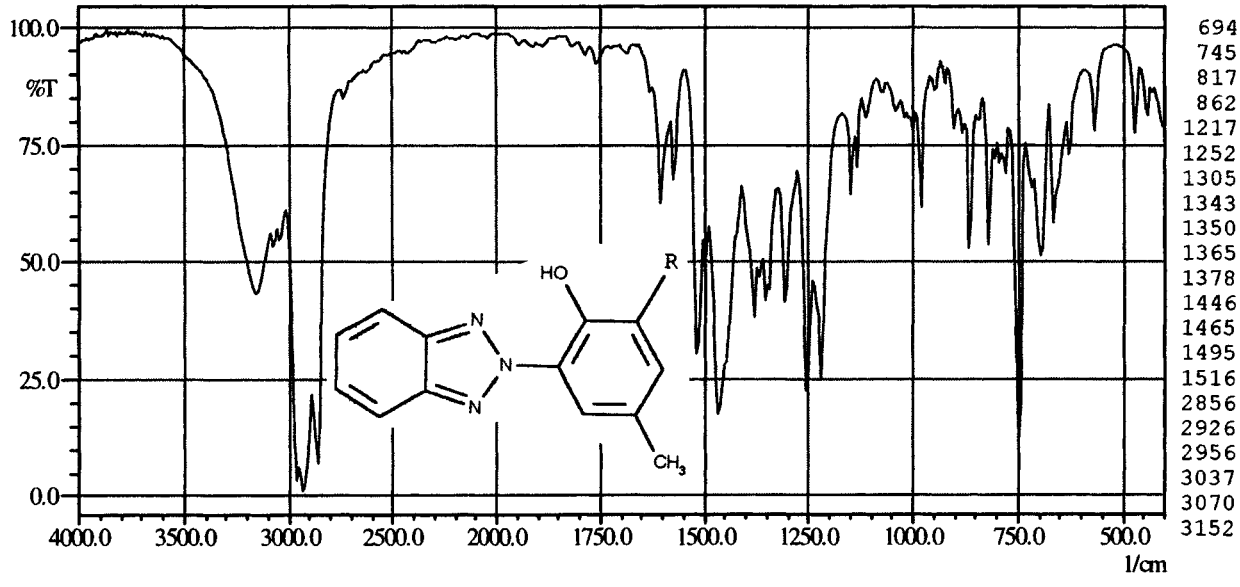
(1) **2-(2-hydroxy-5-methylphenyl)-2H-benzotriazole**
(2) Tinuvin P
(3) Ciba-Geigy
(4) 225.2 g mol^{-1}
(5) light stabiliser for PVC, PS, PU, PC and polyesters
(6) slightly yellowish solid
(13) KBr pellet

132 $C_{17}H_{18}ClN_3O$



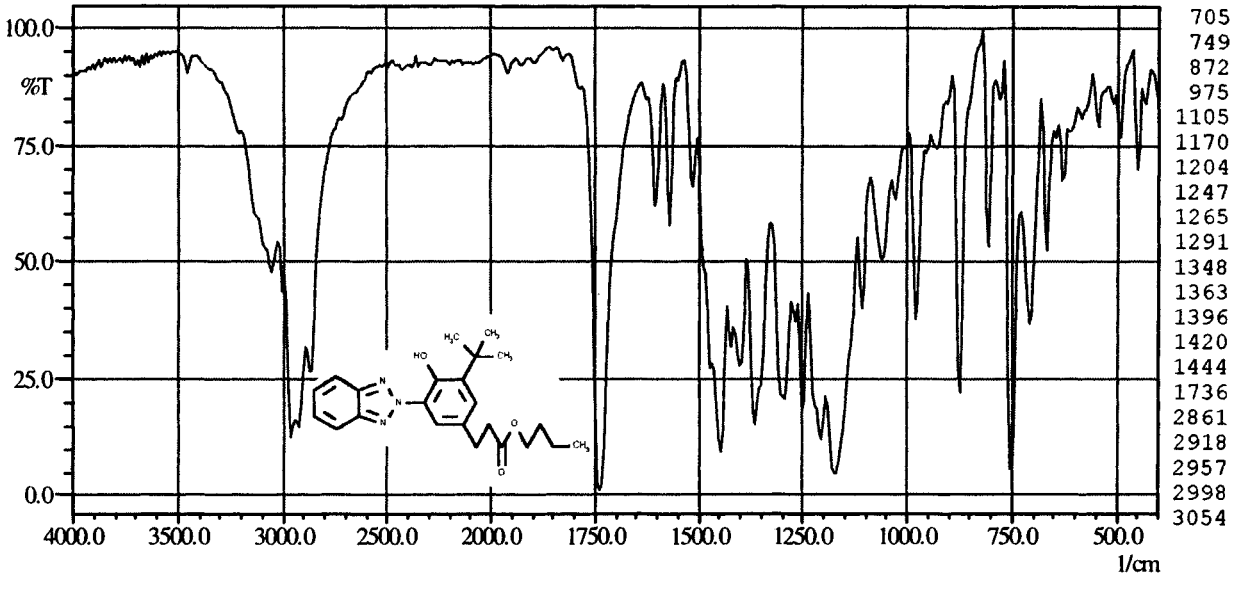
(1) **2-(2'-hydroxy-3'-*t*-butyl-5'-methylphenyl)-5-chlorobenzotriazole**
(2) Tinuvin 326
(3) Ciba-Geigy
(4) 315.7 g mol^{-1}
(5) *UV*-stabiliser
(6) pale yellow solid
(13) KBr pellet

132 $C_{25}H_{35}N_3O$



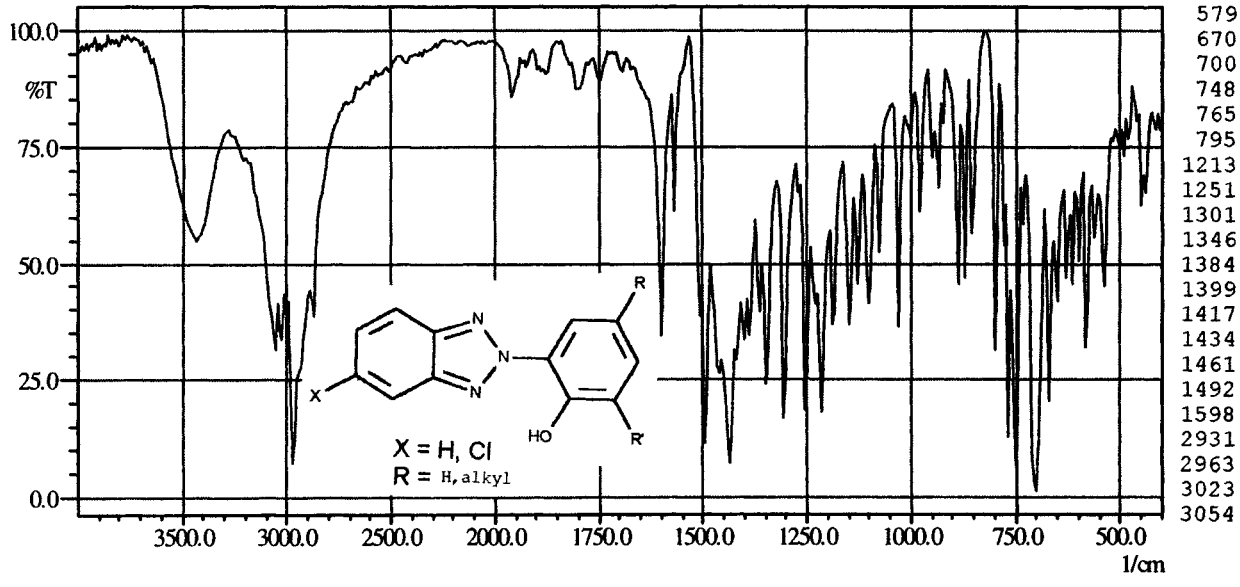
(1) **2-(2'-hydroxy-3'-dodecyl-5'-methylphenyl)benzotriazole**
(2) Tinuvin 571
(3) Ciba-Geigy
(4) 393.6 g mol^{-1}
(5) *UV*-stabiliser
(6) pale-yellow liquid
(9) 1 g cm^{-3}
(10) 1.58
(13) layer btw KBr

132 $C_{44}H_{52}N_6O_6$



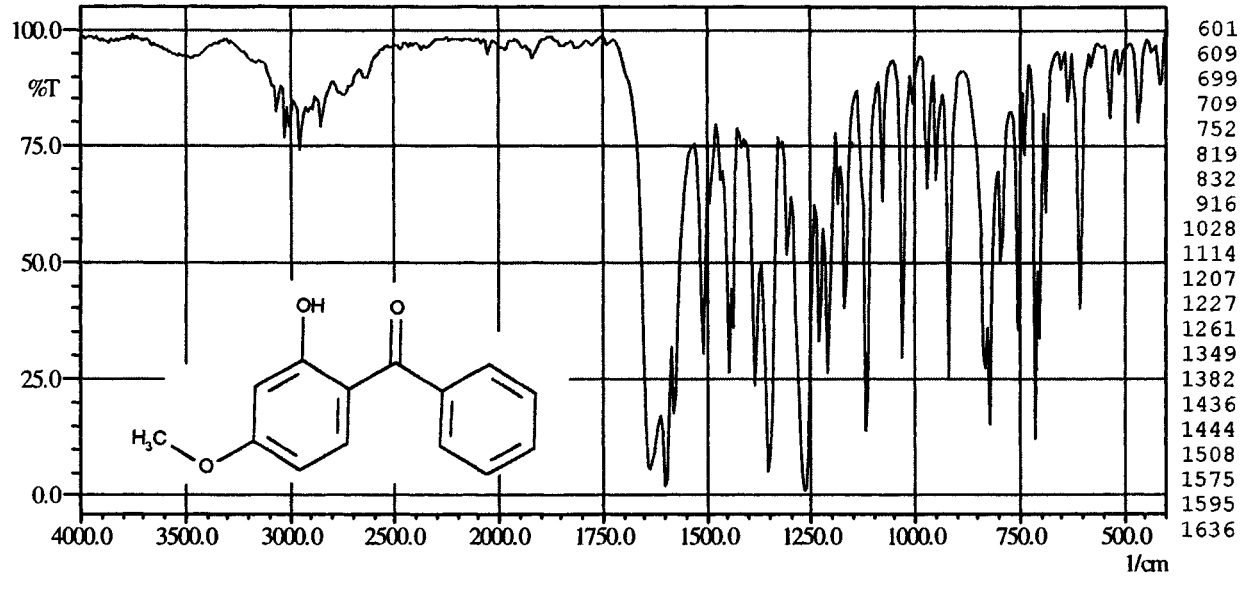
(1) **1,6-hexanediol-*bis*-3-(3-benzotriazole-4-hydroxy-5-*t*-butyl)propionate**
(2) Tinuvin 840
(3) Ciba-Geigy
(4) 760.9 g mol^{-1}
(5) *UV*-stabiliser
(6) slightly yellowish solid
(7) 117 °C
(9) 1.22 g cm^{-3}
(13) KBr pellet

132



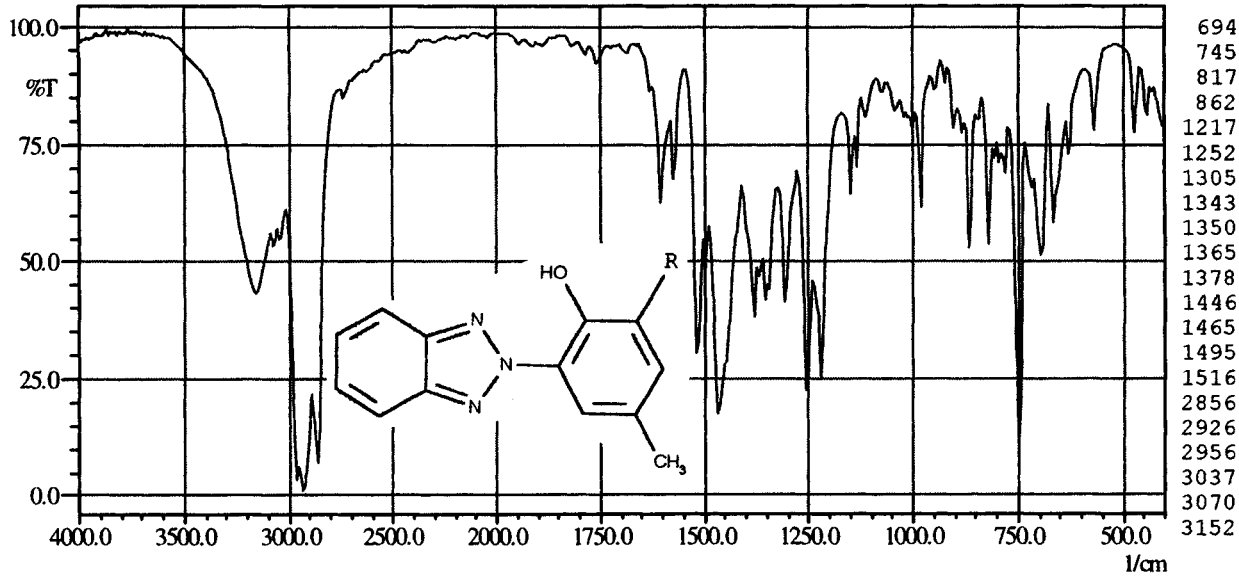
(1) **alkylphenolic benzotriazole derivative**
(2) Tinuvin 234
(3) Ciba-Geigy
(5) light stabiliser for films and fibers
(6) yellowish solid
(13) KBr pellet

134 $C_{14}H_{12}O_3$



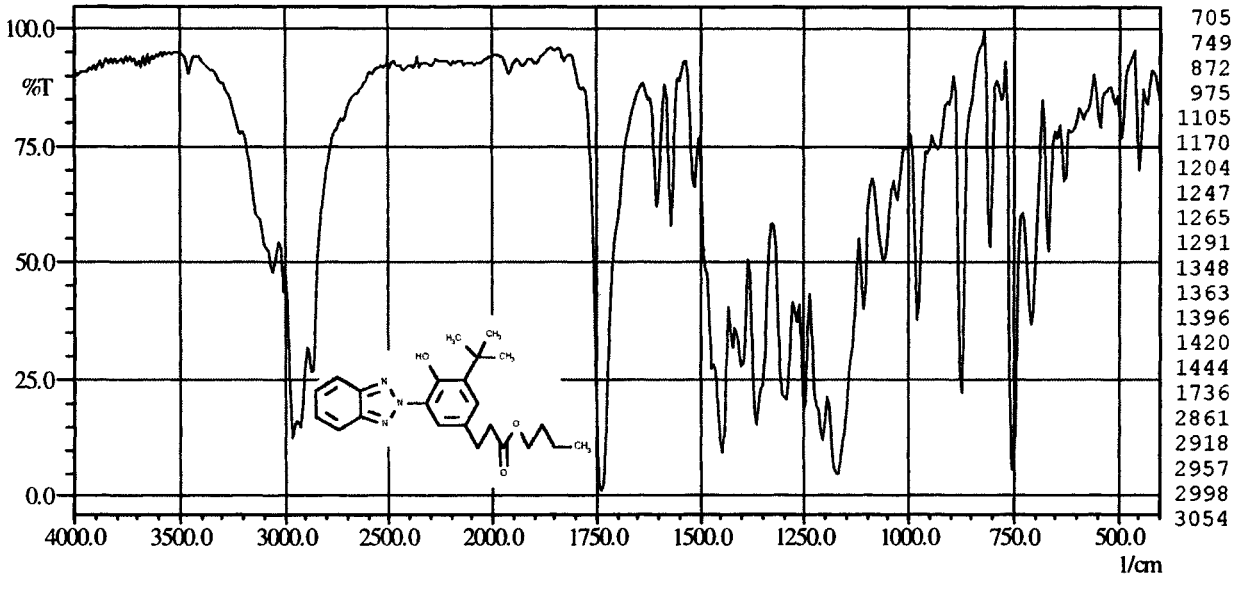
(1) **2-hydroxy-4-methoxybenzophenone**
(2) UV 325
(3) Bayer
(4) 228.3 g mol^{-1}
(5) *UV*-stabiliser
(6) yellowish solid
(13) KBr pellet

132 $C_{25}H_{35}N_3O$



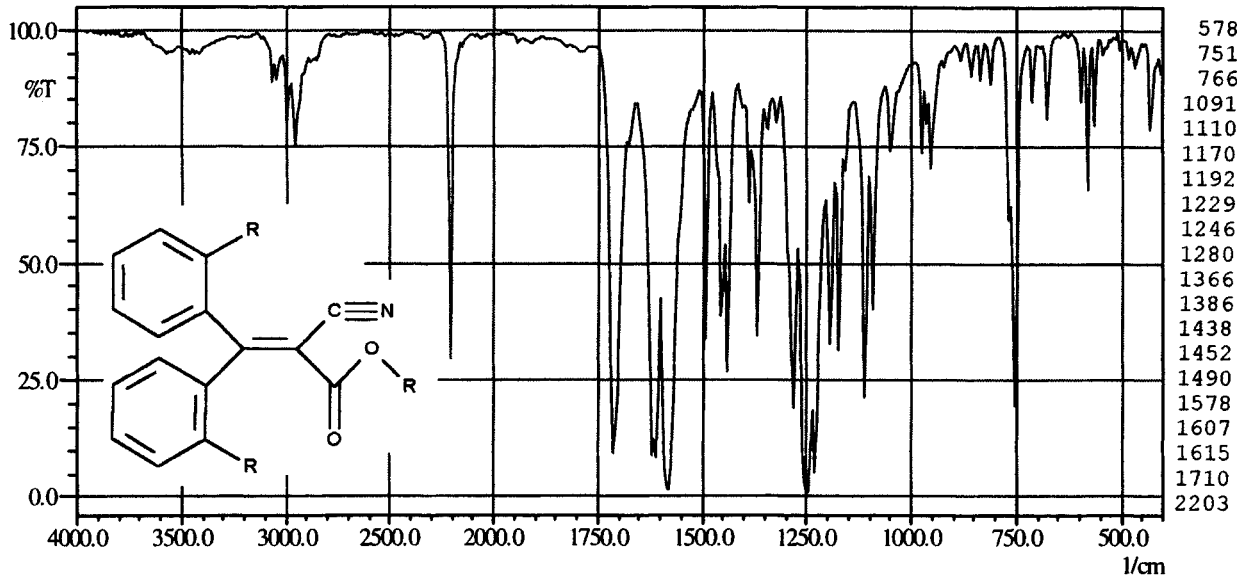
(1) **2-(2'-hydroxy-3'-dodecyl-5'-methylphenyl)benzotriazole**
(2) Tinuvin 571
(3) Ciba-Geigy
(4) 393.6 g mol^{-1}
(5) *UV*-stabiliser
(6) pale-yellow liquid
(9) 1 g cm^{-3}
(10) 1.58
(13) layer btw KBr

132 $C_{44}H_{52}N_6O_6$



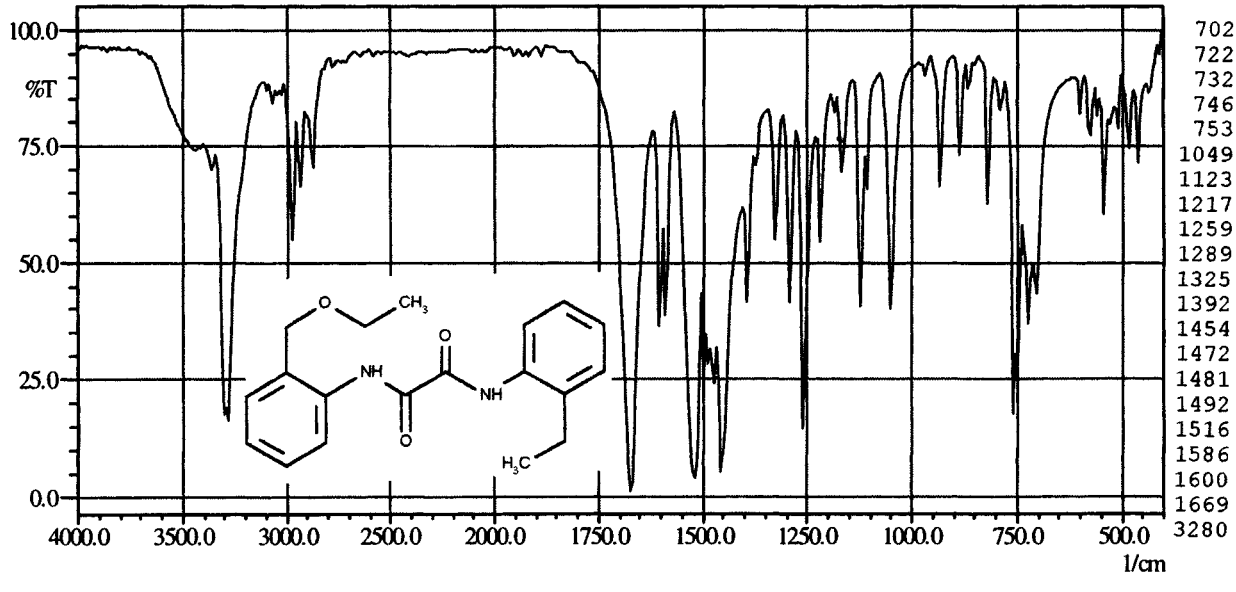
(1) **1,6-hexanediol-*bis*-3-(3-benzotriazole-4-hydroxy-5-*t*-butyl)propionate**
(2) Tinuvin 840
(3) Ciba-Geigy
(4) 760.9 g mol^{-1}
(5) *UV*-stabiliser
(6) slightly yellowish solid
(7) 117 °C
(9) 1.22 g cm^{-3}
(13) KBr pellet

136



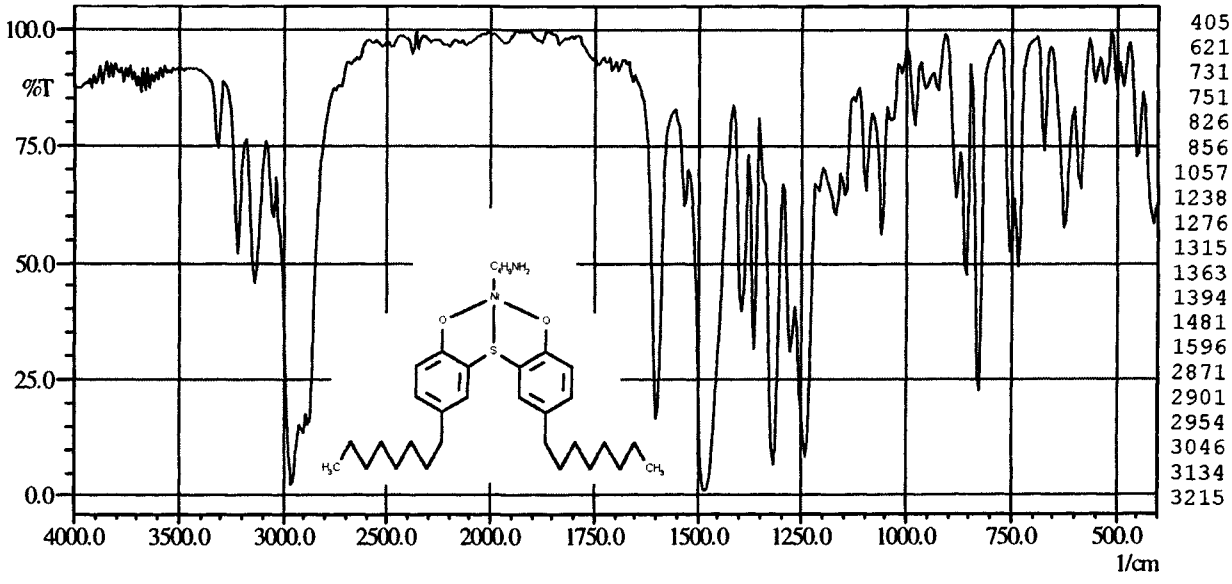
(1) **cyanoacrylate derivative**
(2) UV 340
(3) Bayer
(4) 438.7 g mol^{-1}
(5) *UV*-stabiliser
(6) colourless solid
(13) KBr pellet

137 $C_{18}H_{20}N_2O_3$



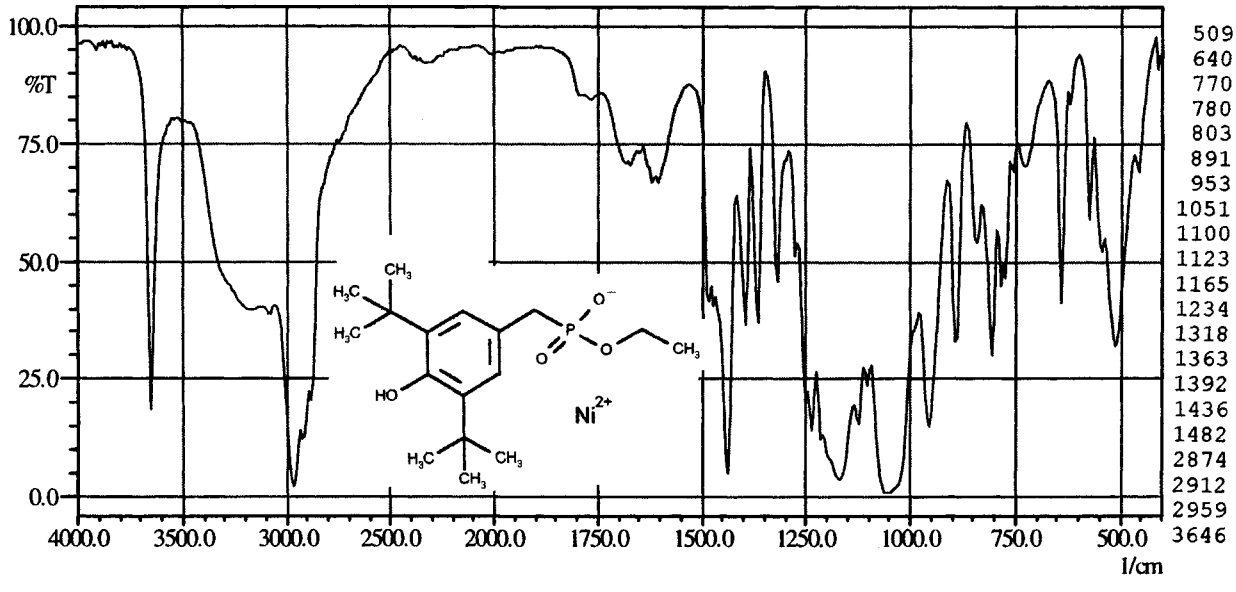
(1) **2-ethoxy-2'-ethyloxalyldianilide**
(2) Baerostab B 200 P
(3) Baerlocher
(4) 312.4 g mol^{-1}
(5) *UV*-stabiliser
(6) colourless solid
(7) 127 °C
(13) KBr pellet

138 $C_{32}H_{51}NO_2SNi$



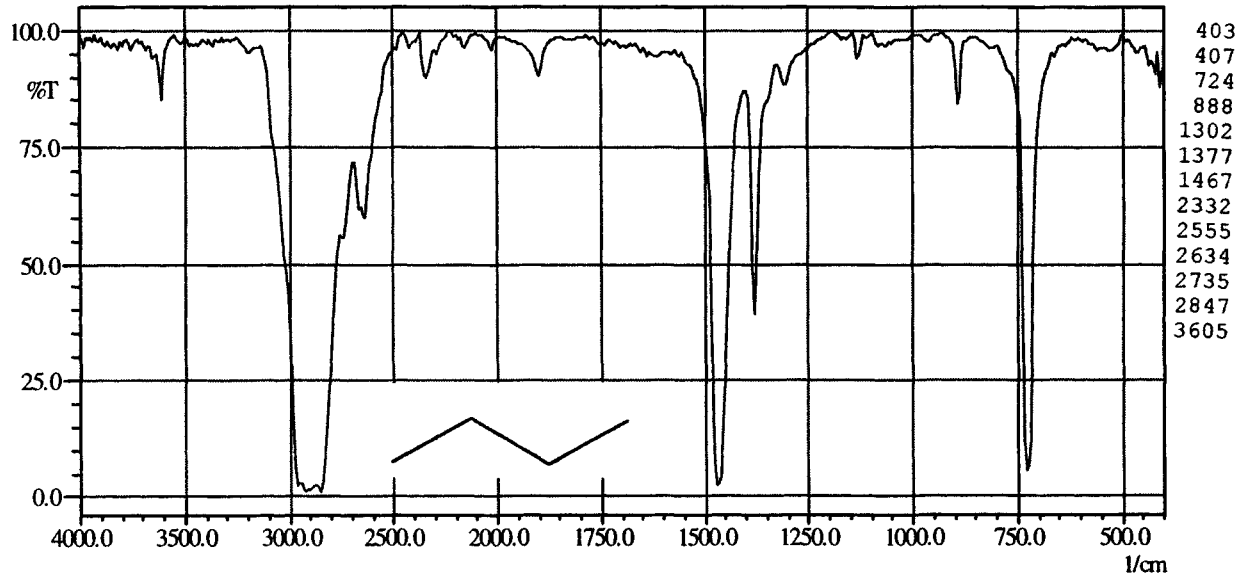
(1) **2,2'-thio-*bis*(4-*t*-octylphenolato)butylamine, Ni-salt**
(2) Chimassorb N-705
(3) Ciba-Geigy
(4) 572.5 g mol^{-1}
(5) *UV*-stabiliser
(6) light-green solid
(7) 278 °C
(13) KBr pellet

138 $C_{34}H_{56}O_8P_2Ni$



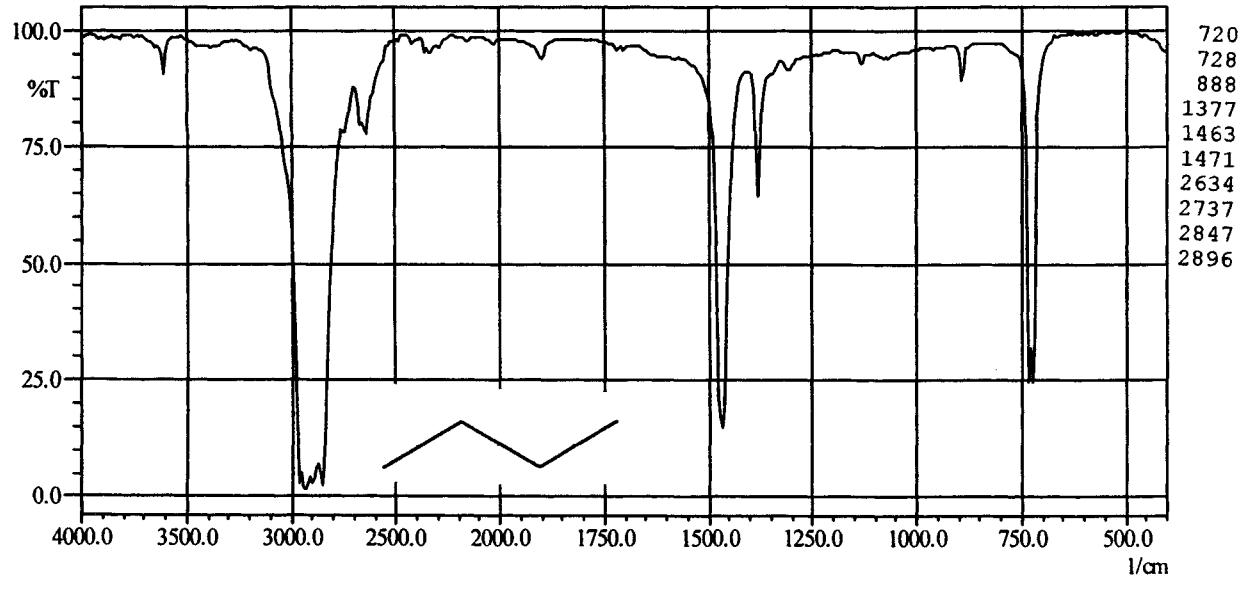
(1) **3,5-di-*t*-butyl-4-hydroxybenzyl phosphonic acid monoethylester, Ni-salt**
(2) Irgastab 2002
(3) Ciba-Geigy
(4) 713.5 g mol^{-1}
(5) stabiliser
(6) pale-yellow to green solid
(13) KBr pellet

139



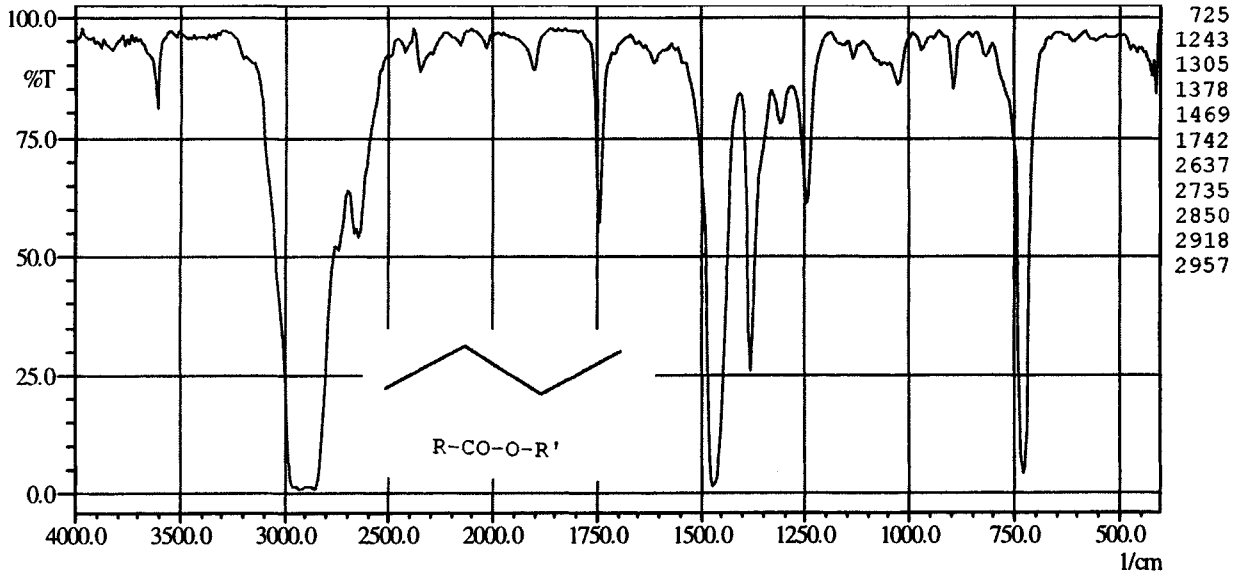
(1) **mixture of higher paraffin hydrocarbons and microwaxes, contains some NH (fatty amine)**
(2) Antilux 610
(3) Rhein-Chemie (Brunne collection)
(5) light stabiliser
(6) yellowish wax
(13) recrystallized film from the melt

139



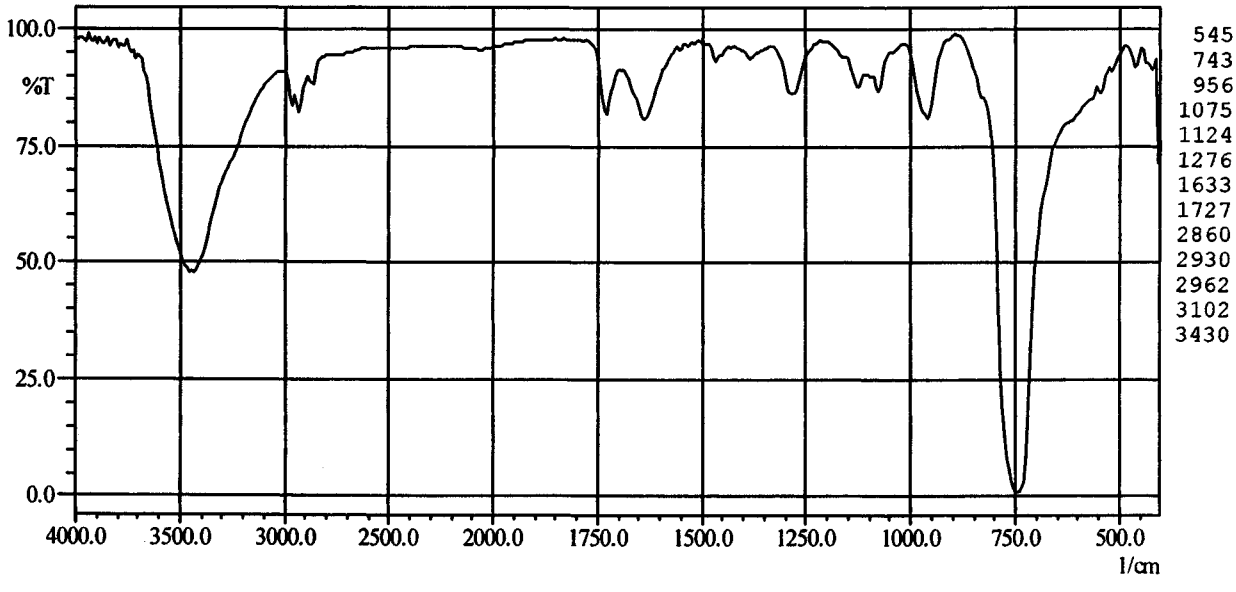
(1) **mixture of high-MW paraffins, contains some NH (fatty amine)**
(2) Antilux 654
(3) Rhein-Chemie (Brunne collection)
(5) antiozonant
(6) white to light-yellow wax
(13) recrystallized film from the melt

139



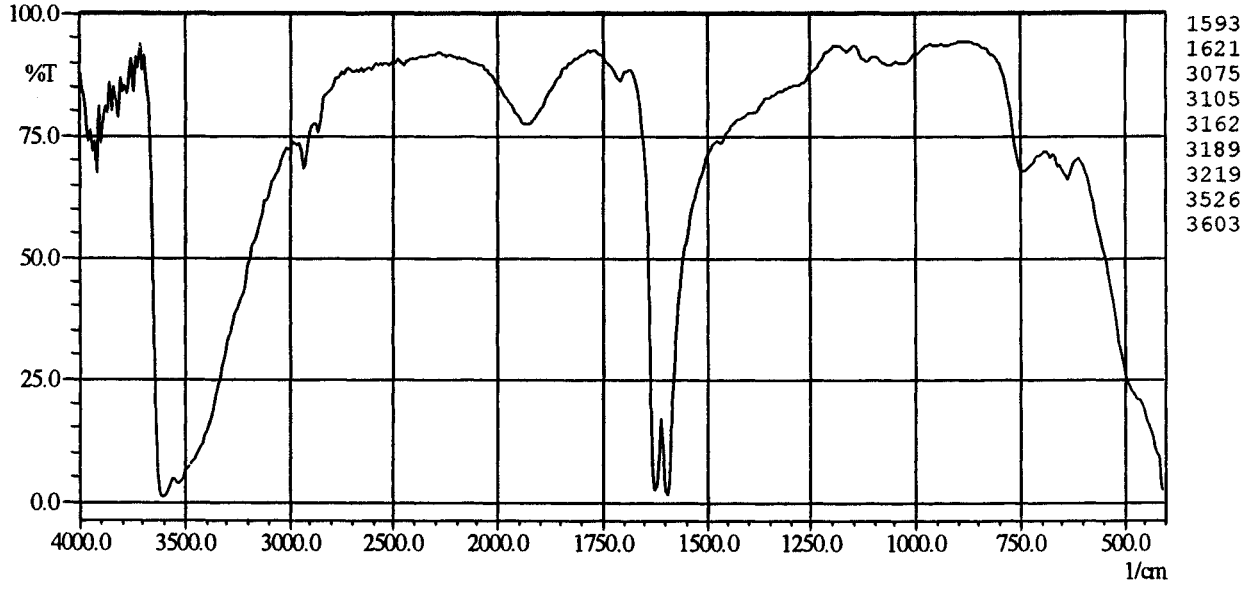
(1) **mixture of higher paraffin hydrocarbons and microwaxes, contains some ester and NH (fatty amine)**
(2) Antilux 750
(3) Rhein-Chemie (Brunne collection)
(5) light stabiliser
(6) yellowish wax
(13) recrystallized film from the melt

1411 Sb_2O_3



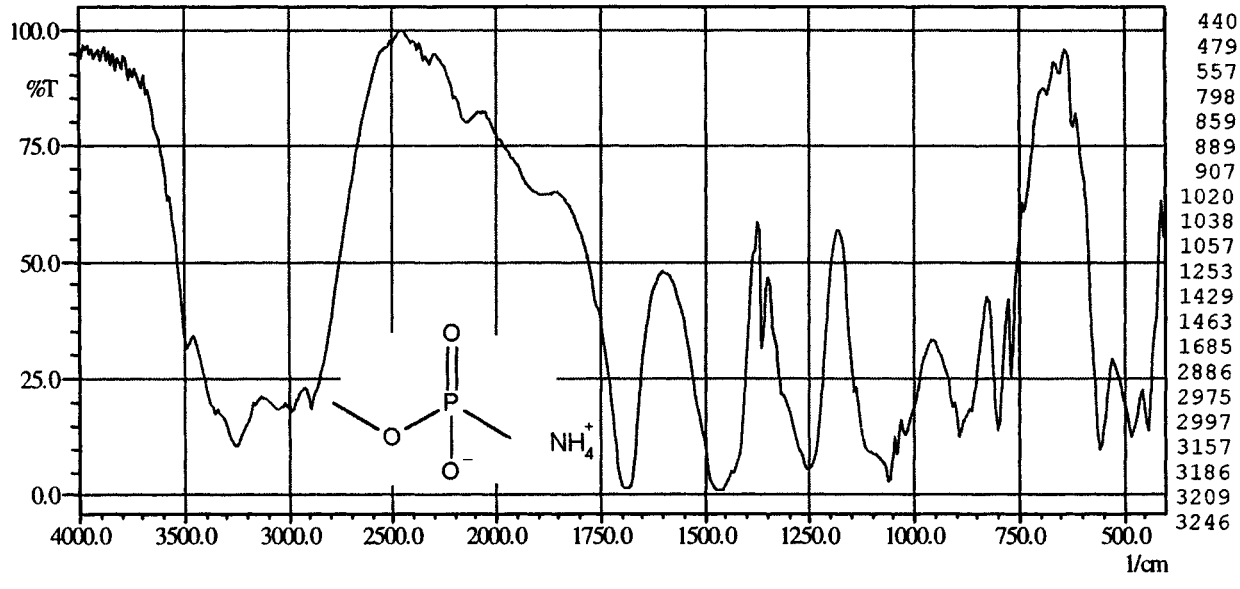
(1) **antimony(III) oxide**
(2) Antimontrioxid Typ Blue
(3) Freudenberg (Brunne collection)
(5) flame retardant
(6) solid
(13) KBr pellet

1412 $SbCl_3$



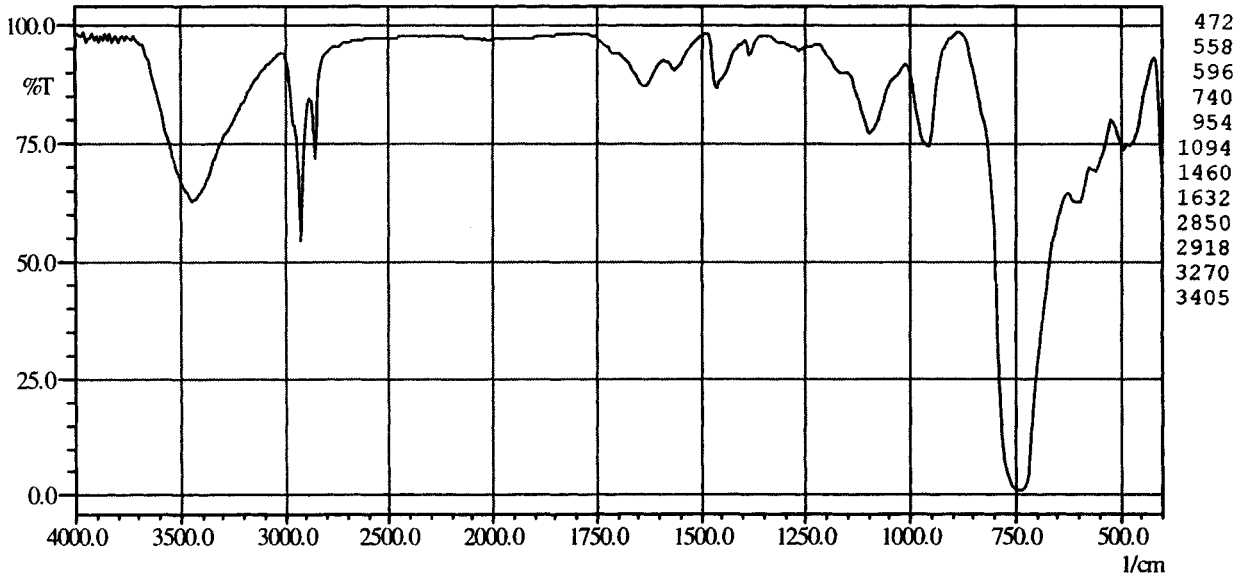
(1) **antimony(III) chloride**
(2) antimony butter
(3) Freudenberg (Brunne collection)
(4) 228.1 g mol^{-1}
(5) flame retardant
(6) soft, hygroscopic mass
(7) 73 °C
(8) 223 °C
(9) 3.14 g cm^{-3}
(13) layer between KBr
(14) partially hydrolysed

1414



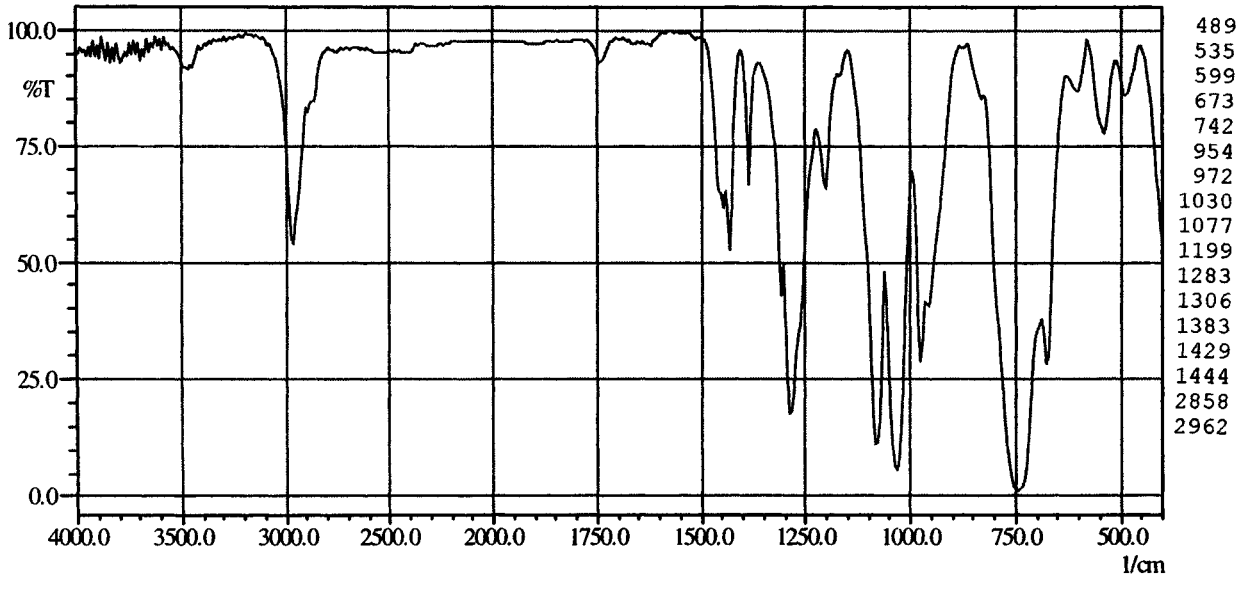
(1) **ammonium polyphosphate**
(2) Exolit VP IFR 23
(3) Hoechst
(5) flame retardant
(6) colourless solid
(9) 1.8 g cm^{-3}
(13) KBr pellet

1415 Sb_2O_3



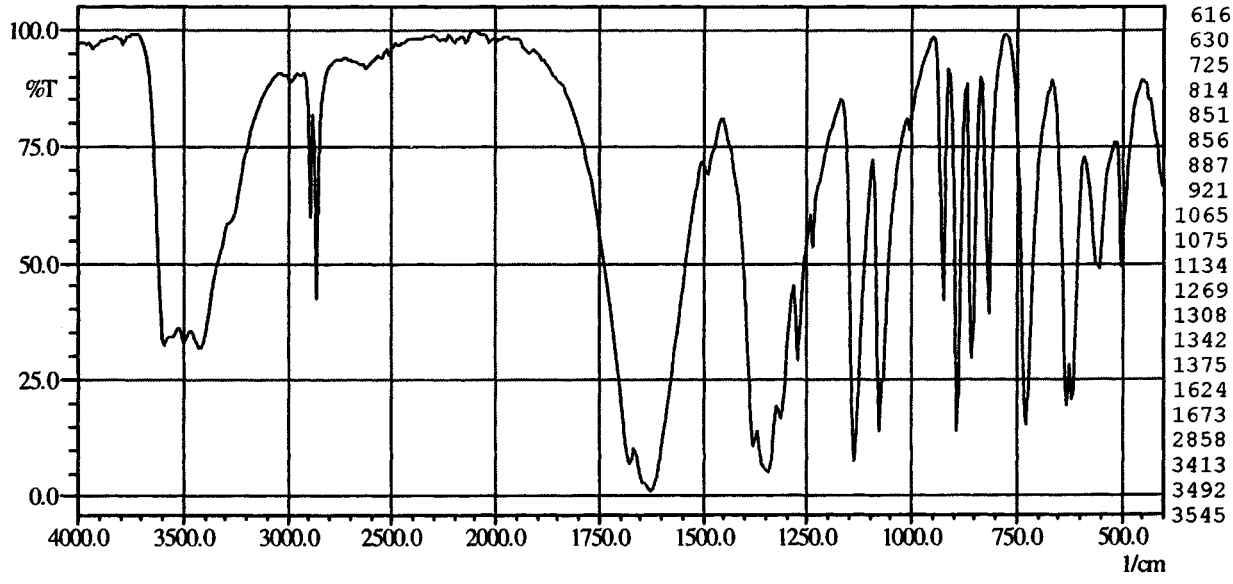
(1) **Sb_2O_3 with mineral oil**
(2) Antiflamm 90/10
(3) Freudenberg (Brunne collection)
(5) flame-inhibiting additive
(6) colourless solid
(13) KBr pellet

1415



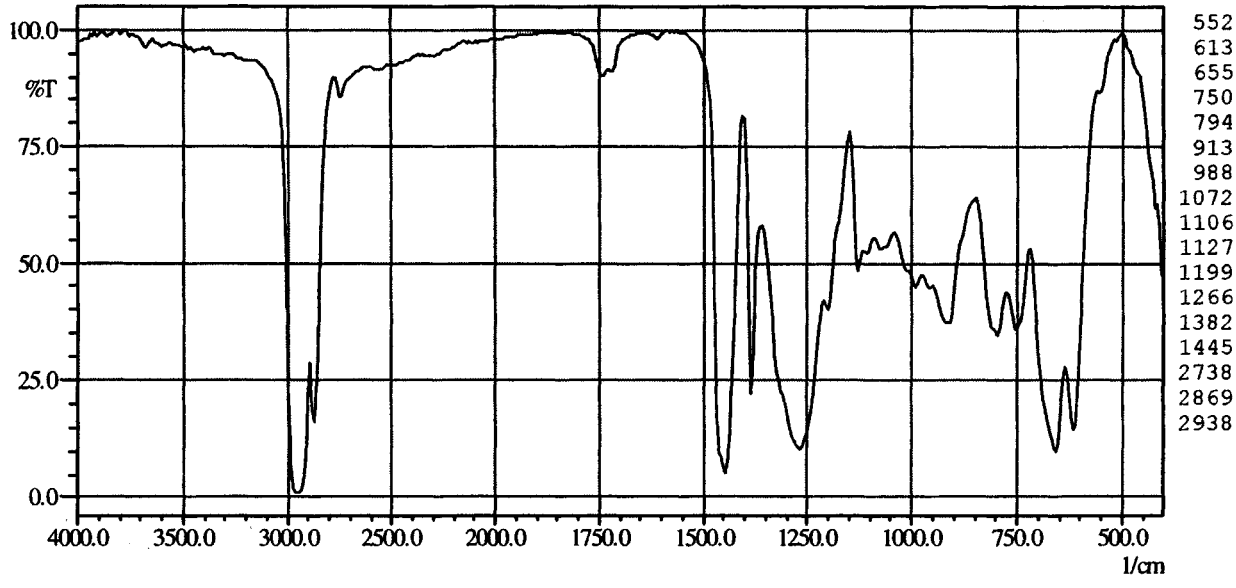
(1) **Sb_2O_3 with chlorinated phosphoric acid ester**
(2) Firex 5718
(3) Dr. Th. Boehme
(5) flame retardant
(6) white sediment (with dispersant)
(13) layer btw KBr

1415 $KSbO_2$



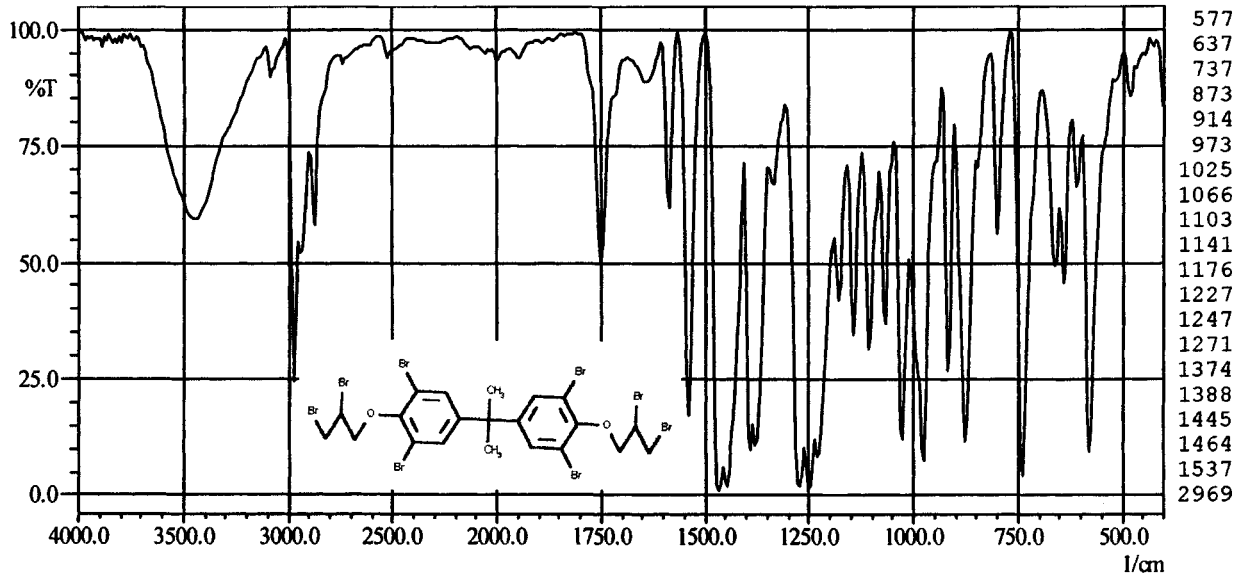
(1) **K antimonate**
(2) potassium antimony(III) oxide
(3) Freudenberg (Brunne collection)
(5) flame-inhibiting additive
(6) colourless solid
(13) KBr pellet

14211



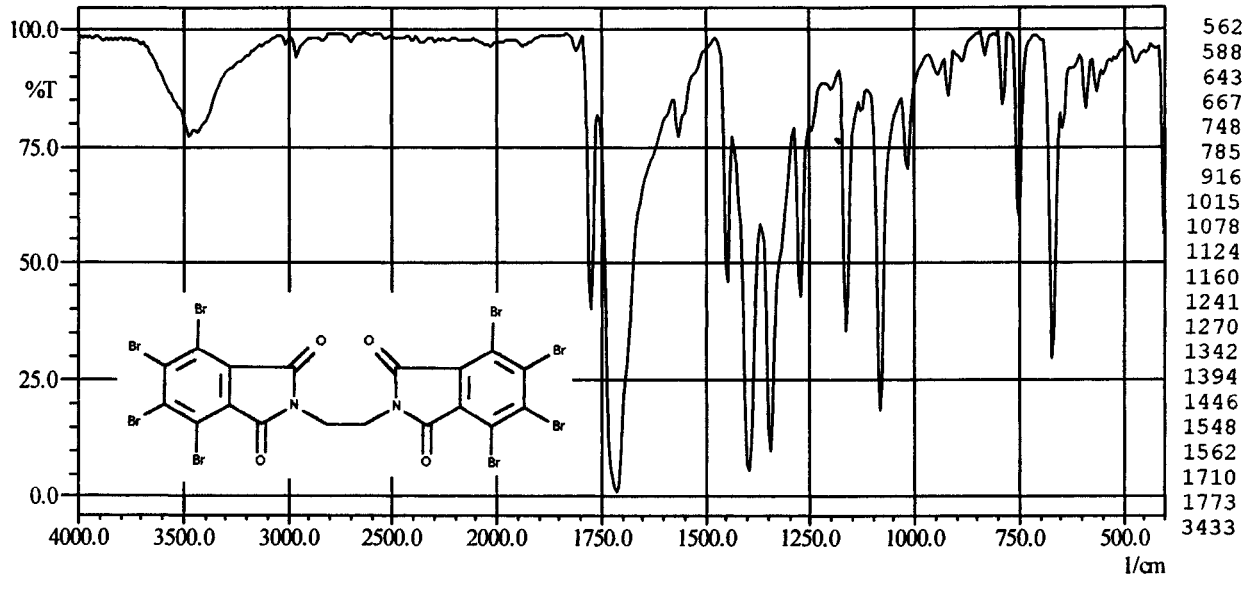
(1) **chlorinated paraffin hydrocarbons**
(2) Cereclor S 52 (Brunne collection)
(3) ICI Petrochemicals and Plastics
(5) flame-retardant additive and plasticiser
(6) yellowish liquid
(13) layer on KBr

14214 $C_{21}H_{20}O_2Br_8$



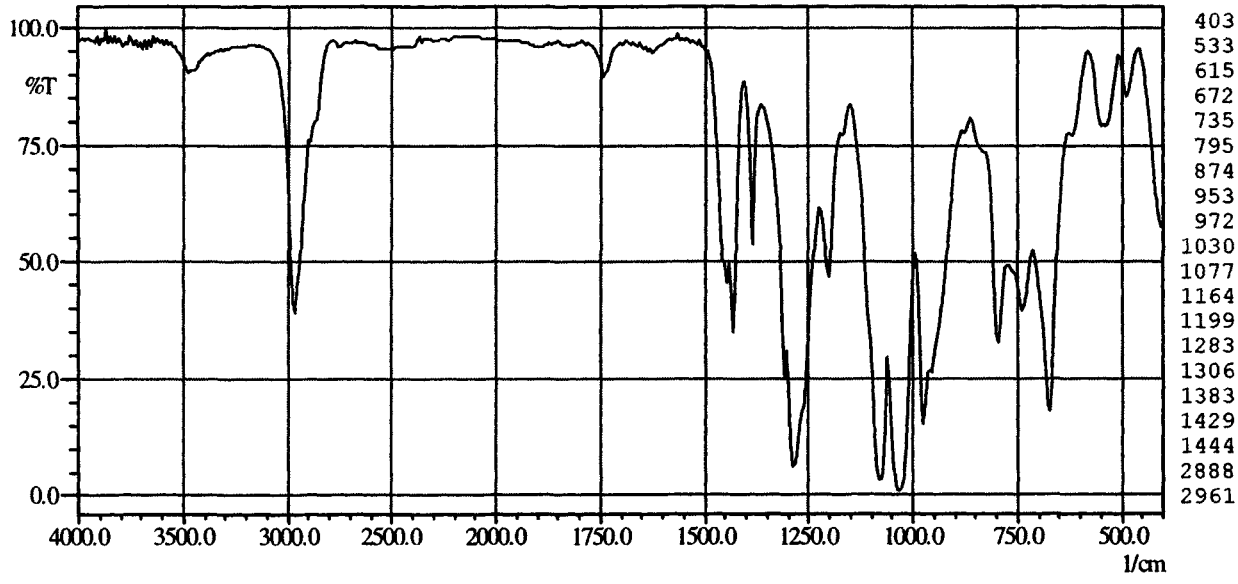
(1) **2,2'-*bis*(4-(2,3-dibromopropoxy)-3,5-dibromophenyl)propane**
(2) Bromkal 66-8
(3) Chem. Fabrik Kalk (Brunne collection)
(4) 835.6 g mol^{-1}
(5) flame retardant
(6) colourless solid
(13) KBr pellet

14215 $C_{18}H_4Br_8N_2O_4$



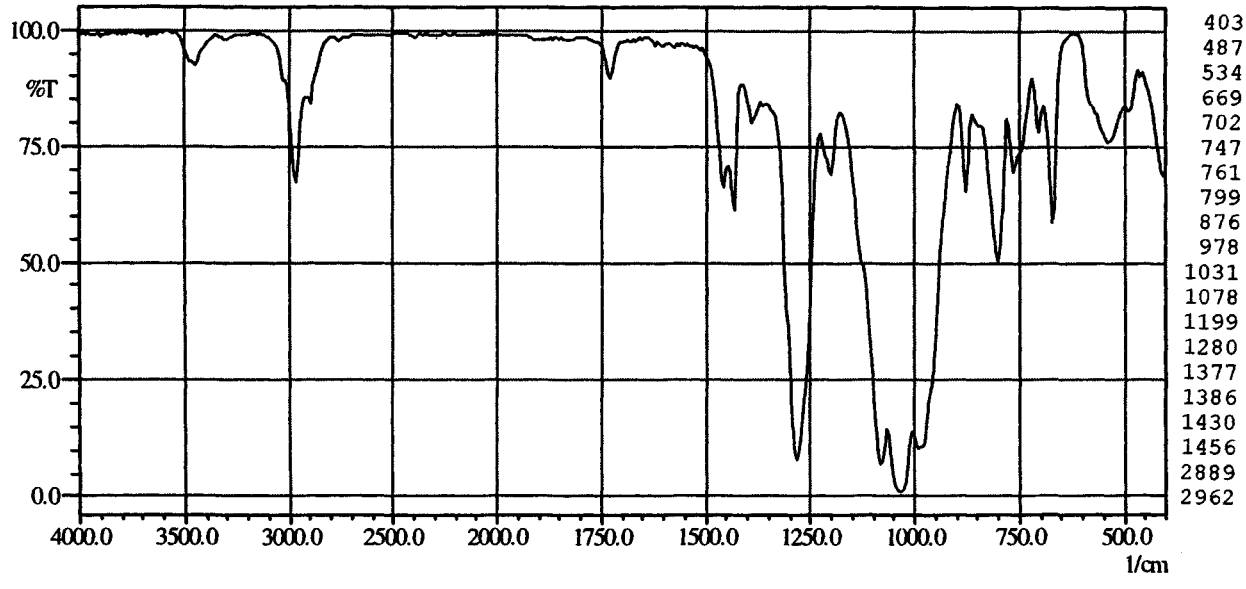
(1) **N,N'-ethylene-*bis*(tetrabromophthalimide)**
(2) Saytex BT 93
(3) Ethyl/Saytech (Brunne collection)
(4) 951.5 g mol^{-1}
(5) flame inhibitor
(6) colourless solid
(13) KBr pellet

14222



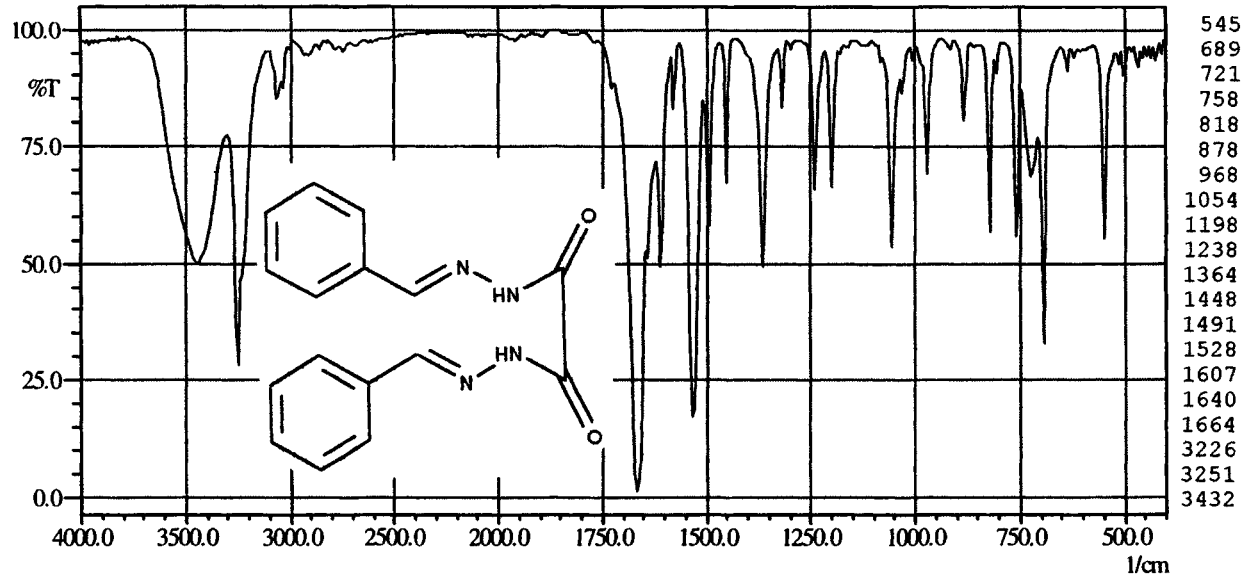
(1) **mixture of Sb_2O_3 with chlorinated phosphoric acid ester**
(2) Firex 5718
(3) Dr. Th. Boehme
(5) flame retardant
(6) white paste
(13) supernatant liquid btw KBr

1423



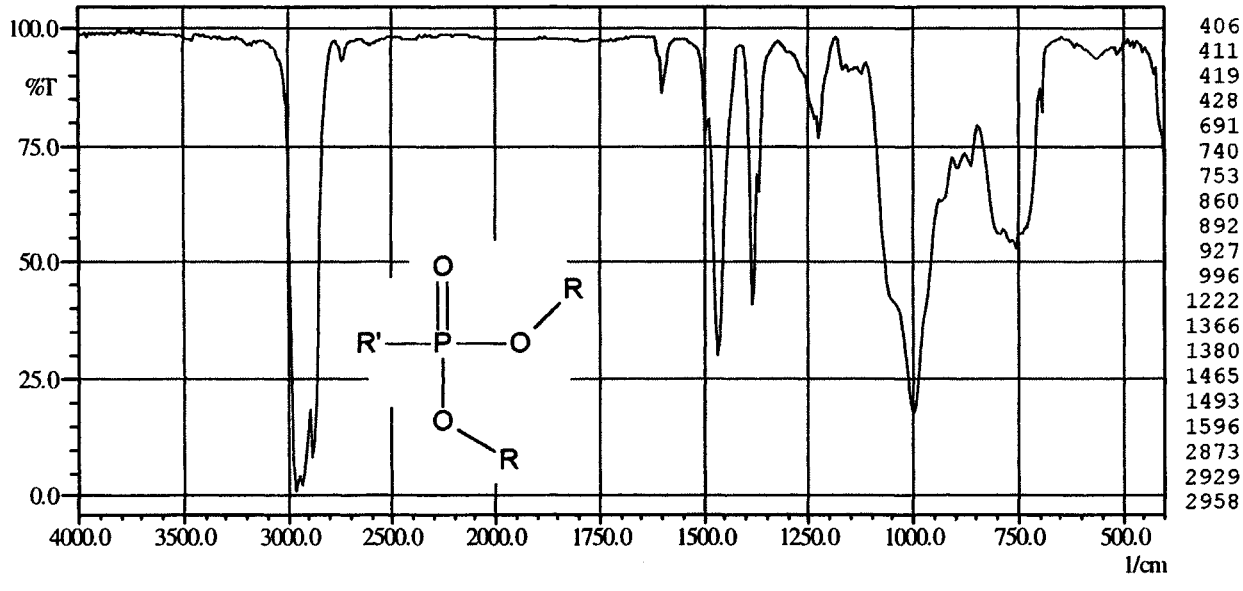
(1) **mixture of oligomeric, chlorinated phosphoric acid ester**
(2) Tego Antiflamm N
(3) Th. Goldschmidt
(5) flame retardant
(6) colourless, clear liquid
(7) 21 °C
(10) 1.462
(13) layer btw KBr

1532 $C_{16}H_{14}N_4O_2$



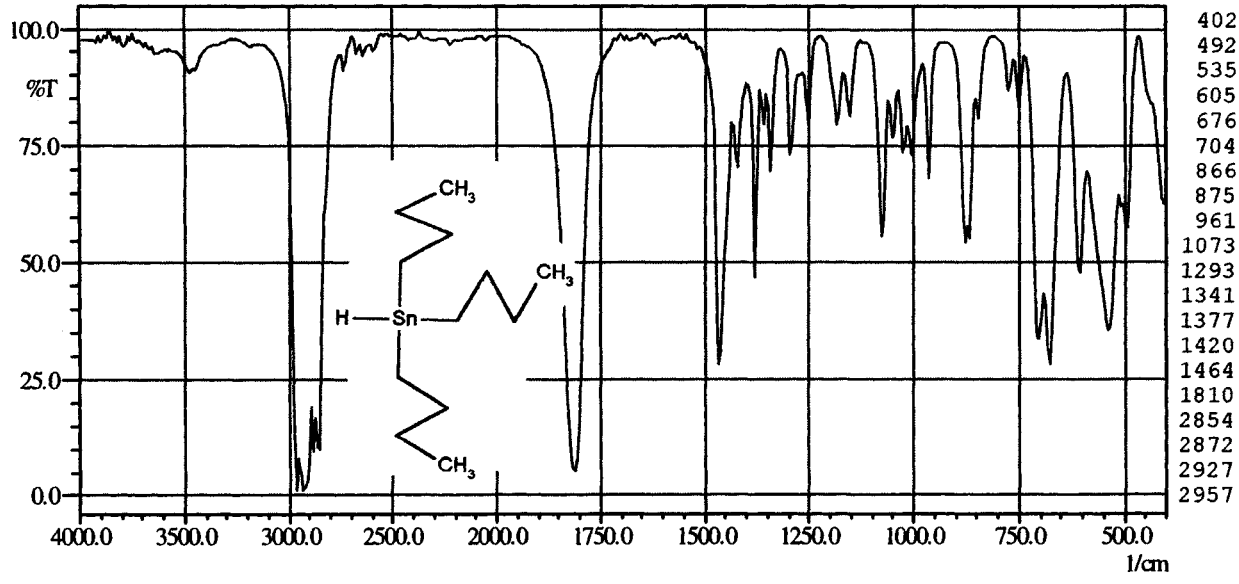
(1) **oxalyl-*bis*(benzylidenehydrazide)**
(2) Eastman OABH-EF
(3) Eastman
(4) 294.2 g mol^{-1}
(5) metal deactivator
(6) colourless, crystalline solid
(13) KBr pellet

155



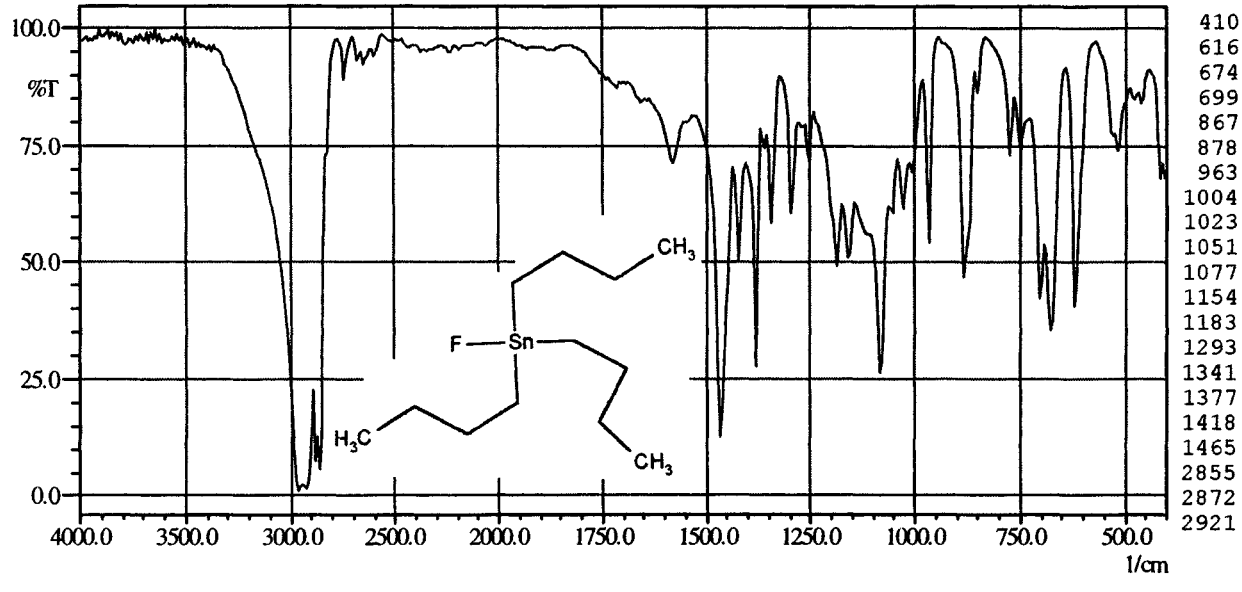
(1) **phosphonic acid ester**
(2) Baerostab CWM 201
(3) Baerlocher
(5) metal deactivator
(6) colourless, clear liquid
(9) 0.89 g cm^{-3}
(10) 1.464
(13) layer btw KBr

16 $C_{12}H_{28}Sn$



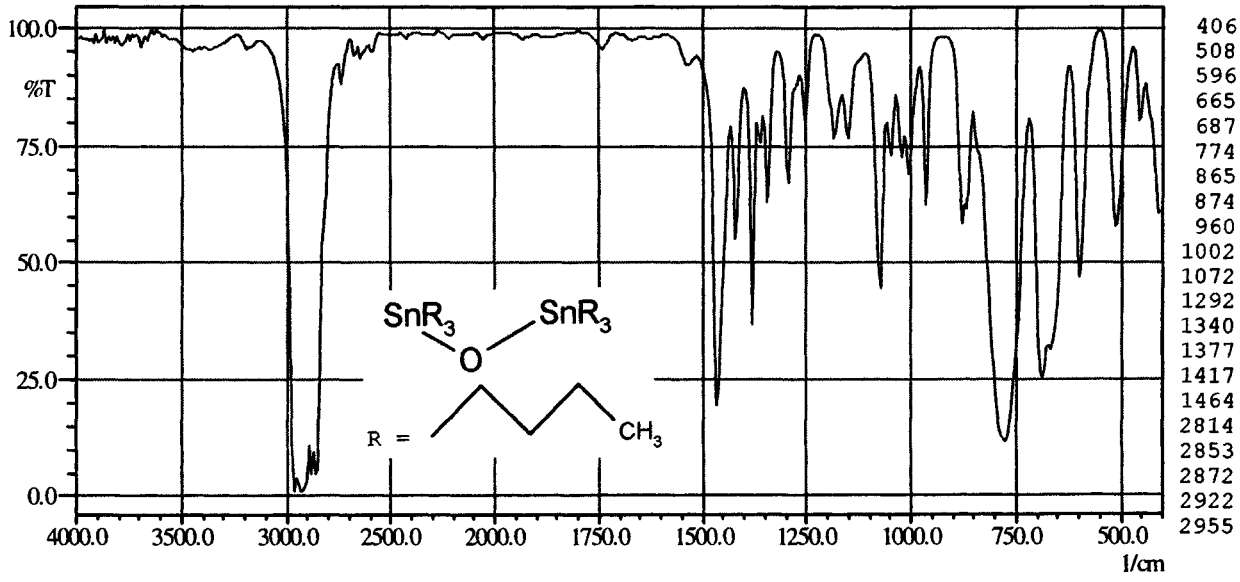
(1) **tributyltin hydride**
(2) XE 9503 (TBTH)
(3) Schering
(4) 291.1 g mol^{-1}
(5) biocide
(6) colourless, clear liquid
(8) 78,5 °C / 12000 Pa
(9) 1.017 g cm^{-3}
(10) 1.472
(13) layer btw KBr

16 $C_{12}H_{27}FSn$



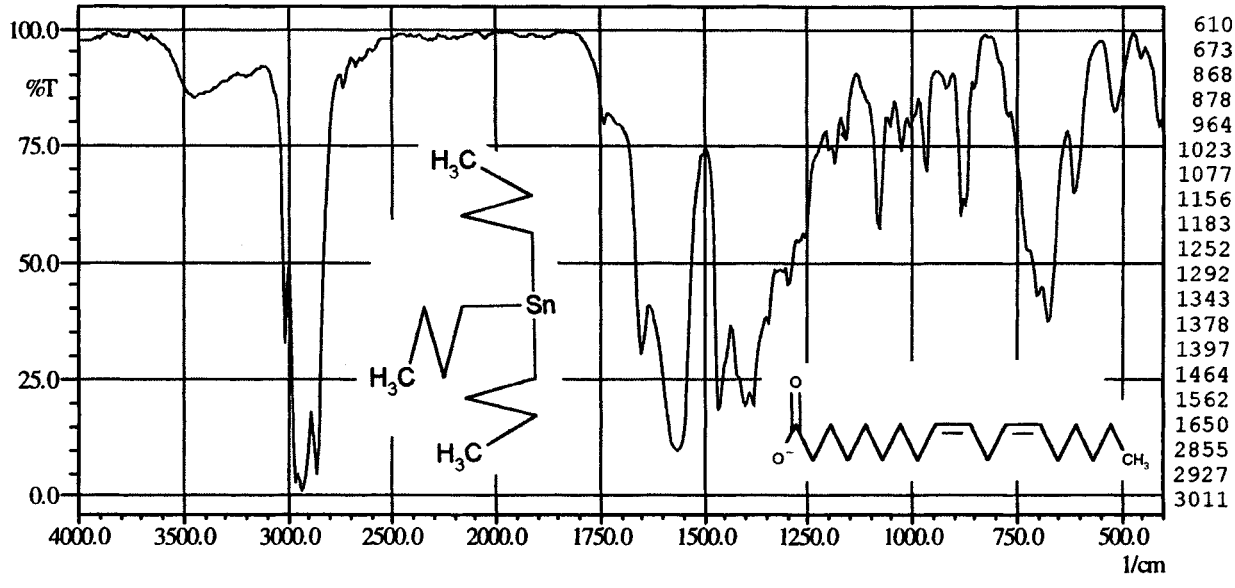
(1) **tributyltin fluoride**
(2) Eurecid 9260 (TBTF)
(3) Schering
(4) 309.1 g mol^{-1}
(5) biocide
(6) colourless solid
(9) 1.25 g cm^{-3}
(13) KBr pellet

16 $C_{24}H_{54}OSn_2$



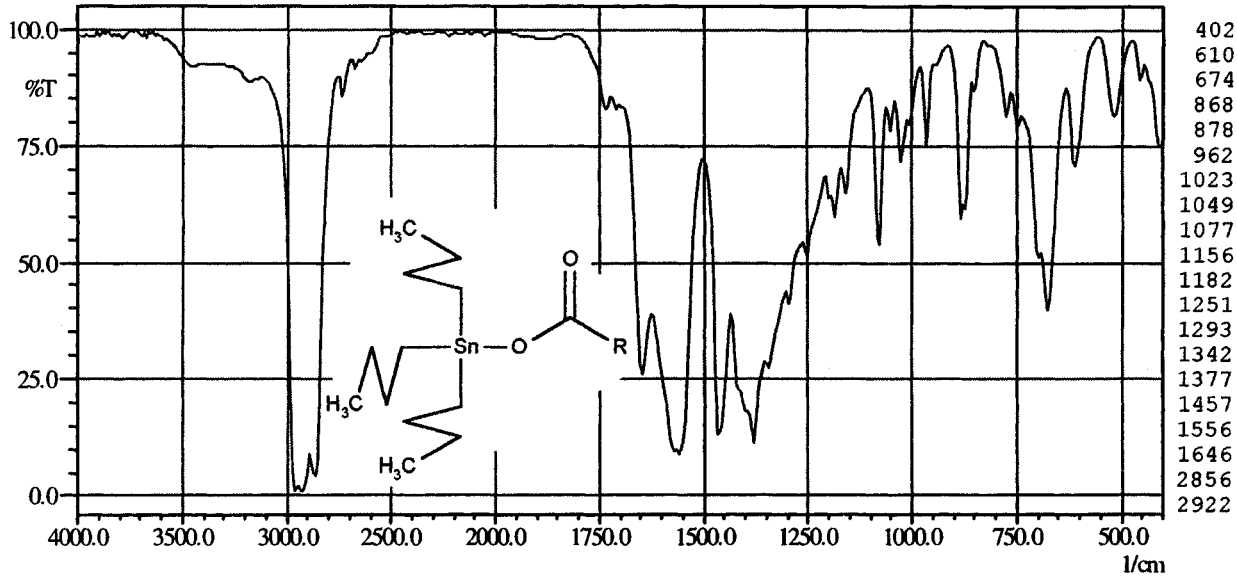
(1) **tributyltin oxide**
(2) Eurecid 9000
(3) Schering
(4) 596.1 g mol^{-1}
(5) biocide
(6) colourless, clear liquid
(8) 173 °C / 17000 Pa
(9) 1.175 g cm^{-3}
(13) layer btw KBr
(14) oxy-*bis*(tributyltin)

16 $C_{30}H_{58}O_2Sn$



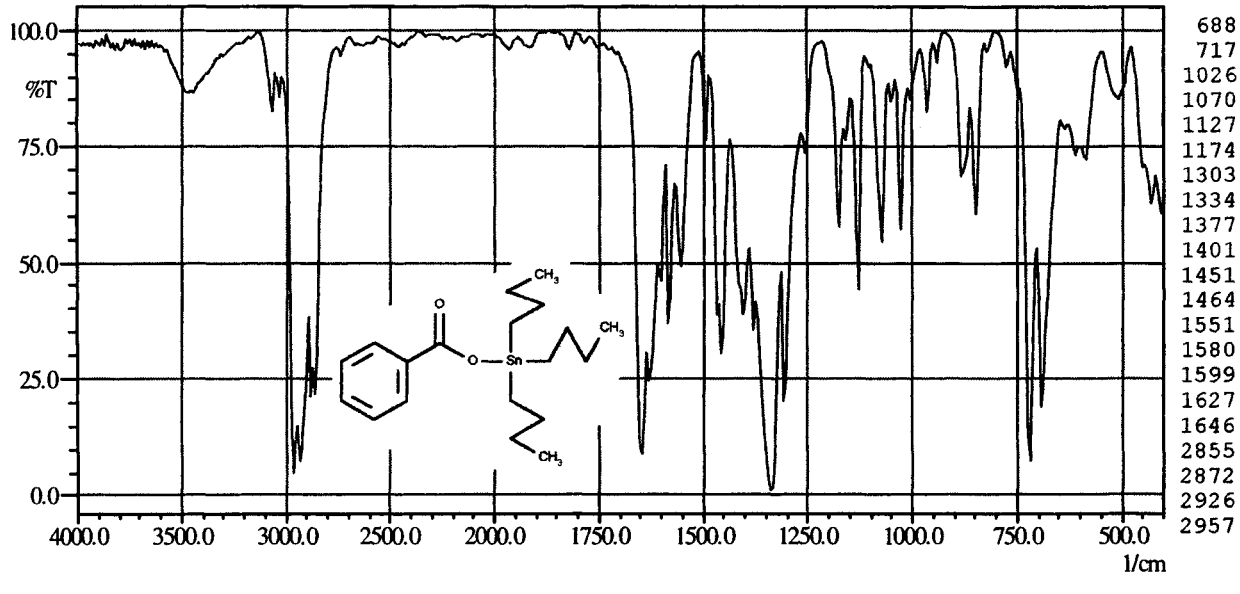
(1) **tributyltin linoleate**
(2) Eurecid 9220 (TBTL)
(3) Schering
(4) 569.5 g mol^{-1}
(5) biocide
(6) yellow, clear liquid
(8) 140 °C / 6600 Pa
(9) 1.055 g cm^{-3}
(13) layer btw KBr

16



(1) **tributyltin naphthenate**
(2) Eurecid 9240 (TBTN)
(3) Schering
(5) biocide
(6) yellow-brown, clear liquid
(8) 125 °C / 6600 Pa
(9) 1.09 g cm^{-3}
(13) layer btw KBr

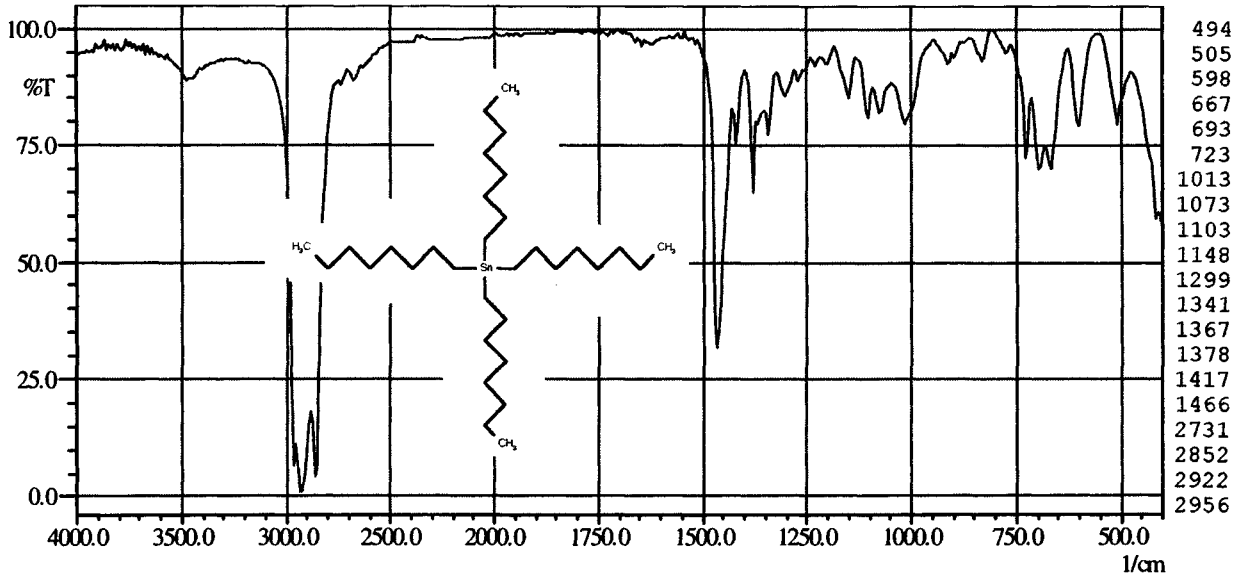
16 $C_{19}H_{32}O_2Sn$



(1) **tributyltin benzoate**
(2) Eurecid 9200 (TBTB)
(3) Schering
(4) 411.2 g mol^{-1}
(5) biocide
(6) colourless, clear liquid
(8) 135 °C / 4000 Pa
(9) 1.185 g cm^{-3}
(13) layer btw KBr

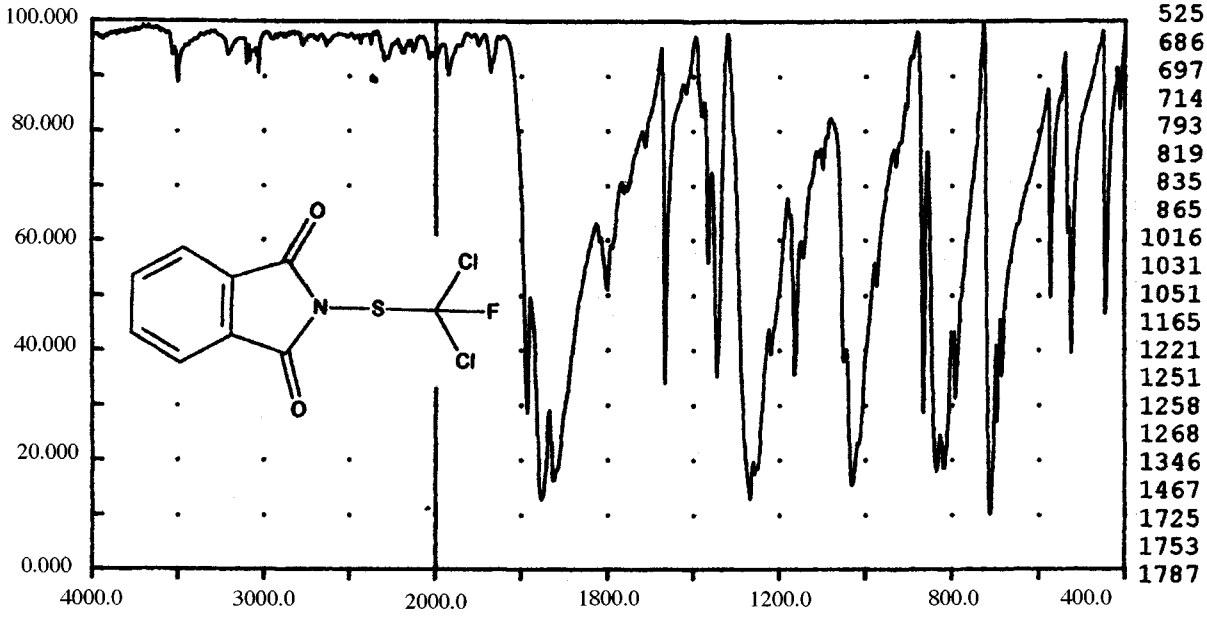
Next Page

16 $C_{32}H_{68}Sn$



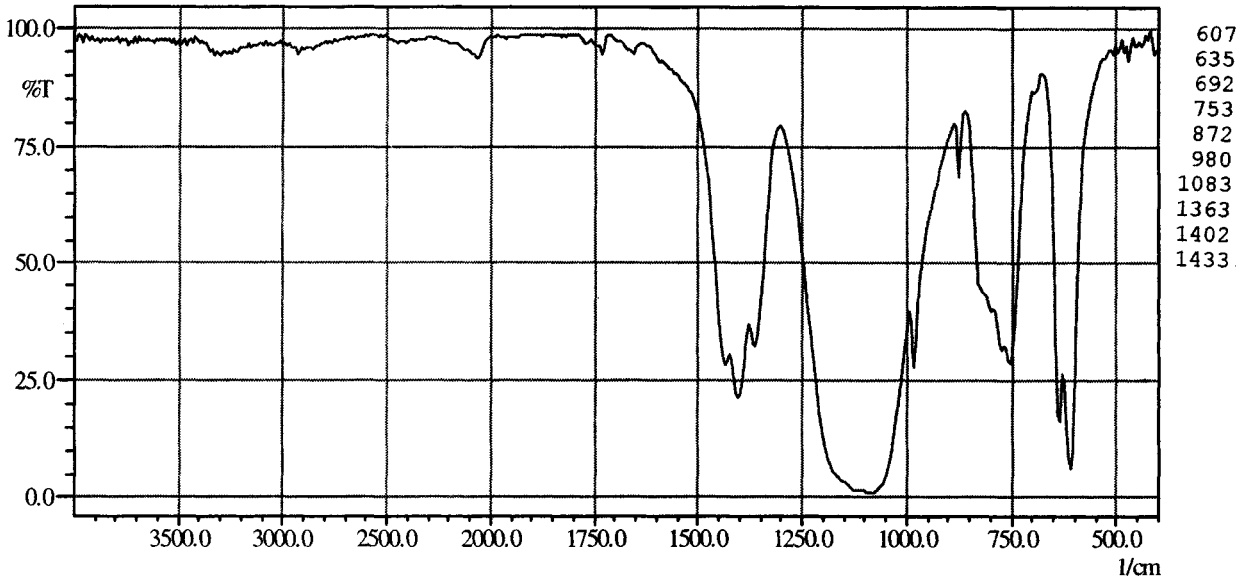
(1) **tetraoctyltin**
(2) Tetra-n-octylzinn, dest. (TOT)
(3) Schering
(4) 571.6 g mol^{-1}
(5) biocide
(6) pale-yellow, clear liquid
(8) 196,5 °C / 1330 Pa
(9) 0.975 g cm^{-3}
(10) 1.474
(13) layer btw KBr

16 $C_9H_4FCl_2NO_2S$



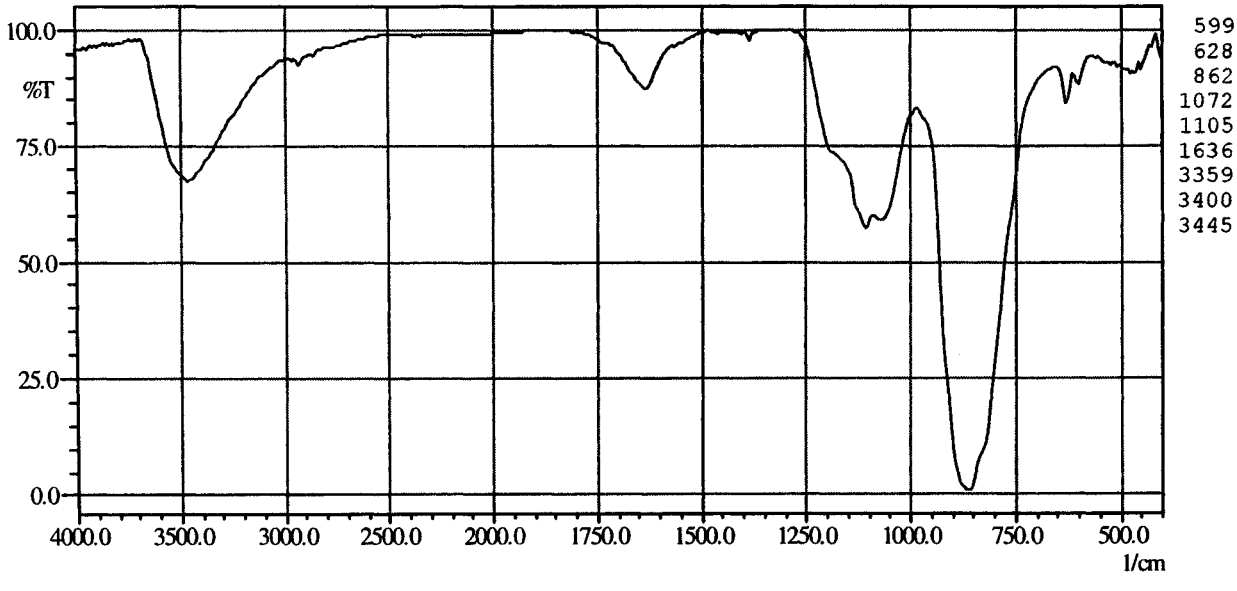
(1) **N-(dichlorofluoromethylthio)phthalimide**
(2) Preventol A3
(3) Bayer
(4) 280.1 g mol^{-1}
(5) biocide
(6) colourless solid

2114 $Ba(MnO_4)_2+BaSO_4$



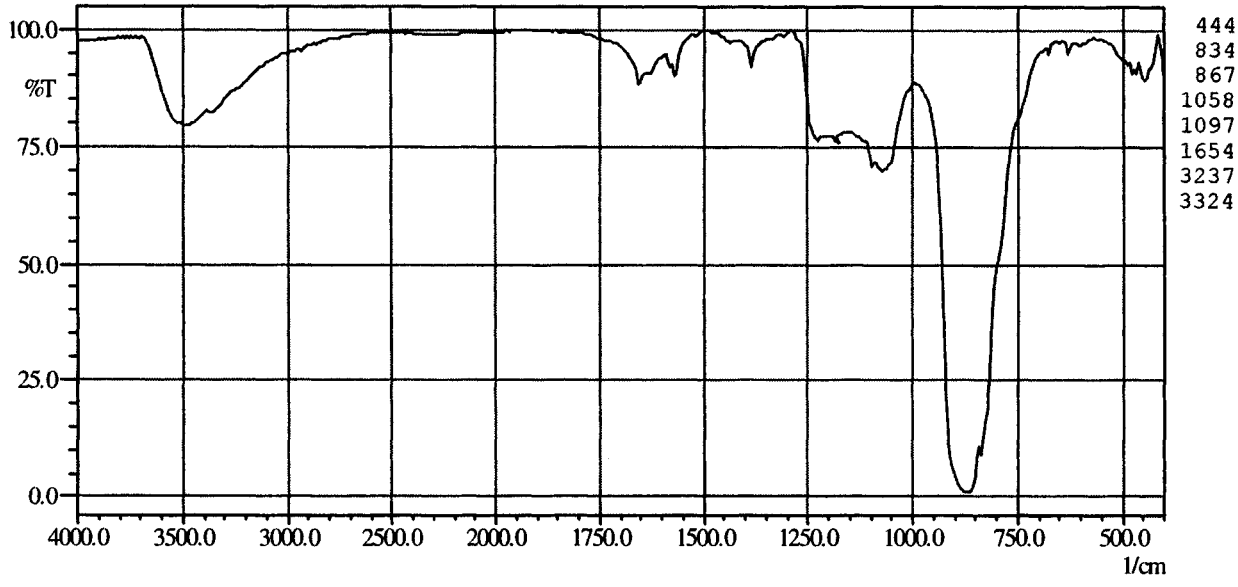
(1) **Ba permanganate mixed crystals with Ba sulfate**
(2) Manganblau
(3) Bayer
(5) pigment for thermoplastics
(6) shining middle-blue solid

2114 $PbCrO_4$



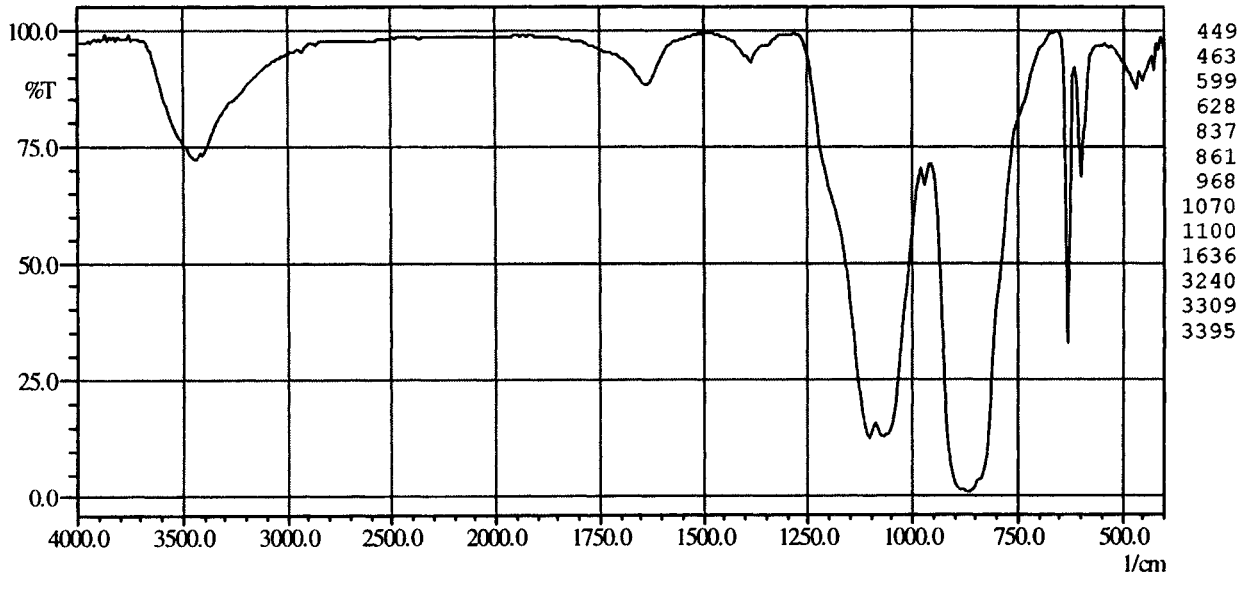
(1) **Pb chromate**
(2) Sicomin Rot L 3130 S
(3) BASF
(5) inorganic pigment
(6) red solid
(13) KBr pellet

2114 $Pb(CrO_4,SO_4)$



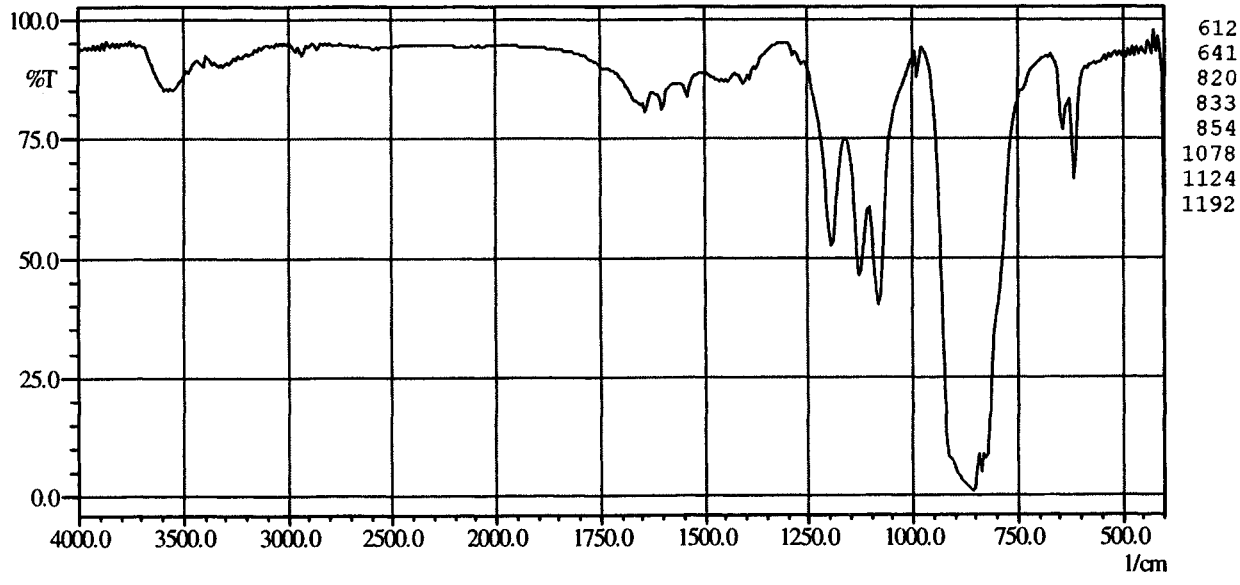
(1) **mixed crystals of Pb chromate-sulfate**
(2) Sicomingelb LD E-55
(3) BASF
(5) organic pigment
(6) yellow solid
(13) KBr pellet

2114 $Pb(CrO_4,SO_4)$



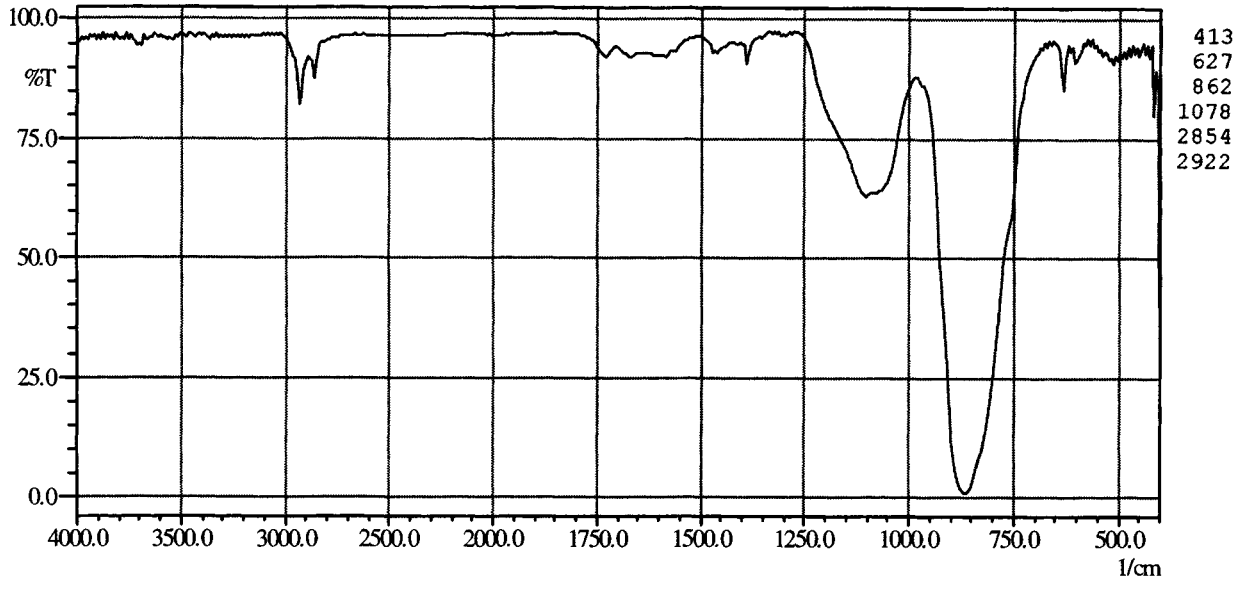
(1) **mixed crystals of Pb chromate-sulfate**
(2) Sicomin Gelb L 1625
(3) BASF
(5) inorganic pigment
(6) yellow solid
(11) Pigment Yellow 34
(12) 7763
(13) KBr pellet

2114 $Pb(CrO_4,SO_4)$



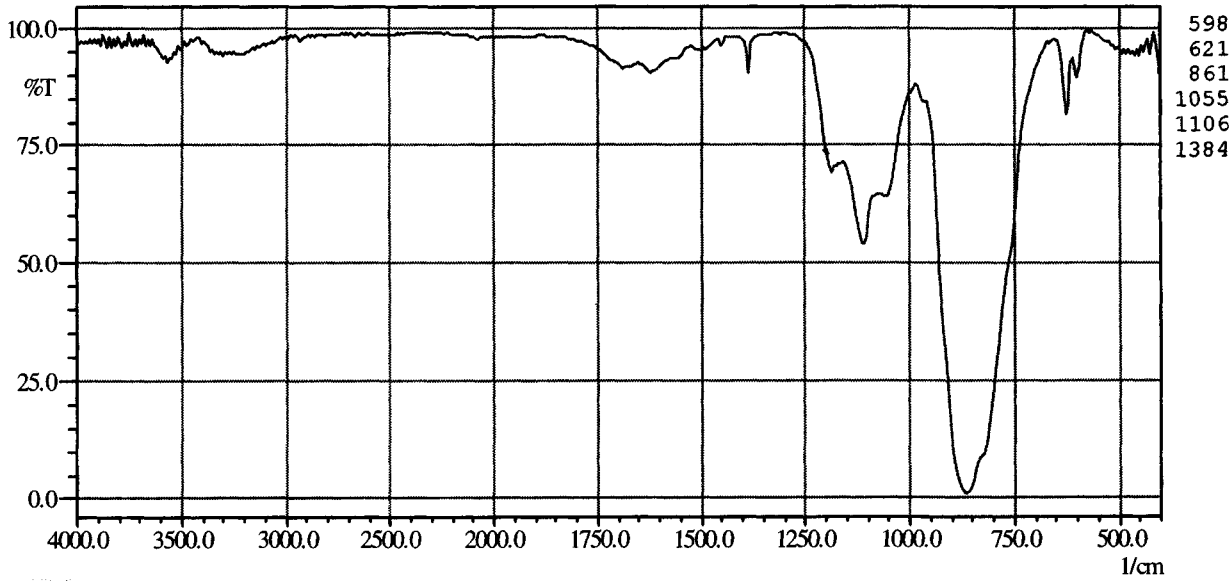
(1) **mixed crystals of Pb chromate-sulfate**
(2) Sicomingelb L 1922
(3) BASF
(5) inorganic pigment
(6) yellow solid
(11) Pigment Yellow 34
(12) 77603
(13) KBr pellet

2114 $Pb(CrO_4,MoO_4)$



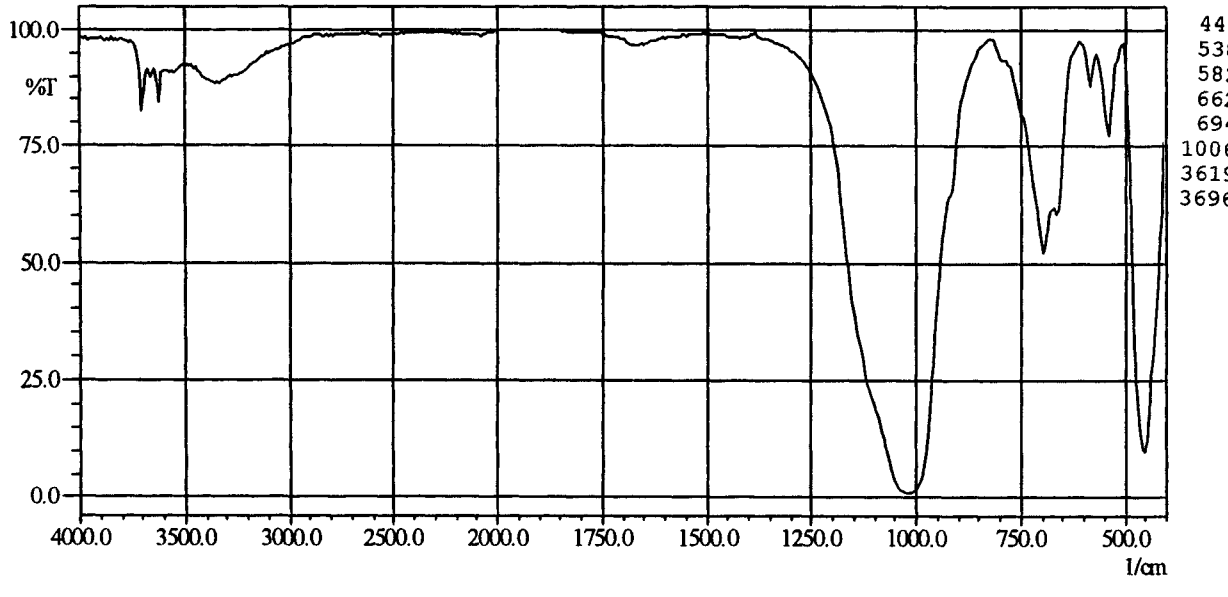
(1) **Pb chromate-molybdate mixed crystals**
(2) Sicomin Rot L 3030 S
(3) BASF
(5) inorganic pigment
(6) red solid
(11) Pigment Red 14
(12) 7765
(13) KBr pellet
(14) contains some sulfate

2114 $Pb(CrO_4,MoO_4,SO_4)$



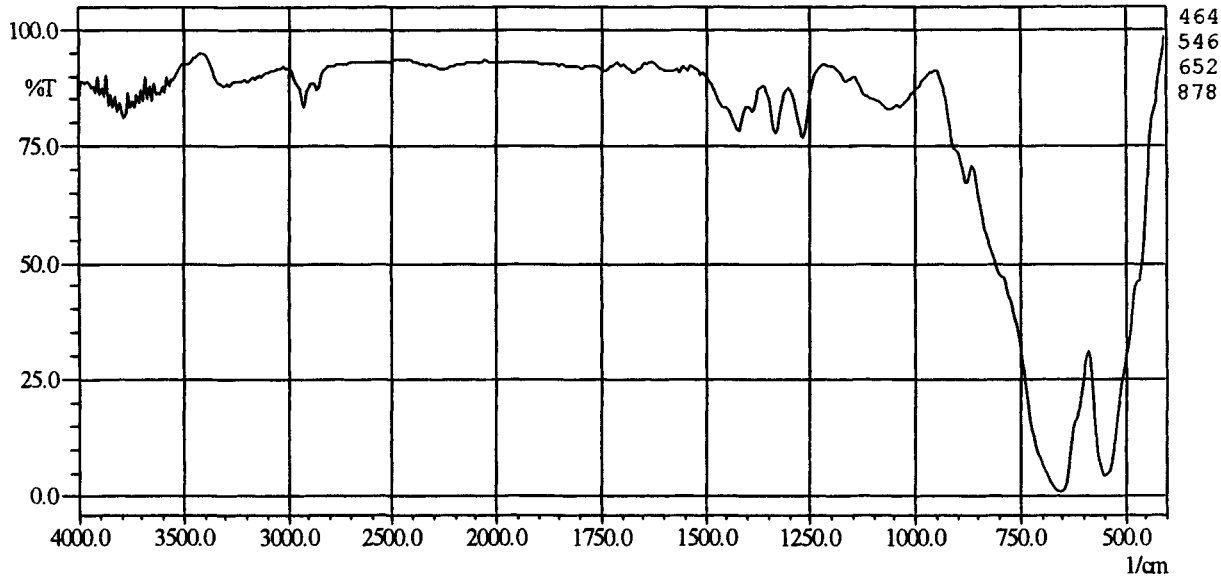
(1) **mixed crystals of Pb chromate-molybdate-sulfate**
(2) Mineralrot B Thiolsol 7947 Z
(3) Cappelle
(5) inorganic pigment
(6) red solid
(11) Pigment Red 104
(12) 77605
(13) KBr pellet

2114 $Na_8(Al_6Si_6O_{24})Sx$



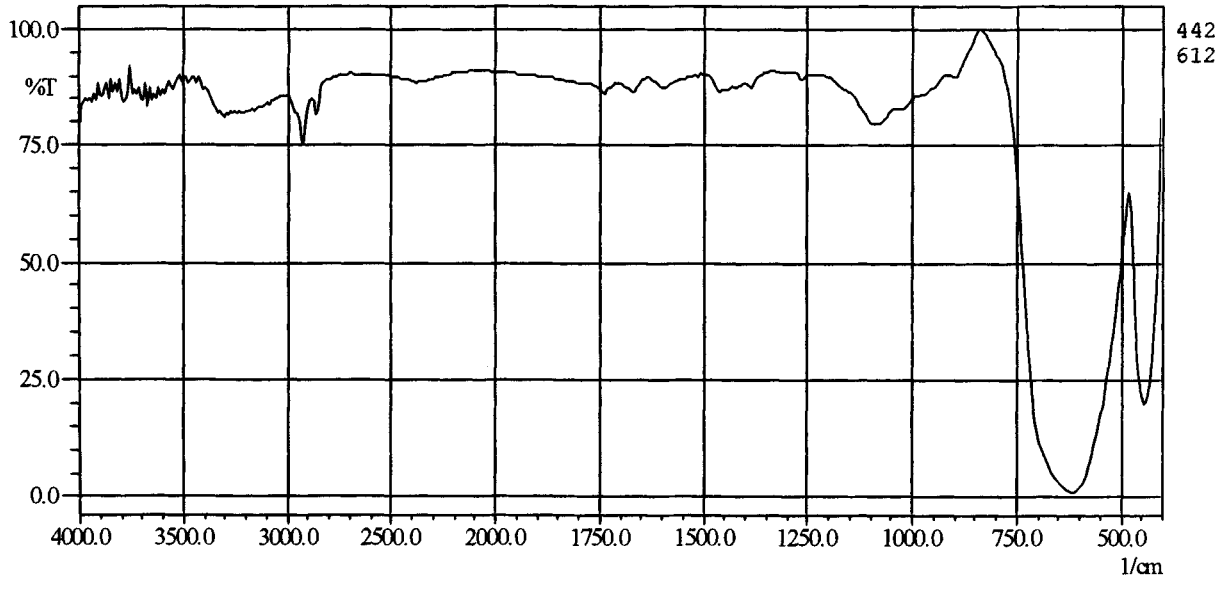
(1) **S-containing Na Al silicate**
(2) Ultramarin Blau
(3) BASF (Brunne collection)
(5) inorganic pigment
(6) blue solid
(11) Pigment Blue 29
(13) KBr pellet, H_2O subtracted

2115 $Co(Cr, Al)_2O_4$



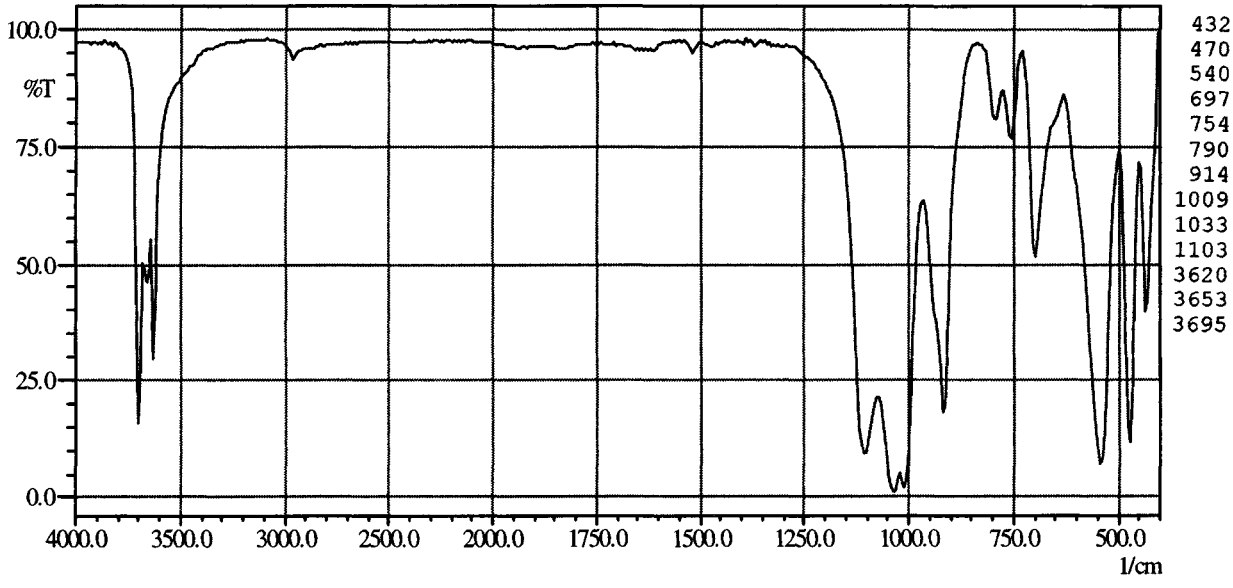
(1) **Co chromate-aluminate, spinell structure**
(2) Lichtblau 100 Standard 9515
(3) Bayer
(5) inorganic pigment
(6) blue solid
(11) Pigment Blue 28
(12) 77346
(13) KBr pellet

2115 $(Co, Ni, Zn)_2(Ti, Al)O_4$



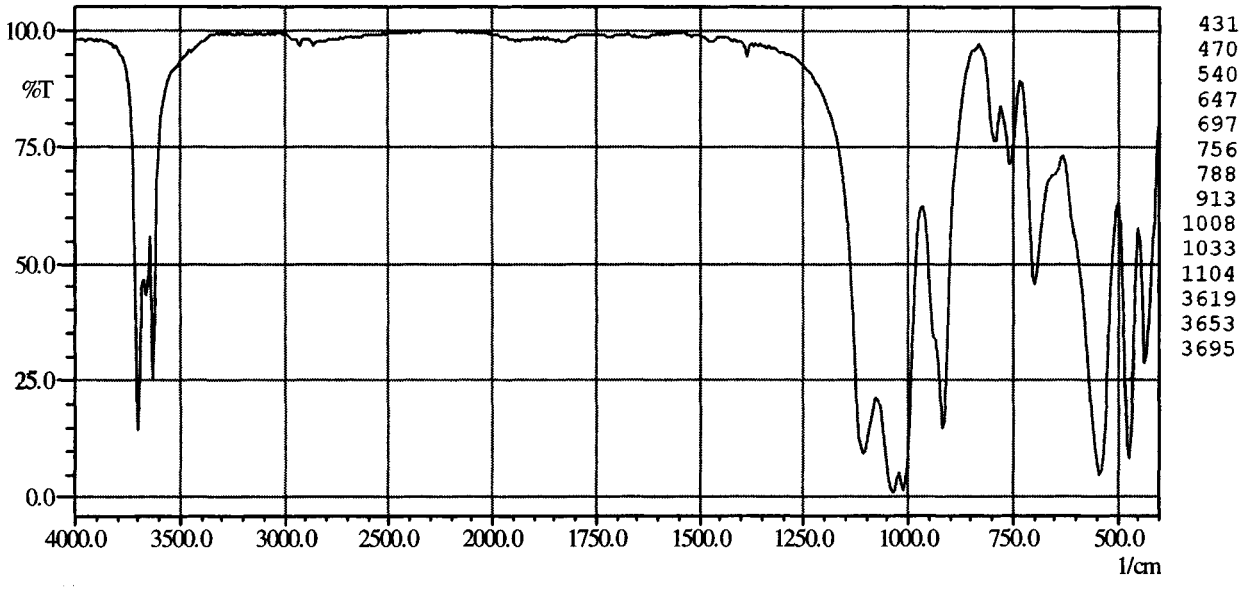
(1) **Co Ni Zn titanate aluminate, inverse spinell**
(2) Lichtgruen 5 G Standard 9270
(3) Bayer
(5) inorganic pigment
(6) green solid
(11) Pigment Green 14
(12) 77346
(13) KBr pellet

2116 $Al_4H_8O_{18}Si_4$



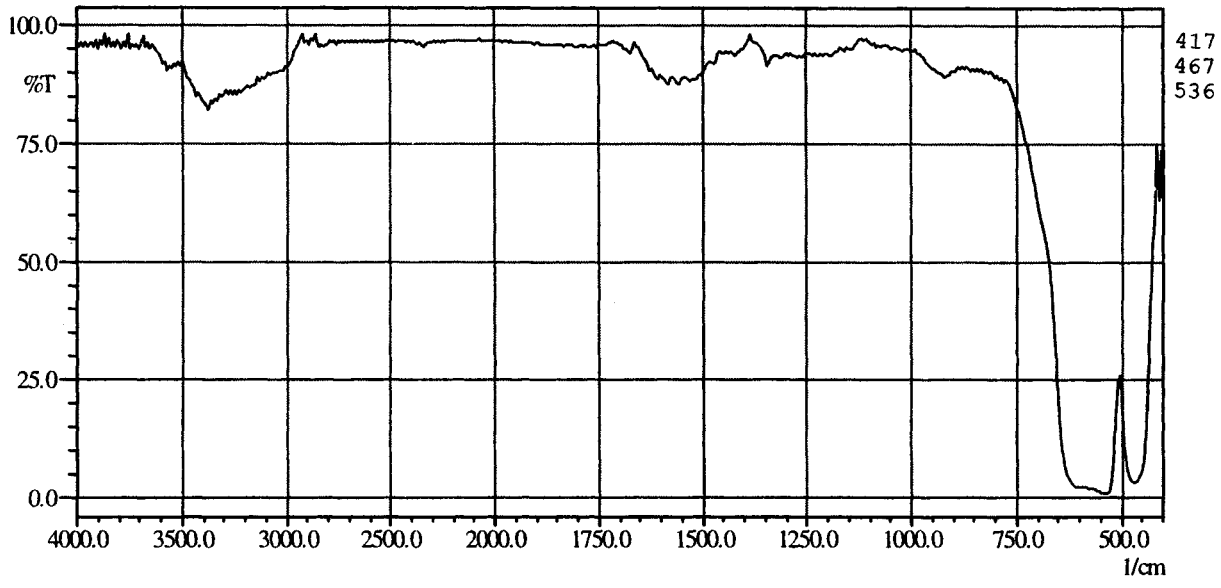
(1) **Al silicate, hydrated**
(2) Dixie Clay
(3) C.H. Erbsloeh, (Vanderbilt)
(4) 516.3 g mol^{-1}
(5) filler
(6) beige solid
(9) 2.62 g cm^{-3}
(13) KBr pellet
(14) kaolinite, hard clay

2116 $Al_4H_8O_{18}Si_4$



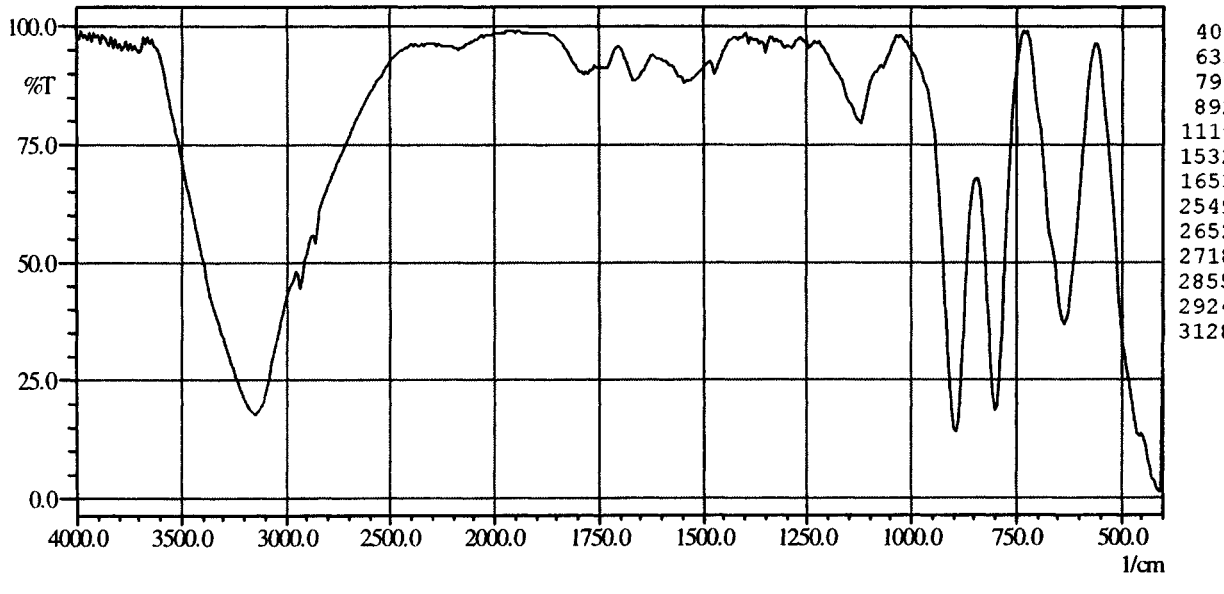
(1) **Al silicate, hydrated**
(2) Mc Namee Clay
(3) C.H. Erbsloeh (Vanderbilt)
(4) 516.3 g mol^{-1}
(5) filler
(6) beige solid
(9) 2.62 g cm^{-3}
(13) KBr pellet
(14) kaolin, kaolinite, soft clay

214 FeO(OH)



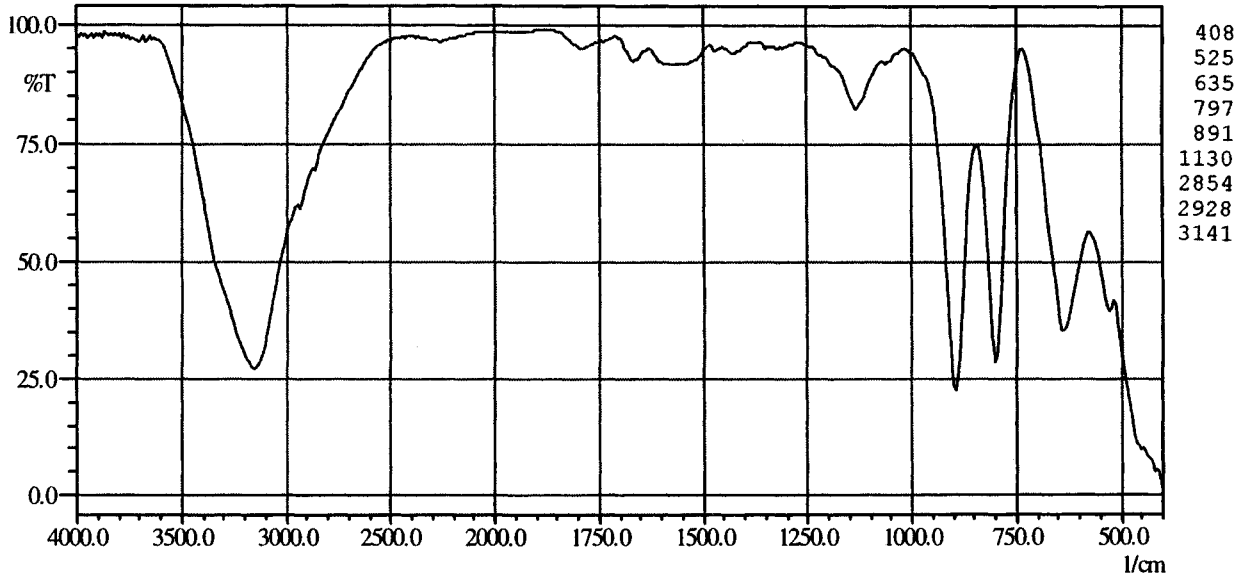
(1) **Fe oxide**
(2) Sicotrans Rot L 2915 D
(3) BASF
(5) inorganic pigment
(6) red solid
(11) Pigment Red 11
(12) 77491
(13) KBr pellet

214 $FeO(OH), H_2O$



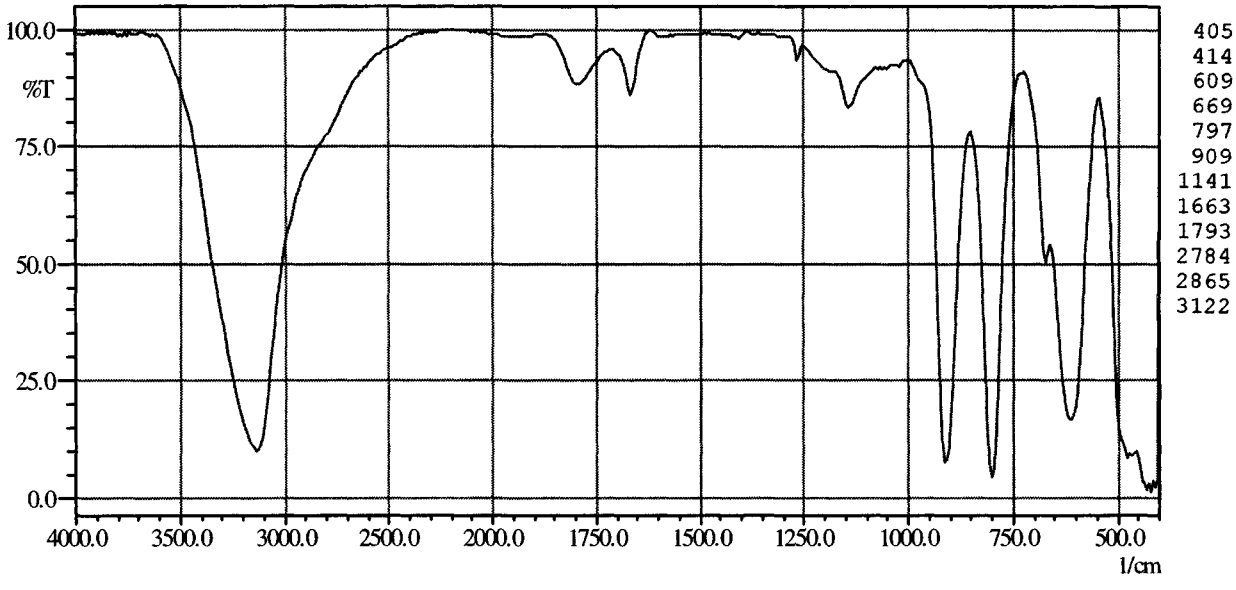
(1) **Fe oxide hydrate**
(2) Sicotrans Gelb L 1916
(3) BASF
(5) inorganic pigment
(6) yellow solid
(11) Pigment Yellow 42
(12) 77492
(13) KBr pellet

214 $FeO(OH), H_2O$



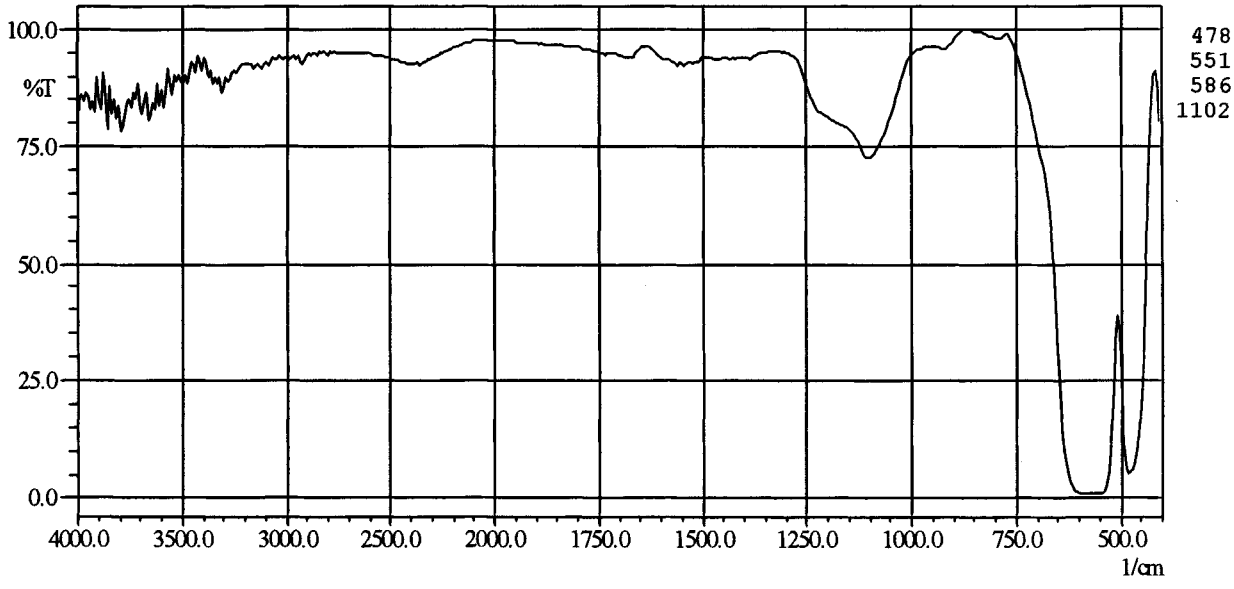
(1) **Fe oxide hydrate**
(2) Sicotrans Orange L 2416
(3) BASF
(5) inorganic pigment
(6) orange solid
(13) KBr pellet

214 $FeO(OH), H_2O$



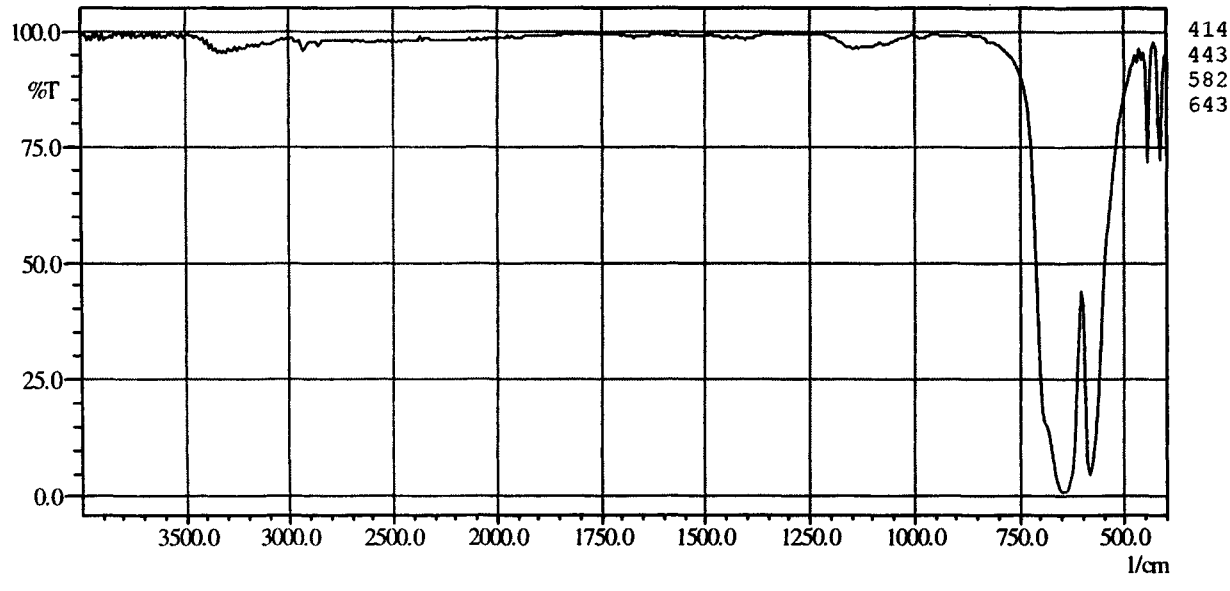
(1) **Fe oxide hydrate**
(2) Bayferrox 920
(3) Bayer
(5) inorganic pigment
(6) red solid
(13) KBr pellet

214 Fe_3O_4



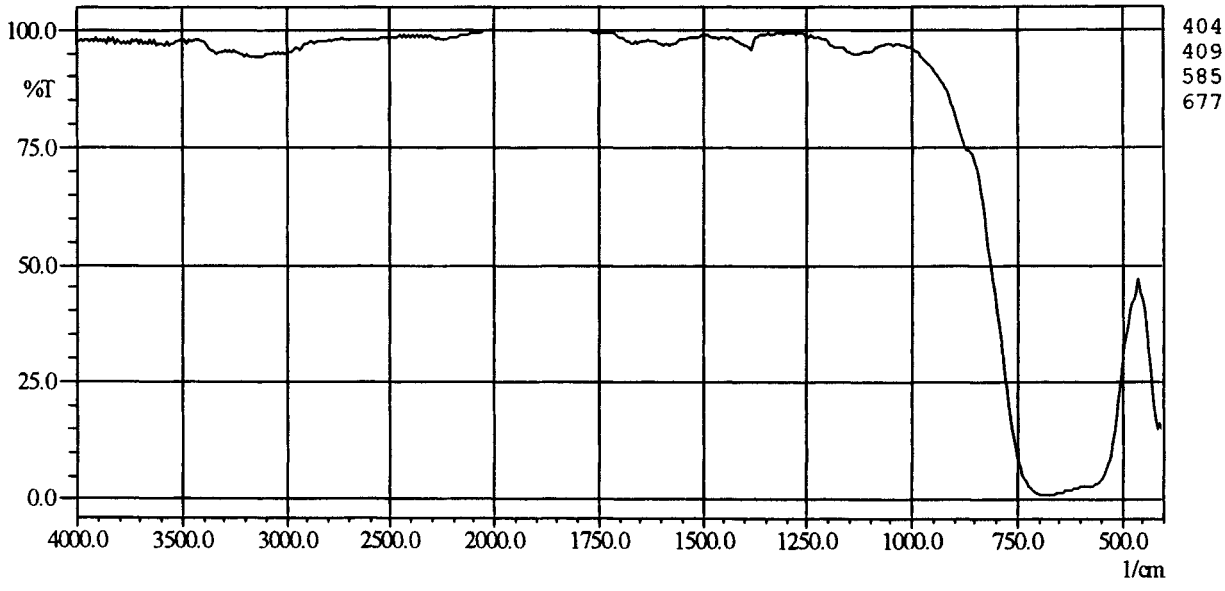
(1) **iron(II, III) oxide, magnetite structure**
(2) Bayferrox 318, Standard 86
(3) Bayer
(4) 231.6 g mol^{-1}
(5) inorganic pigment
(6) black solid
(11) Pigment Black 11
(12) 77499
(13) KBr pellet

214 Cr_2O_3



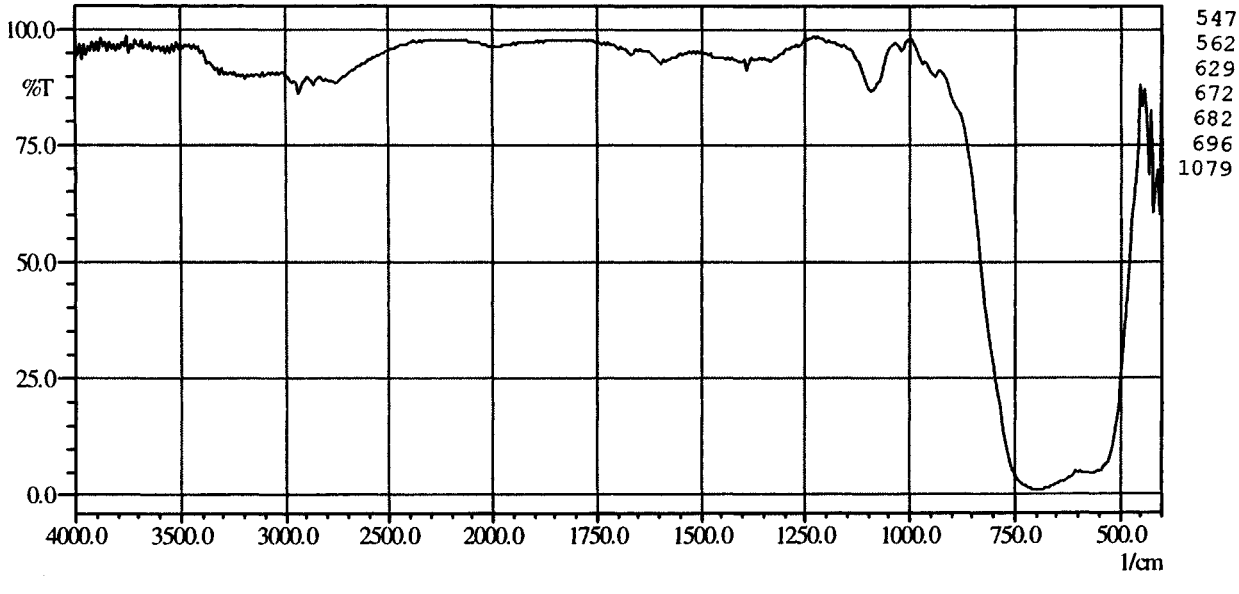
(1) **chromium(III) oxide, corundum structure**
(2) Chromoxidgruen GN
(3) Bayer
(5) pigment for thermoplastics
(6) green solid

214 Cr_2O_3-Sb_2O_3-TiO_2



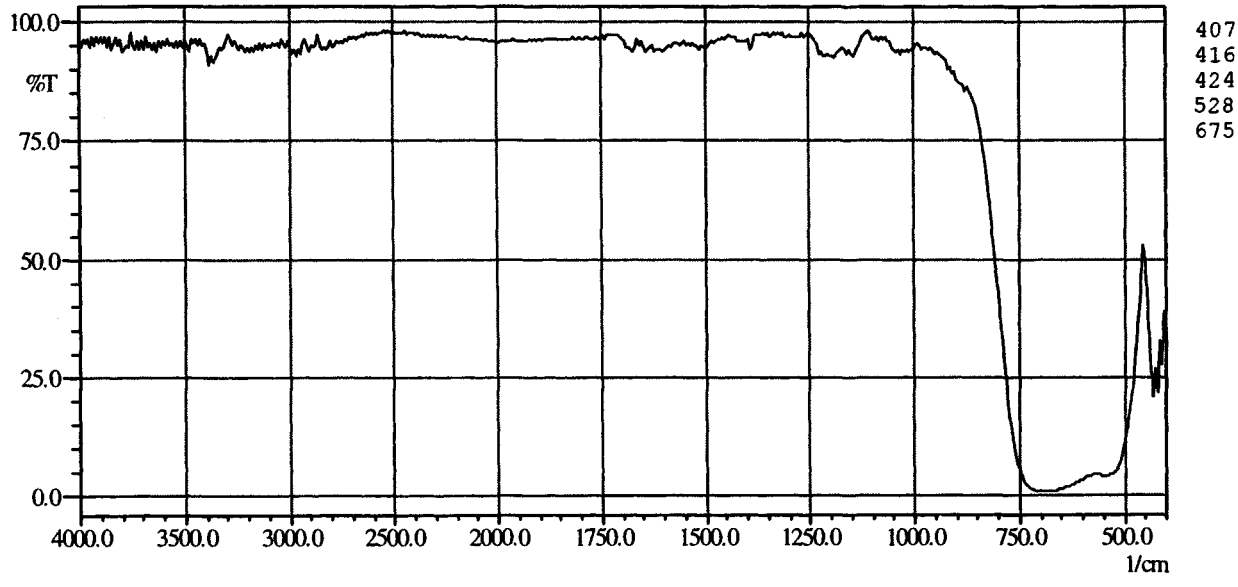
(1) **Cr-Sb-Ti oxide mixed phase system**
(2) Sicotrans Gelb L 1910
(3) BASF
(5) inorganic pigment
(6) yellow solid
(11) Pigment Brown 24
(12) 77310
(13) KBr pellet
(14) rutile structure

214 Sb_2O_3,NiO,TiO_2



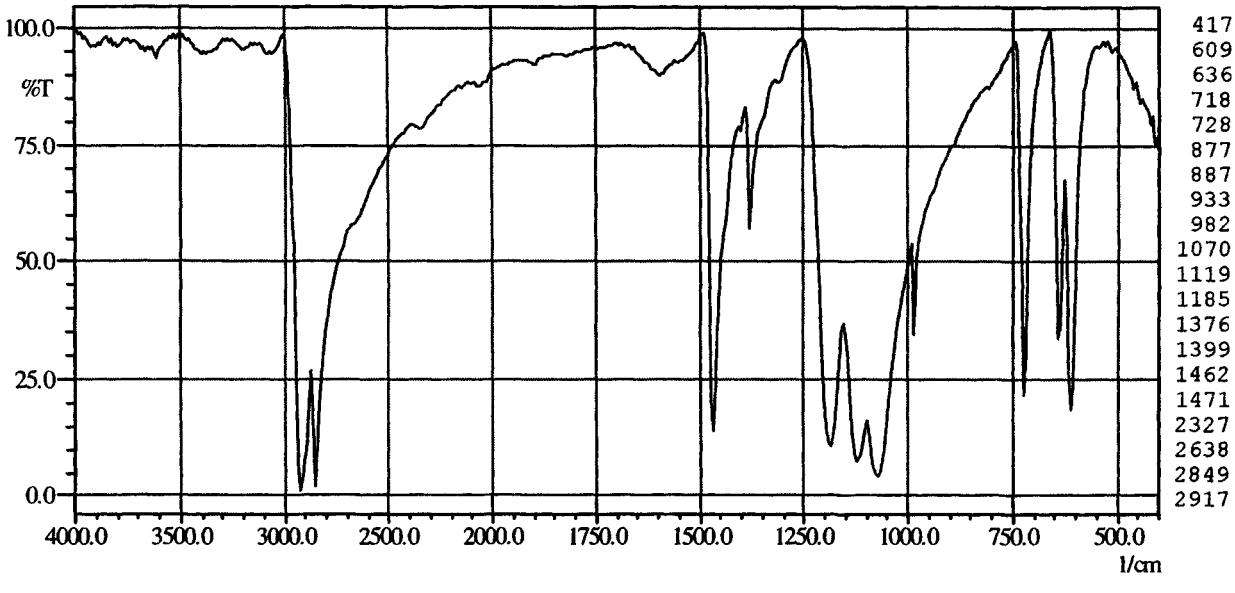
(1) **Sb Ni Ti oxide**
(2) Lichtgelb 7 G
(3) Bayer
(5) inorganic pigment
(6) yellow solid
(11) Pigment Yellow 53
(12) 77788
(13) KBr pellet

214 TiO_2



(1) **titanium dioxide**
(2) Tioxide R-CR-2
(3) Worlee
(4) 79.88 g mol^{-1}
(5) inorganic pigment
(6) white solid
(11) Pigment White 6
(12) 77891
(13) KBr pellet
(14) rutile

214 CdS-CdSe+$BaSO_4$



(1) **calcined coprecipitation of CdS and CdSe, extended with $BaSO_4$**
(2) Cadmium Red
(3) Cerdec
(5) inorganic pigment for ABS and engineering polymers
(6) red solid
(11) Red 108
(13) KBr

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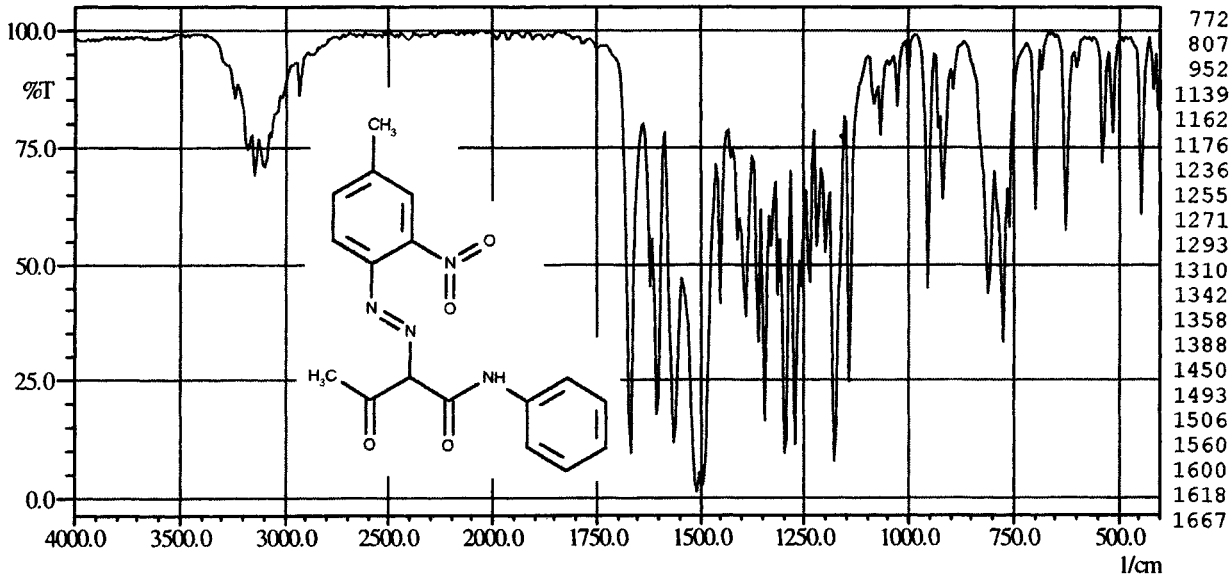
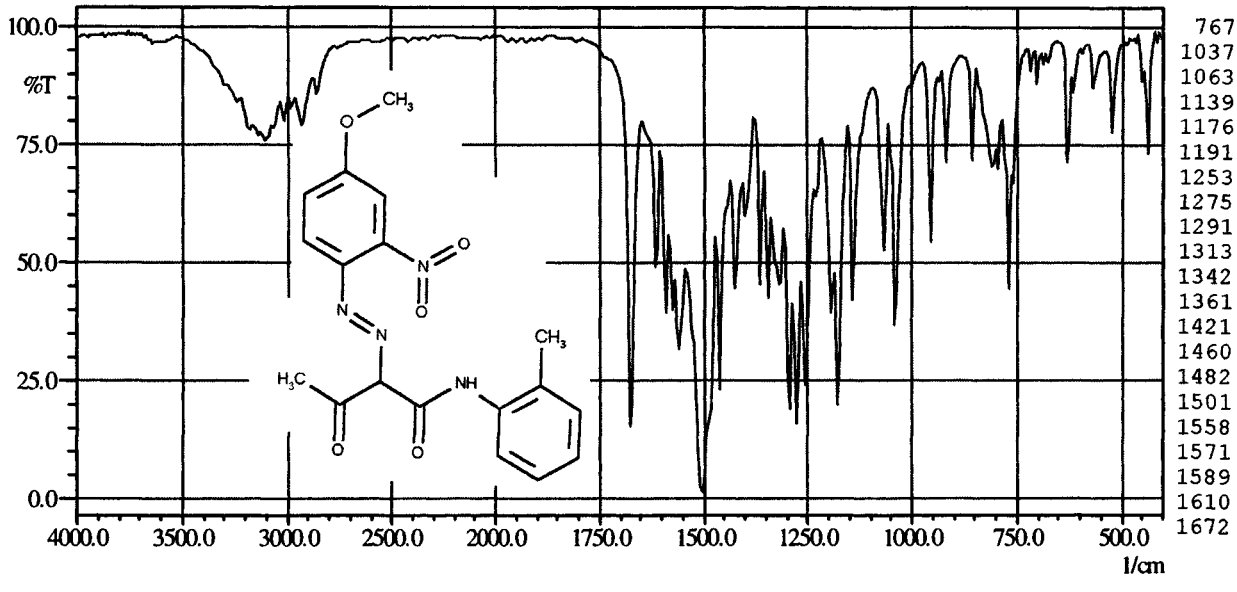
2211 $C_{17}H_{16}N_4O_4$



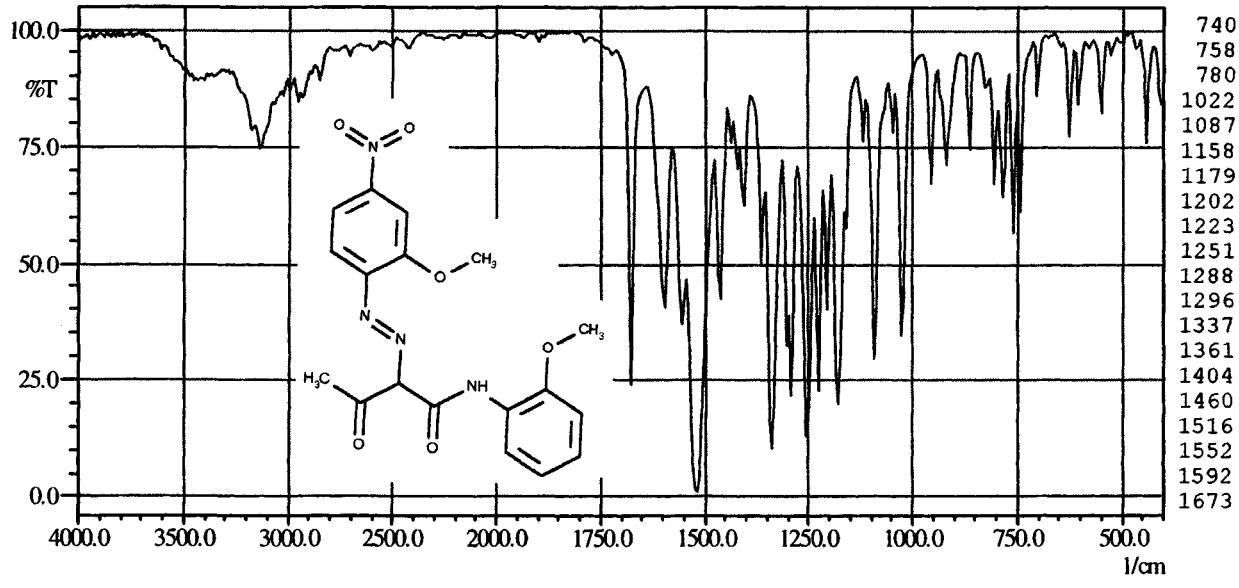
(1) **3-nitro-4-toluidine -> acetoacetic arylide-anilide**
(2) Hansa Gelb G
(3) Hoechst
(4) 340.3 g mol^{-1}
(5) organic pigment
(6) yellow solid
(11) Pigment Yellow 1
(12) 11680
(13) KBr pellet

2211 $C_{18}H_{18}N_4O_5$



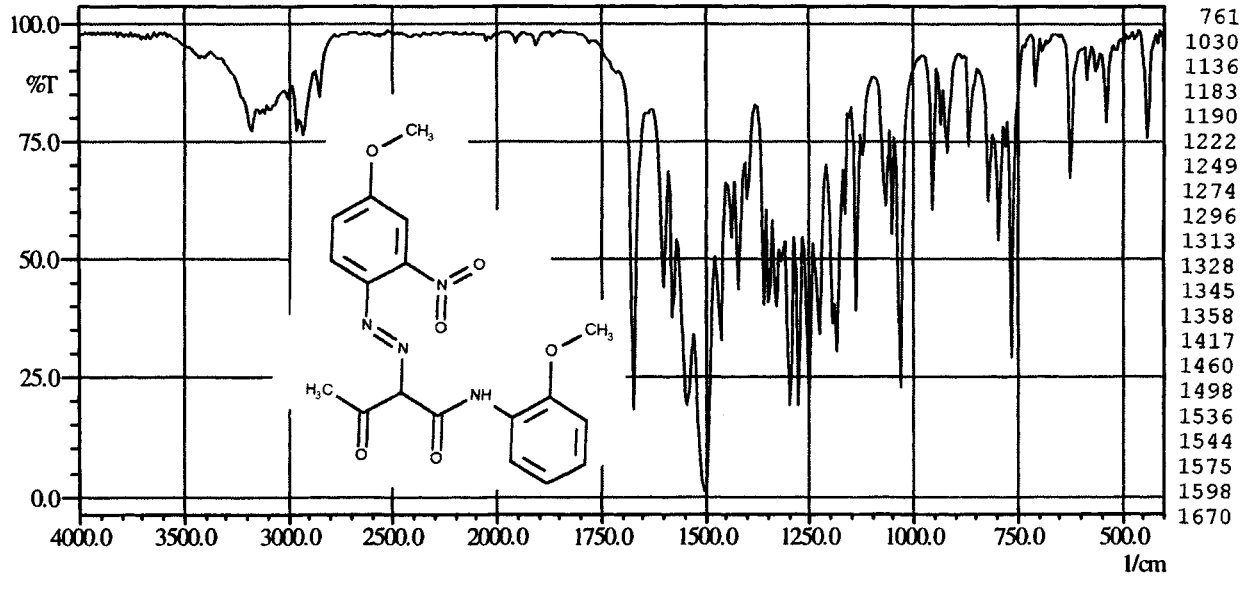
(1) **4-methoxy-2-nitroaniline -> acetoacetic arylide-2-methylanilide**
(2) Hansa Gelb 3R
(3) Hoechst
(4) 370.4 g mol^{-1}
(5) organic pigment
(6) yellow solid
(11) Pigment Orange 1
(12) 11725
(13) KBr pellet

2211 $C_{18}H_{18}N_4O_6$



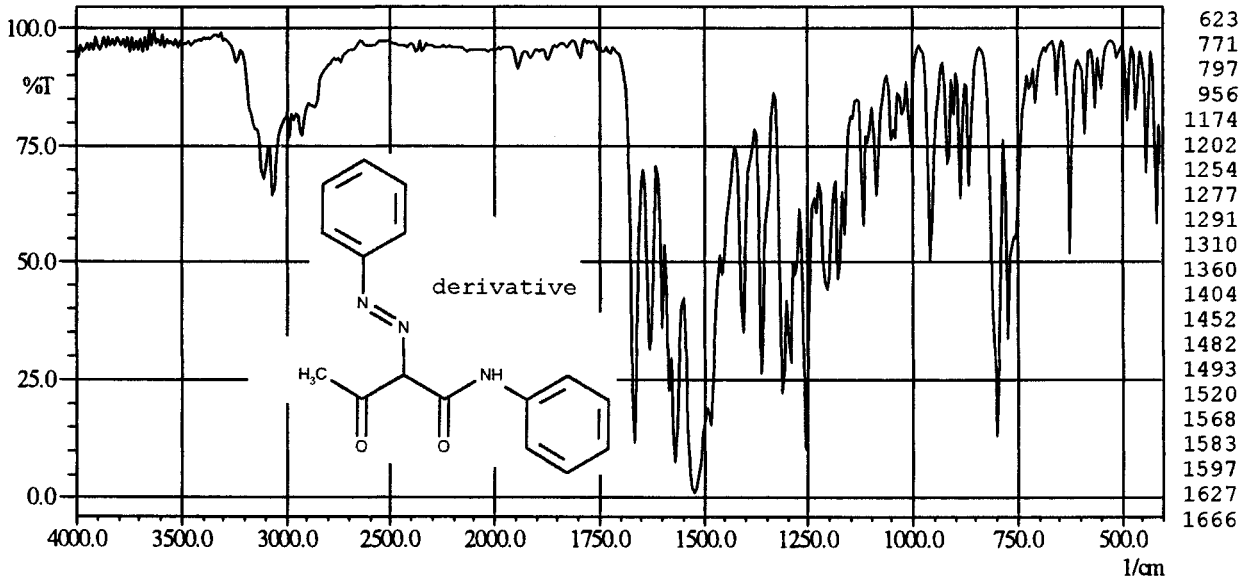
(1) **2-methoxy-4-nitroaniline -> acetoacetic arylide-2-methoxyanilide**
(2) Monolite Yellow 2G
(3) ICI
(4) 386.4 g mol^{-1}
(5) organic pigment
(6) yellow solid
(11) Pigment Yellow 74
(12) 11741
(13) KBr pellet

2211 $C_{18}H_{18}N_4O_6$



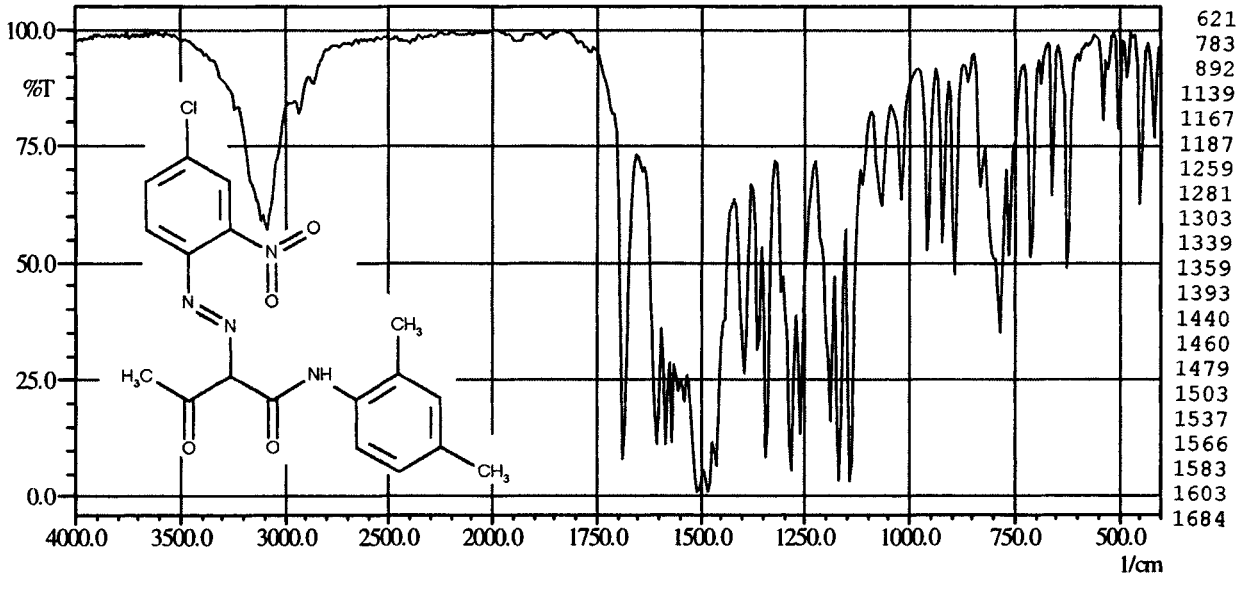
(1) **4-methoxy-2-nitroaniline -> acetoacetic arylide-2-methoxyanilide**
(2) Hansa Gelb RN
(3) Hoechst
(4) 386.3 g mol^{-1}
(5) organic pigment
(6) yellow solid
(11) Pigment Yellow 65
(12) 11740
(13) KBr pellet

2211 $C_{21}H_{18}ClN_3O_2$



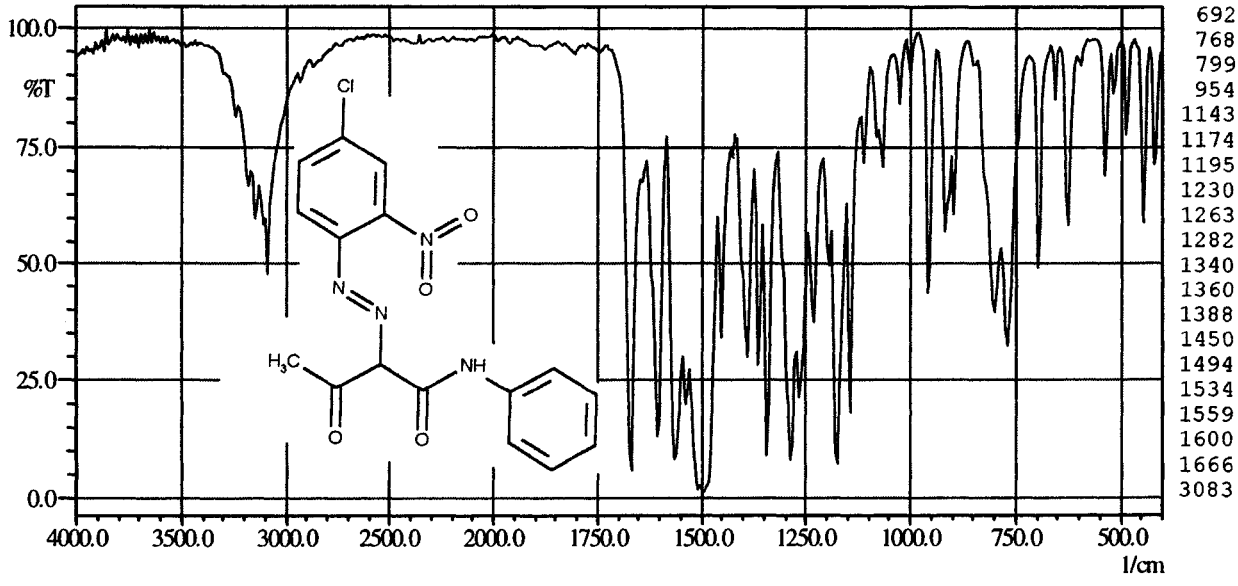
(1) **4-chloro-2-toluidine -> acetoacetic arylide-1-naphthylimide**
(2) Helio Echtgelb 8G
(3) Bayer
(4) 379.8 g mol^{-1}
(5) organic pigment
(6) yellow solid
(11) Pigment Yellow 25
(13) KBr pellet
(14) other source:aniline-ACAA anilide, $C_{16}H_{15}N_3O_2$

2211 $C_{17}H_{14}Cl_2N_4O_4$



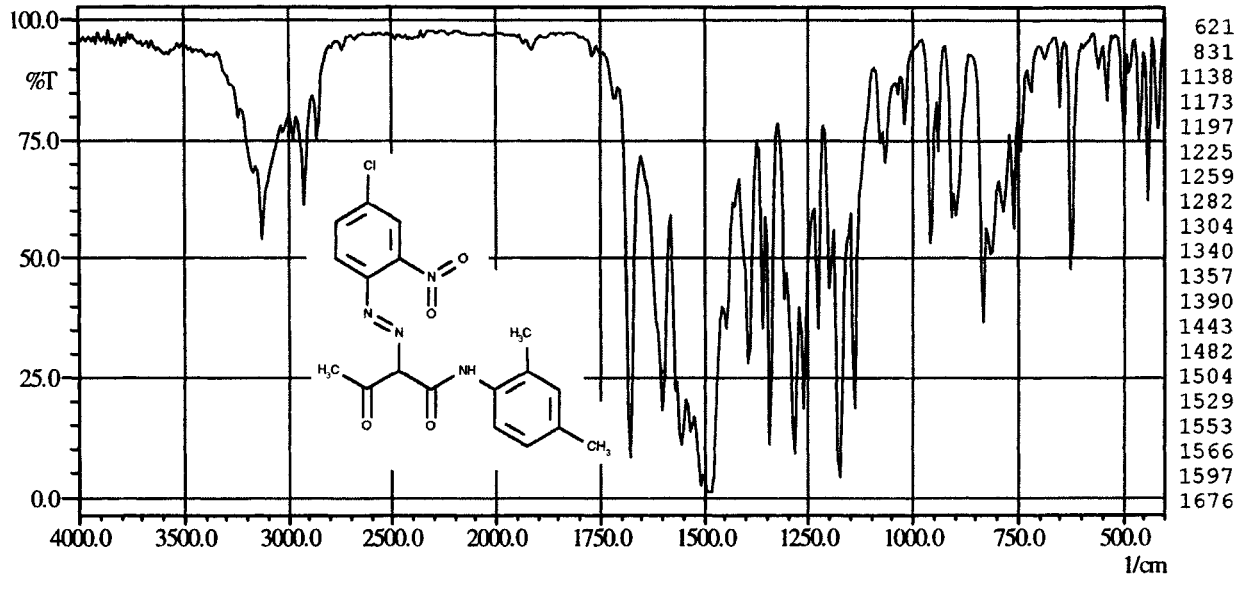
(1) **4-chloro-2-nitroaniline -> acetoacetic arylide-6-chloro-2-methylanilide**
(2) Hansa Gelb 8G
(3) Hoechst
(4) 409.2 g mol^{-1}
(5) organic pigment
(6) yellow solid
(11) Pigment Yellow 82
(13) KBr pellet

2211 $C_{16}H_{13}ClN_4O_4$



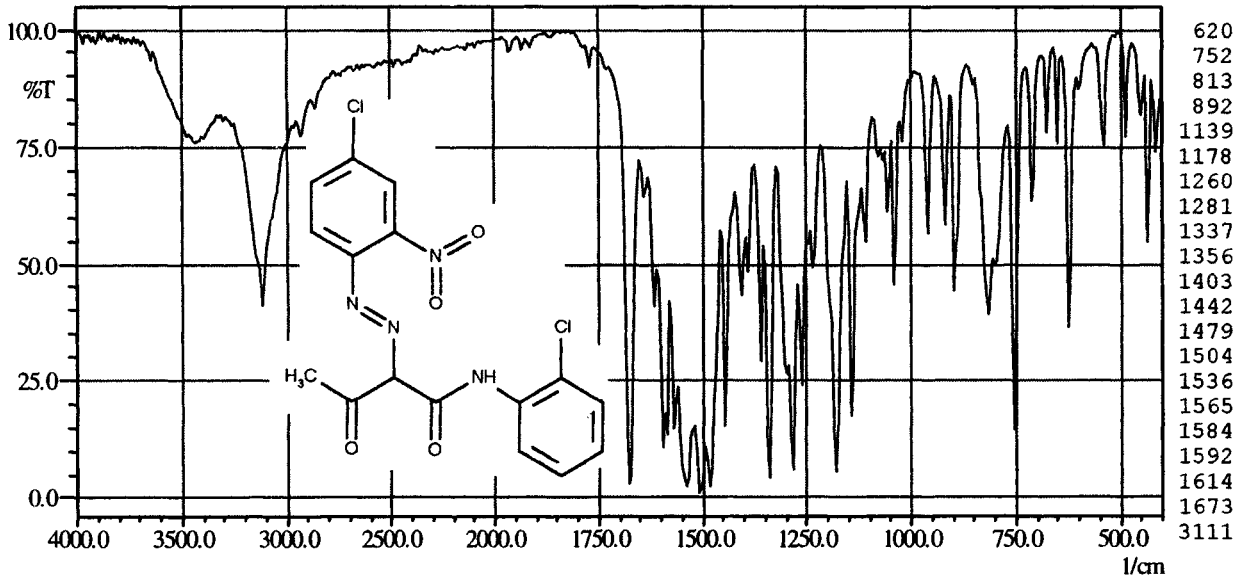
(1) **4-chloro-2-nitroaniline -> acetoacetic arylide-anilide**
(2) Hansa Gelb 3G
(3) Hoechst
(4) 360.7 g mol^{-1}
(5) organic pigment
(6) yellow solid
(11) Pigment Yellow 6
(12) 11670
(13) KBr pellet

2211 $C_{18}H_{17}ClN_4O_4$



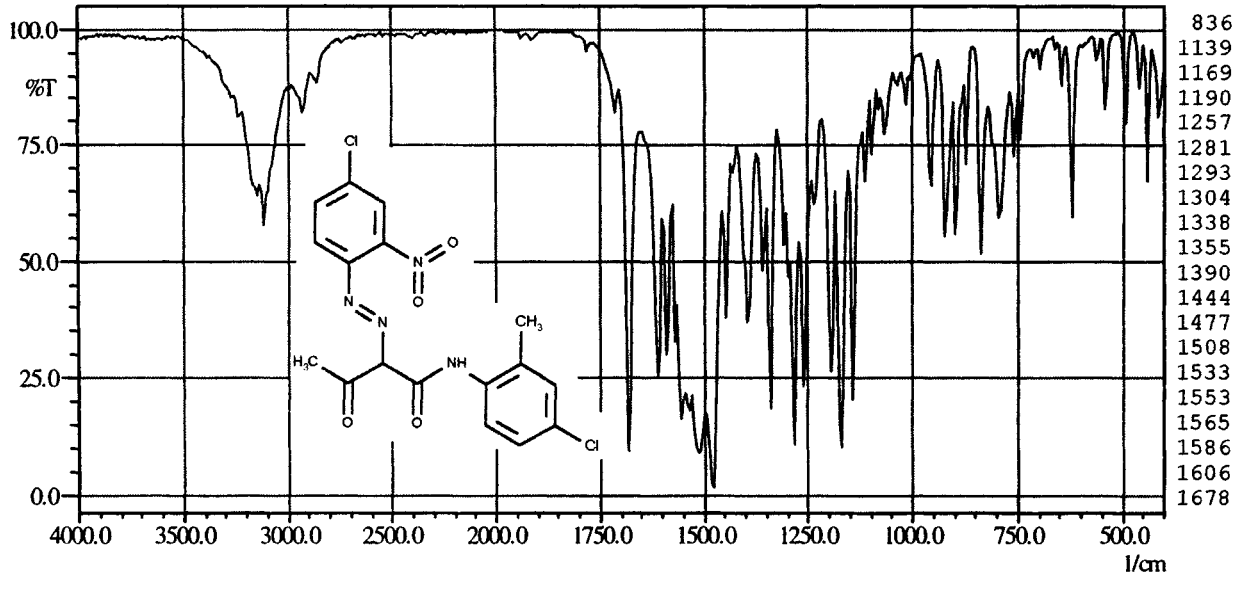
(1) **4-chloro-2-nitroaniline -> acetoacetic arylide-2,4-dimethylanilide**
(2) Hansa Gelb GR
(3) Hoechst
(4) 388.8 g mol^{-1}
(5) organic pigment
(6) yellow solid
(11) Pigment Yellow 2
(12) 11730
(13) KBr pellet

2211 $C_{16}H_{12}Cl_2N_4O_4$



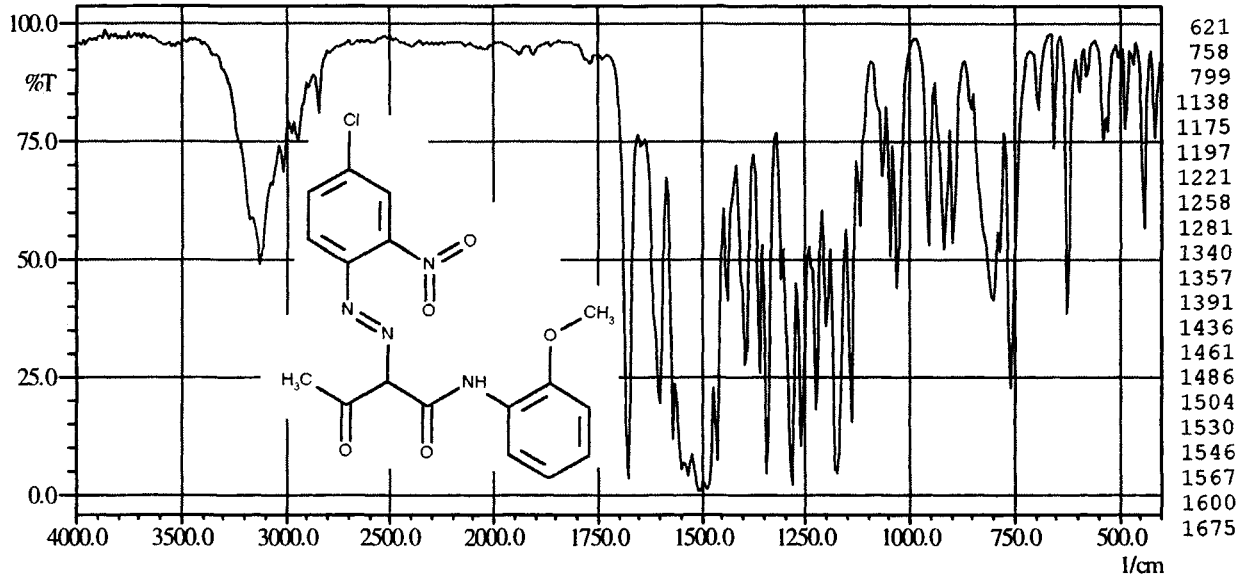
(1) **4-chloro-2-nitroaniline -> acetoacetic arylide-2-chloroanilide**
(2) Monolite Yellow 10 GE
(3) ICI
(4) 395.2 g mol^{-1}
(5) organic pigment
(6) yellow solid
(11) Pigment Yellow 3
(12) 11710
(13) KBr pellet

2211 $C_{17}H_{14}Cl_2N_4O_4$



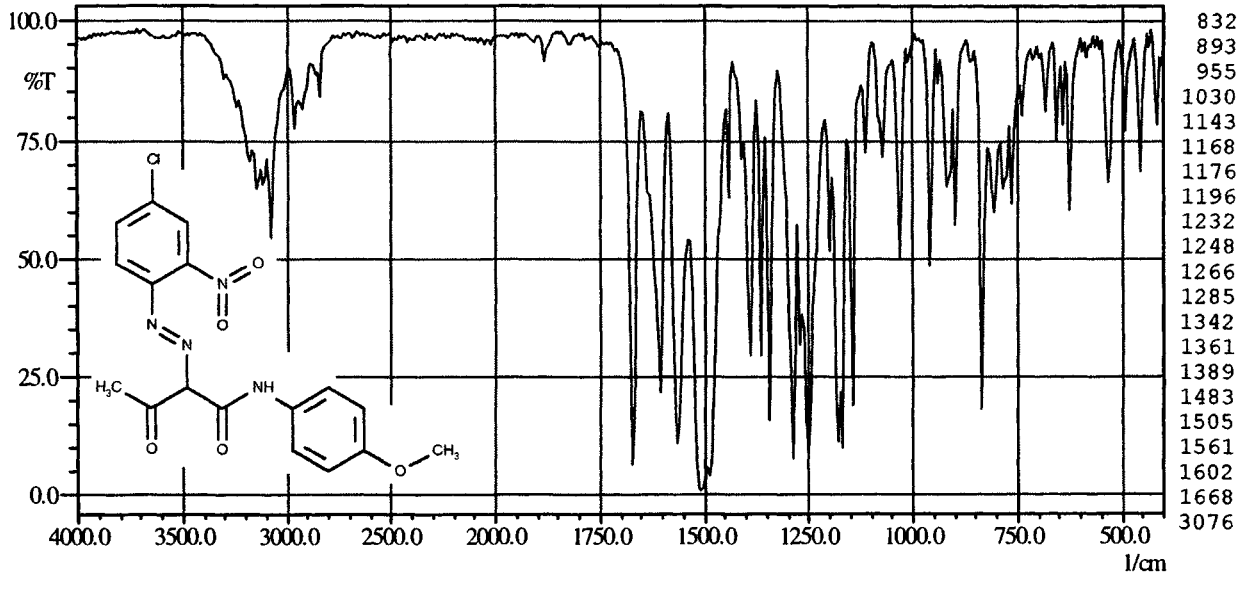
(1) **4-chloro-2-nitroaniline -> acetoacetic arylide-4-chloro-2-methylanilide**
(2) Hansa Brillantgelb 10 GX
(3) Hoechst
(4) 409.2 g mol^{-1}
(5) organic pigment
(6) yellow solid
(11) Pigment Yellow 98
(12) 11727
(13) KBr pellet

2211 $C_{17}H_{15}ClN_4O_5$



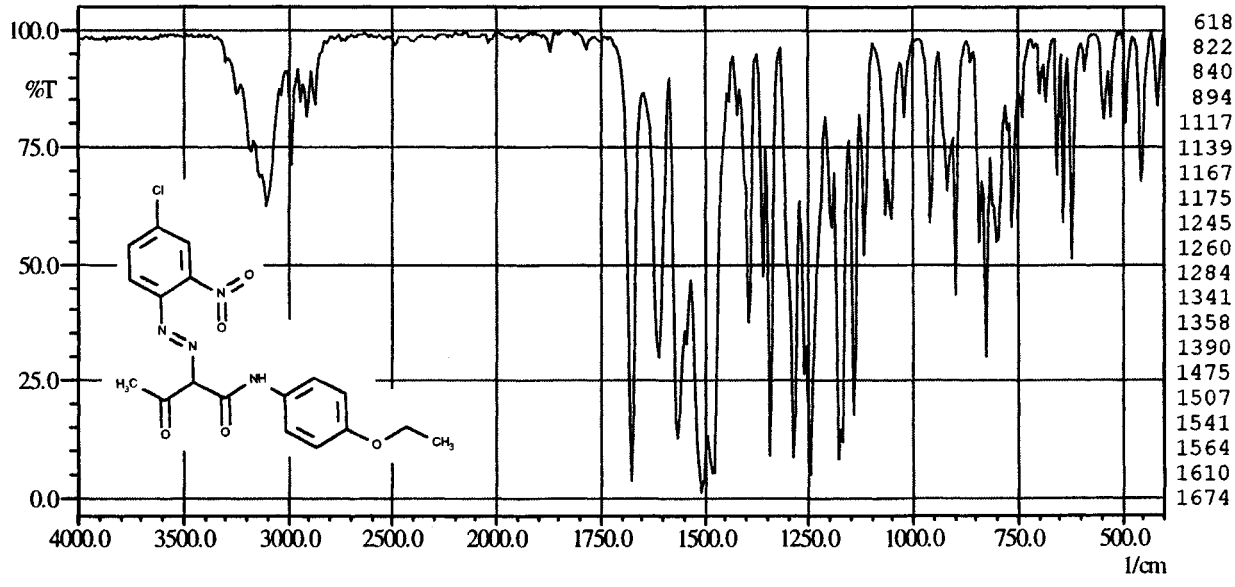
(1) **4-chloro-2-nitroaniline -> acetoacetic arylide-2-methoxyanilide**
(2) Hansa Brillantgelb 4GX
(3) Hoechst
(4) 390.8 g mol^{-1}
(5) organic pigment
(6) yellow solid
(11) Pigment Yellow 73
(12) 11738
(13) KBr pellet

2211 $C_{17}H_{15}ClN_4O_5$



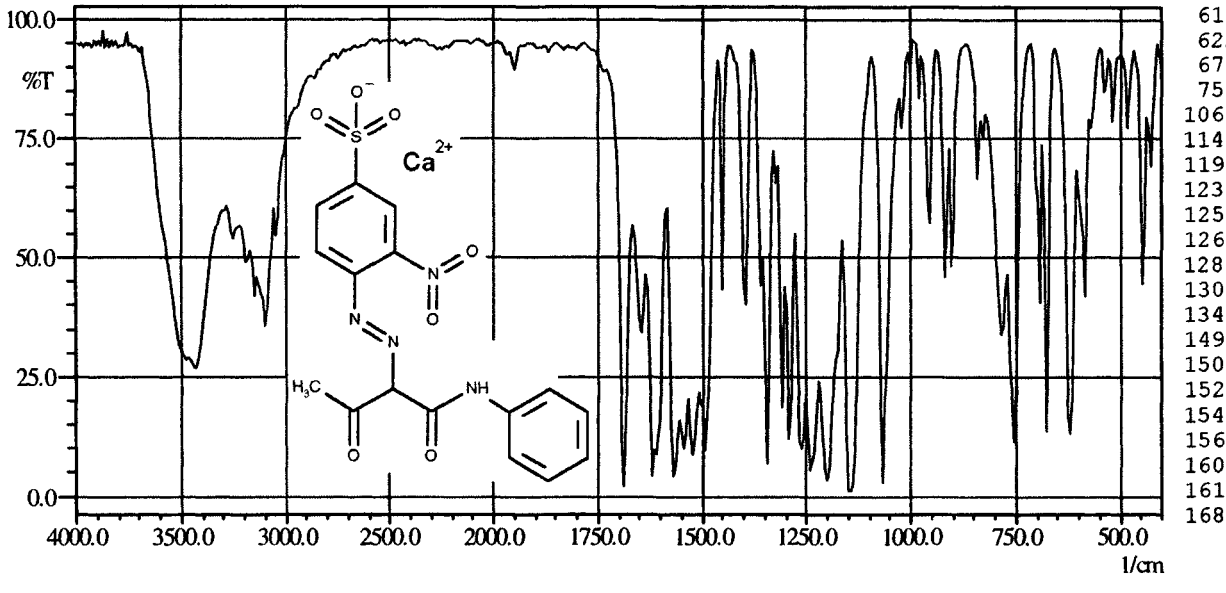
(1) **4-chloro-2-nitroaniline -> acetoacetic arylide-4-methoxyanilide**
(2) Symuler Fast Yellow 4119
(3) DIC
(4) 390.8 g mol^{-1}
(5) organic pigment
(6) yellow solid
(11) Pigment Yellow 130
(13) KBr pellet

2211 $C_{17}H_{17}ClN_4O_5$



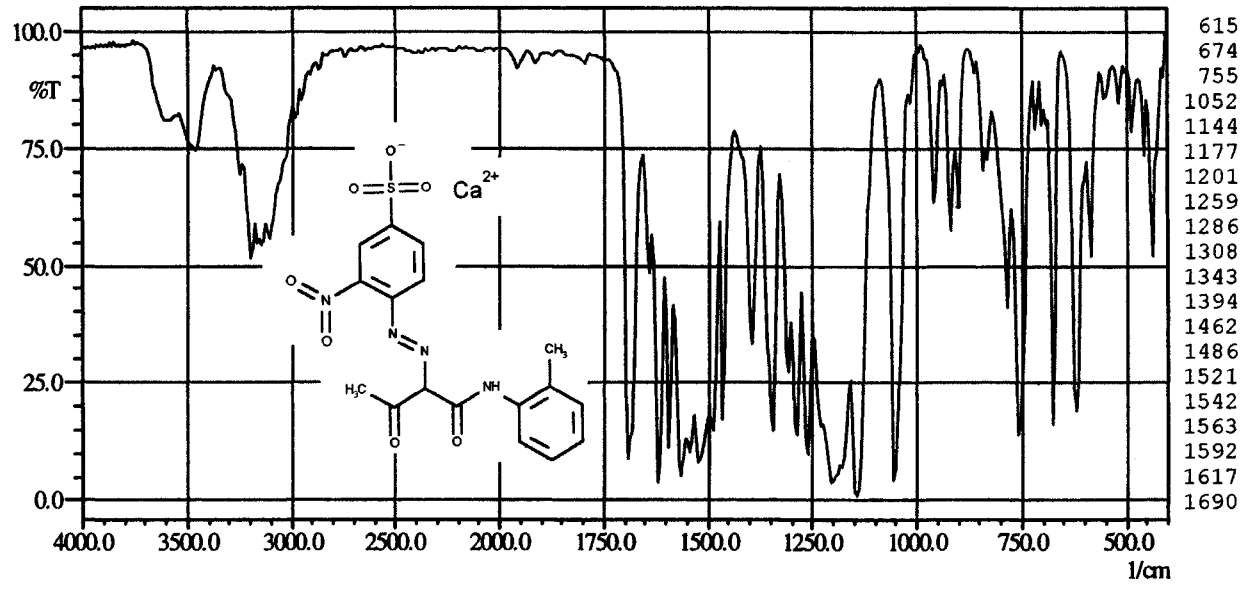
(1) **4-chloro-2-nitroaniline -> acetoacetic arylide-4-ethoxyanilide**
(2) Hansa Gelb XT
(3) Hoechst
(4) 392.8 g mol^{-1}
(5) organic pigment
(6) yellow solid
(11) Pigment Yellow 75
(12) 11770
(13) KBr pellet

2211 $C_{32}H_{24}N_8O_{14}S_2Ca$



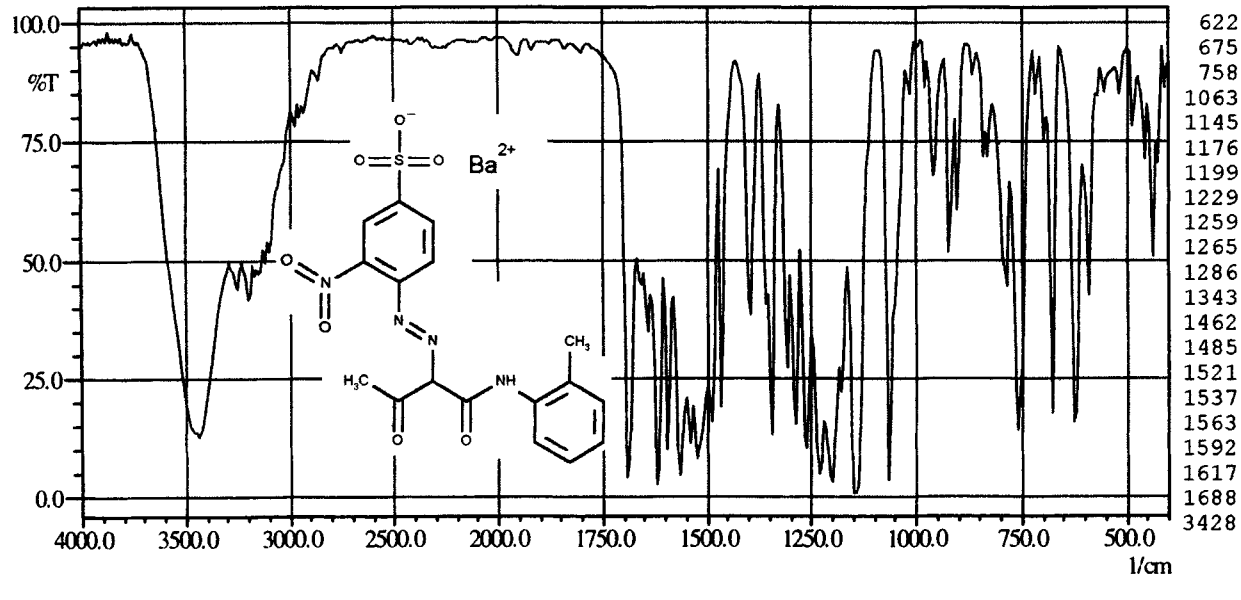
(1) **4-amino-5-nitrobenzenesulfonic acid -> acetoacetic arylide-anilide, Ca-salt**
(2) Irgalite Yellow WSC
(3) Ciba-Geigy
(4) 848.7 g mol^{-1}
(5) organic pigment
(6) yellow solid
(11) Pigment Yellow 61:1
(12) 13880
(13) KBr pellet

2211 $C_{34}H_{30}N_8O_{14}S_2Ca$



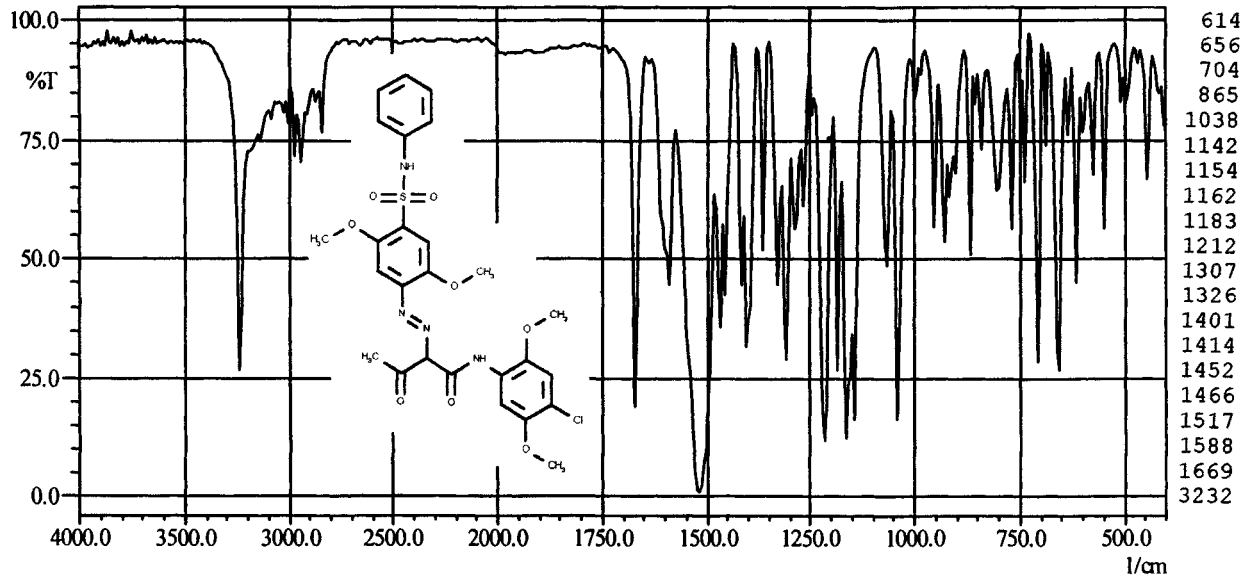
(1) **4-amino-3-nitrobenzenesulfonic acid -> acetoacetic arylide-2-methylanilide, Ca-salt**
(2) Irgaplast Gelb R
(3) Ciba-Geigy
(4) 878.9 g mol^{-1}
(5) organic pigment
(6) yellow solid
(11) Pigment Yellow 62:1
(12) 13940:1
(13) KBr pellet

2211 $C_{34}H_{30}N_8O_{14}S_2Ba$



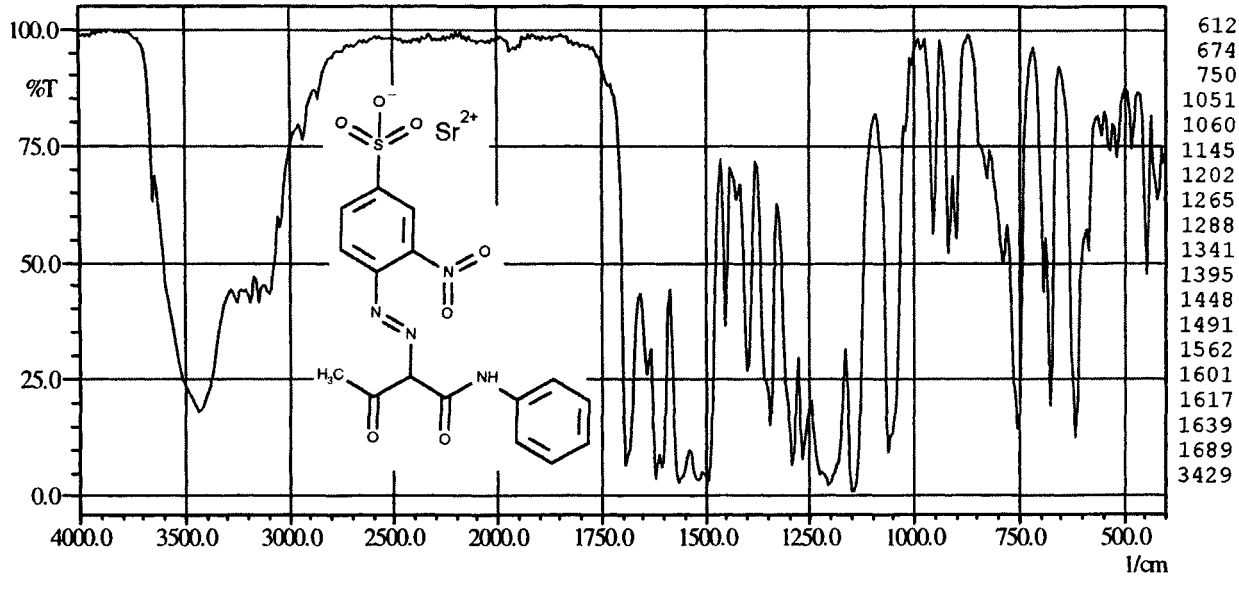
(1) **4-amino-3-nitrobenzenesulfonic acid -> acetoacetic arylide-2-methylanilide, Ba-salt**
(2) Irgalite Yellow WSR
(3) Ciba-Geigy
(4) 976.1 g mol^{-1}
(5) organic pigment
(6) yellow solid
(11) Pigment Yellow 62:1
(12) 13940:1
(13) KBr pellet

2211 $C_{26}H_{27}ClN_4O_8S$



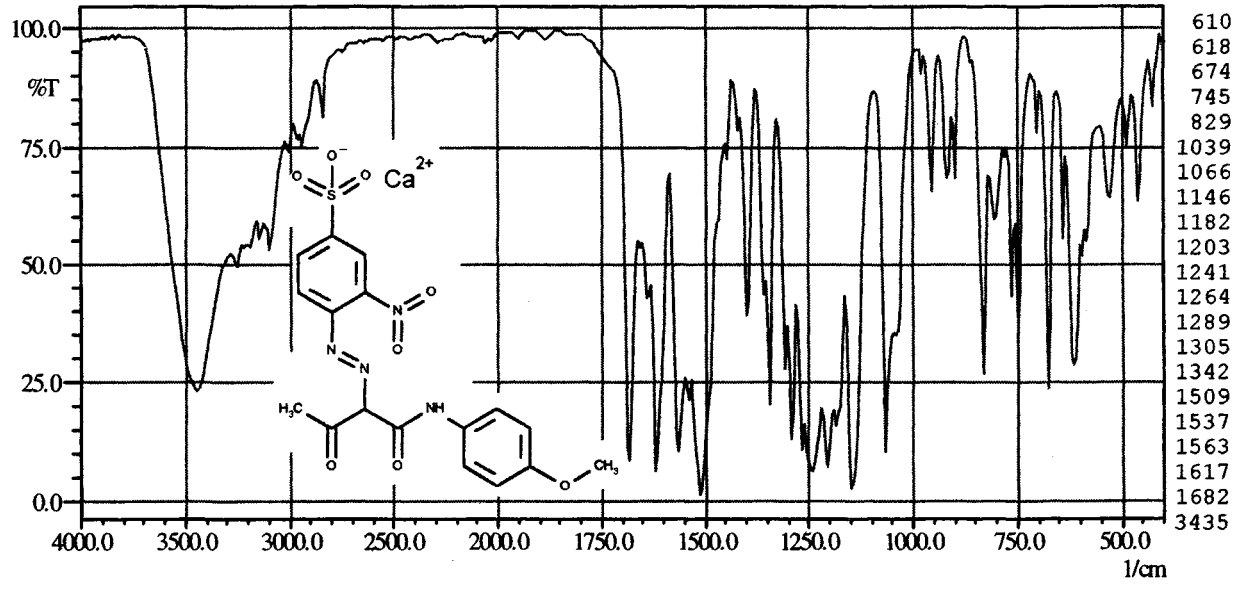
(1) **2,5-dimethoxy-4-N-phenylsulfonamidoaniline -> acetoacetic arylide-4-chloro-2,5-dimethoxyanilide**
(2) Novoperm Gelb FGL
(3) Hoechst
(4) 591.0 g mol^{-1}
(5) organic pigment
(6) yellow solid
(11) Pigment Yellow 97
(12) 11767
(13) KBr pellet

2211 $C_{32}H_{24}N_8O_{14}S_2Sr$



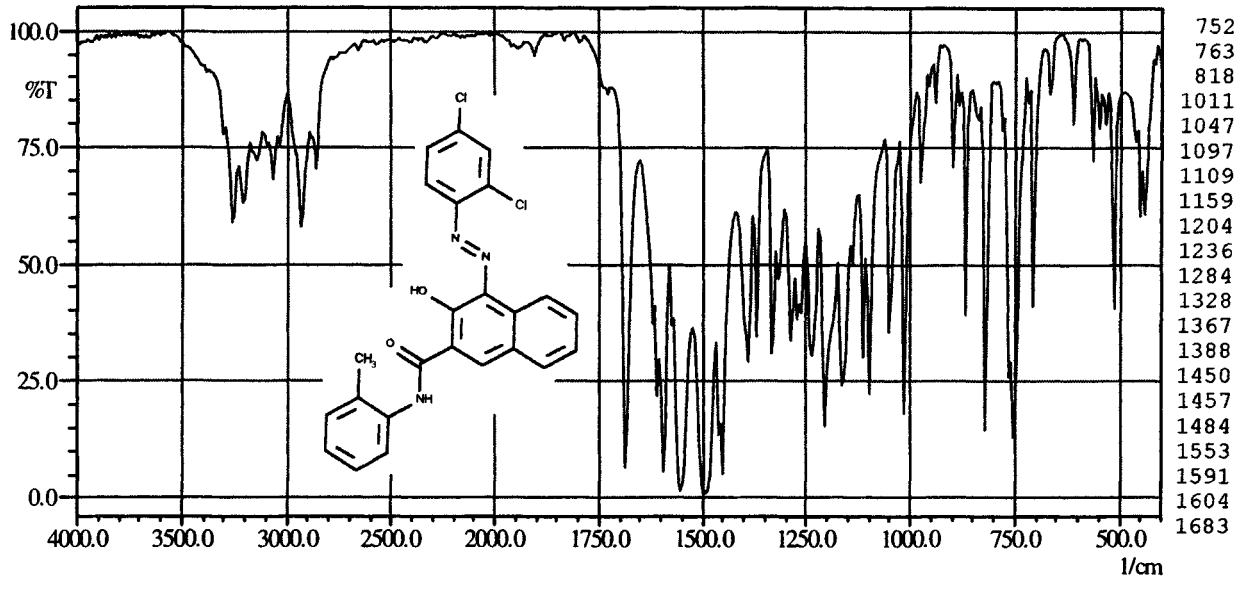
(1) **3-nitrosulfanilic acid -> acetoacetic arylide-anilide, Sr-salt**
(2) Symuler Lake Fast Yellow 6G
(3) DIC
(4) 896.3 g mol^{-1}
(5) organic pigment
(6) yellow solid
(11) Pigment Yellow 133
(13) KBr pellet

2211 $C_{34}H_{30}N_8O_{16}S_2Ca$



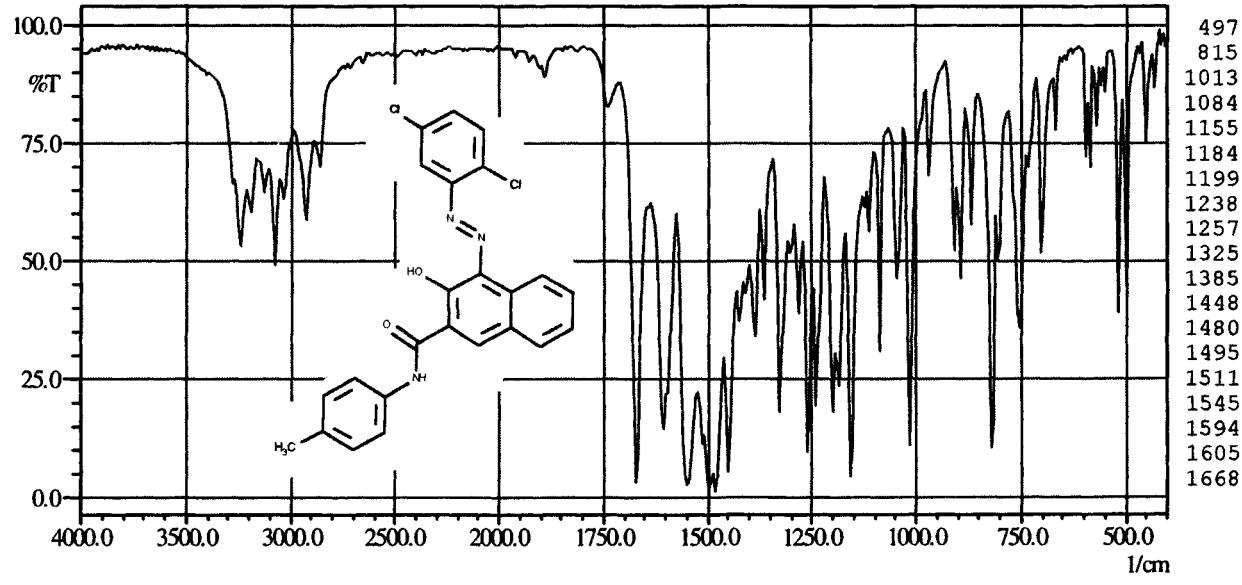
(1) **3-nitrosulfanilic acid -> acetoacetic arylide-4-methoxyanilide**
(2) Symuler Yellow 3056
(3) DIC
(4) 910.9 g mol^{-1}
(5) organic pigment
(6) yellow solid
(11) Pigment Yellow 169
(12) 13955
(13) KBr pellet

2212 $C_{24}H_{17}Cl_2N_3O_2$



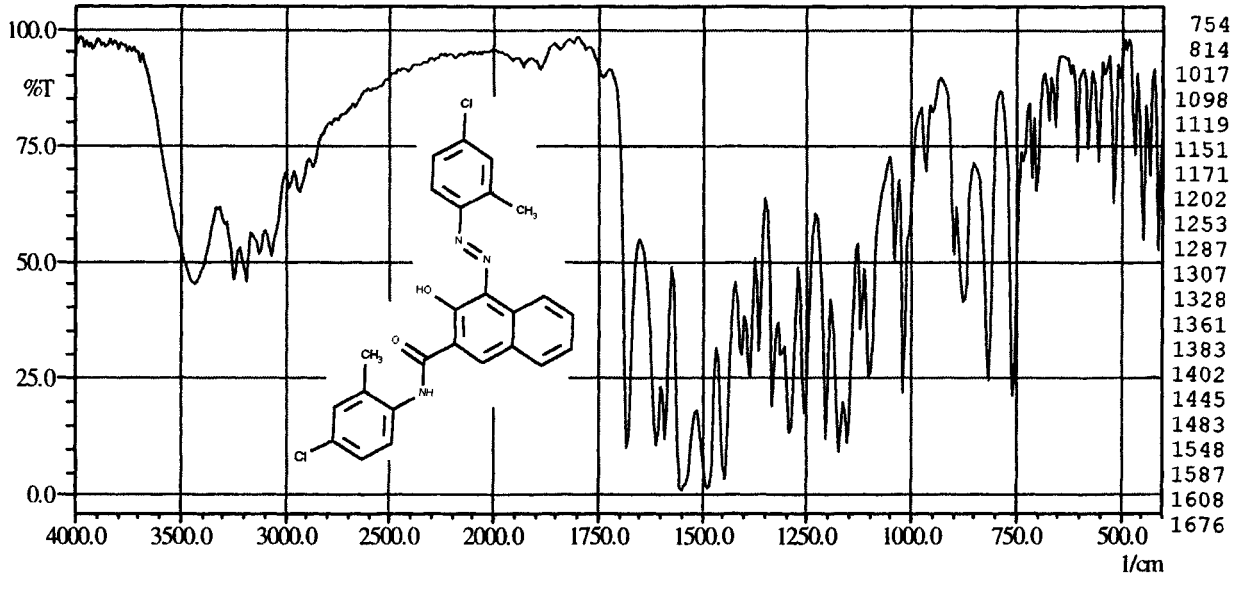
(1) **2,4-dichloroaniline -> 2-hydroxynaphthoic arylide-2-methylanilide**
(2) Permanent Rot FGG
(3) Hoechst
(4) 450.3 g mol^{-1}
(5) organic pigment
(6) red solid
(11) Pigment Red 148
(13) KBr pellet

2212 $C_{24}H_{17}Cl_2N_3O_2$



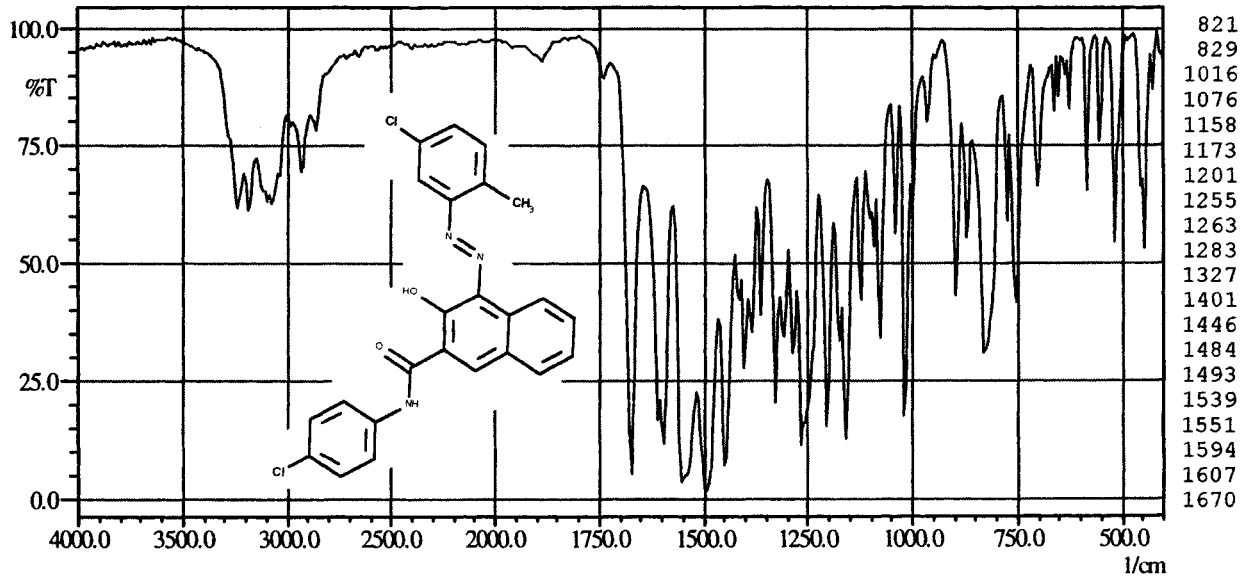
(1) **2,5-dichloroaniline -> 2-hydroxynaphthoic arylide-4-methylanilide**
(2) Permanent Rot FRL
(3) Hoechst
(4) 450.3 g mol^{-1}
(5) organic pigment
(6) red solid
(11) Pigment Red 10
(12) 12440
(13) KBr pellet

2212 $C_{25}H_{19}Cl_2N_3O_2$



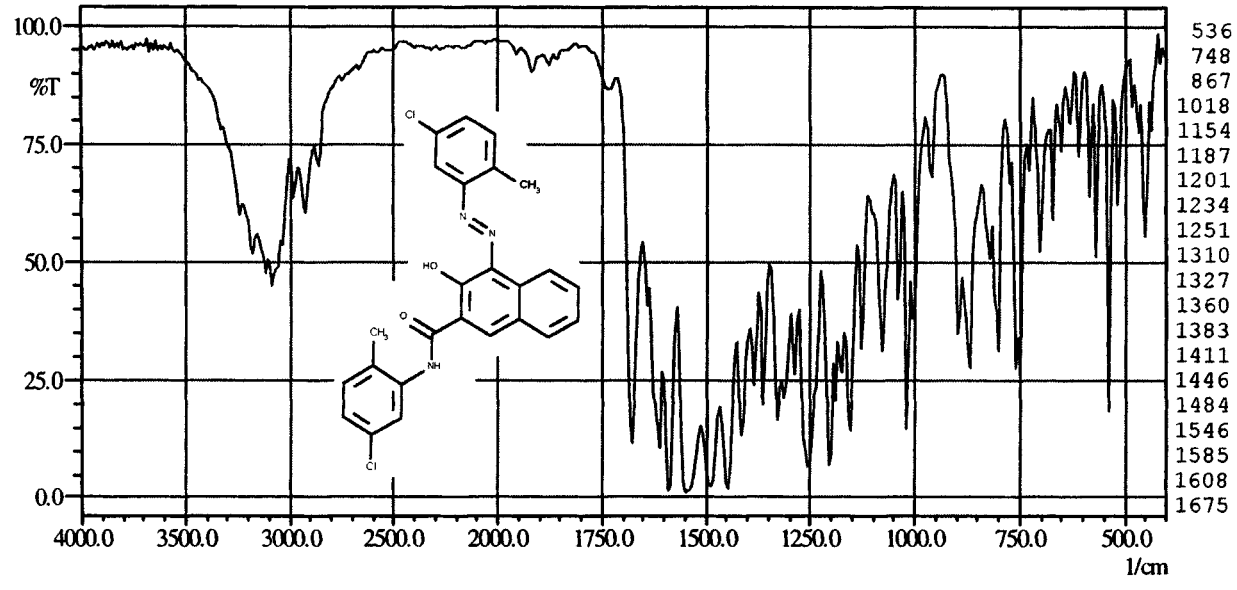
(1) **4-chloro-2-toluidine -> 2-hydroxynaphthoic arylide-4-chloro-2-methylanilide**
(2) Monolite Red 4RH
(3) ICI
(4) 464.4 g mol^{-1}
(5) organic pigment
(6) red solid
(11) Pigment Red 7
(12) 12420
(13) KBr pellet

2212 $C_{24}H_{17}Cl_2N_3O_2$



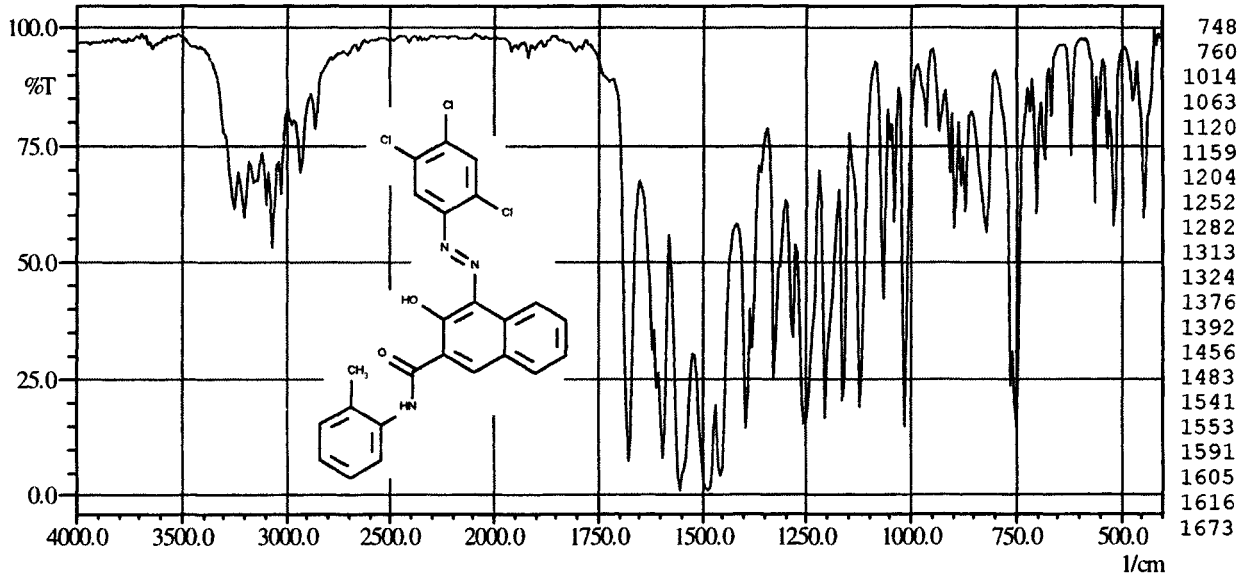
(1) **5-chloro-2-toluidine -> 2-hydroxynaphthoic arylide-4-chloroanilide**
(2) Helio Echtcarmin B
(3) Bayer
(4) 450.3 g mol^{-1}
(5) organic pigment
(6) red solid
(11) Pigment Red 96
(13) KBr pellet

2212 $C_{25}H_{18}Cl_3N_3O_2$



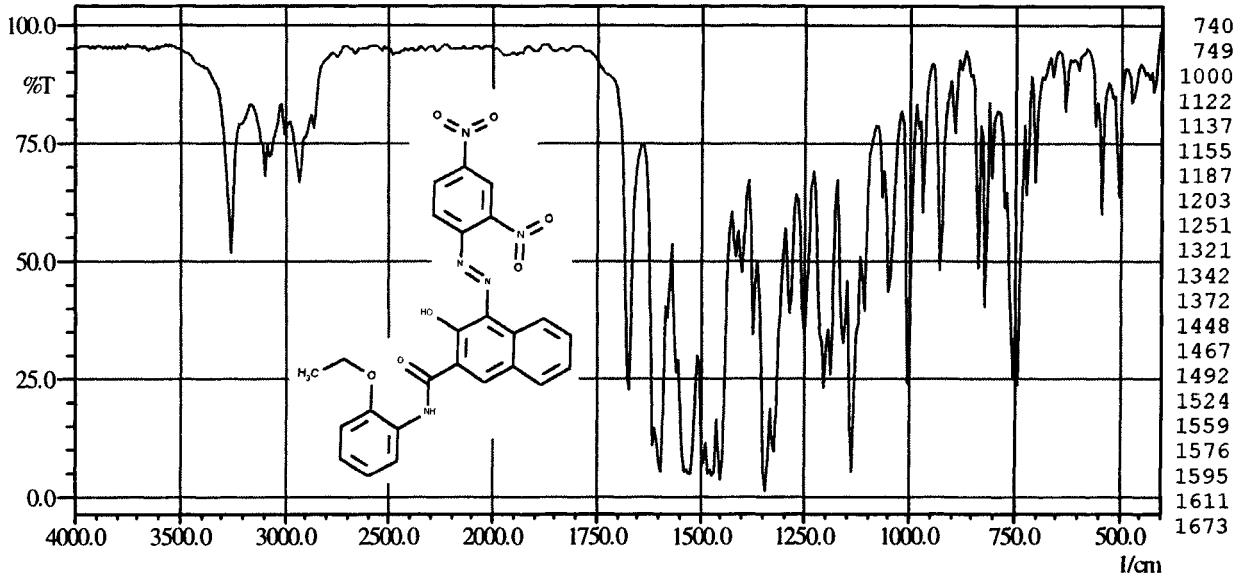
(1) **5-chloro-2-toluidine -> 2-hydroxynaphthoic arylide-5-chloro-2-methylanilide**
(2) Permanent Rubin FBH
(3) Hoechst
(4) 498.8 g mol^{-1}
(5) organic pigment
(6) dark-red solid
(11) Pigment Red 11
(12) 12430
(13) KBr pellet

2212 $C_{24}H_{16}Cl_3N_3O_2$



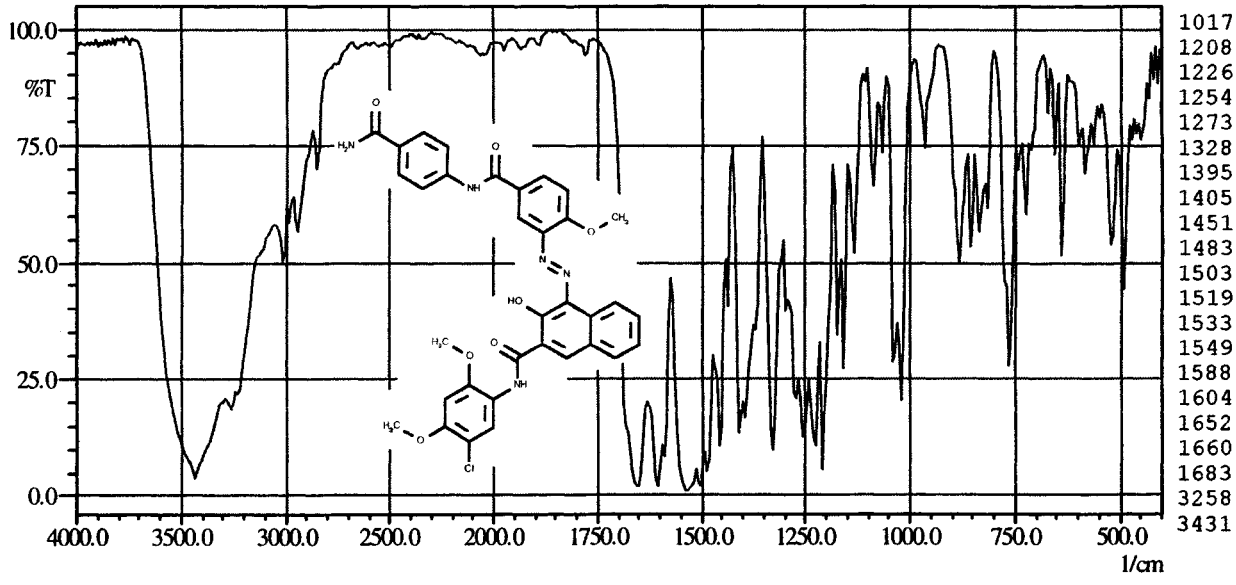
(1) **2,4,5-trichloroaniline -> 2-hydroxynaphthoic arylide-2-methylanilide**
(2) Permanent Rot FGR 70
(3) Hoechst
(4) 484.8 g mol^{-1}
(5) organic pigment
(6) red solid
(11) Pigment Red 112
(12) 12370
(13) KBr pellet

2212 $C_{25}H_{19}N_5O_7$



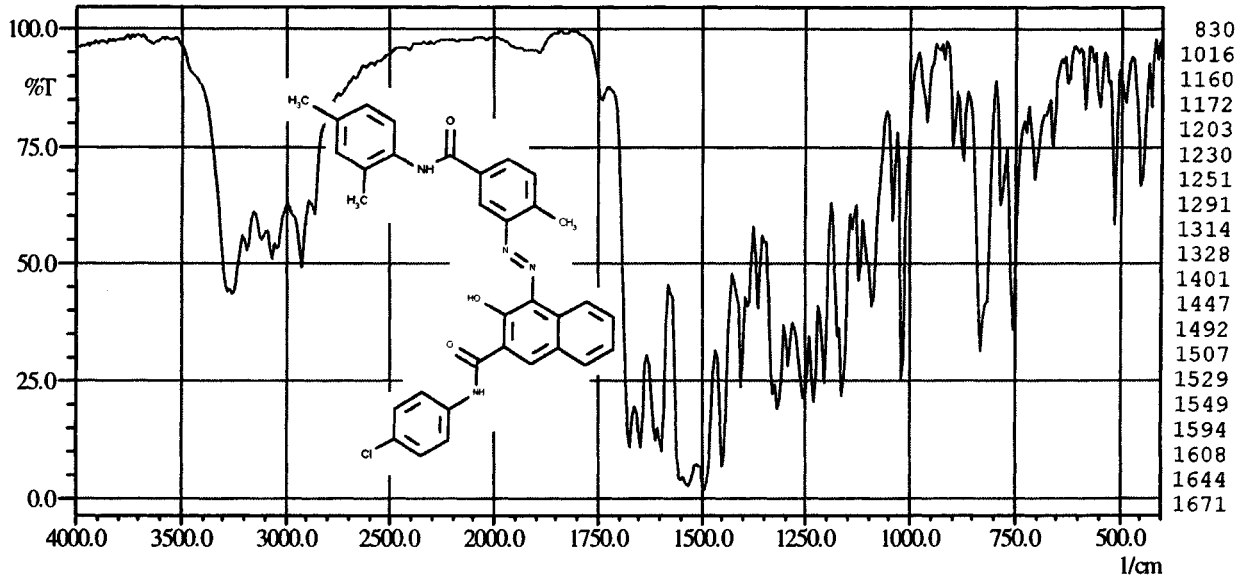
(1) **2,4-dinitroaniline -> 2-hydroxynaphthoic arylide-2-ethoxyanilide**
(2) Helio Echtbordo RR
(3) Bayer
(4) 501.5 g mol^{-1}
(5) organic pigment
(6) dark-red solid
(11) Pigment Red 136
(13) KBr pellet

2212 $C_{34}H_{28}ClN_5O_7$



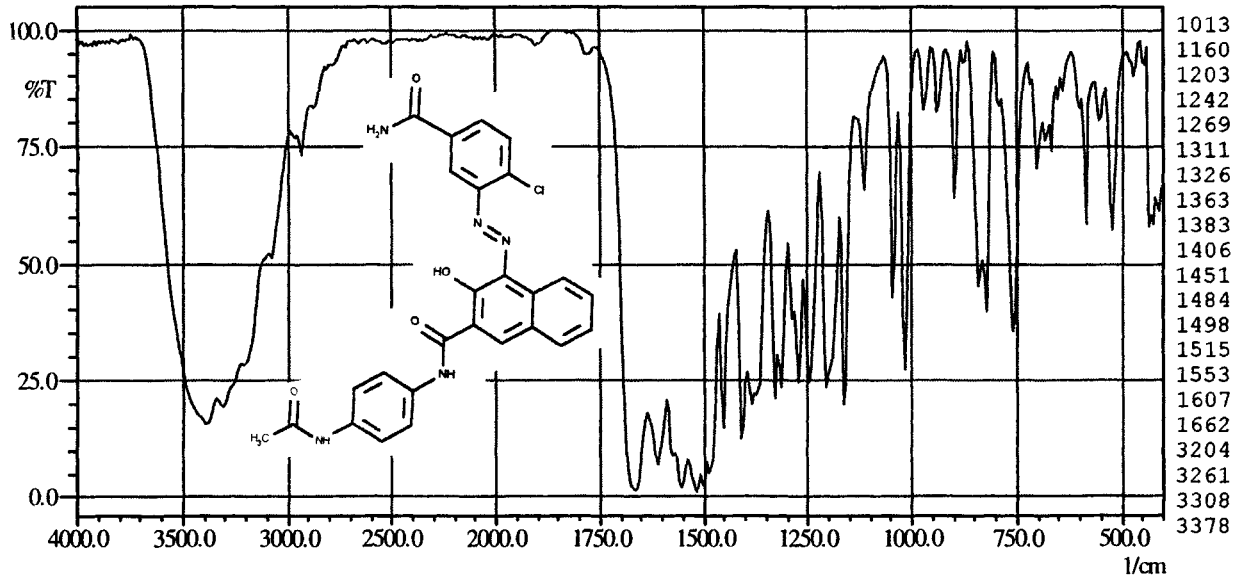
(1) **3-amino-4-methoxy-N(4'-benzamide)benzamide -> 2-hydroxynaphthoic arylide-2,4-dimethoxy-5-chloranilide**
(2) PV-Echtrot HF4B
(3) Hoechst
(4) 654.1 g mol^{-1}
(5) organic pigment
(6) red solid
(11) Pigment Red 187
(12) 12486
(13) KBr pellet

2212 $C_{33}H_{27}ClN_4O_3$



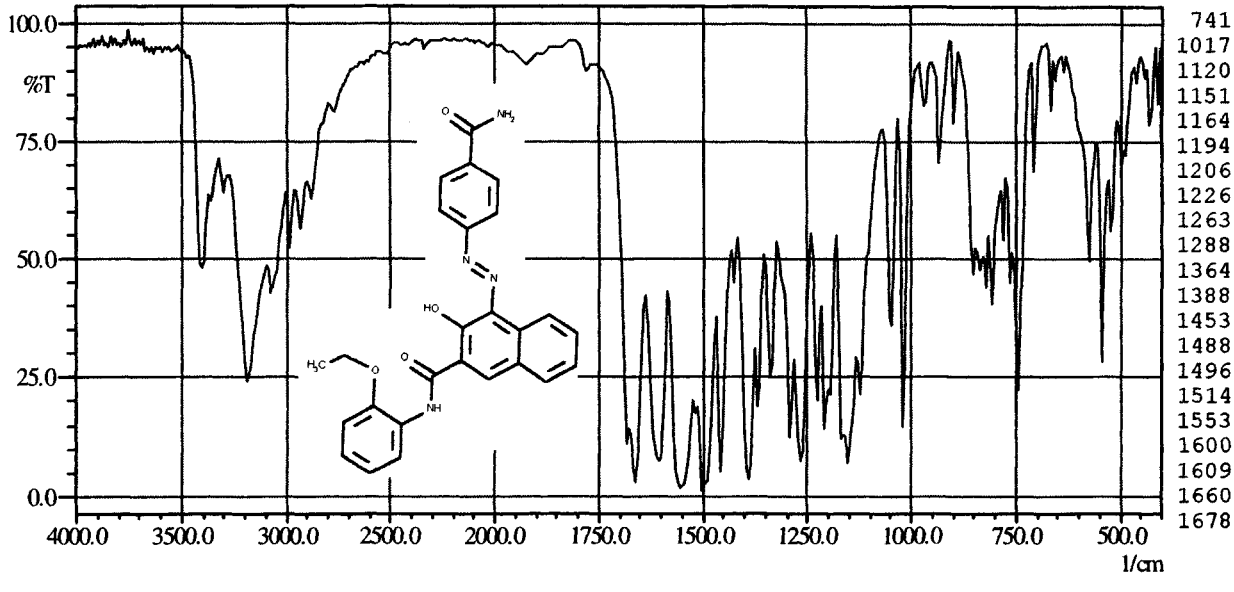
(1) **3-amino-4-methyl-N-(2',4'-xylyl)benzamide -> 2-hydroxynaphthoic arylide-4-chloroanilide**
(2) Vulkan Echtrosa G
(3) Hoechst
(4) 563.0 g mol^{-1}
(5) organic pigment
(6) pink solid
(11) Pigment Red 30
(12) 12330
(13) KBr pellet

2212 $C_{26}H_{20}ClN_5O_4$



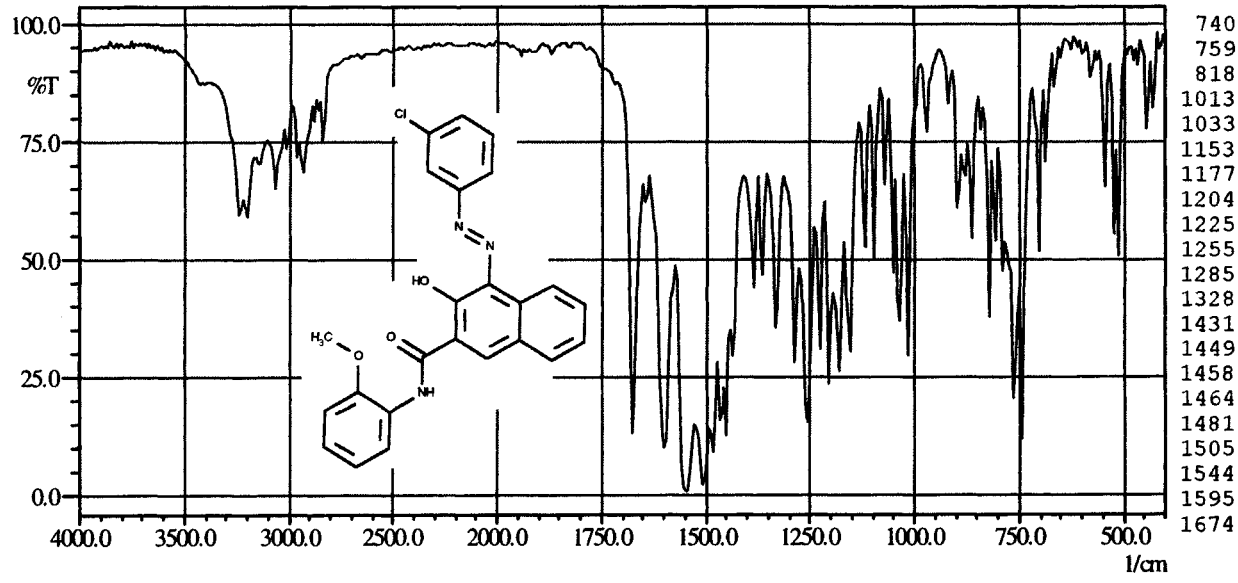
(1) **3-amino-4-chlorobenzamide -> 2-hydroxynaphthoic arylide-4-aminoacetylanilide**
(2) Novoperm Rot HFG
(3) Hoechst
(4) 501.9 g mol^{-1}
(5) organic pigment
(6) red solid
(11) Pigment Orange 38
(12) 12367
(13) KBr pellet

2212 $C_{26}H_{22}N_4O_4$



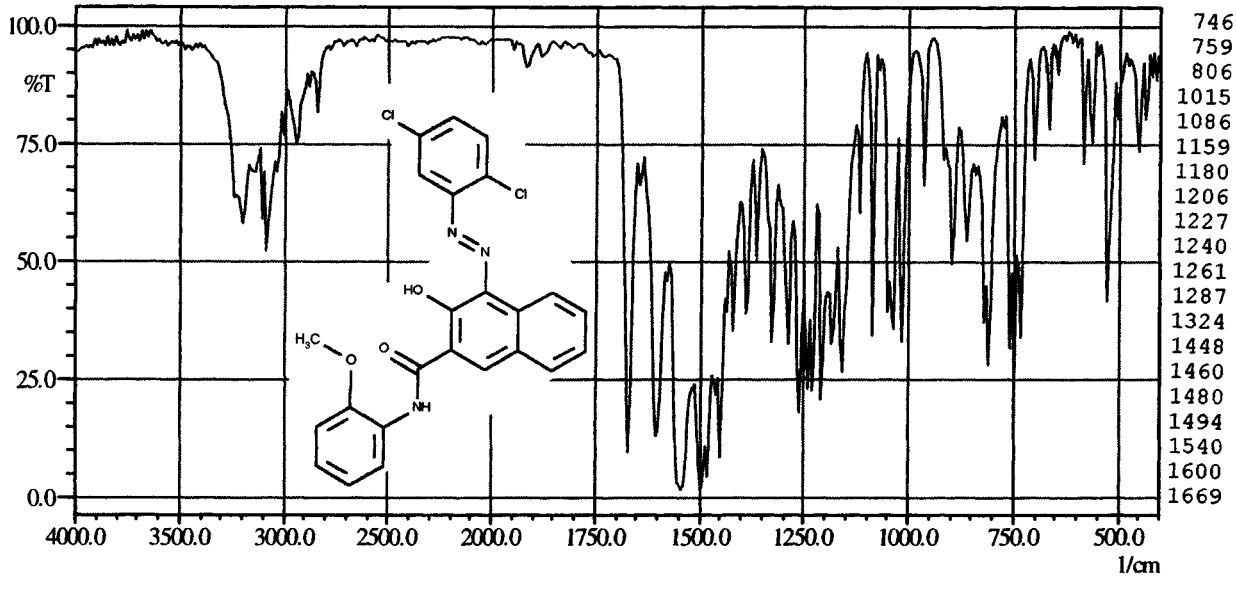
(1) **4-aminobenzamide -> 2-hydroxynaphthoic arylide-2-ethoxyanilide**
(2) Novoperm Rot F5RK
(3) Hoechst
(4) 454.5 g mol^{-1}
(5) organic pigment
(6) red solid
(11) Pigment Red 170
(12) 12475
(13) KBr pellet

2212 $C_{24}H_{18}Cl_3N_3O_3$



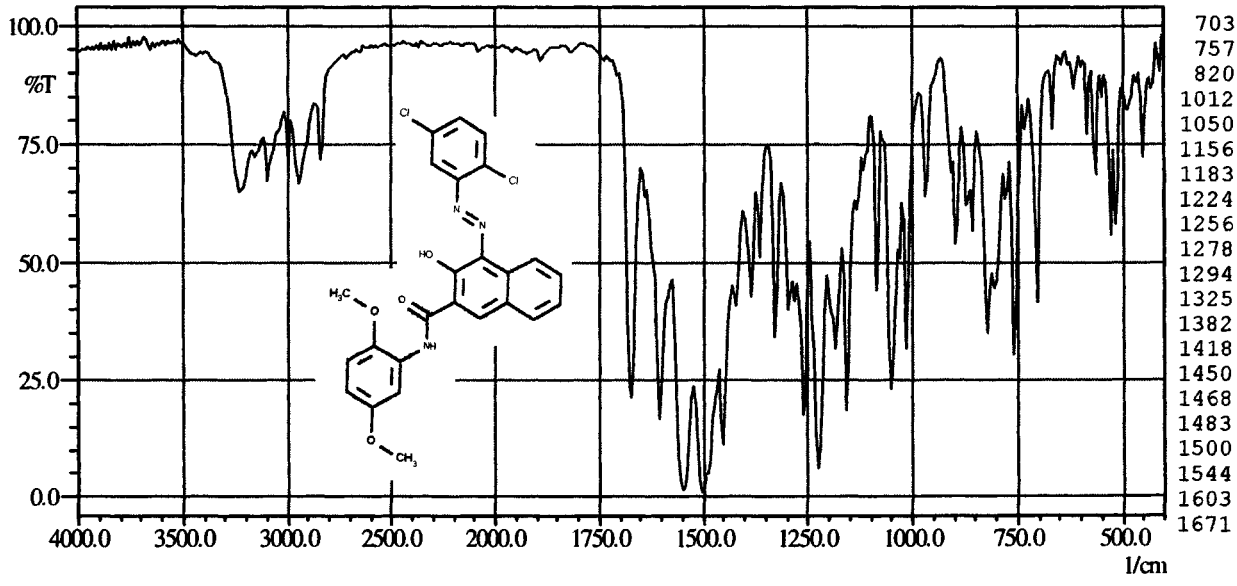
(1) **3-chloroaniline -> 2-hydroxynaphthoic arylide-2-methoxyanilide**
(2) Helio Echtorange G
(3) Bayer
(4) 502.8 g mol^{-1}
(5) organic pigment
(6) orange solid
(11) Pigment Orange 4
(12) 12459
(13) KBr pellet

2212 $C_{24}H_{17}Cl_2N_3O_3$



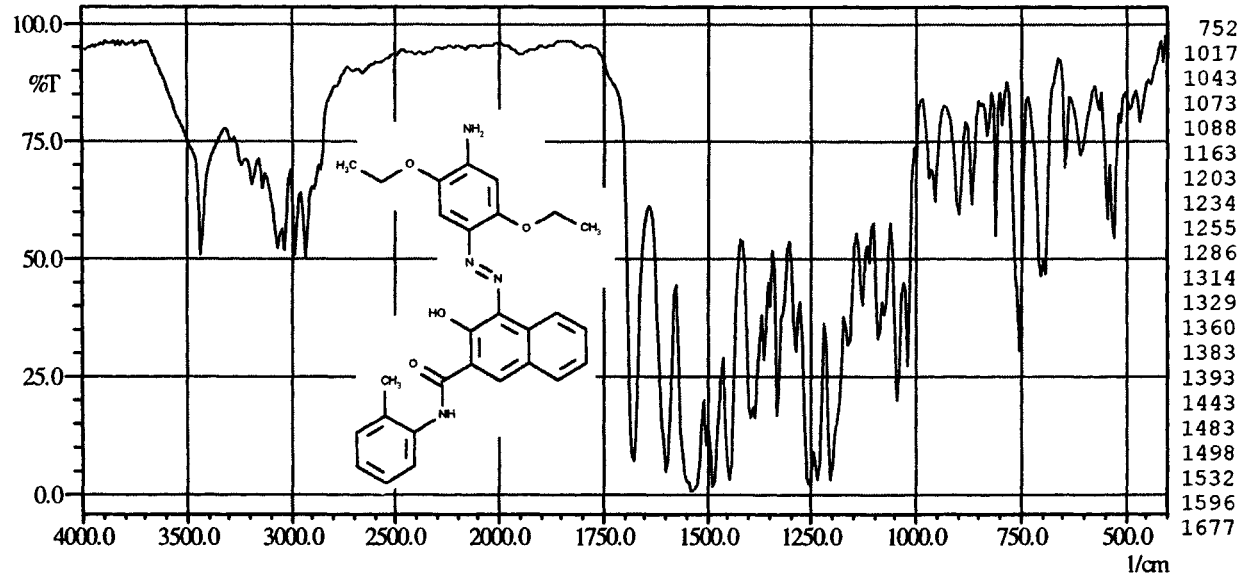
(1) **2,5-dichloroaniline -> 2-hydroxynaphthoic arylide-2-methoxyanilide**
(2) Permanent Rot FRLL
(3) Hoechst
(4) 466.3 g mol^{-1}
(5) organic pigment
(6) red solid
(11) Pigment Red 9
(12) 12460
(13) KBr pellet

2212 $C_{25}H_{19}Cl_2N_3O_4$



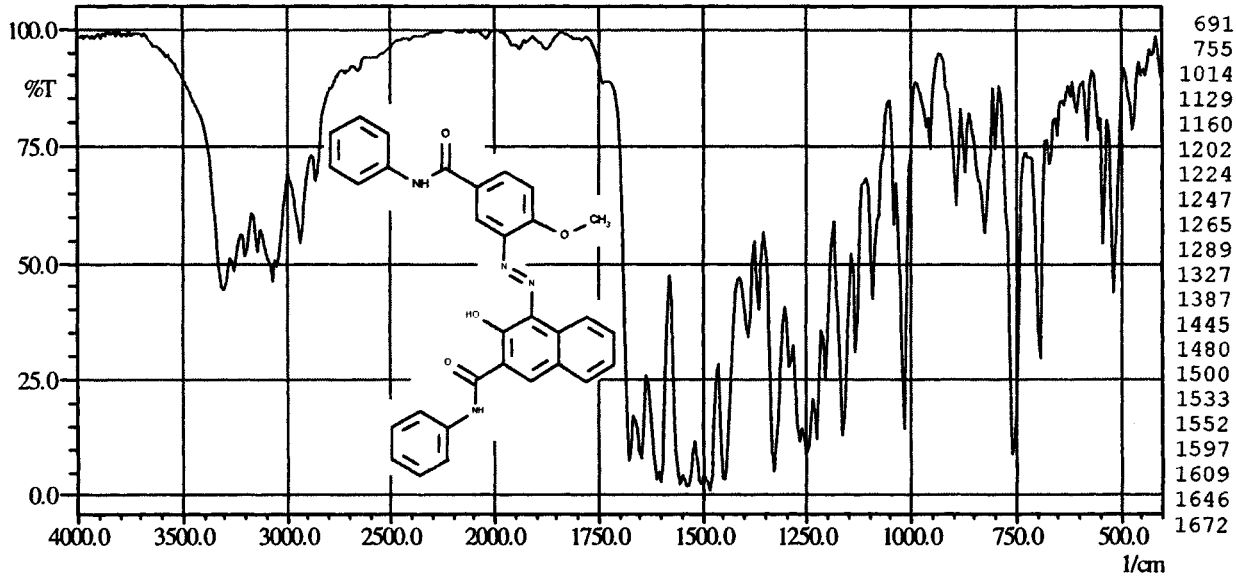
(1) **2,5-dichloroaniline -> 2-hydroxynaphthoic arylide-2,5-dimethoxyanilide**
(2) Permanent Braun FG
(3) Hoechst
(4) 496.4 g mol^{-1}
(5) organic pigment
(6) brown solid
(11) Pigment Brown 1
(12) 12480
(13) KBr pellet

2212 $C_{28}H_{28}N_4O_4$



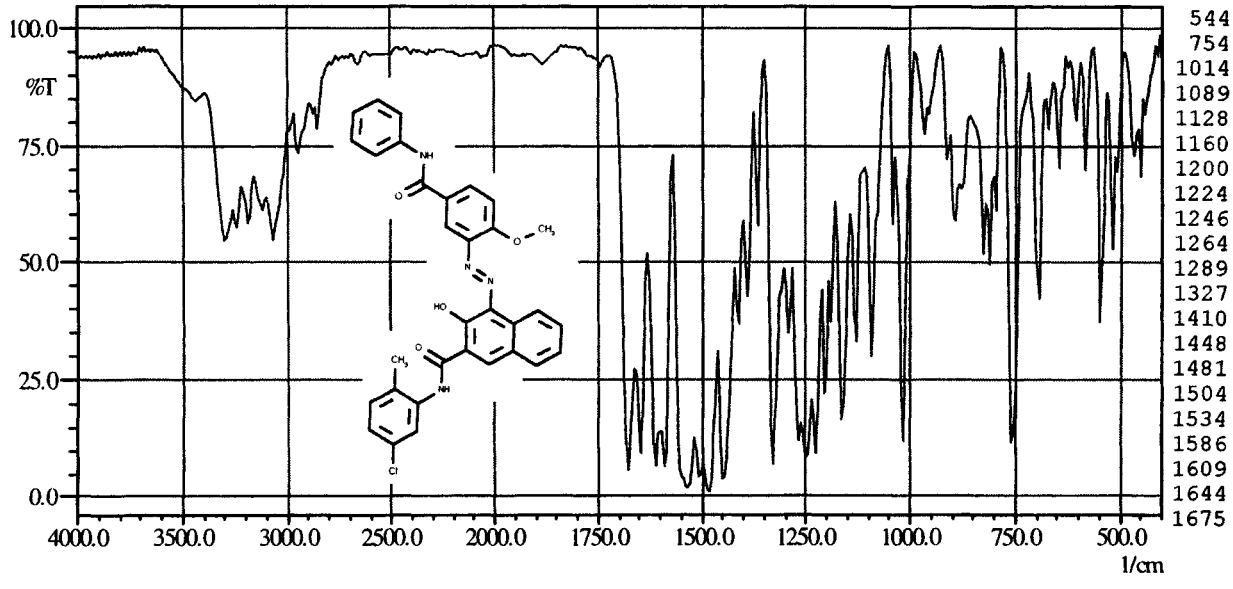
(1) **4-amino-2,5-diethoxybenzanilide -> 2-hydroxynaphthoic arylide-2-methylanilide**
(2) Helio Echtbrilliantblau RR
(3) Bayer
(4) 484.5 g mol^{-1}
(5) organic pigment
(6) blue solid
(11) Pigment Blue 23
(13) KBr pellet

2212 $C_{31}H_{24}N_4O_4$



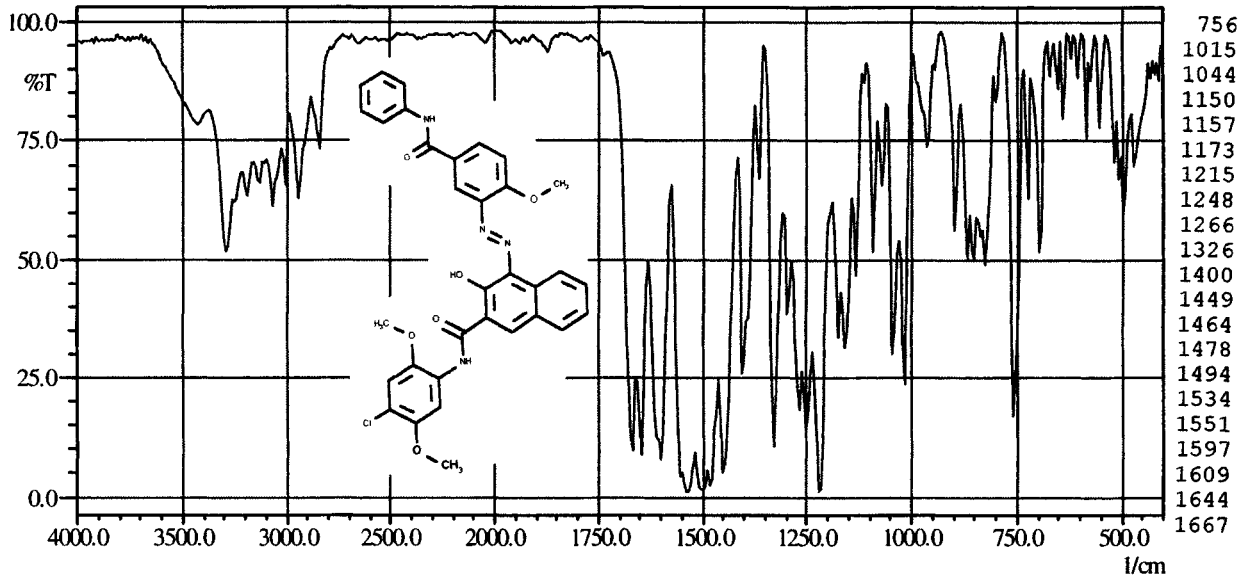
(1) **3-amino-4-methoxybenzanilide -> 2-hydroxynaphthoic arylide-anilide**
(2) Vulkan Echtrubin B
(3) Hoechst
(4) 516.5 g mol^{-1}
(5) organic pigment
(6) ruby solid
(11) Pigment Red 32
(12) 12320
(13) KBr pellet

2212 $C_{32}H_{25}ClN_4O_4$



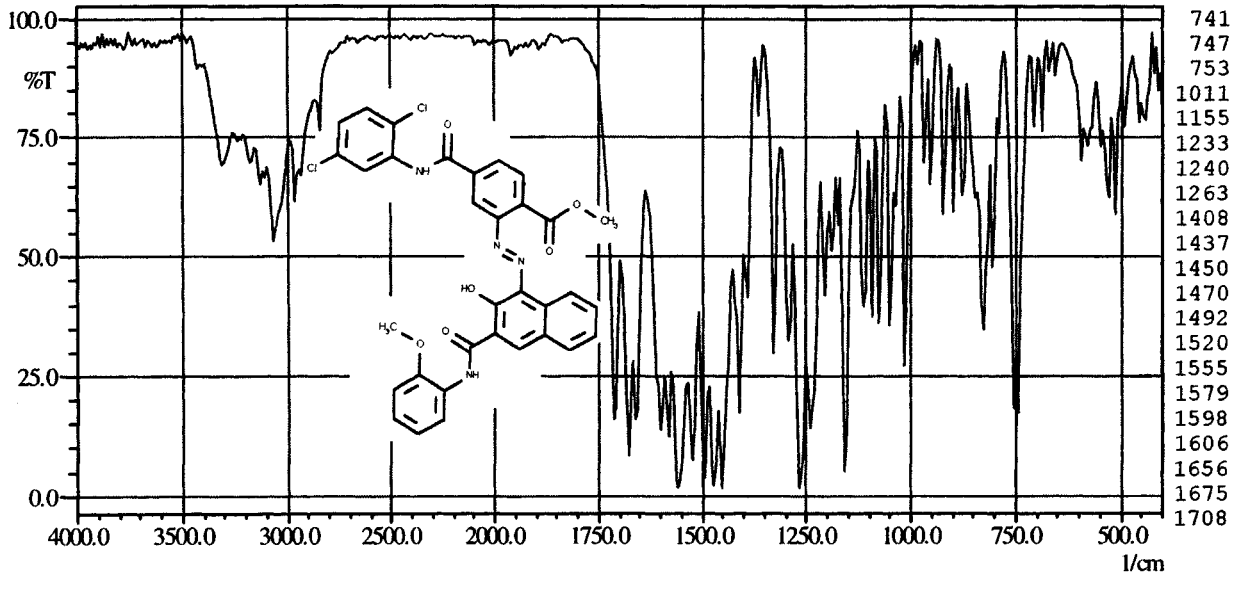
(1) **3-amino-4-methoxybenzanilide -> 2-hydroxynaphthoic arylide-4-chloro-2-methylanilide**
(2) Permanent Rosa F3B
(3) Hoechst
(4) 565.0 g mol^{-1}
(5) organic pigment
(6) pink solid
(11) Pigment Red 147
(12) 12433
(13) KBr pellet

2212 $C_{32}H_{27}ClN_4O_6$



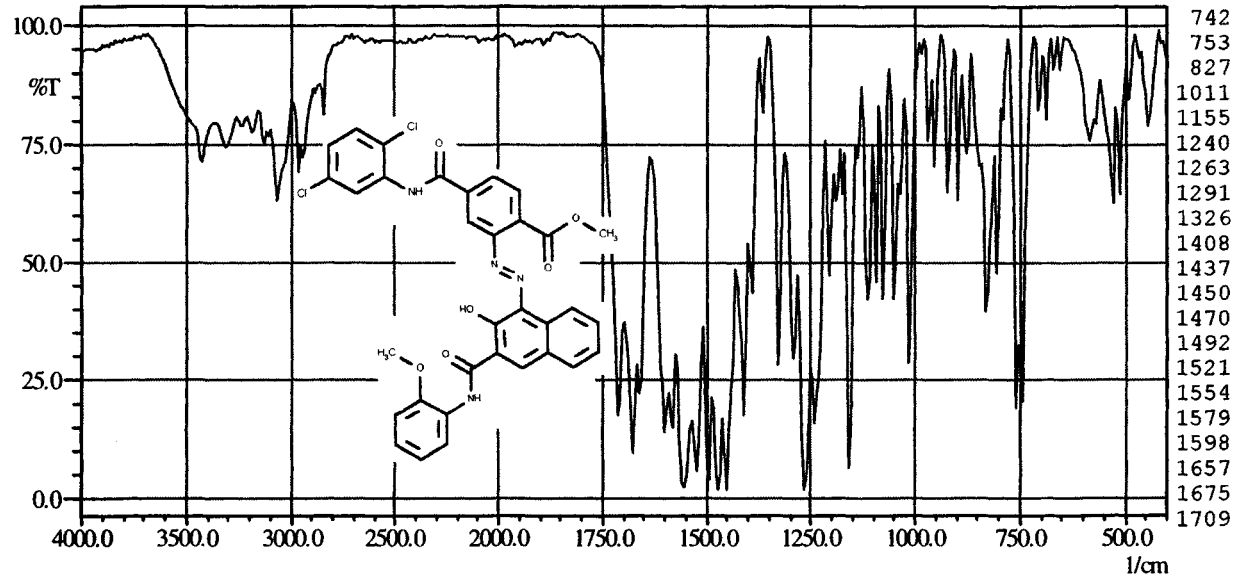
(1) **3-amino-4-methoxybenzanilide -> 2-hydroxynaphthoic arylide-4-chloro-2,5-dimethoxyanilide**
(2) Permanent Carmin FBB02
(3) Hoechst
(4) 599.0 g mol^{-1}
(5) organic pigment
(6) dark-red solid
(11) Pigment Red 146
(12) 12485
(13) KBr pellet

2212 $C_{33}H_{24}Cl_2N_4O_6$



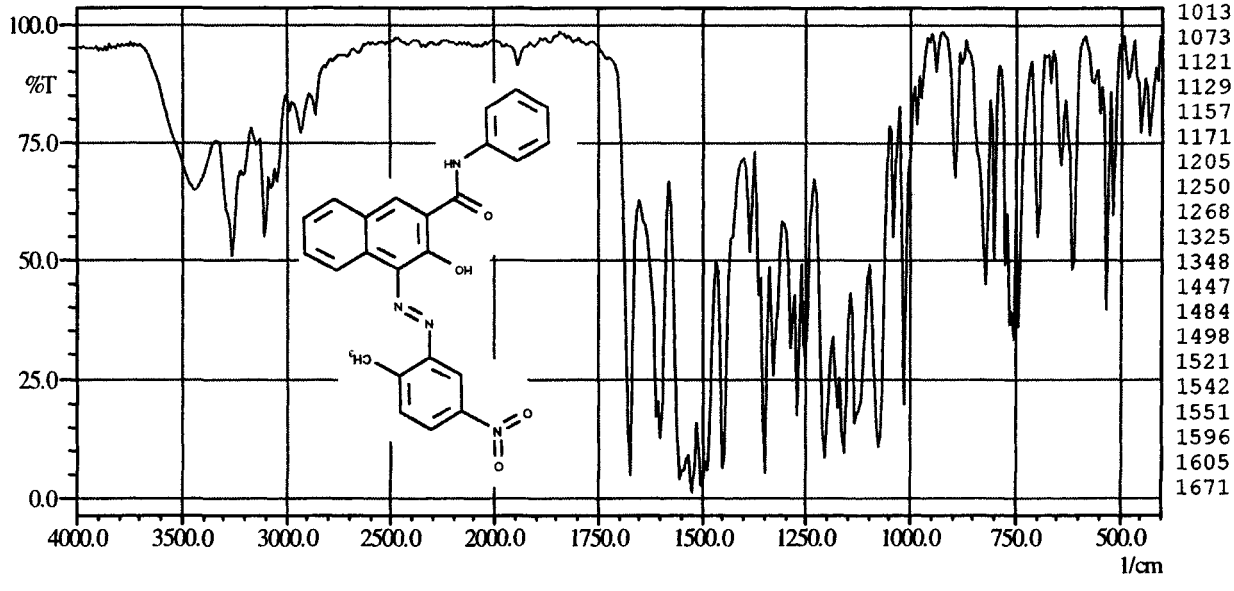
(1) **2-amino-4-(2,5-dichloroanilido)benzoic methylester -> 2-hydroxynaphthoic arylide-2-anisidide**
(2) Novoperm Rot HF 3570
(3) Hoechst
(4) 643.5 g mol^{-1}
(5) organic pigment
(6) red solid
(13) KBr pellet

2212 $C_{33}H_{24}Cl_2N_4O_6$



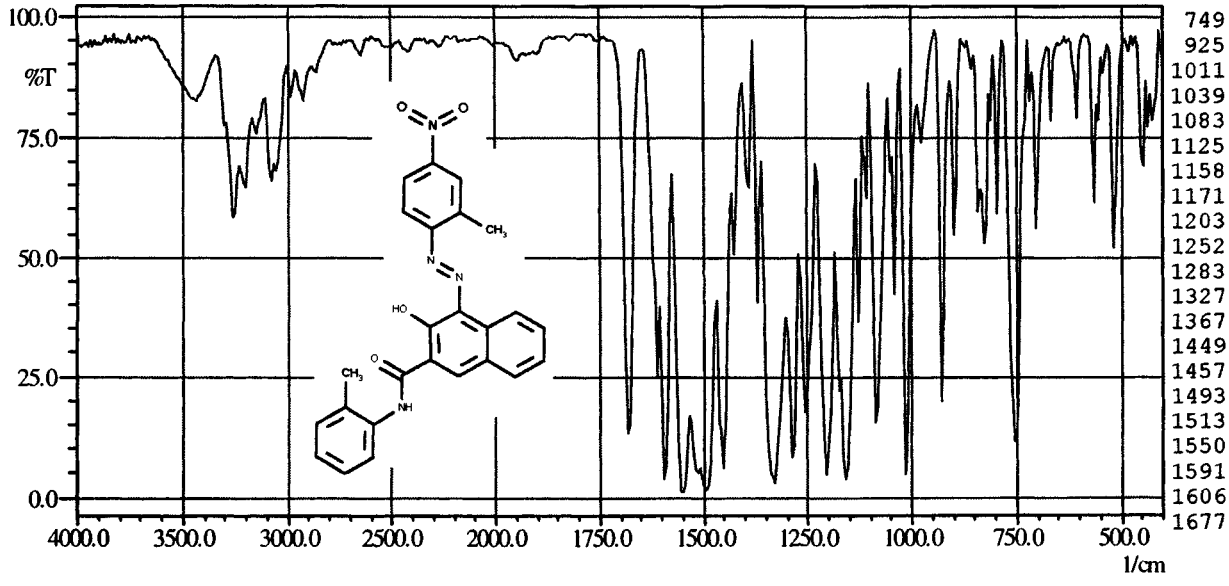
(1) **2-amino-4-(2,5-dichloroanilido)benzoic methylester -> 2-hydroxynaphthoic arylide-2-anisidide**
(2) Novoperm Rot HF3S
(3) Hoechst
(4) 643.5 g mol^{-1}
(5) organic pigment
(6) red solid
(11) Pigment Red 188
(12) 12467
(13) KBr pellet

2212 $C_{24}H_{18}N_4O_4$



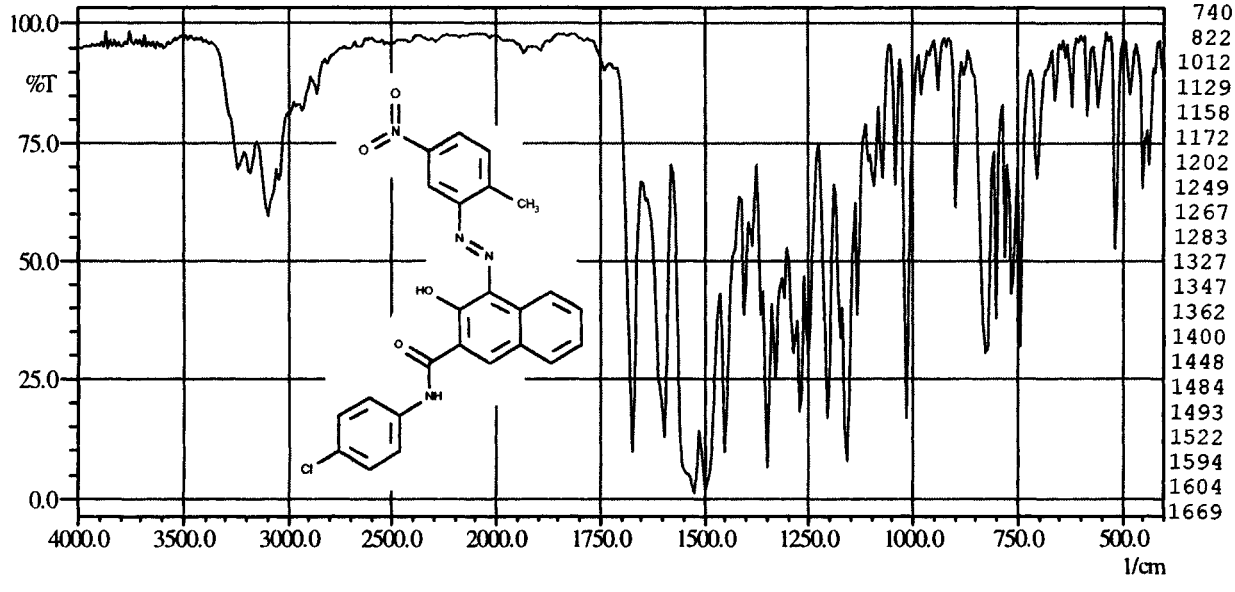
(1) **5-nitro-2-toluidine -> 2-hydroxynaphthoic arylide-anilide**
(2) Symuler Fast Scarlet BGT
(3) DIC
(4) 426.4 g mol^{-1}
(5) organic pigment
(6) scarlet solid
(11) Pigment Red 22
(12) 12315
(13) KBr pellet

2212 $C_{25}H_{20}N_4O_4$



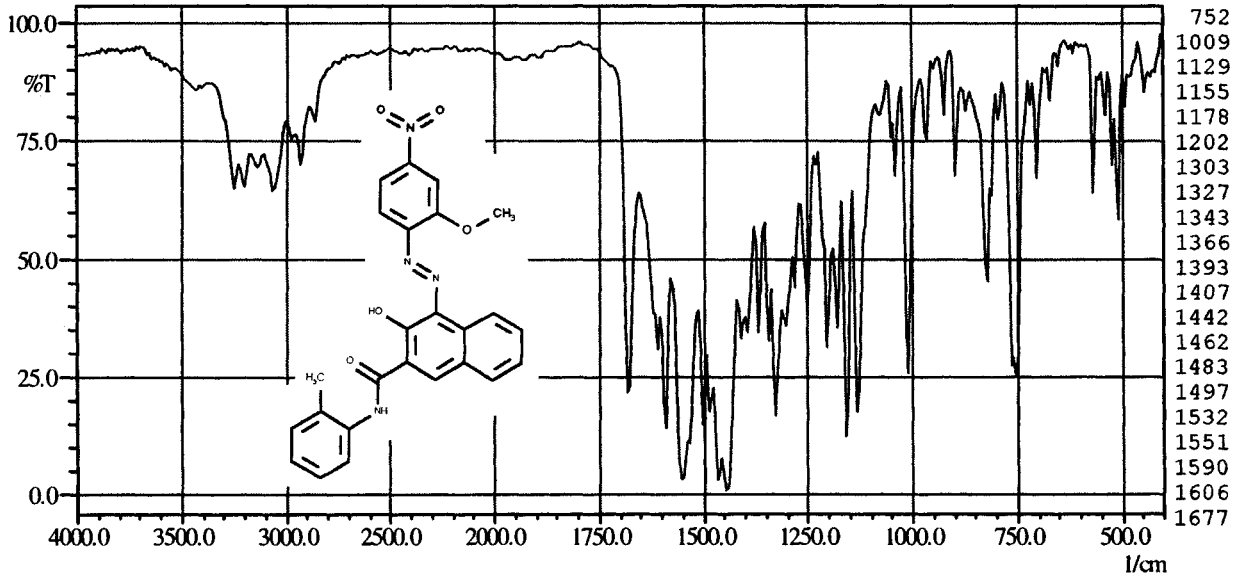
(1) **4-nitro-2-toluidine -> 2-hydroxynaphthoic arylide-2-methylanilide**
(2) Permanent Bordo FRR
(3) Hoechst
(4) 440.5 g mol^{-1}
(5) organic pigment
(6) dark-red solid
(11) Pigment Red 12
(12) 12385
(13) KBr pellet

2212 $C_{24}H_{17}ClN_4O_4$



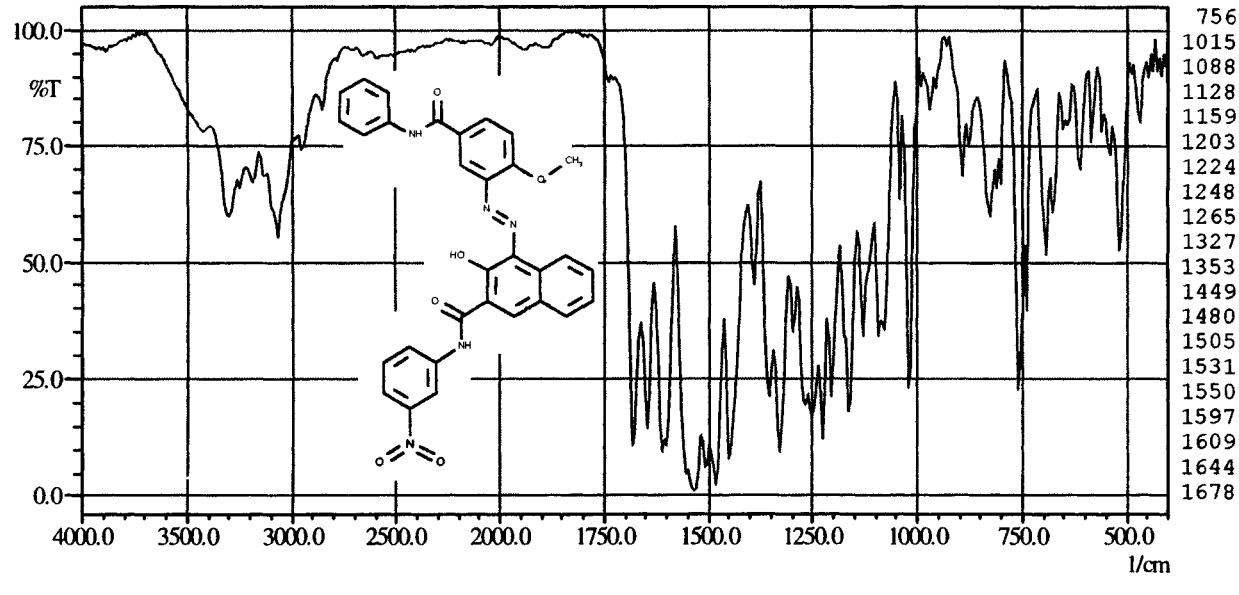
(1) **5-nitro-2-toluidine -> 2-hydroxynaphthoic arylide-4-chloroanilide**
(2) Permanent Rot F4R
(3) Hoechst
(4) 460.9 g mol^{-1}
(5) organic pigment
(6) red solid
(11) Pigment Red 8
(12) 12335
(13) KBr pellet

2212 $C_{25}H_{20}N_4O_5$



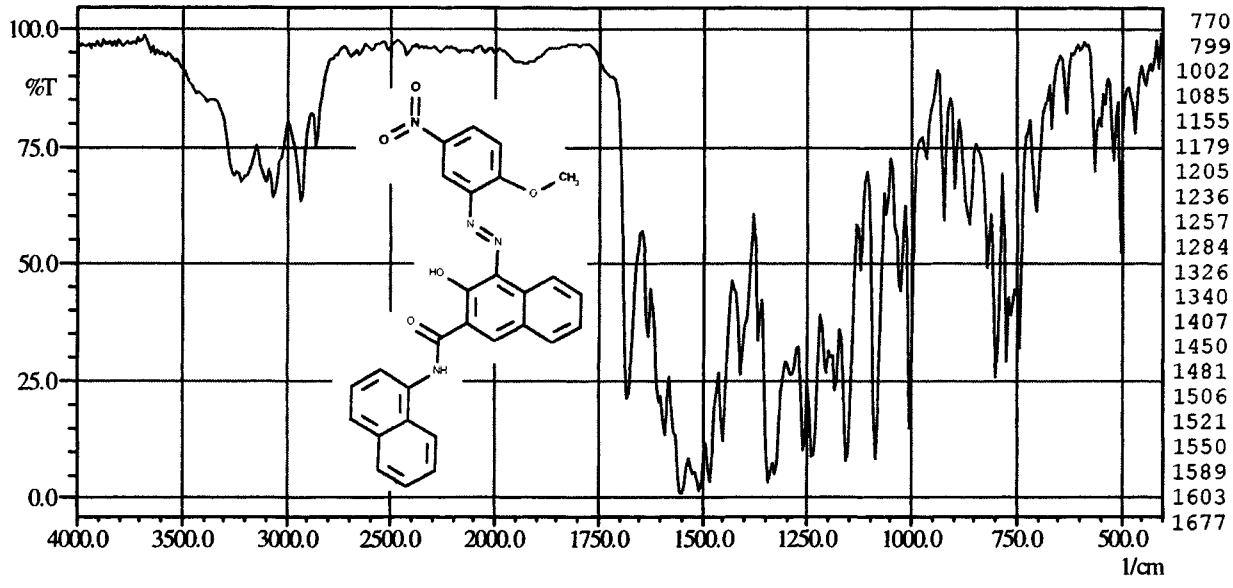
(1) **2-methoxy-4-nitroaniline -> 2-hydroxynaphthoic arylide-2-methylanilide**
(2) Toluidine Maroon RT-530-D
(3) DuPont
(4) 456.4 g mol^{-1}
(5) organic pigment
(6) dark-red solid
(11) Pigment Red 19
(13) KBr pellet

2212 $C_{31}H_{23}N_5O_6$



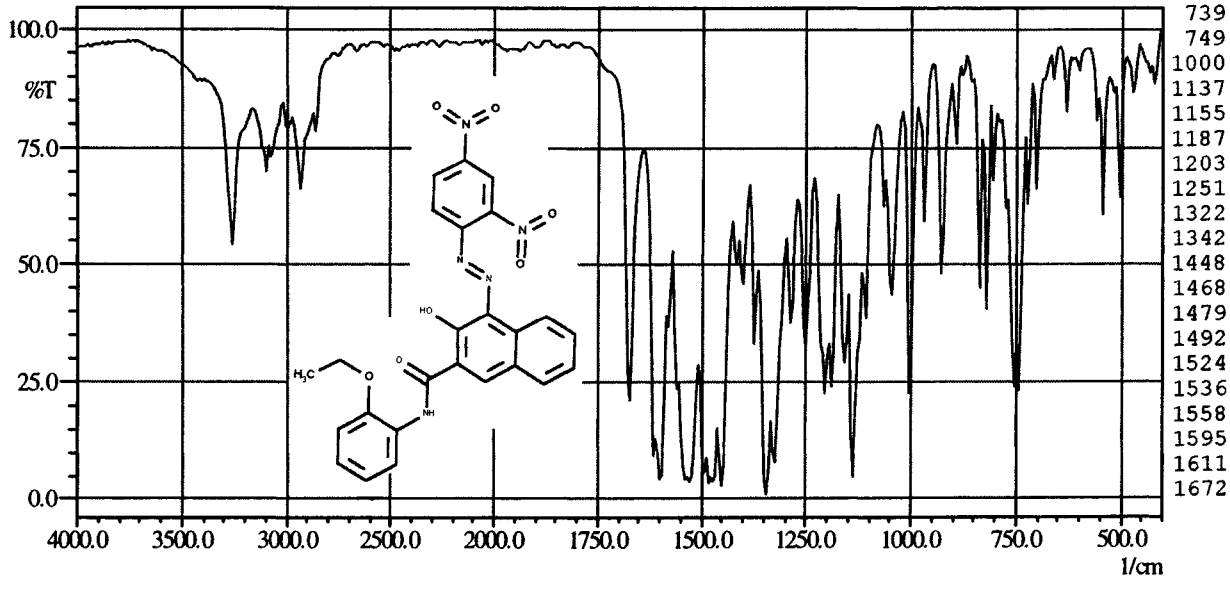
(1) **3-amino-4-methoxybenzanilide -> 2-hydroxynaphthoic arylide-3-nitroanilide**
(2) Symuler Fast Red 4085
(3) DIC
(4) 561.6 g mol^{-1}
(5) organic pigment
(6) red solid
(11) Pigment Red 31
(12) 12360
(13) KBr pellet

2212 $C_{28}H_{19}N_3O_5$



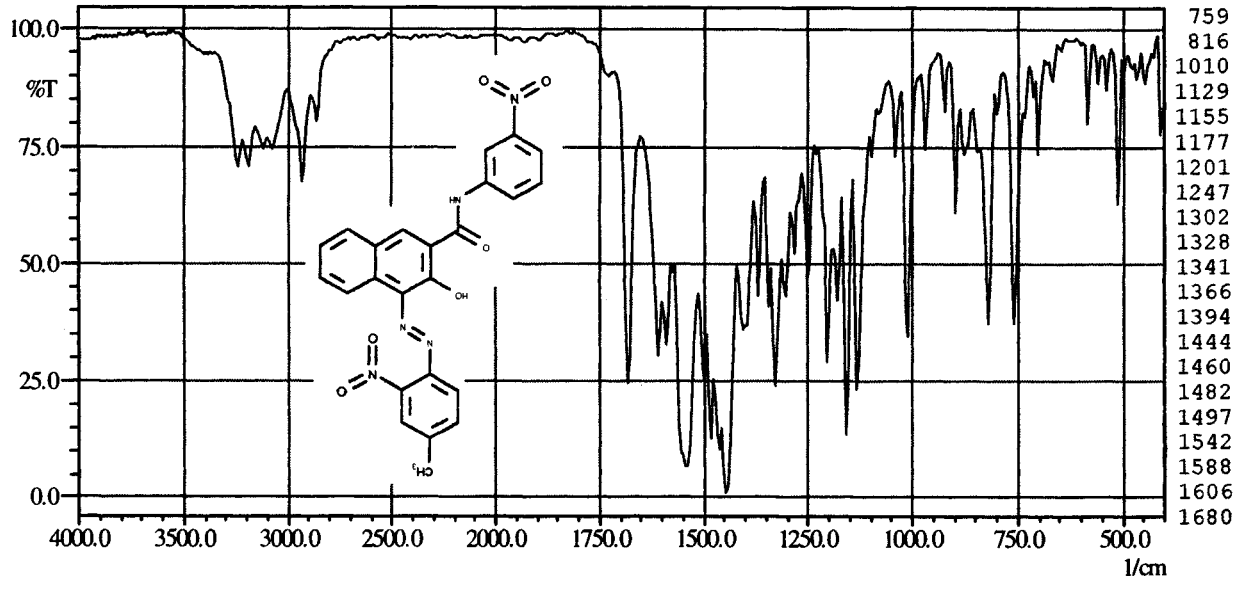
(1) **2-methoxy-4-nitroaniline -> 2-hydroxynaphthoic arylide-1-naphthylamide**
(2) Permanent Bordo F3R
(3) Hoechst
(4) 477.5 g mol^{-1}
(5) organic pigment
(6) dark-red solid
(11) Pigment Red 16
(12) 12500
(13) KBr pellet

2212 $C_{25}H_{19}N_5O_7$



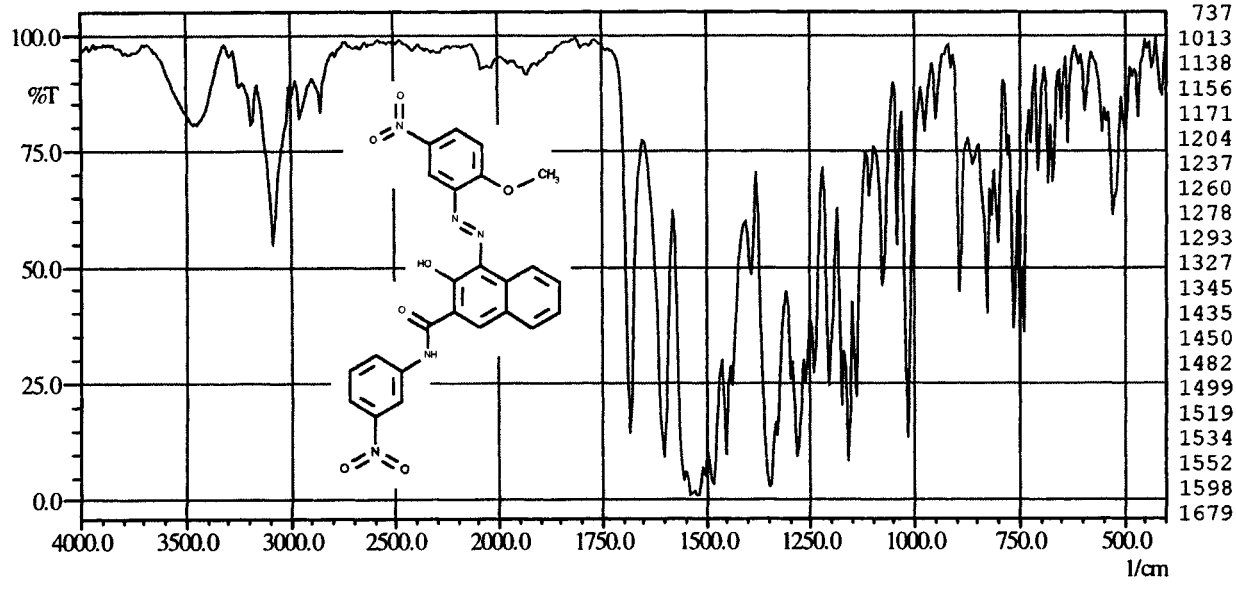
(1) **2,4-dinitroaniline -> 2-hydroxynaphthoic arylide-2-ethoxyanilide**
(2) Helio Echtbrilliantrot 3B
(3) Bayer
(4) 501.5 g mol^{-1}
(5) organic pigment
(6) red solid
(11) Pigment Red 136
(13) KBr pellet

2212 $C_{24}H_{17}N_5O_6$



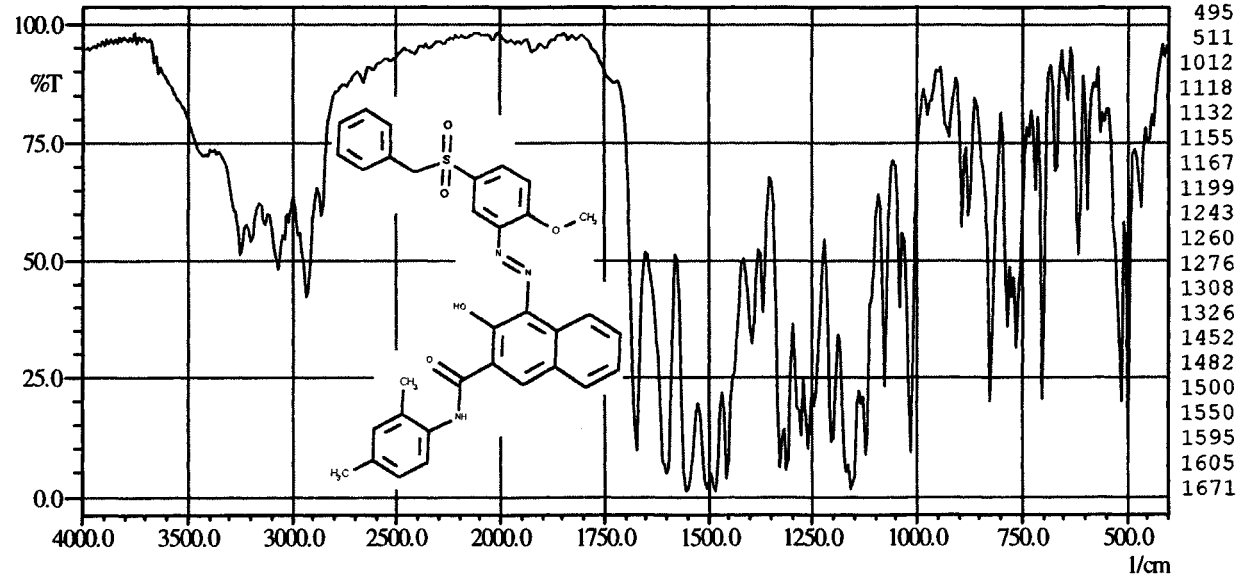
(1) **2-nitro-4-toluidine -> 2-hydroxynaphthoic arylide-3-nitroanilide**
(2) Sico Echtmaroon BMD dunkel
(3) BASF
(4) 471.4 g mol^{-1}
(5) organic pigment
(6) red-brown solid
(11) Pigment Red 18
(12) 12350
(13) KBr pellet

2212 $C_{24}H_{17}N_5O_7$



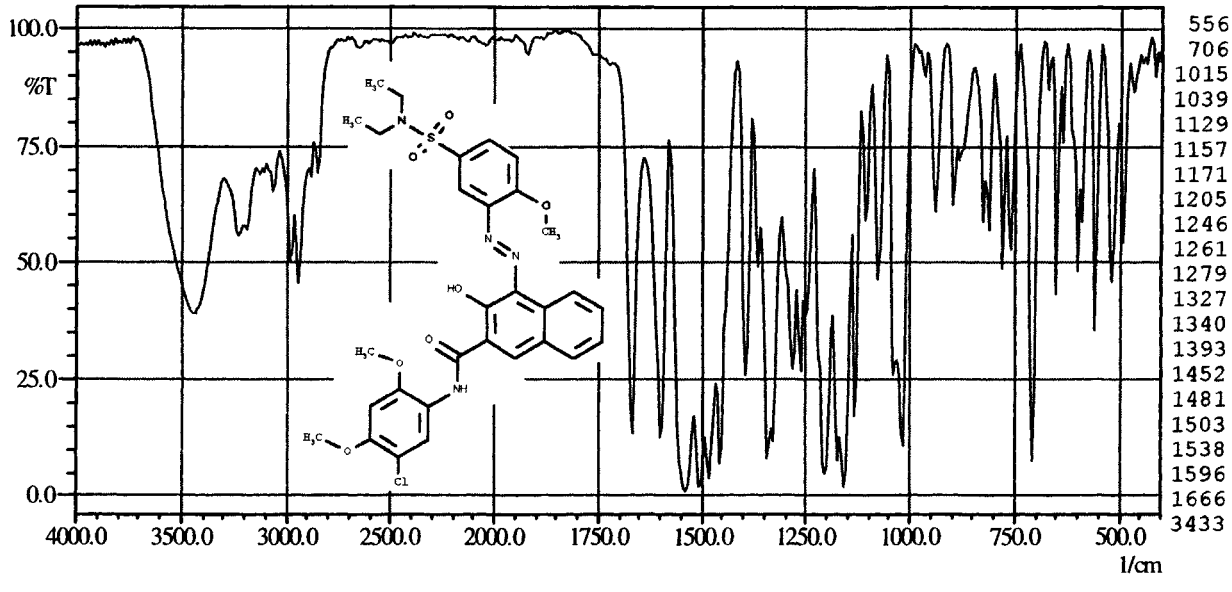
(1) **2-methoxy-5-nitroaniline -> 2-hydroxynaphthoic arylide-3-nitroanilide**
(2) Symuler Fast Red 4015
(3) DIC
(4) 487.4 g mol^{-1}
(5) organic pigment
(6) red solid
(11) Pigment Red 23
(12) 12355
(13) KBr pellet

2212 $C_{33}H_{29}N_3O_5S$



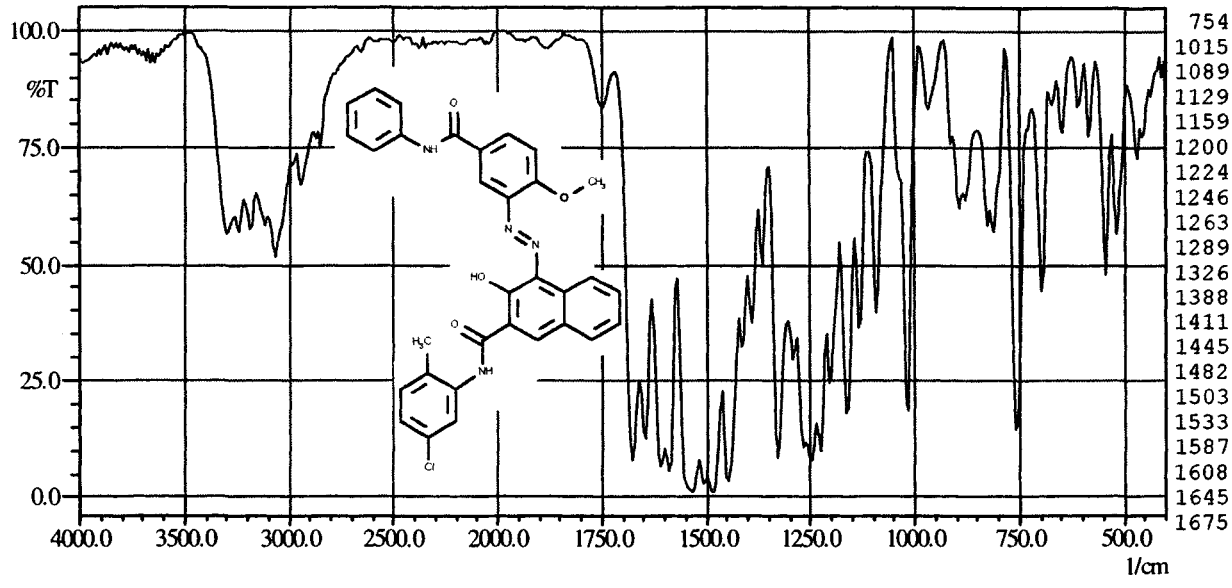
(1) **3-amino-4-methoxyphenylbenzyl sulfone -> 2-hydroxynaphthoic arylide-2,3-dimethylanilide**
(2) Hansa Rottoner R
(3) Hoechst
(4) 579.7 g mol^{-1}
(5) organic pigment
(6) red solid
(11) Pigment Red 163
(12) 12455
(13) KBr pellet

2212 $C_{30}H_{31}ClN_4O_7S$



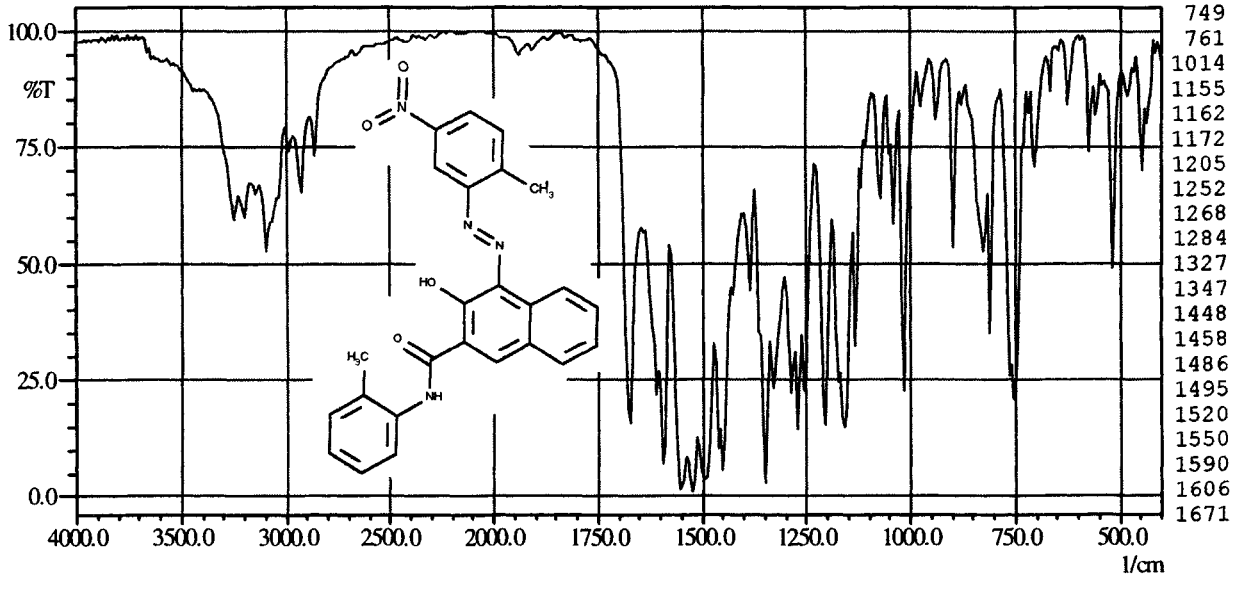
(1) **2-methoxy-5-N,N-dimethylsulfonamidoaniline -> 2-hydroxynaphthoic arylide-5-chloro-2,4-dimethoxyanilide**
(2) Permanent Carmin FB01
(3) Hoechst
(4) 627.1 g mol^{-1}
(5) organic pigment
(6) dark-red solid
(11) Pigment Red 5
(12) 12490
(13) KBr pellet

2212 $C_{32}H_{25}ClN_4O_4$



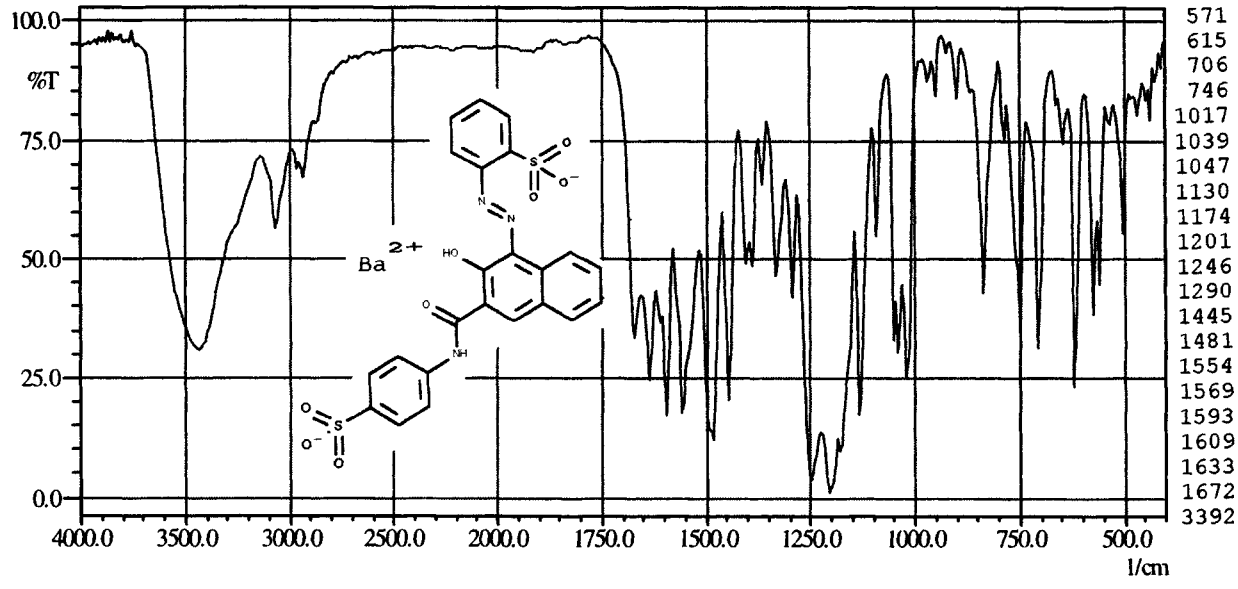
(1) **3-amino-4-methoxybenzoanilide -> 2-hydroxynaphthoic acid-4-chloro-2-methylanilide**
(2) Permanent Rosa
(3) Hoechst
(4) 565.0 g mol^{-1}
(5) organic pigment
(6) pink solid
(11) Pigment Red 147
(13) KBr pellet

2212 $C_{25}H_{20}N_4O_4$



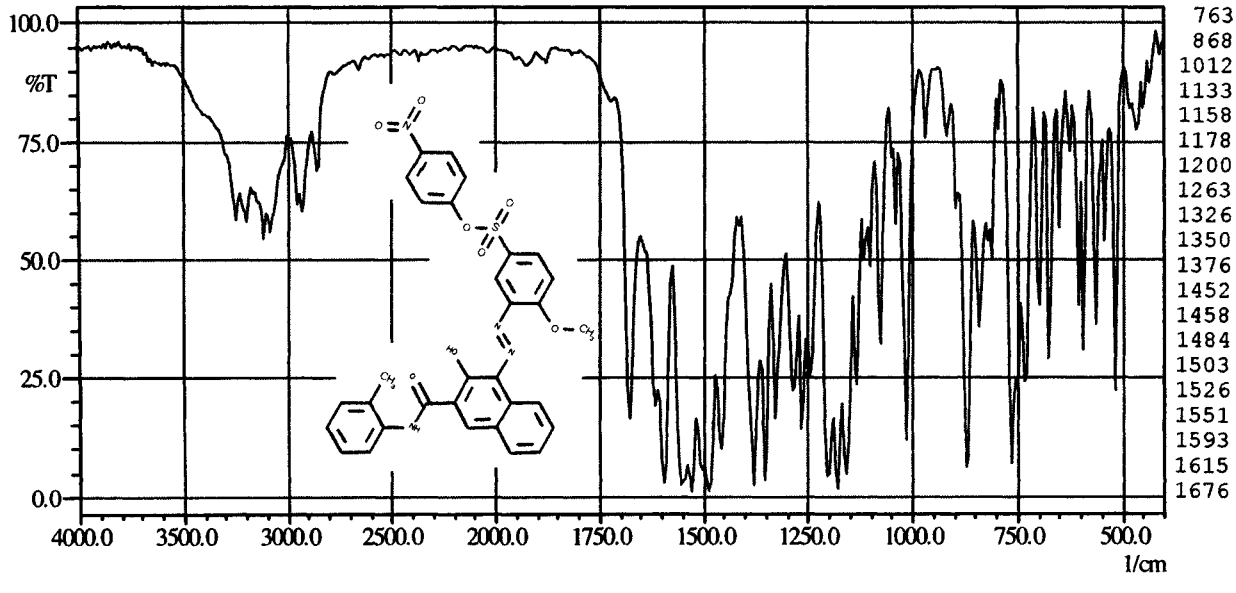
(1) **5-nitro-2-toluidine -> 2-hydroxynaphthoic arylide-2-methylanilide**
(2) Montclair Red Medium 235–7700
(3) Sun
(4) 440.4 g mol^{-1}
(5) organic pigment
(6) red solid
(11) Pigment Red 17
(12) 12390
(13) KBr pellet

2212 $C_{23}H_{15}N_3O_8S_2Ba$



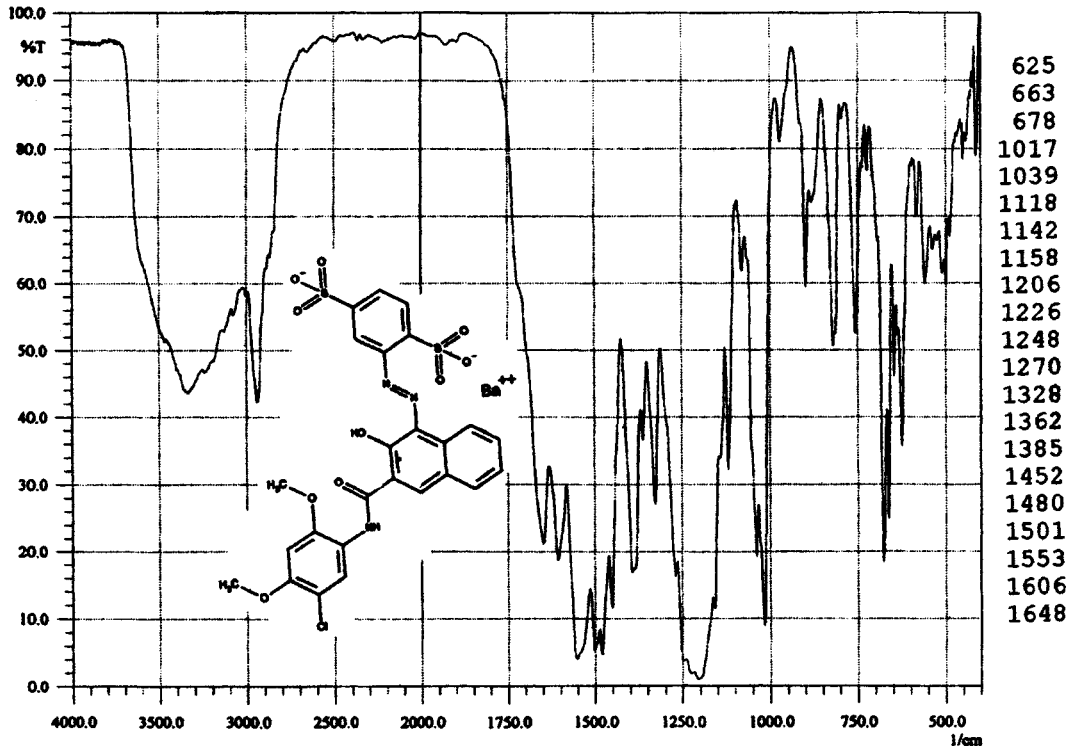
(1) **2-aminobenzenesulfonic acid -> 2-hydroxynaphthoic arylide-4-sulfonic acid anilide, Ba-salt**
(2) PV-Rot H4B 01
(3) Hoechst
(4) 662.9 g mol^{-1}
(5) organic pigment
(6) red solid
(11) Pigment Red 151
(12) 15892
(13) KBr pellet

2212 $C_{31}H_{24}N_4O_8S$



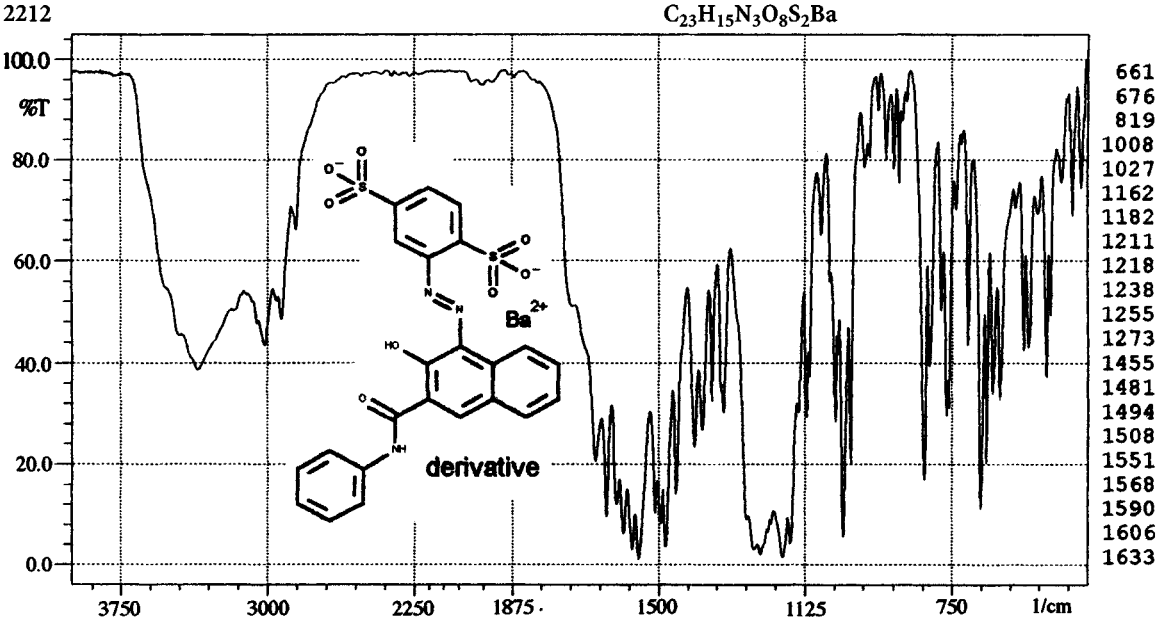
(1) **4'-nitrophenyl(3-amino-4-methoxyphenyl)sulfonate -> 2-hydroxynaphthoic arylide-2-methylanilide**
(2) Helio Echtcarmin G
(3) Bayer
(4) 612.6 g mol^{-1}
(5) organic pigment
(6) red solid
(11) Pigment Red 95
(13) KBr pellet

2212 $C_{25}H_{18}ClN_3O_{10}S_2Ba$



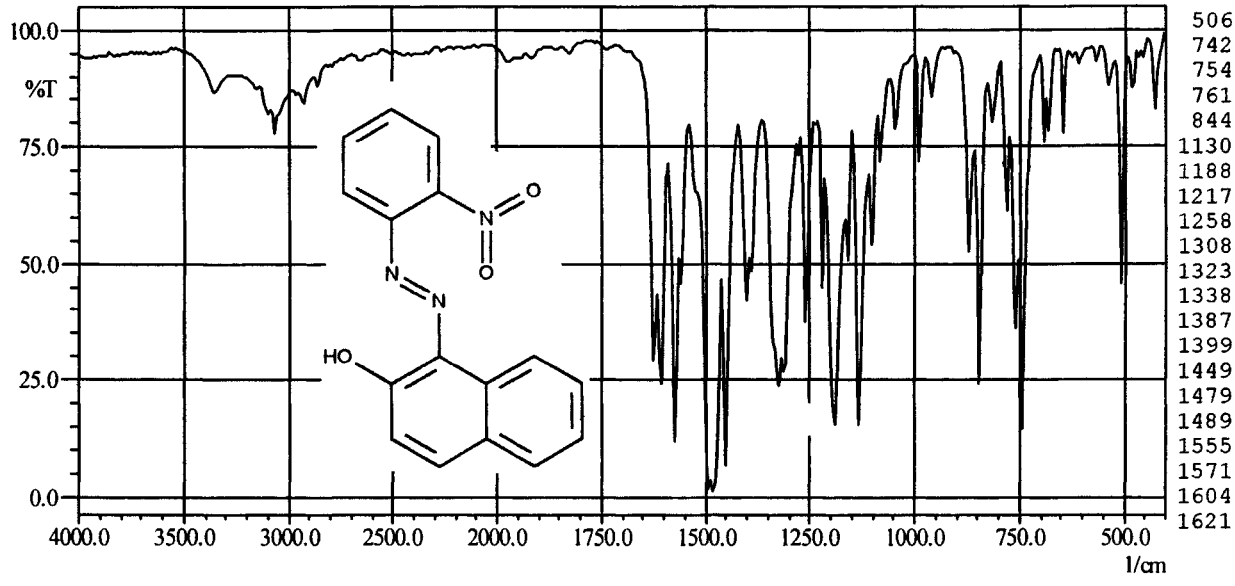
(1) **2-amino-1,4-benzenedisulfonic acid->2-hydroxynaphthoic arylide-2, 4-dimethoxy-5-chloro-anilide, Ba salt**
(2) Irgaplast Rot HGL
(3) Ciba-Geigy
(4) 757.3 g mol^{-1}
(5) organic pigment
(6) red solid
(11) Pigment Red 134
(13) KBr pellet

2212 $C_{23}H_{15}N_3O_8S_2Ba$



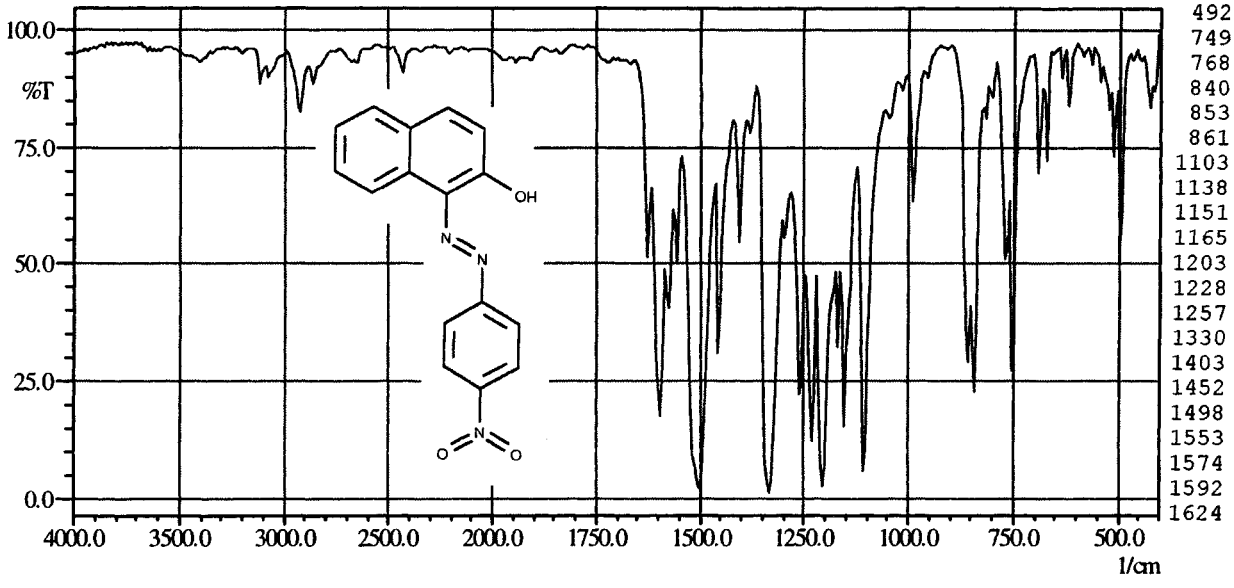
(1) **2-amino-1,4-benzenedisulfonic acid->2-hydroxynaphthoic arylide-2-naphthylamide, Ba salt**
(2) Irgaplast Rot HBL
(3) Ciba-Geigy
(4) 662.8 g mol^{-1}
(5) organic pigment
(6) red solid
(11) Pigment Red 133
(13) KBr pellet

2213 $C_{16}H_{11}N_3O_3$



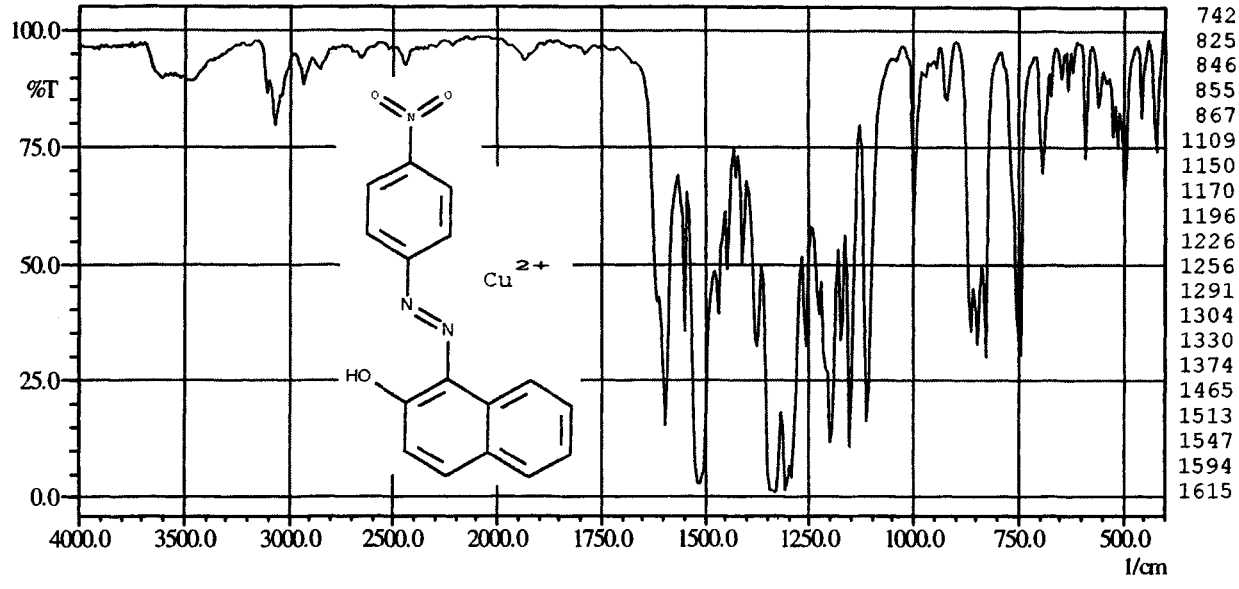
(1) **2-nitroaniline -> 2-naphthol**
(2) Ortho Nitranilinorange
(3) commercial
(4) 293.3 g mol^{-1}
(5) organic pigment
(6) orange solid
(11) Pigment Orange 2
(12) 12060
(13) KBr pellet

2213 $C_{16}H_8N_3O_3$



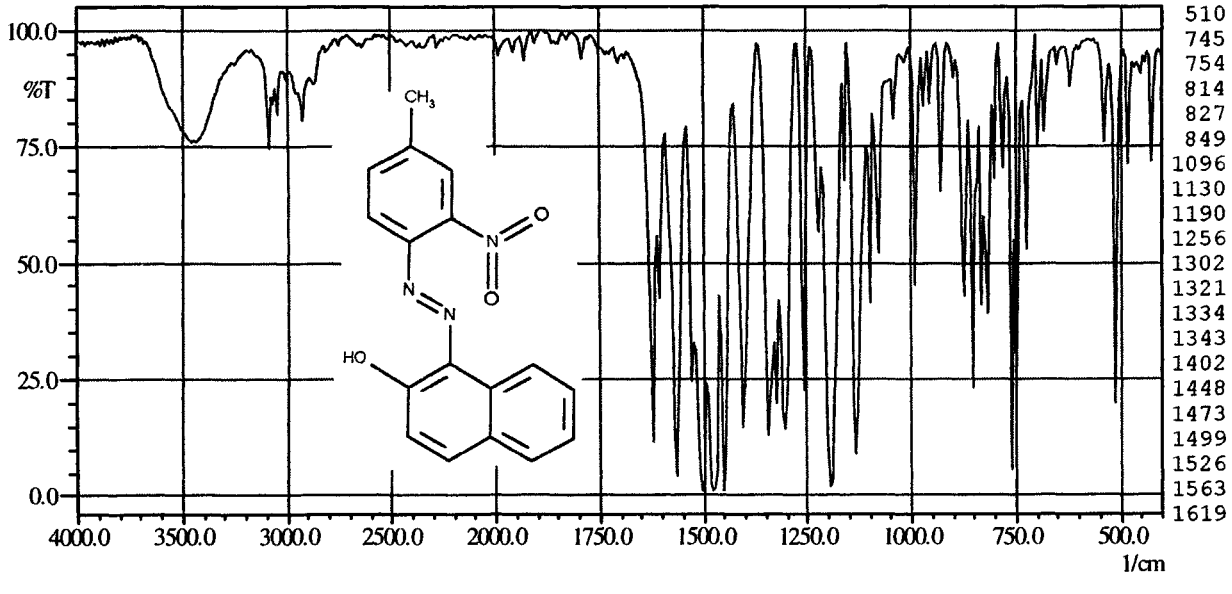
(1) **4-nitroaniline -> 2-naphthol**
(2) Pigmentrot B
(3) Hoechst
(4) 290.3 g mol^{-1}
(5) organic pigment
(6) red solid
(11) Pigment Red 1
(12) 12070
(13) KBr pellet

2213 $C_{16}H_{12}N_2O$



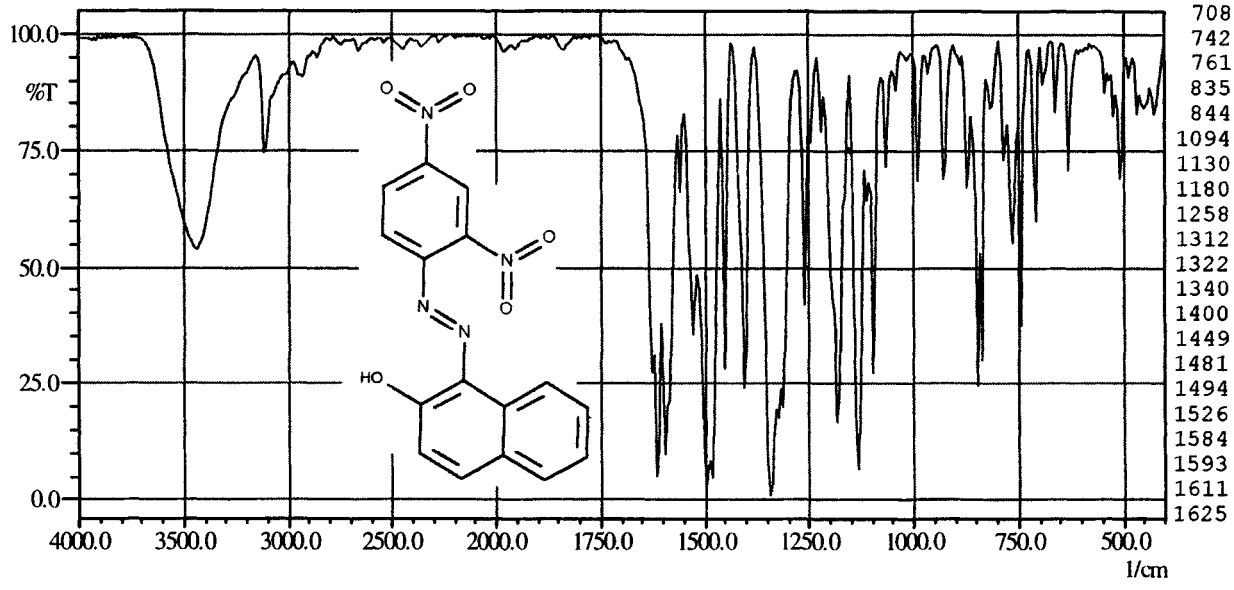
(1) **4-nitroaniline -> 2-naphthol, Cu-complex**
(2) Tiefdruckbraun 30
(3) commercial
(4) 248.3 g mol^{-1}
(5) organic pigment
(6) brown solid
(11) Pigment Brown 2
(12) 12071
(13) KBr pellet

2213 $C_{17}H_{13}N_3O_3$



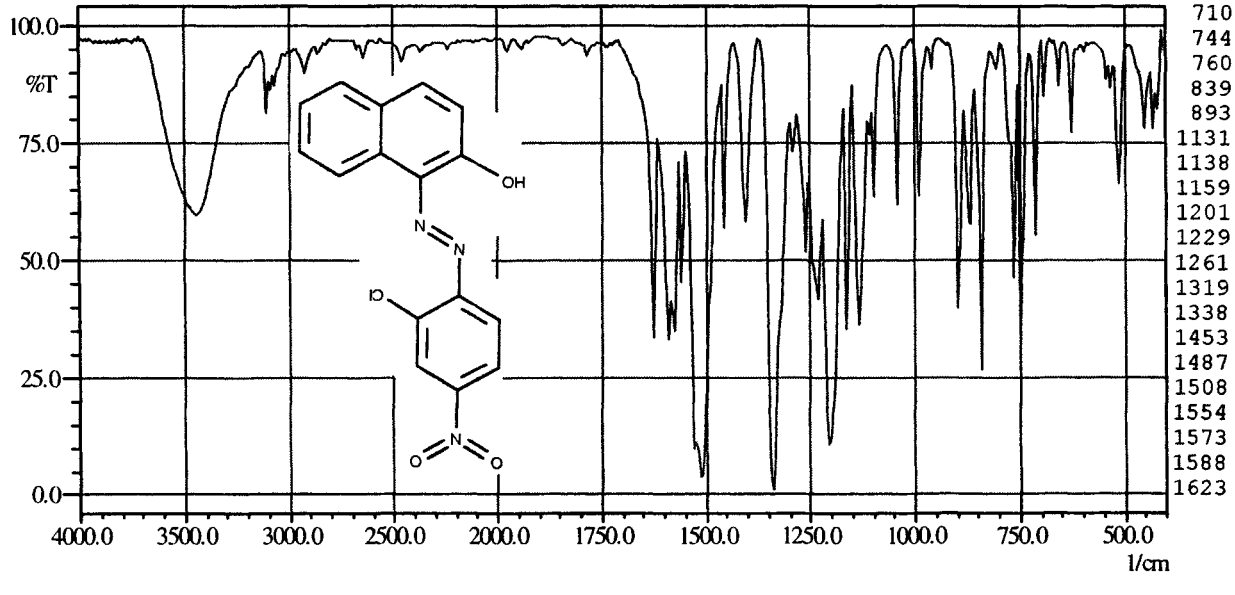
(1) **4-methyl-2-nitroaniline -> 2-naphthol**
(2) Hansa Scharlach RNC
(3) Hoechst
(4) 307.3 g mol^{-1}
(5) organic pigment
(6) scarlet solid
(11) Pigment Red 3
(12) 12120
(13) KBr pellet

2213 $C_{16}H_{10}N_4O_5$



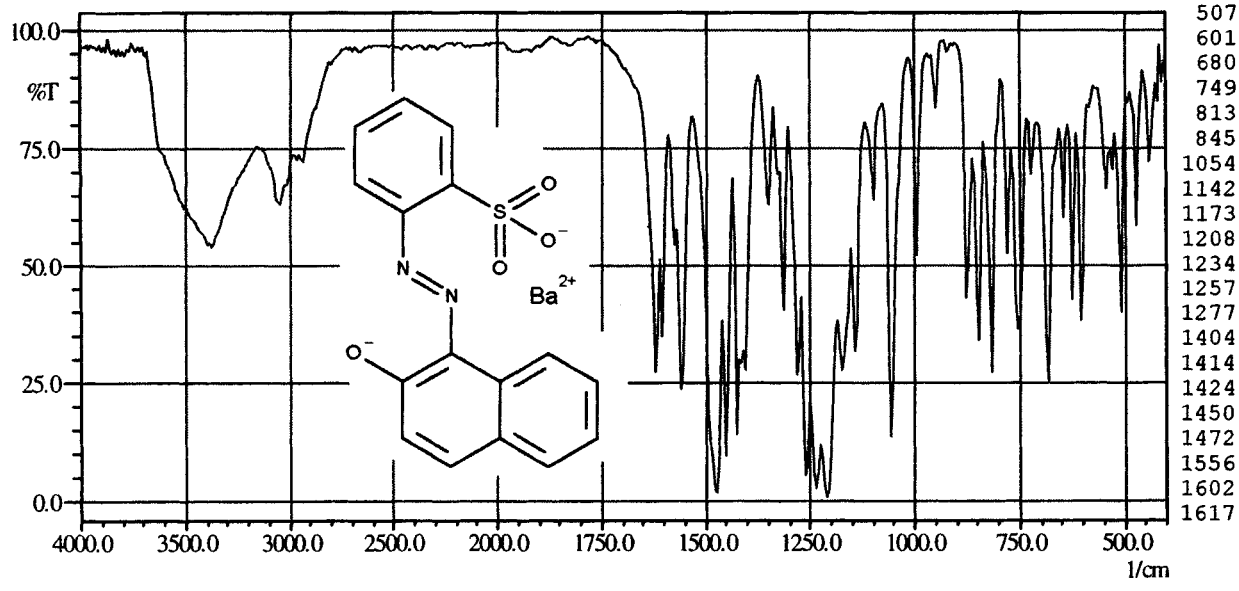
(1) **2,4-dinitroaniline -> 2-naphthol**
(2) Hansa Rot GG
(3) Hoechst
(4) 338.3 g mol^{-1}
(5) organic pigment
(6) red solid
(11) Pigment Orange 5
(12) 12075
(13) KBr pellet

2213 $C_{16}H_{10}ClN_3O_3$



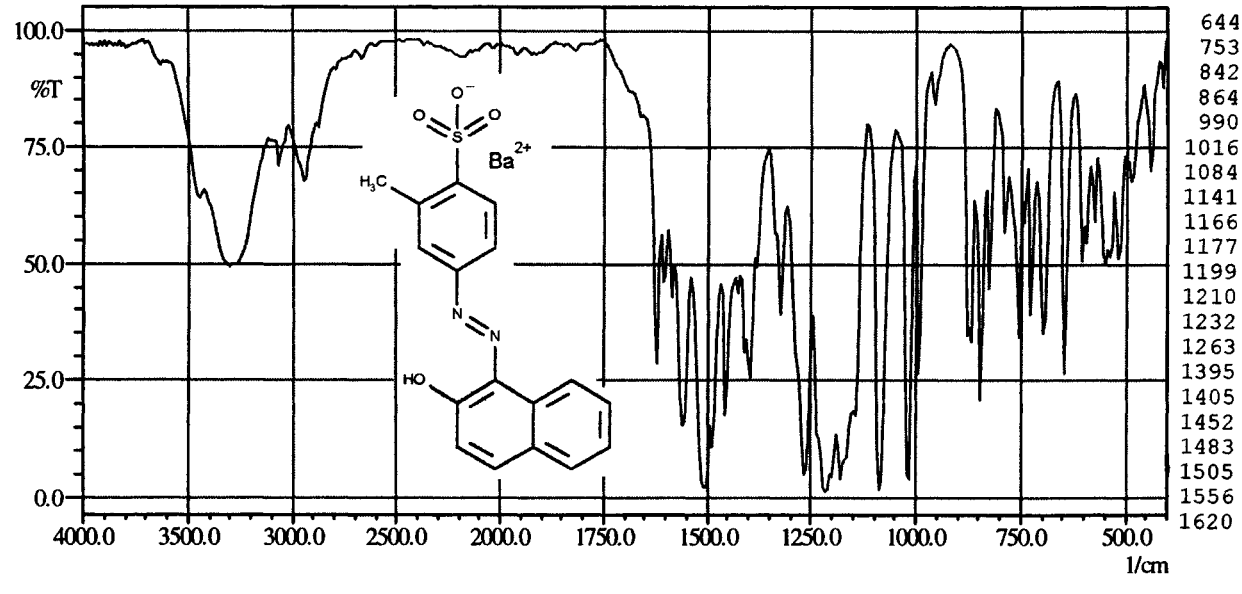
(1) **2-chloro-4-nitroaniline -> 2-naphthol**
(2) Hansa Rot R
(3) Hoechst
(4) 327.7 g mol^{-1}
(5) organic pigment
(6) red solid
(11) Pigment Red 4
(12) 12085
(13) KBr pellet

2213 $C_{16}H_{10}N_2O_4SBa$



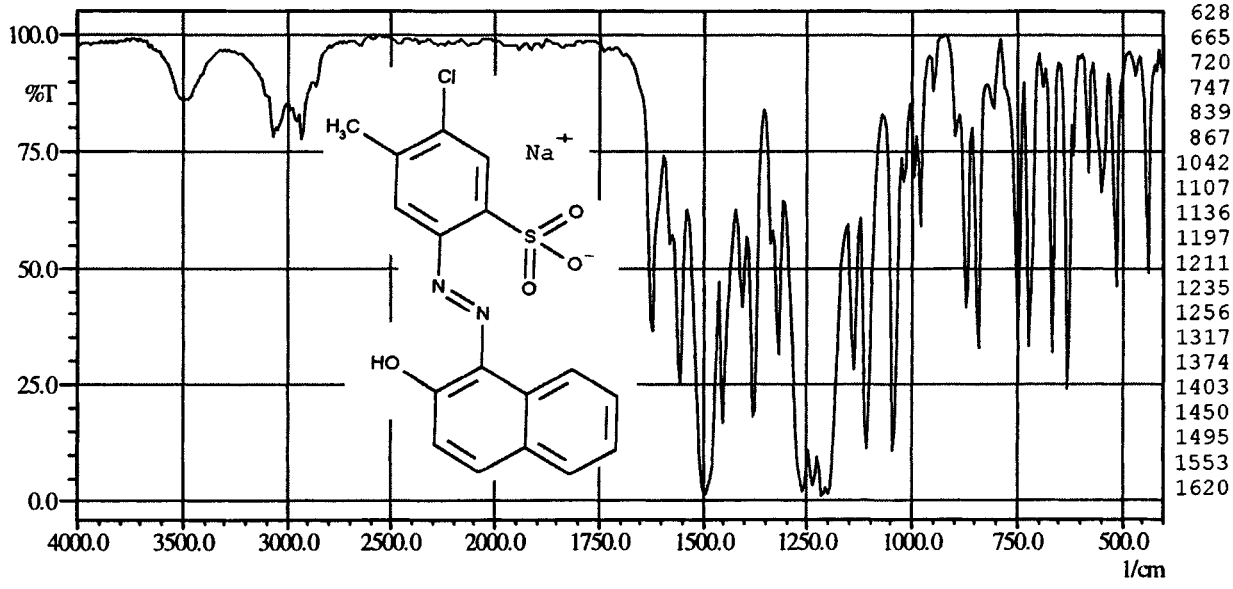
(1) **2-naphthylamine-1-sulfonic acid -> 2-naphthol, Ba-salt**
(2) Tobithol Red B
(3) Capelle
(4) 463.6 g mol^{-1}
(5) organic pigment
(6) red solid
(11) Pigment Red 49:1
(12) 15630:1
(13) KBr pellet

2213 $C_{17}H_{10}N_2O_4Ba$



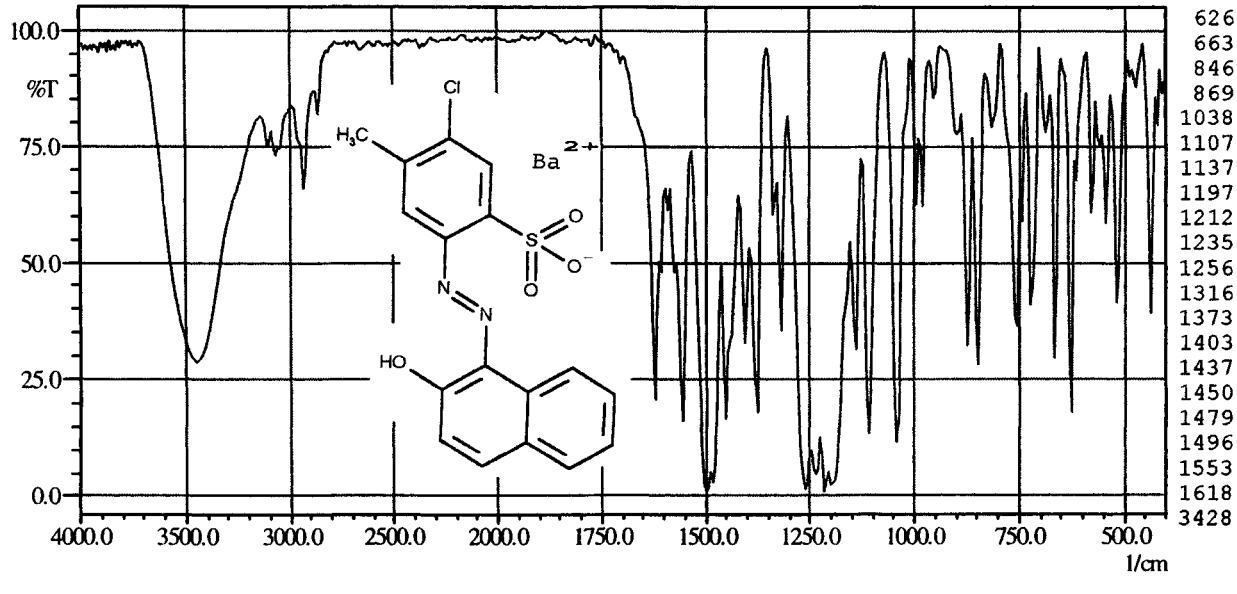
(1) **2-methylsulfanilic acid -> 2-naphthol, Ba-salt**
(2) Lithol Rot RMT
(3) BASF
(4) 443.6 g mol^{-1}
(5) organic pigment
(6) red solid
(11) Pigment Red 51
(12) 15580
(13) KBr pellet

2213 $C_{17}H_{11}ClN_2O_4SNa_2$



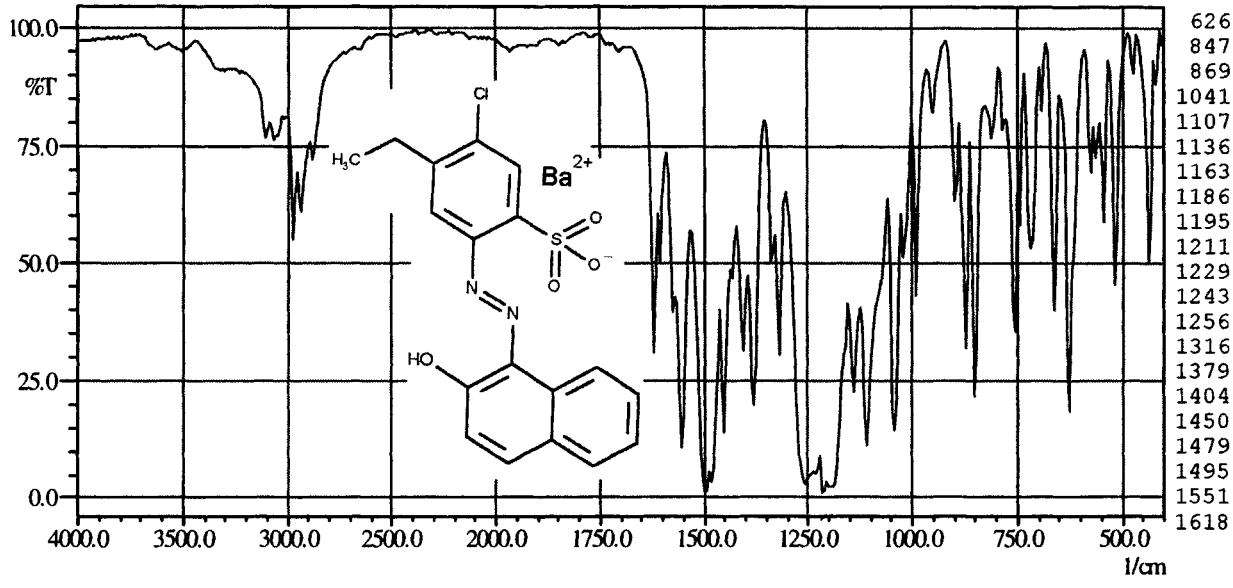
(1) **4-chloro-3-toluidine-6-sulfonic acid -> 2-naphthol, Na-salt**
(2) Lackrot C
(3) Hoechst
(4) 420.8 g mol^{-1}
(5) organic pigment
(6) red solid
(11) Pigment Red 53
(12) 15585
(13) KBr pellet

2213 $C_{34}H_{24}Cl_2N_4O_8Ba$



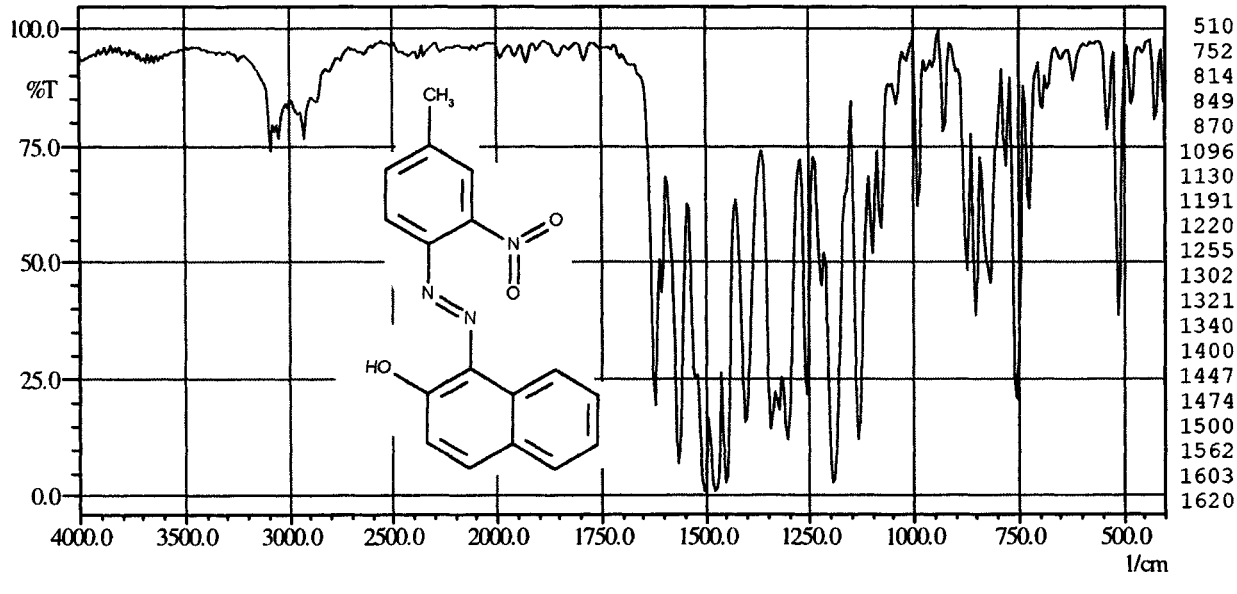
(1) **4-chloro-3-toluidine-6-sulfonic acid -> 2-naphthol, Ba-salt**
(2) Permanent Lackrot LCLL
(3) Hoechst
(4) 824.8 g mol^{-1}
(5) organic pigment
(6) red solid
(11) Pigment Red 53:1
(12) 15585:1
(13) KBr pellet

2213 $C_{18}H_{13}ClN_2O_4SBa$



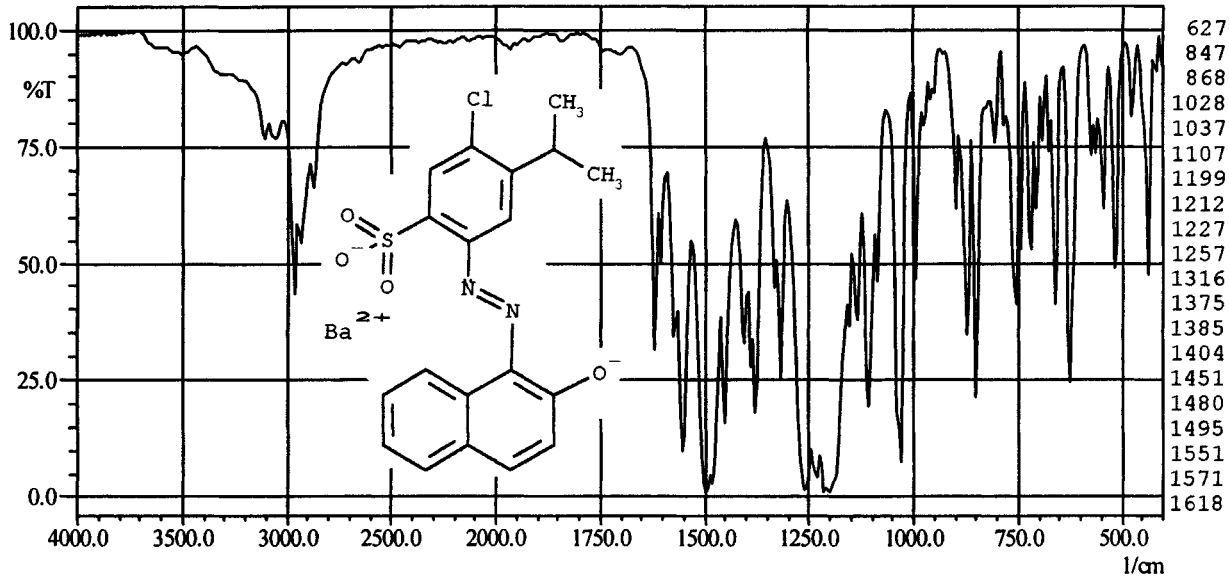
(1) **2-amino-4-ethyl-5-chlorobenzenesulfonic acid -> 2-naphthol, Ba-salt**
(2) Clarion Red 20-7155
(3) American Cyanamid
(4) 526.1 g mol^{-1}
(5) organic pigment
(6) red solid
(11) Pigment Orange 46
(12) 15602
(13) KBr pellet

2213 $C_{17}H_{13}N_3O_3$



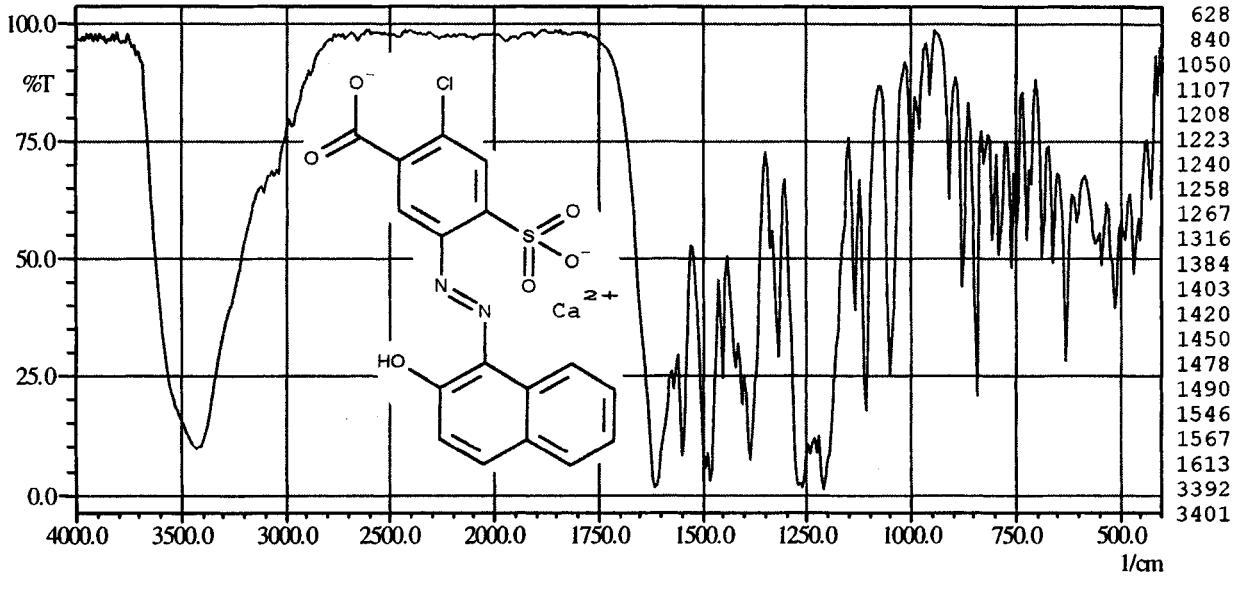
(1) **1-(4-methyl-2-nitro-1-phenyl)azo-2-naphthol**
(2) Hansascharlach RNC
(3) Hoechst
(4) 307.3 g mol^{-1}
(5) organic pigment
(6) dark-red solid
(11) Pigment Red 3
(12) 12120
(13) KBr pellet

2213 $C_{196}H_{14}N_2O_4SBa$



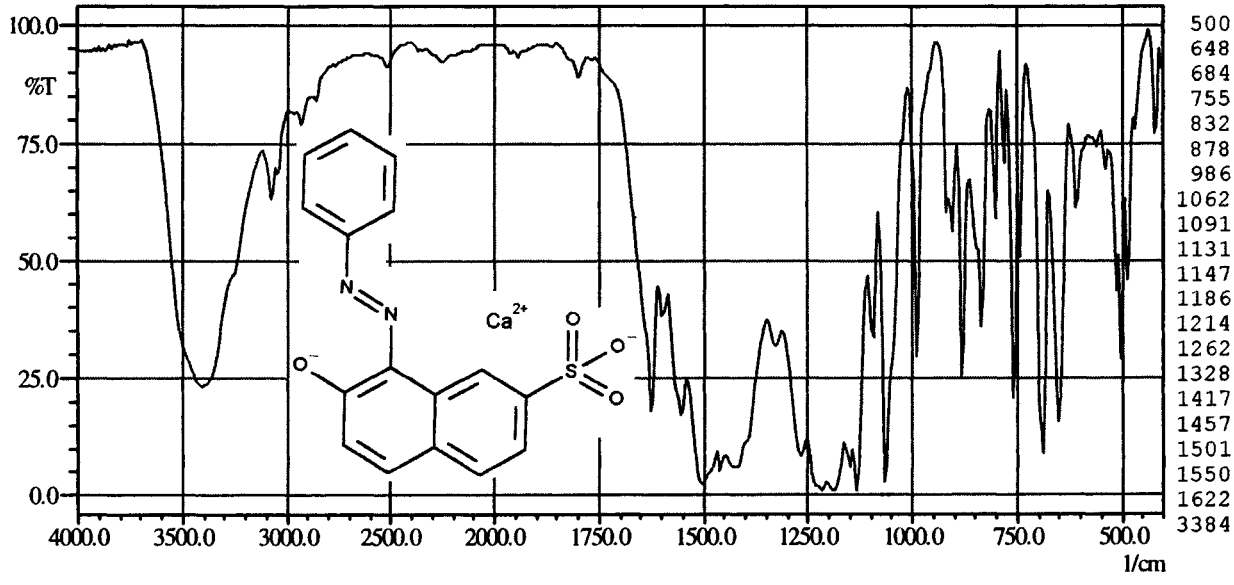
(1) **2-amino-5-chloro-4-i-propylbenzenesulfonic acid -> 2-naphthol, Ba-salt**
(2) Arcturus Red
(3) commercial
(4) 539.1 g mol^{-1}
(5) organic pigment
(6) red solid
(11) Pigment Red 117
(12) 1563
(13) KBr pellet

2213 $C_{17}H_9ClN_2O_6SCa$



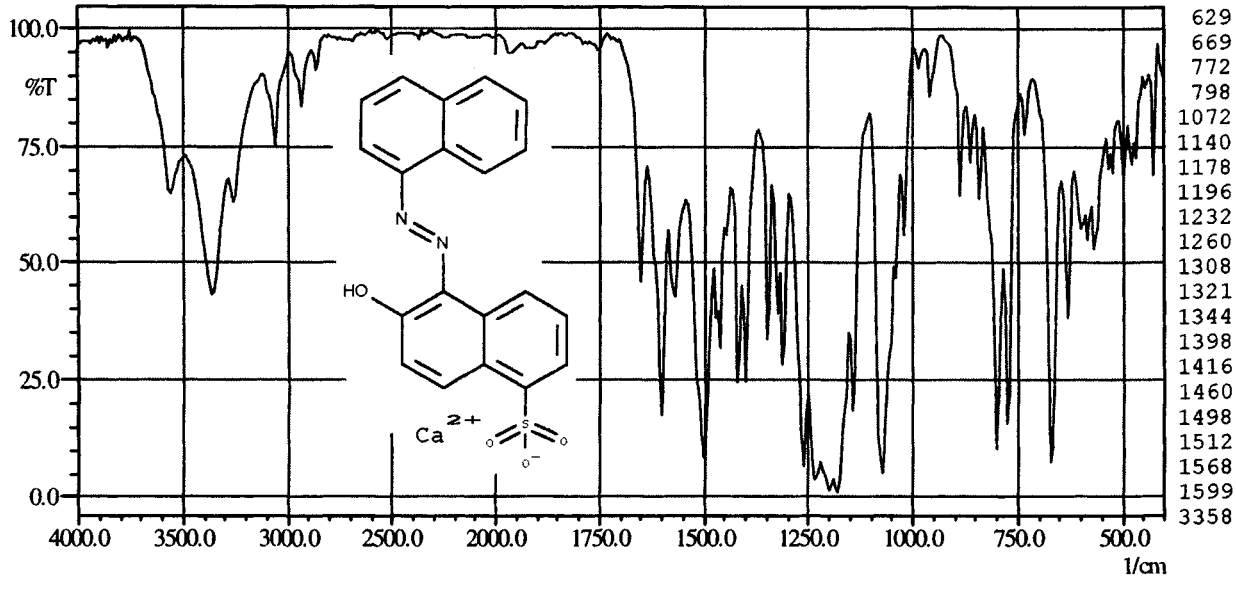
(1) **2-amino-4-carboxy-5-chlorobenzenesulfonic acid -> 2-naphthol, Ca-salt**
(2) PV-Rot NCR
(3) Hoechst
(4) 444.8 g mol^{-1}
(5) organic pigment
(6) red solid
(11) Pigment Red 68
(12) 15525
(13) KBr pellet

2213 $C_{16}H_{10}N_2O_4SCa$



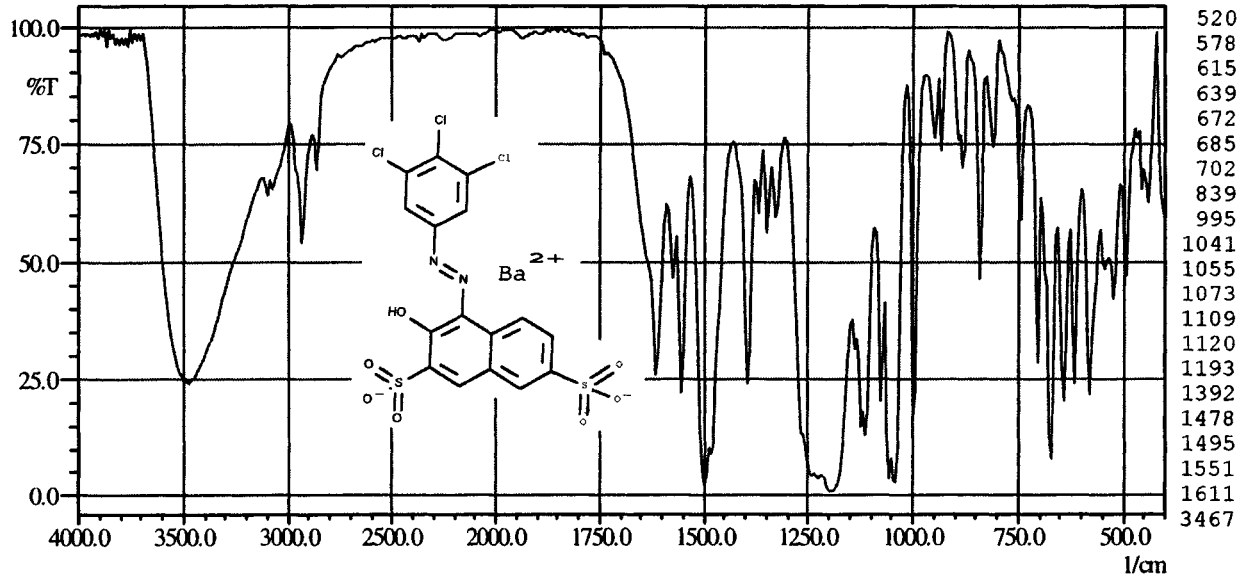
(1) **aniline -> 2-naphthol-6-sulfonic acid, Ca-salt**
(2) Helio Orange CAG
(3) Hoechst
(4) 334.3 g mol^{-1}
(5) organic pigment
(6) orange solid
(11) Pigment Orange 18
(12) 15970
(13) KBr pellet

2213 $C_{20}H_{12}N_2O_4Ca$



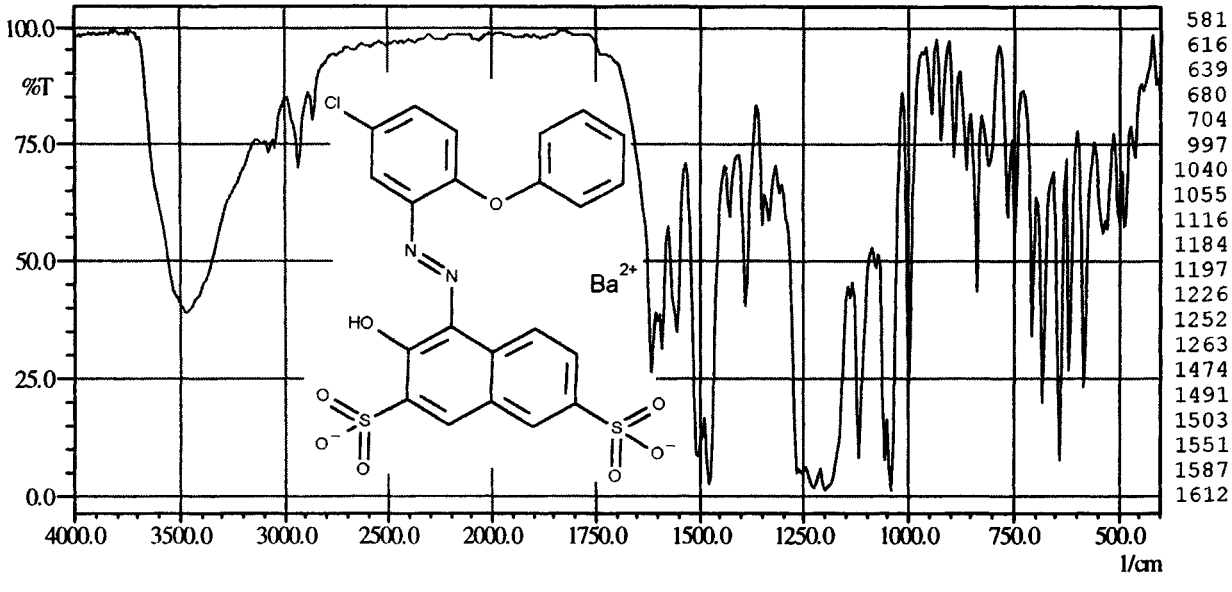
(1) **1-naphthylamine -> 2-naphthol-5-sulfonic acid, Ca-salt**
(2) Helio Bordo BL
(3) Hoechst
(4) 384.4 g mol^{-1}
(5) organic pigment
(6) dark-red solid
(11) Pigment Red 54:1
(12) 14830:1
(13) KBr pellet

2213 $C_{16}H_7Cl_3N_2O_7S_2Ba$



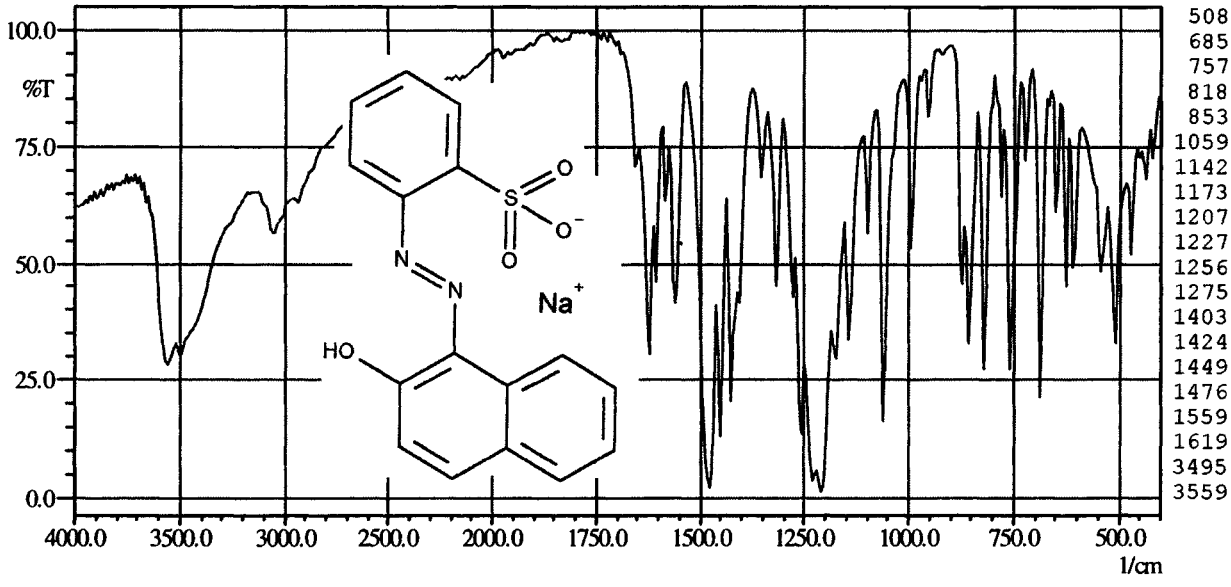
(1) **3,4,5-trichloroaniline -> 2-naphthol-3,6-disulfonic acid, Ba-salt**
(2) Helio Echtrottoner R
(3) Bayer
(4) 647.0 g mol^{-1}
(5) organic pigment
(6) red solid
(11) Pigment Red 120
(13) KBr pellet

2213 $C_{22}H_{13}ClN_2O_8S_2Ba$



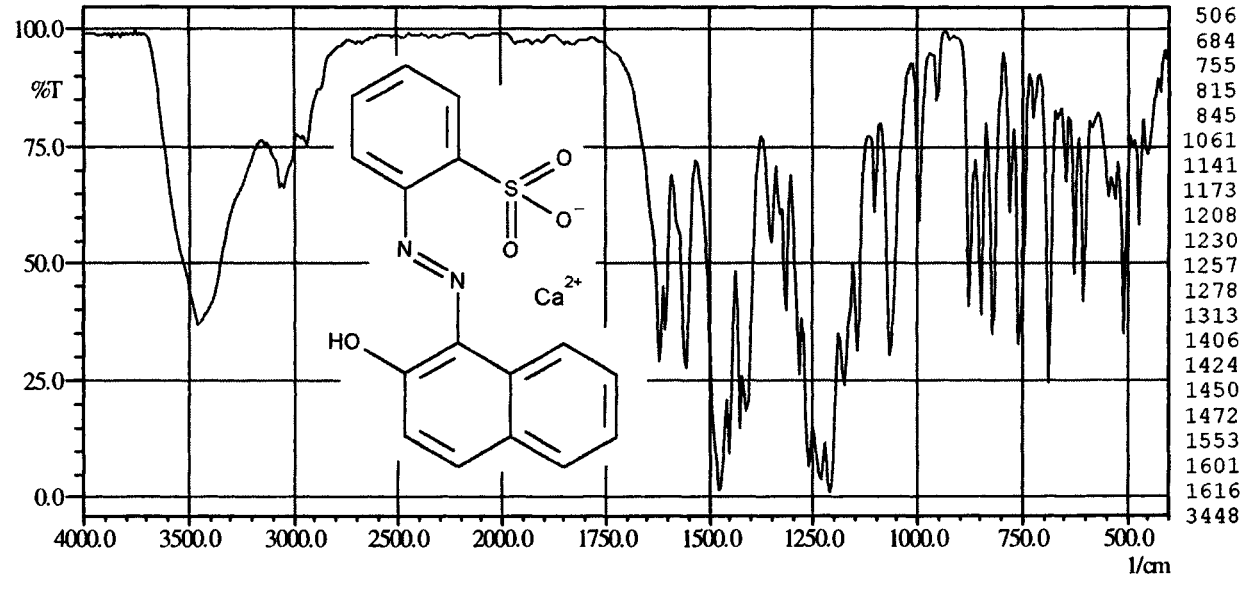
(1) **5-chloro-2-phenoxyaniline -> 2-naphthol-3,6-disulfonic acid, Ba-salt**
(2) Helio Echtrottoner 3B
(3) Bayer
(4) 670.2 g mol^{-1}
(5) organic pigment
(6) red solid
(11) Pigment Red 94
(13) KBr pellet

2213 $C_{20}H_{12}N_2O_4SNa_2$



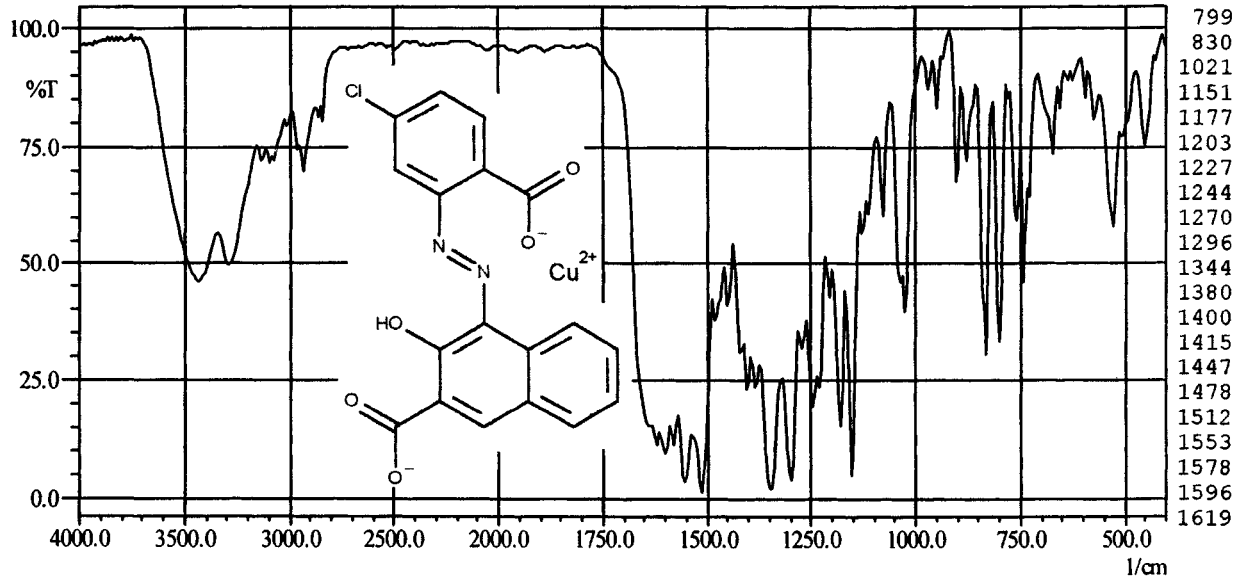
(1) **2-naphthylamine-1-sulfonic acid -> 2-naphthol, Na-salt**
(2) Lithol Rot RS
(3) BASF
(4) 422.4 g mol^{-1}
(5) organic pigment
(6) red solid
(11) Pigment Red 49
(12) 15630
(13) KBr pellet

2213 $C_{20}H_{12}N_2O_4SCa$



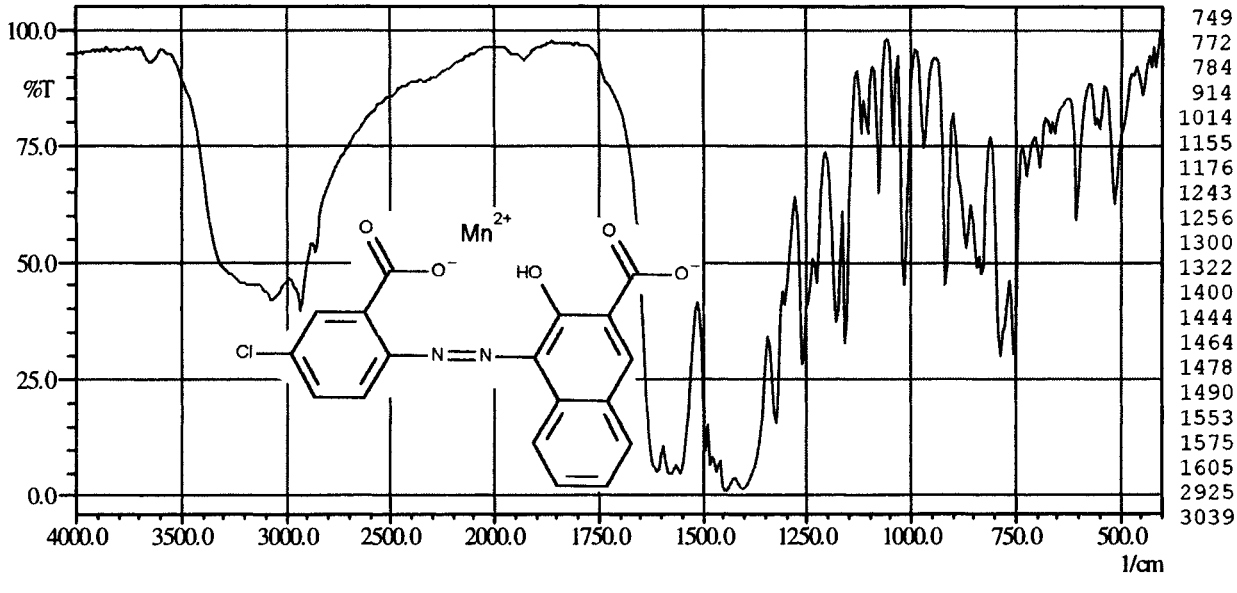
(1) **2-naphthylamine-1-sulfonic acid -> 2-naphthol, Ca-Salt**
(2) Lithol Rot RBKX (Brillianttoner CS)
(3) BASF
(4) 416.5 g mol^{-1}
(5) organic pigment
(6) red solid
(11) Pigment Red 49:2
(12) 15630:2
(13) KBr pellet

2214 $C_{18}H_9ClN_2O_5Cu$



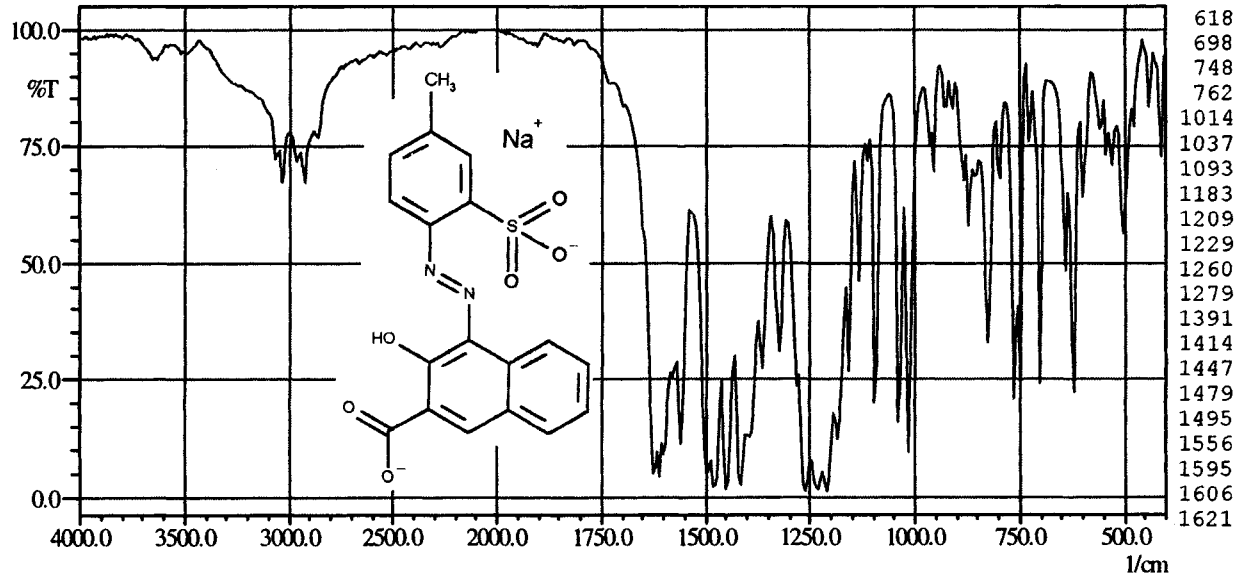
(1) **2-amino-5-chlororbenzoic acid -> 2-hydroxynaphthoic arylide, Cu-salt**
(2) Newport Maroon RT-647-D
(3) Newport
(4) 420.3 g mol^{-1}
(5) organic pigment
(6) brown solid
(11) Pigment Red 55
(12) 15820
(13) KBr pellet

2214 $C_{18}H_9ClN_2O_5Mn$



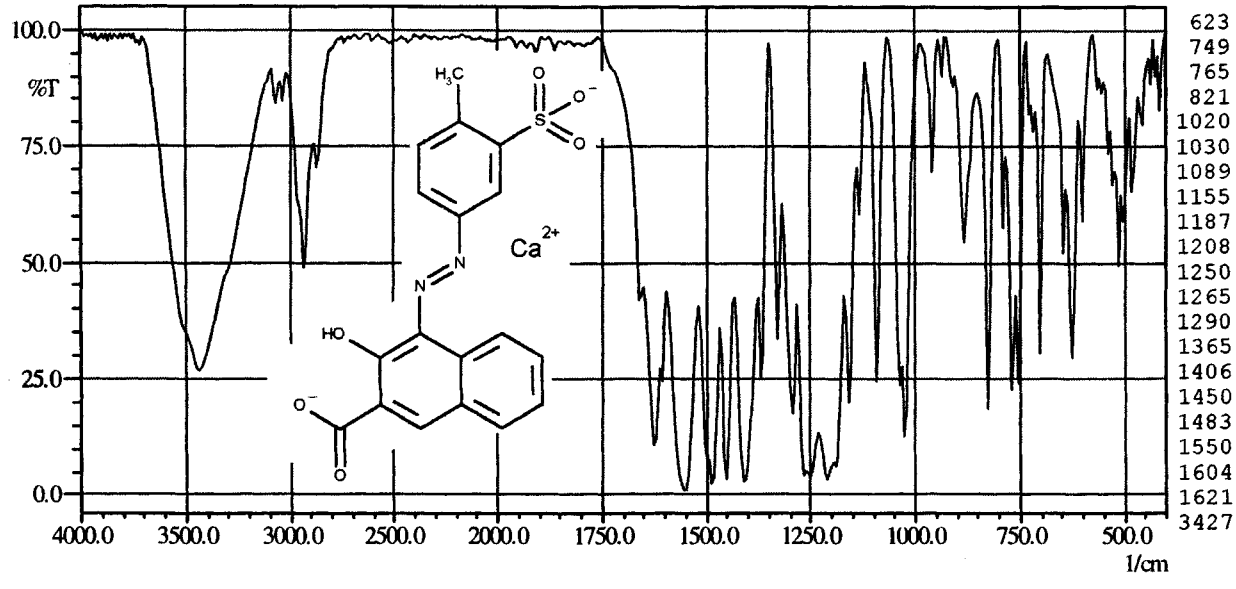
(1) **2-amino-5-chlororbenzoic acid -> 2-hydroxynaphthoic arylide, Mn-salt**
(2) Maroon Gold IRT-608-D
(3) Du Pont
(4) 411.7 g mol^{-1}
(5) organic pigment
(6) brown solid
(11) Pigment Red 55
(12) 15820
(13) KBr pellet

2214 $C_{18}H_{12}N_2O_6SNa_2$



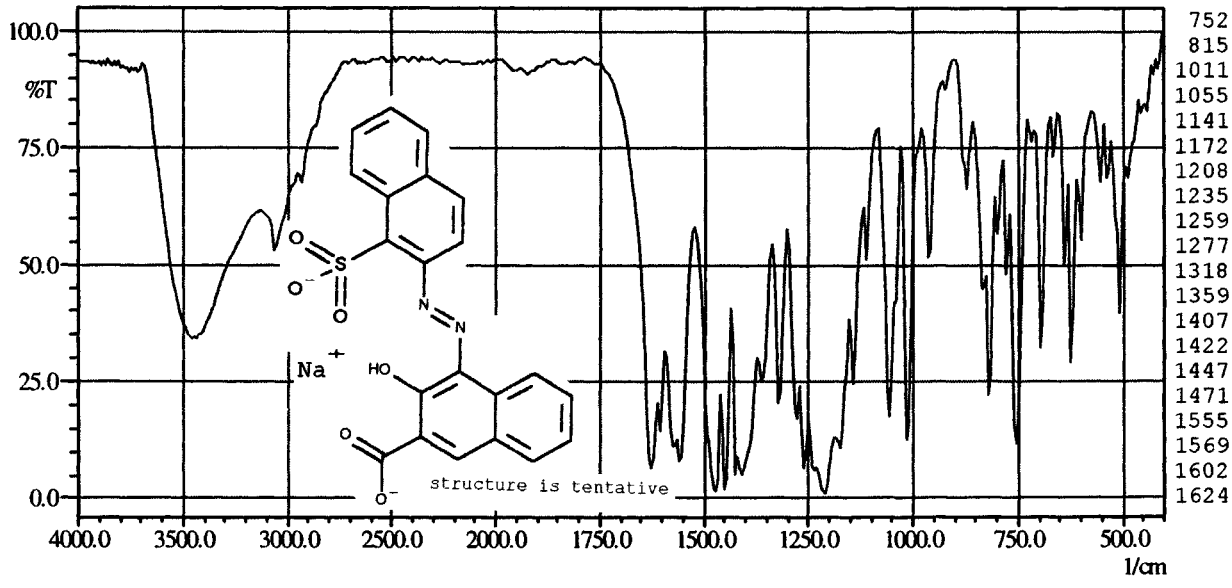
(1) **4-toluidine-3-sulfonic acid -> 2-hydroxynaphthoic arylide, Na-salt**
(2) Lithol Rubin BN
(3) BASF
(4) 430.4 g mol^{-1}
(5) organic pigment
(6) ruby solid
(11) Pigment Red 57
(12) 15850
(13) KBr pellet

2214 $C_{17}H_{12}N_2O_6SCa$



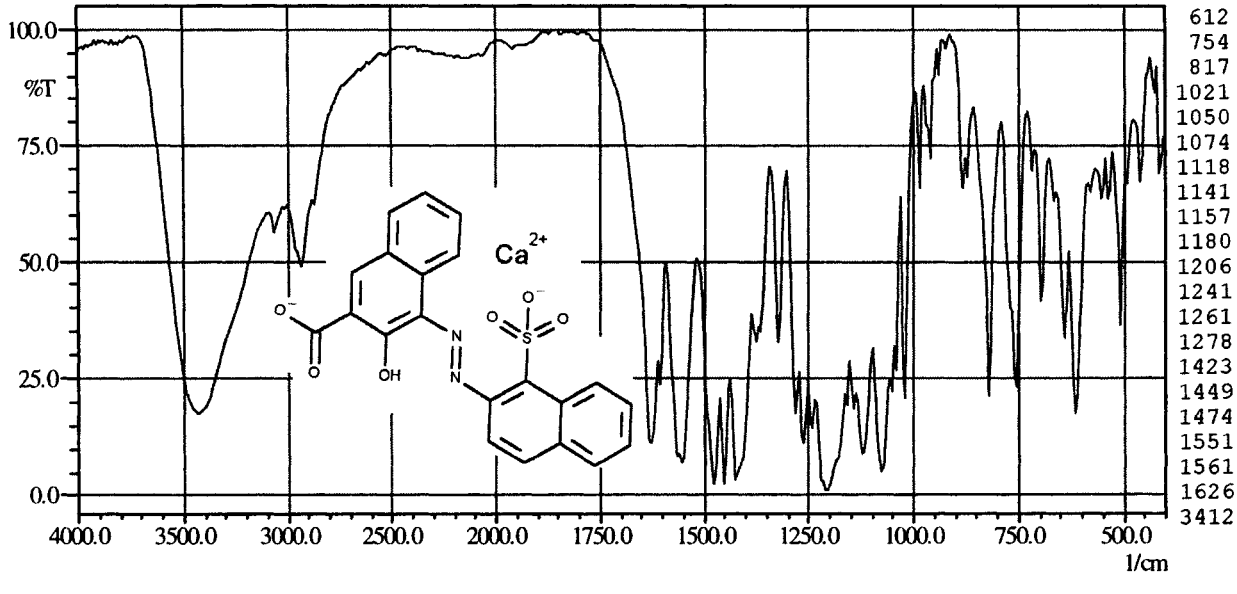
(1) **4-toluidine-2-sulfonic acid -> 2-hydroxynaphthoic arylide, Ca-salt**
(2) Irgalite Rubine 4BP
(3) Ciba-Geigy
(4) 412.4 g mol^{-1}
(5) organic pigment
(6) dark-red solid
(11) Pigment Red 57:1
(12) 15850:1
(13) KBr pellet

2214 $C_{21}H_{12}N_2O_6SNa_2$



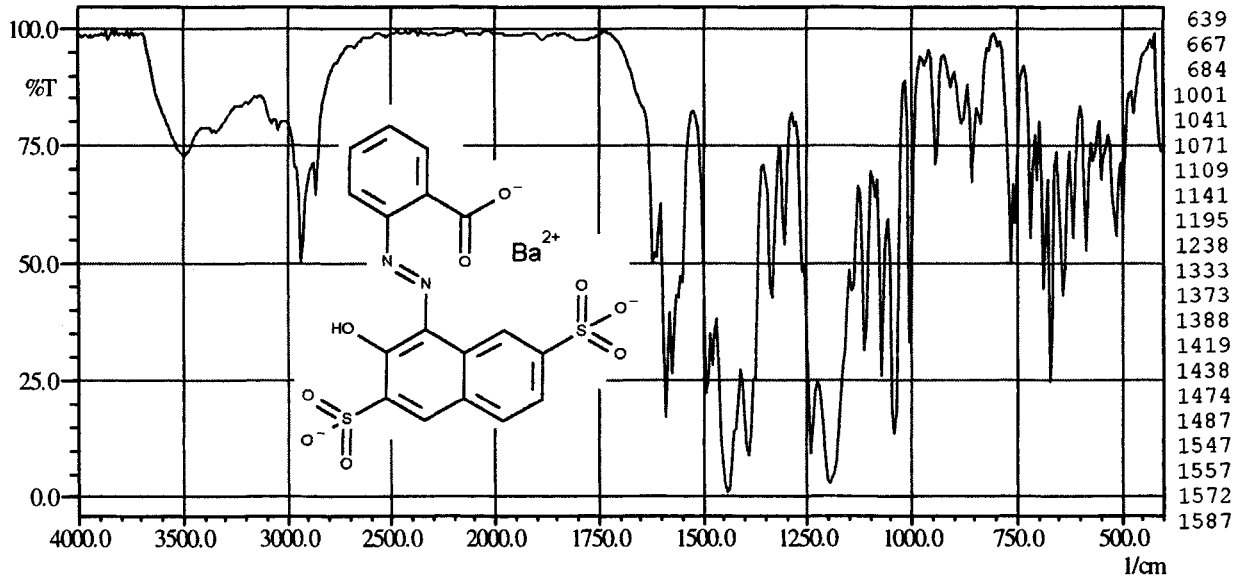
(1) **2-amino-1-naphthalenesulfonic acid -> 2-hydroxynaphthoic arylide, Na-salt**
(2) Lithol Bordeaux BNS
(3) BASF
(4) 466.4 g mol^{-1}
(5) organic pigment
(6) dark-red solid
(11) Pigment Red 63
(12) 15580
(13) KBr pellet

2214 $C_{21}H_{12}N_2O_6SCa$



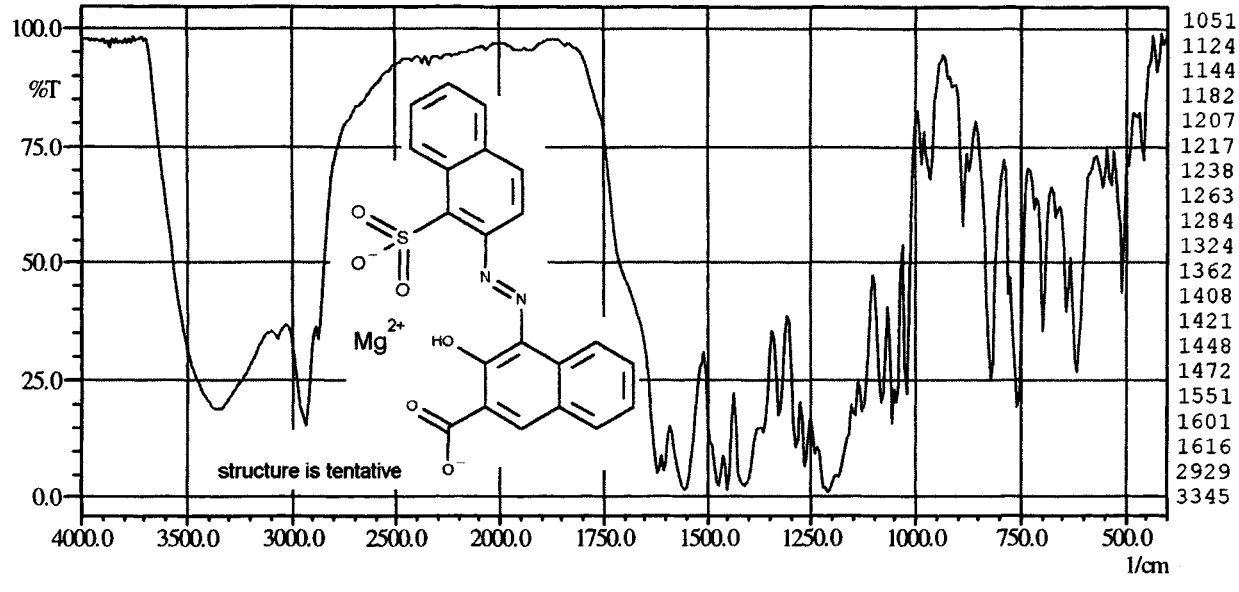
(1) **2-amino-1-naphthalenesulfonic acid -> 2-hydroxynaphthoic arylide, Ca-salt**
(2) Symuler Lake Bordeaux 10 B 310
(3) DIC
(4) 460.5 g mol^{-1}
(5) organic pigment
(6) dark-red solid
(11) Pigment Red 63:1
(12) 15880:1
(13) KBr pellet

2214 $C_{17}H_8N_2O_9S_2Ba$



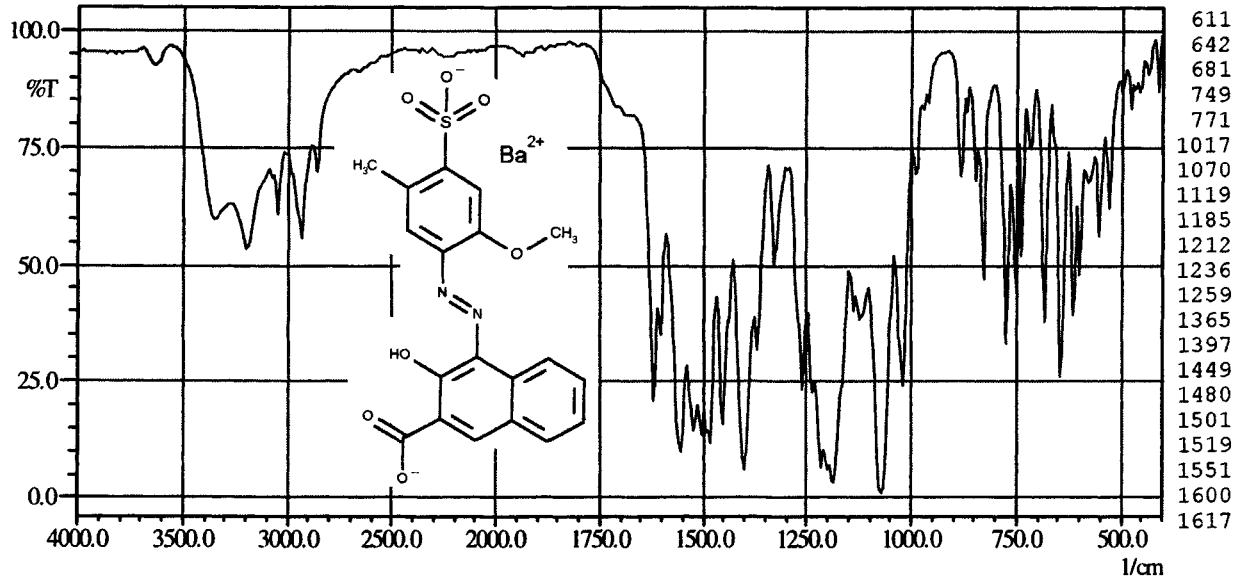
(1) ***o*-aminobenzoic acid -> 2-hydroxy-3,6-naphthalenedisulfonic acid, Ba-salt**
(2) Pigmentscharlach 3 B
(3) Hoechst
(4) 585.7 g mol^{-1}
(5) organic pigment
(6) scarlet solid
(11) Pigment Red 60:1
(12) 16105
(13) KBr pellet

2214 $C_{21}H_{12}N_2O_6SMn$



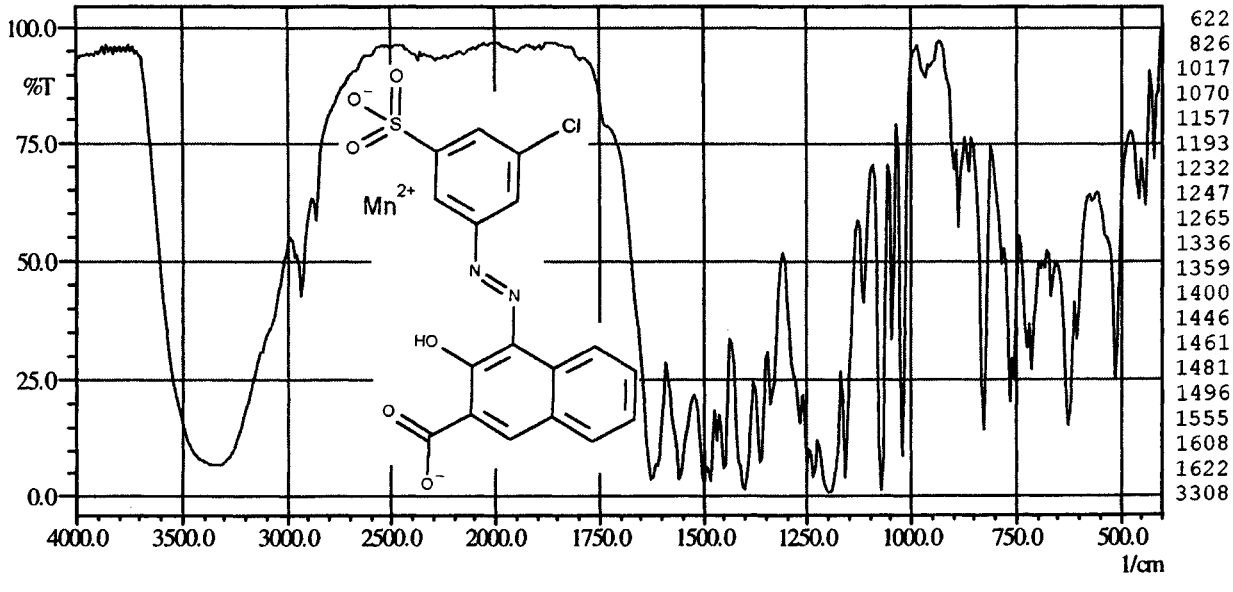
(1) **2-amino-1-naphthalenesulfonic acid -> 2-hydroxynaphthoic arylide, Mn-salt**
(2) Maroon Toner BB
(3) BASF
(4) 475.4 g mol^{-1}
(5) organic pigment
(6) brown solid
(11) Pigment Red 63:2
(12) 15580:2
(13) KBr pellet

2214 $C_{19}H_{14}N_2O_7SBa$



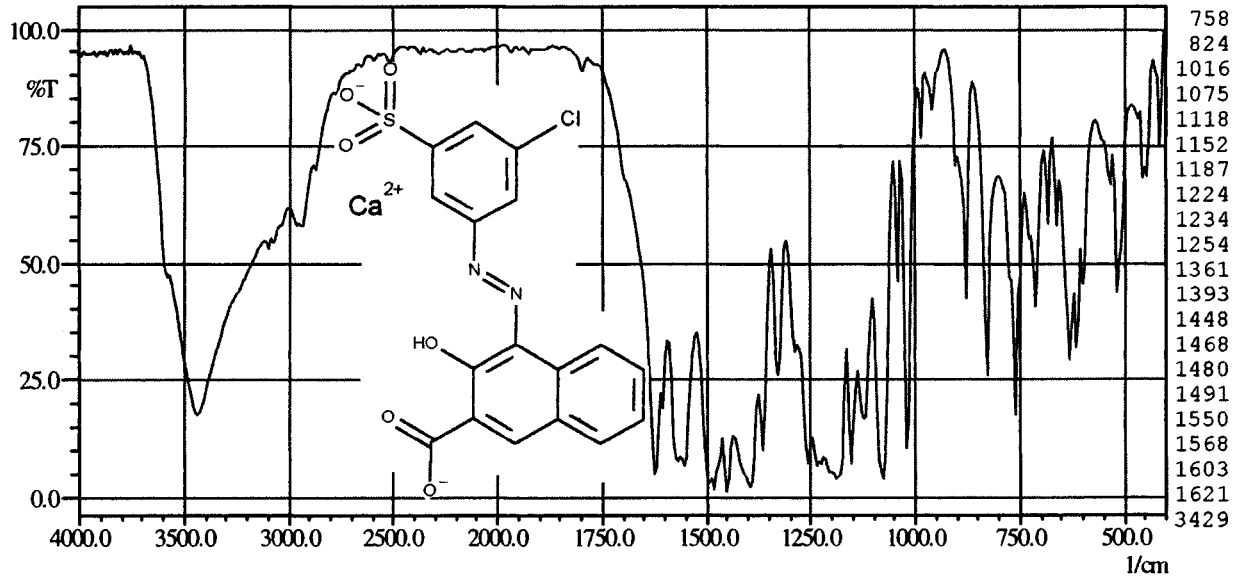
(1) **2-methyl-5-methoxysulfanilic acid -> 2-hydroxynaphthoic arylide, Ba-salt**
(2) Permanent Bordo RN
(3) Hoechst
(4) 551.7 g mol^{-1}
(5) organic pigment
(6) dark-red solid
(11) Pigment Red 56
(12) 15870
(13) KBr pellet

2214 $C_{17}H_9ClN_2O_6SMn$



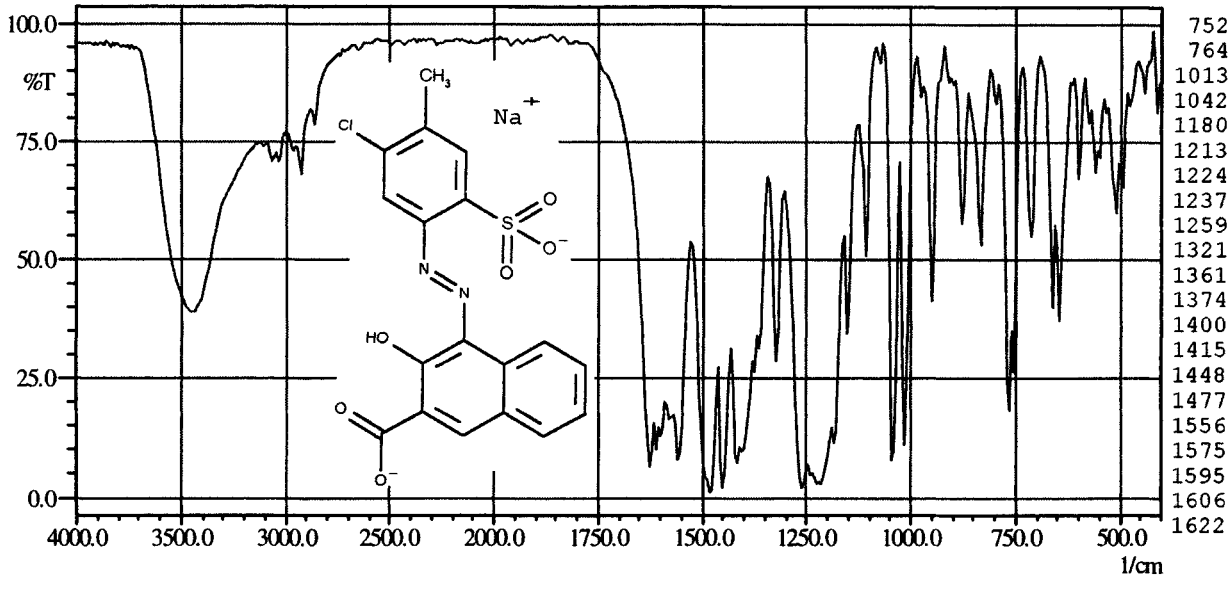
(1) **3-amino-6-chlorobenzenesulfonic acid -> 2-hydroxynaphthoic arylide, Mn-salt**
(2) Sico Maroon BM hell
(3) BASF
(4) 459.7 g mol^{-1}
(5) organic pigment
(6) dark-red solid
(11) Pigment Red 58:4
(12) 15825:4
(13) KBr pellet

2214 $C_{17}H_9ClN_2O_6SCa$



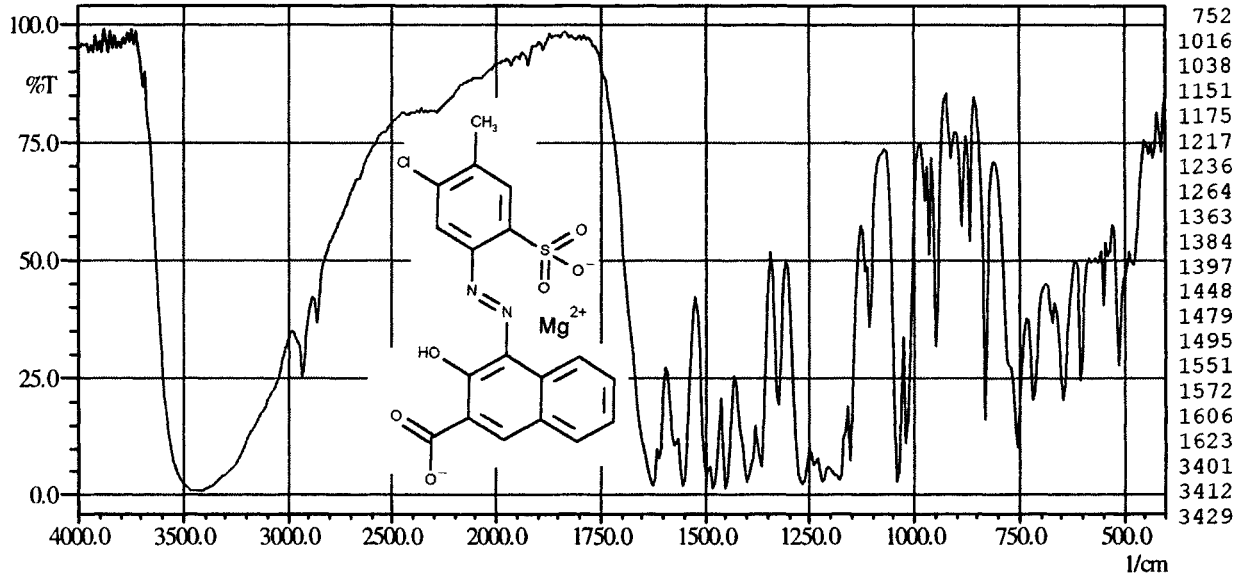
(1) **3-amino-5-chlorobenzenesulfonic acid -> 2-hydroxynaphthoic arylide, Ca-salt**
(2) Lithol Rubin GK
(3) BASF
(4) 444.9 g mol^{-1}
(5) organic pigment
(6) ruby solid
(11) Pigment Red 58:2
(12) 15825:2
(13) KBr pellet

2214 $C_{18}H_{11}ClN_2O_6SNa_2$



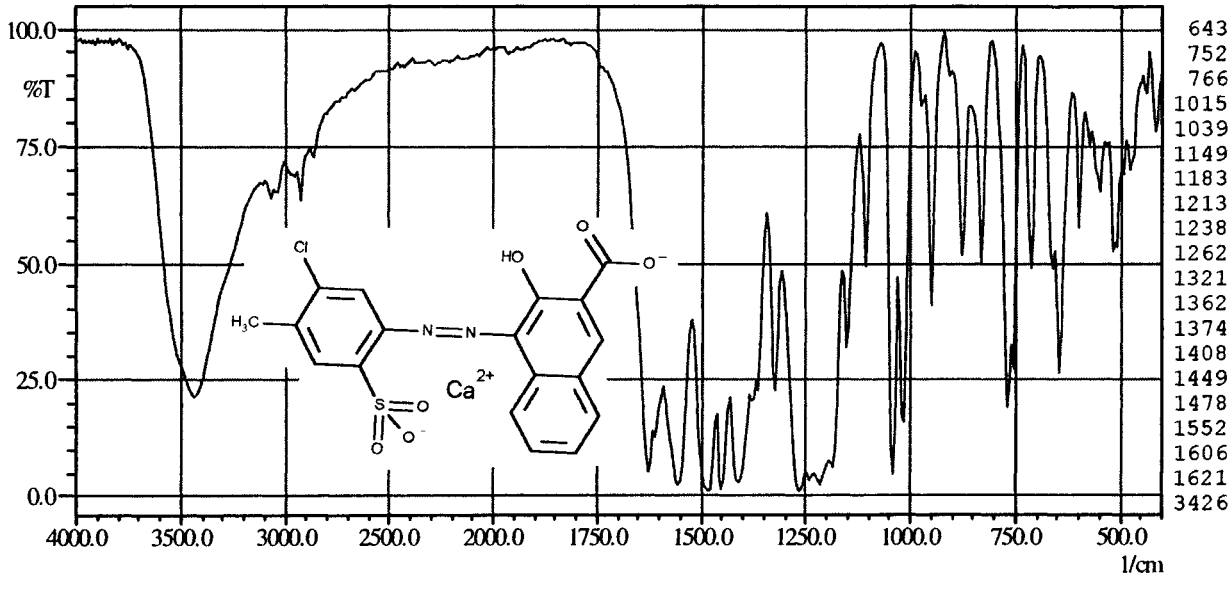
(1) **5-chloro-4-toluidine-2-sulfonic acid -> 2-hydroxynaphthoic arylide, Na-salt**
(2) Permanent Rot 2B
(3) Hoechst
(4) 464.8 g mol^{-1}
(5) organic pigment
(6) red solid
(11) Pigment Red 48
(12) 15865
(13) KBr pellet

2214 $C_{18}H_{11}ClN_2O_6Mg$



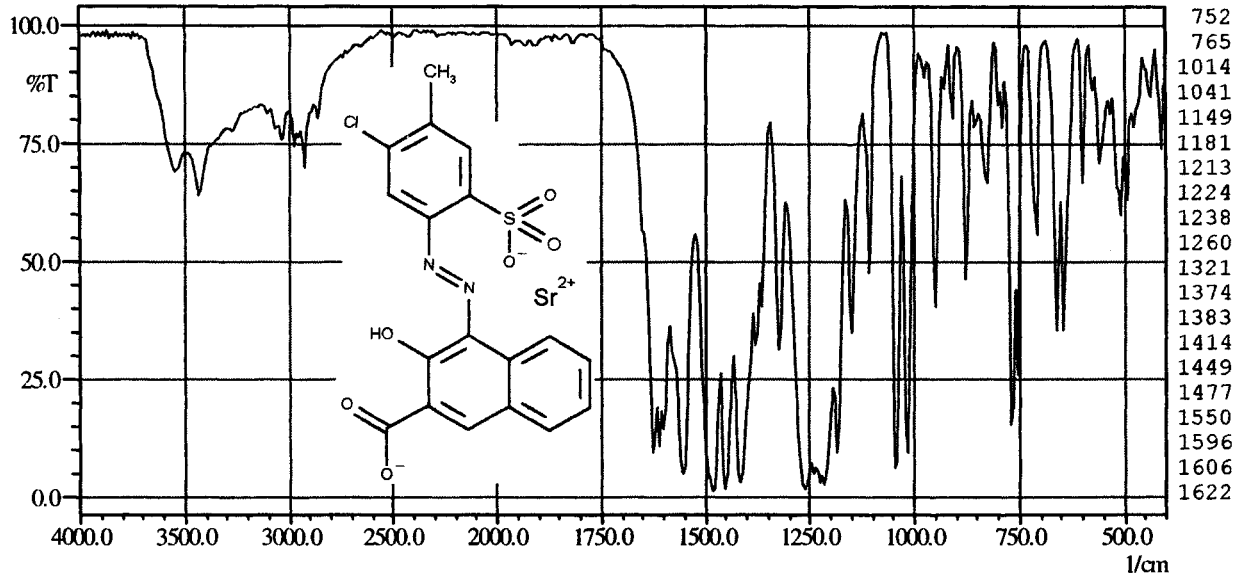
(1) **5-chloro-4-toluidine-2-sulfonic acid -> 2-hydroxynaphthoic arylide, Mg-salt**
(2) Irgalite Red MGP
(3) Ciba-Geigy
(4) 443.1 g mol^{-1}
(5) organic pigment
(6) red solid
(11) Pigment Red 48:5
(12) 15865:5
(13) KBr pellet

2214 $C_{18}H_{11}ClN_2O_6SCa$



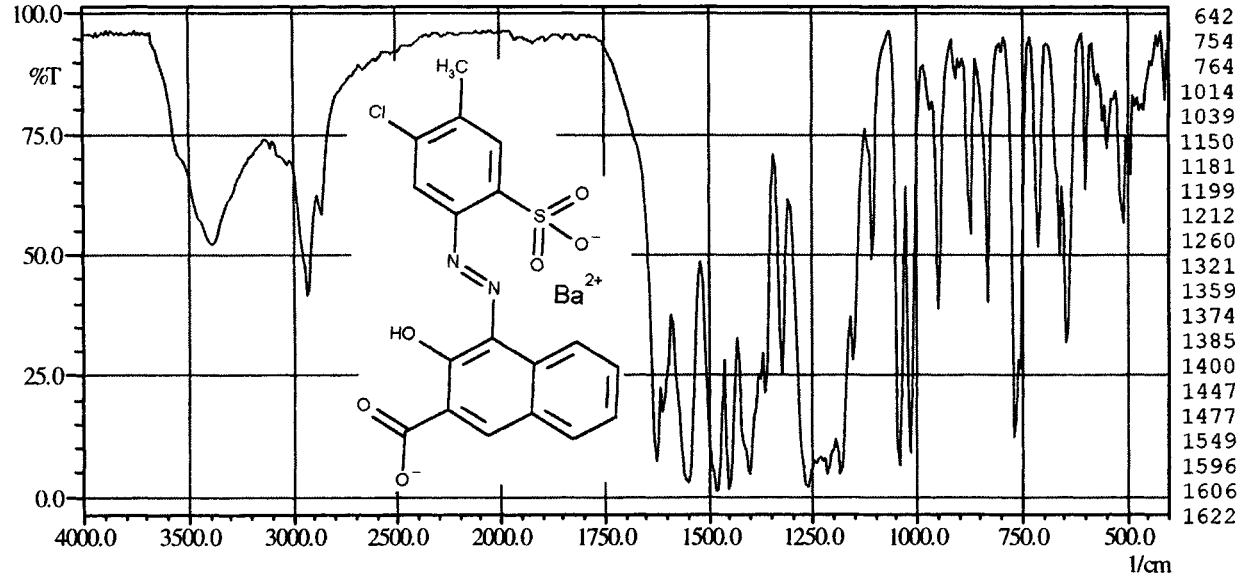
(1) **5-chloro-4-toluidine-2-sulfonic acid -> 2-hydroxynaphthoic arylide, Ca-salt**
(2) Rubine Toner 2BO
(3) ICI
(4) 458.9 g mol^{-1}
(5) organic pigment
(6) dark-red solid
(11) Pigment Red 48:2
(12) 15865:2
(13) KBr pellet

2214 $C_{18}H_{11}ClN_2O_6Sr$



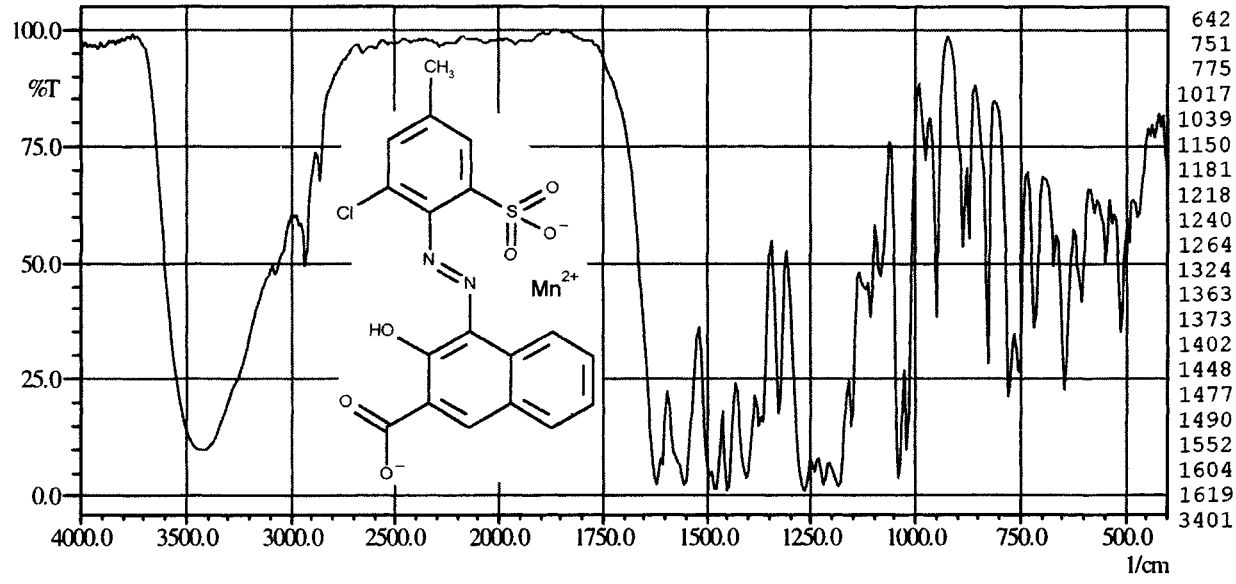
(1) **5-chloro-4-toluidine-2-sulfonic acid -> 2-hydroxynaphthoic arylide, Sr-salt**
(2) Irgalite Red 2BY
(3) Ciba-Geigy
(4) 506.4 g mol^{-1}
(5) organic pigment
(6) red solid
(11) Pigment Red 48:3
(12) 15865:3
(13) KBr pellet

2214 $C_{18}H_{11}ClN_2O_6Ba$



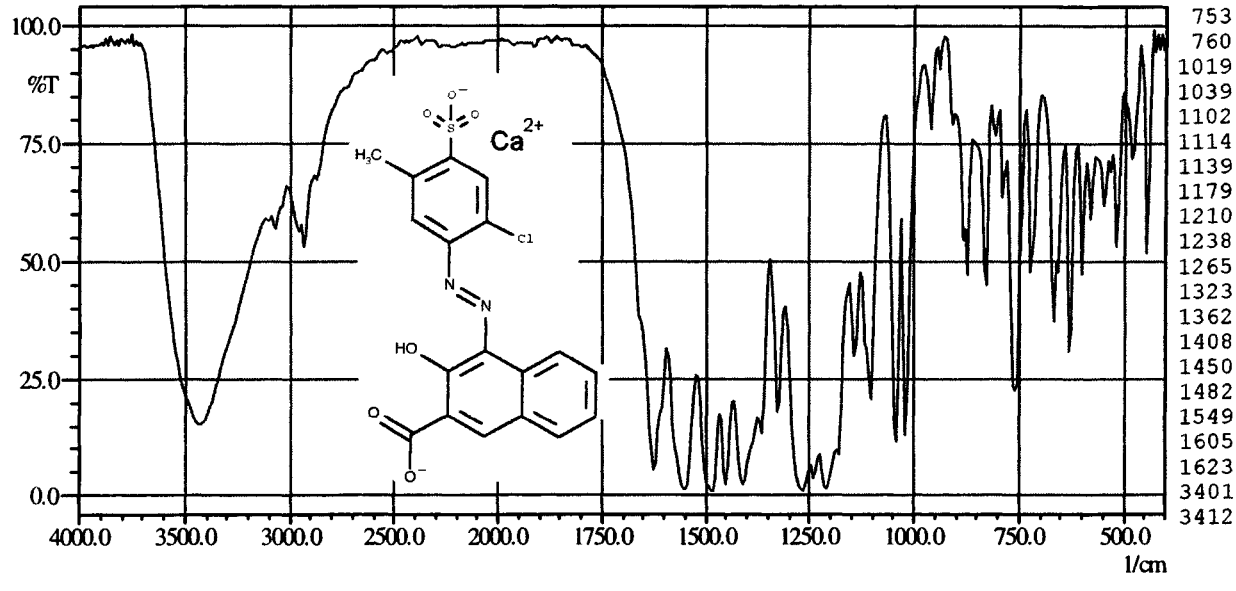
(1) **5-chloro-4-toluidine-2-sulfonic acid -> 2-hydroxynaphthoic arylide, Ba-salt**
(2) Irgalite Red NBSP
(3) Ciba-Geigy
(4) 556.1 g mol^{-1}
(5) organic pigment
(6) red solid
(11) Pigment Red 48:1
(12) 15865:1
(13) KBr pellet

2214 $C_{18}H_{11}ClN_2O_6SMn$



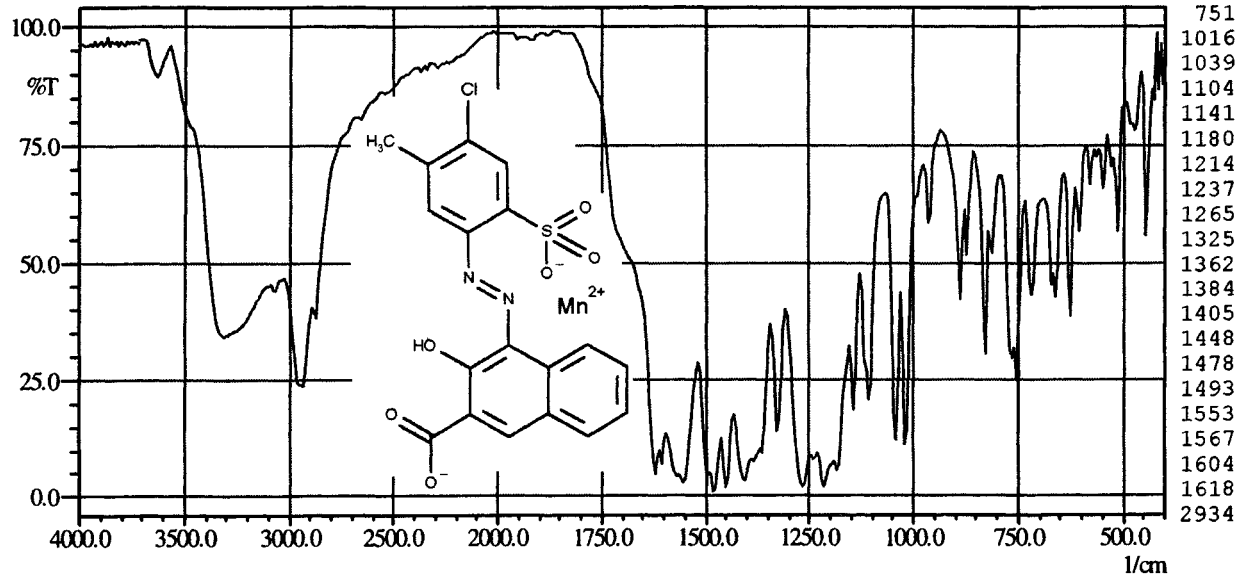
(1) **5-chloro-4-toluidine-2-sulfonic acid -> 2-hydroxynaphthoic arylide, Mn-salt**
(2) Lithol Echtscharlach L 4260
(3) BASF
(4) 473.7 g mol^{-1}
(5) organic pigment
(6) scarlet solid
(11) Pigment Red 48:4
(12) 15865:4
(13) KBr pellet

2214 $C_{18}H_{11}ClN_2O_6SCa$



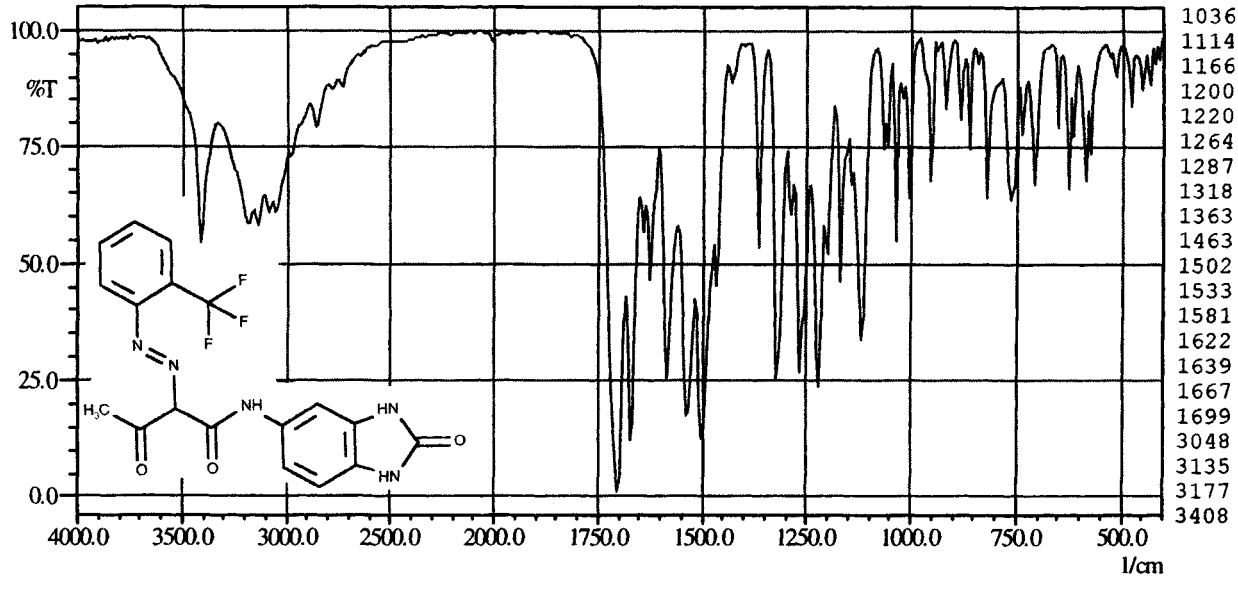
(1) **6-chloro-3-toluidine-4-sulfonic acid -> 2-hydroxynaphthoic arylide, Ca-salt**
(2) Macatawa Red
(3) commercial
(4) 458.9 g mol^{-1}
(5) organic pigment
(6) red solid
(11) Pigment Red 52:1
(12) 15860
(13) KBr pellet

2214 $C_{18}H_{11}ClN_2O_6SMn$



(1) **6-chloro-3-toluidine-4-sulfonic acid -> 2-hydroxynaphthoic arylide, Mn-salt**
(2) Sico Maroon 33 M
(3) BASF
(4) 473.7 g mol^{-1}
(5) organic pigment
(6) dark-red solid
(11) Pigment Red 52:2
(12) 15860
(13) KBr pellet

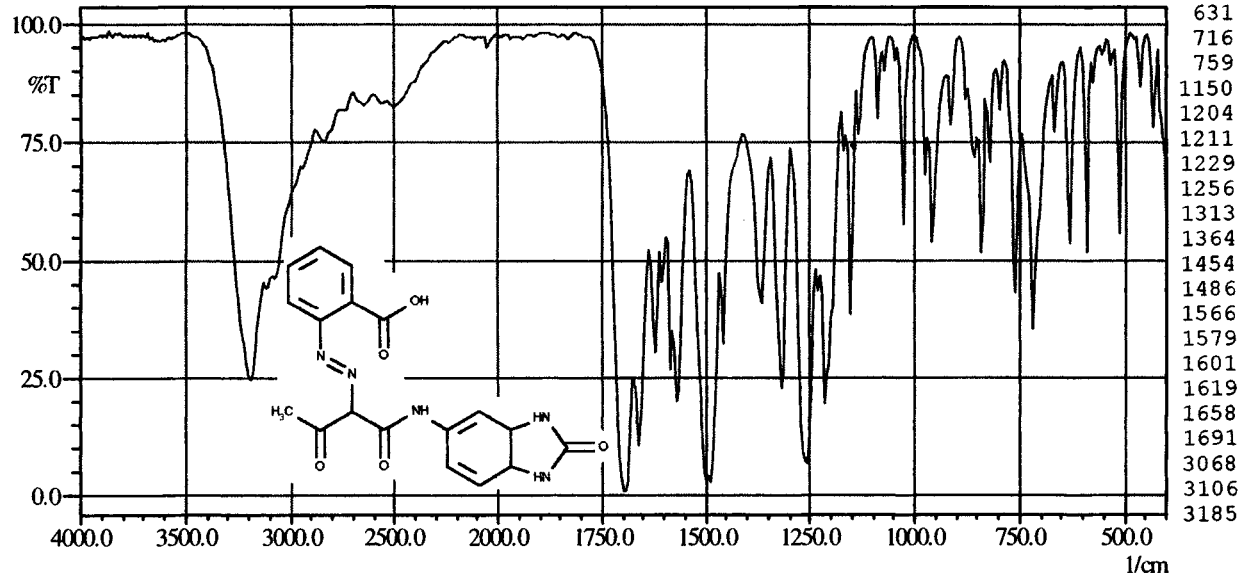
2215 $C_{18}H_{14}F_3N_5O_3$



(1) **2-trifluoromethylaniline -> 5-N-acetoacetylamino-benzimidazolone**
(2) Hostaperm Gelb H3G
(3) Hoechst
(4) 405.3 g mol^{-1}
(5) organic pigment
(6) yellow solid
(11) Pigment Yellow 154
(12) 11781
(13) KBr pellet

2215

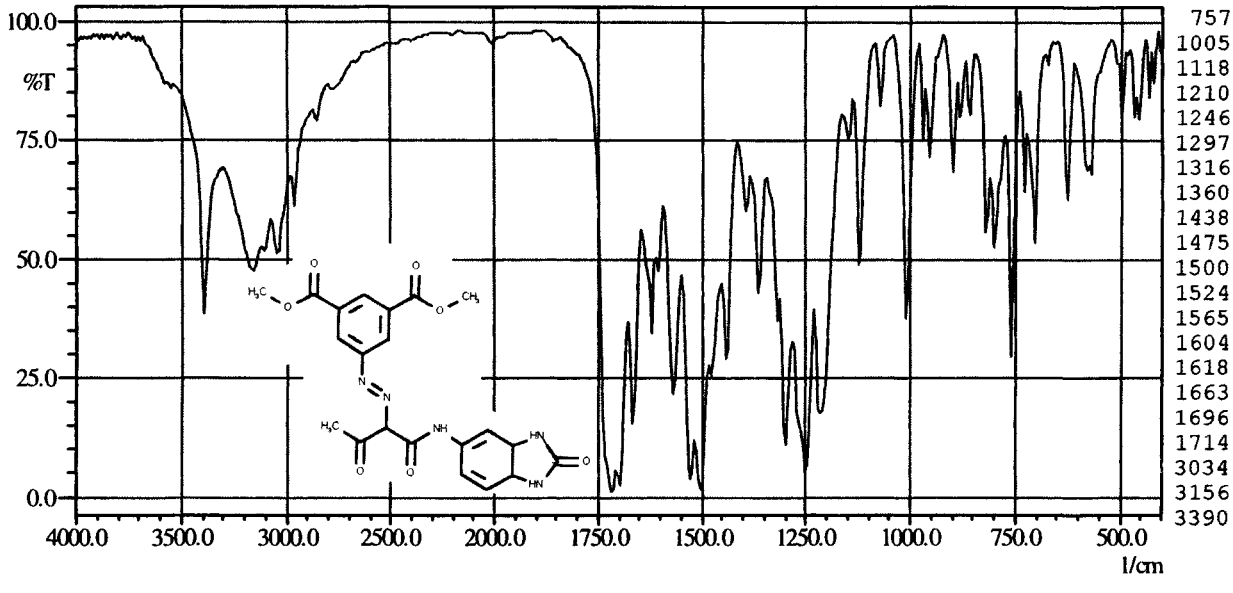
$C_{18}H_{15}N_5O_5$



(1) **2-carboxyaniline -> 5-N-acetoacetylaminobenzimidazolone**
(2) Hostaperm Gelb H4G
(3) Hoechst
(4) 381.3 g mol^{-1}
(5) organic pigment
(6) yellow solid
(11) Pigment Yellow 151
(12) 13980
(13) KBr pellet

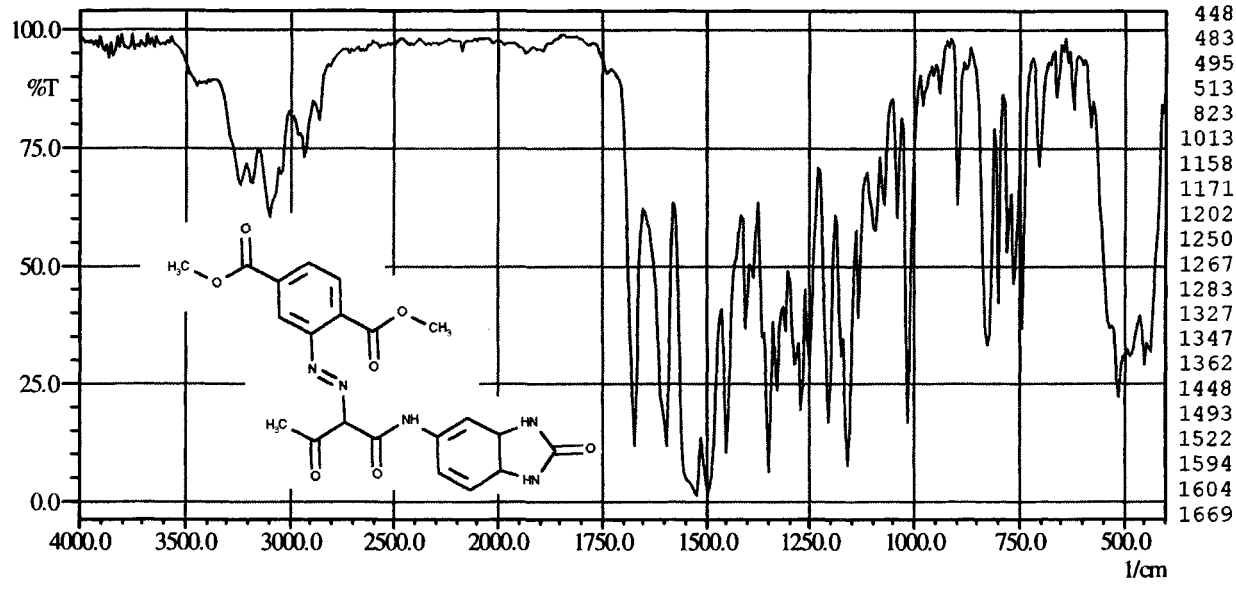
2215

$C_{21}H_{19}N_5O_7$



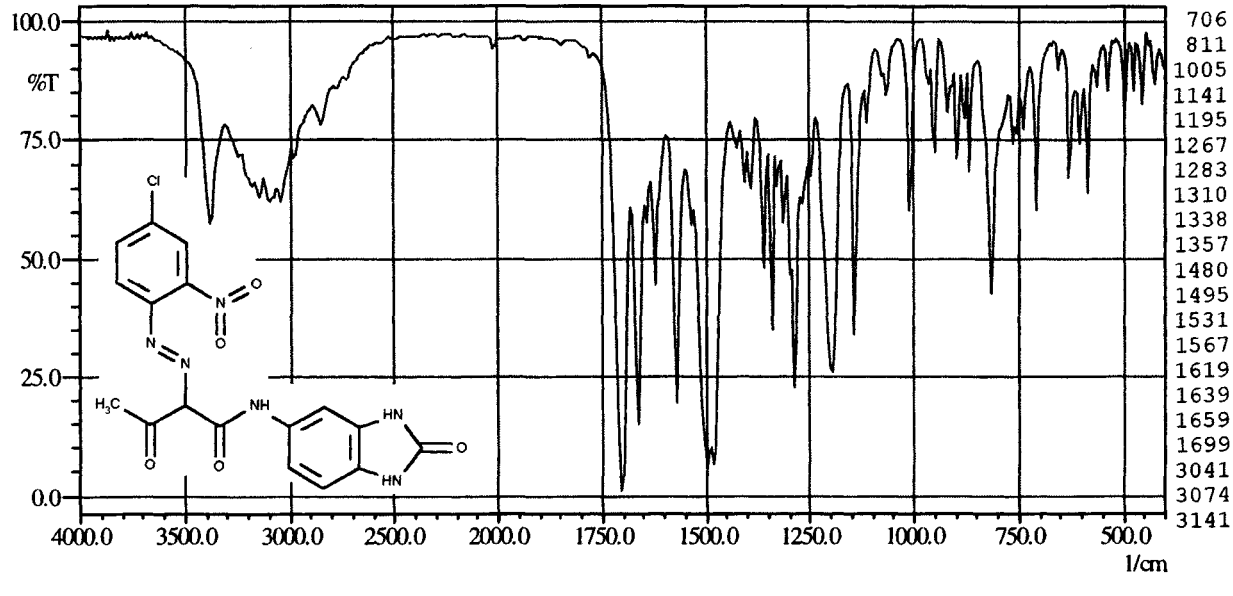
(1) **3,5-dicarboxymethylaniline -> 5-N-acetoacetylaminobenzimidazolone**
(2) PV-Echt-Gelb H2G01
(3) Hoechst
(4) 453.4 g mol^{-1}
(5) organic pigment
(6) yellow solid
(11) Pigment Yellow 120
(12) 11783
(13) KBr pellet

2215 $C_{21}H_{19}N_5O_7$



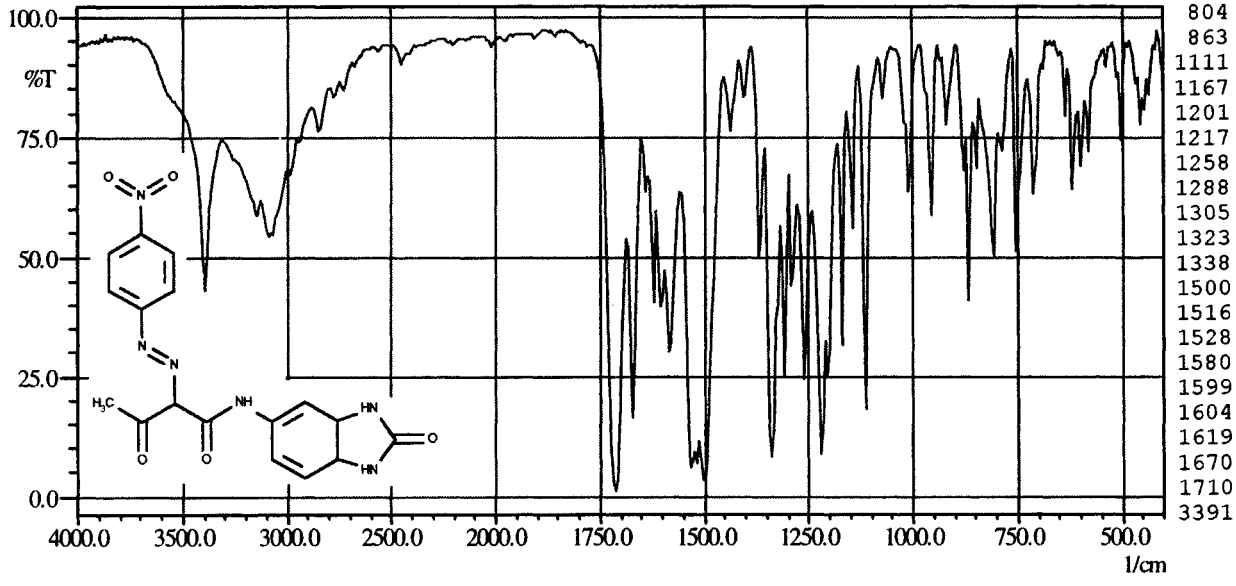
(1) **2,5-dimethoxycarbonylaniline -> 5-N-acetoacetyl-aminobenzimidazolone**
(2) Hostaperm Gelb H6G
(3) Hoechst
(4) 453.4 g mol^{-1}
(5) organic pigment
(6) yellow solid
(11) Pigment Yellow 175
(12) 11784
(13) KBr pellet

2215 $C_{17}H_{13}ClN_6O_5$



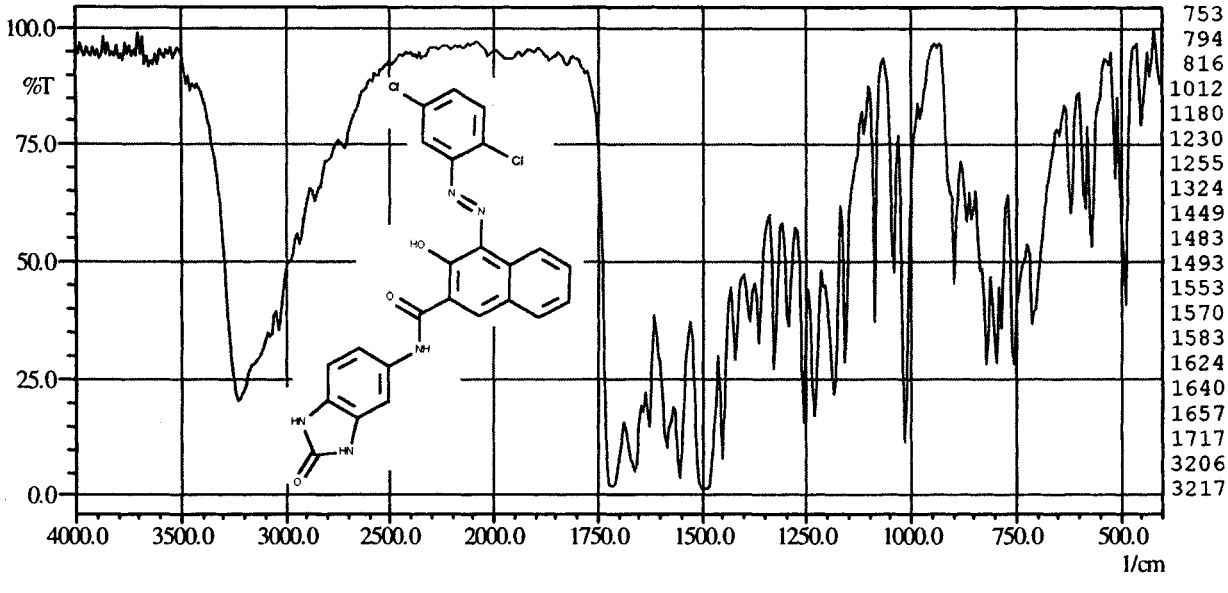
(1) **4-chloro-2-nitroaniline -> 5-N-acetoacetylaminobenz-imidazolone**
(2) Novoperm Orange HL70
(3) Hoechst
(4) 416.8 g mol^{-1}t
(5) organic pigmen
(6) orange solid
(11) Pigment Orange 36
(12) 11780
(13) KBr pellet

2215 $C_{17}H_{14}N_6O_5$



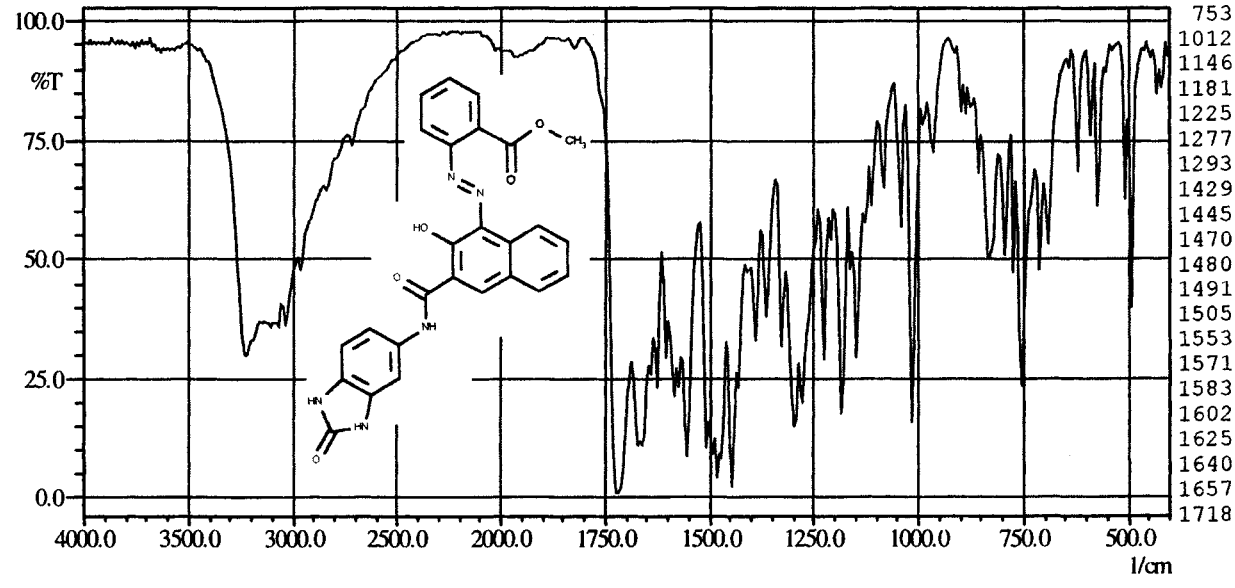
(1) **4-nitroaniline -> 5-N-acetoacetylaminobenzimidazolone**
(2) Novoperm Orange H5G70
(3) Hoechst
(4) 382.3 g mol^{-1}
(5) organic pigment
(6) orange solid
(11) Pigment Orange 62
(12) 11775
(13) KBr pellet

2215 $C_{24}H_{15}Cl_2N_5O_3$



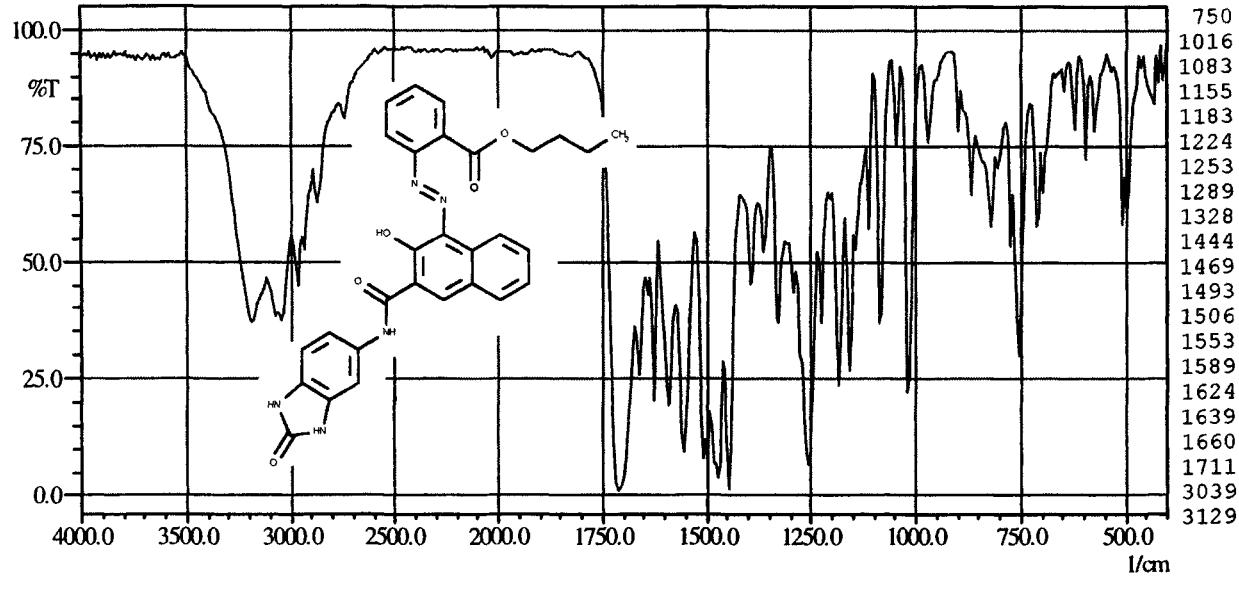
(1) **2,5-dichloroaniline -> 2'-hydroxy-3'-naphthoyl-5-amino-benzimidazolone**
(2) Hostaperm Braun HFR
(3) Hoechst
(4) 492.3 g mol^{-1}
(5) organic pigment
(6) brown solid
(11) Pigment Brown 25
(12) 12510
(13) KBr pellet

2215 $C_{26}H_{19}N_5O_5$



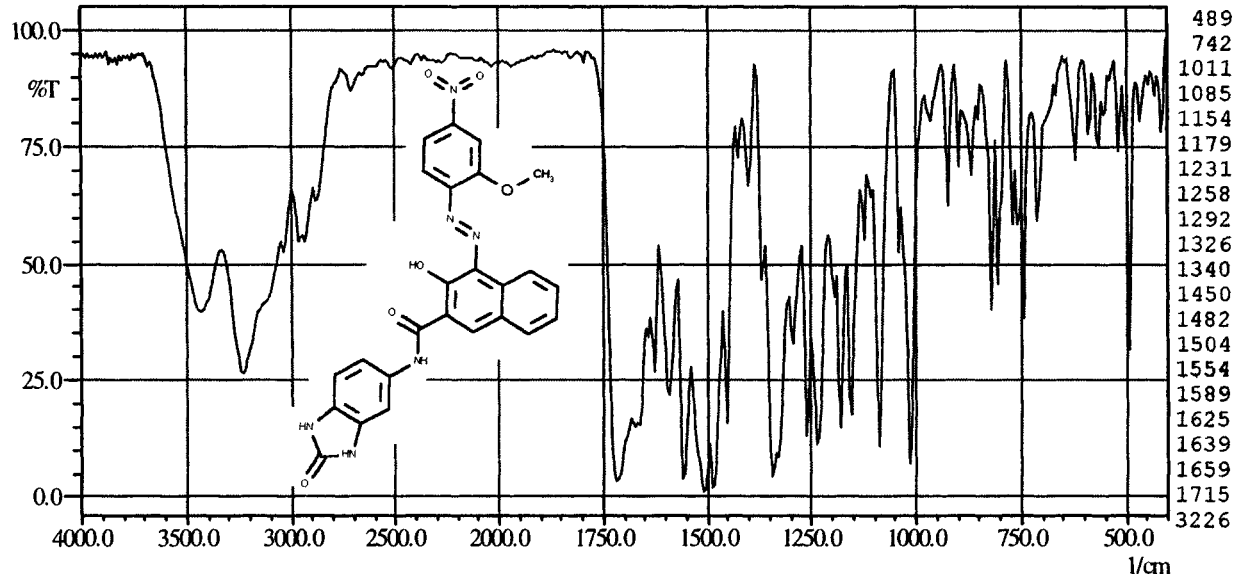
(1) **2-carboxymethylaniline -> 2'-hydroxy-3'-naphthoyl-5-aminobenzimidazolone**
(2) Novoperm Rot HFT
(3) Hoechst
(4) 481.5 g mol^{-1}
(5) organic pigment
(6) red solid
(11) Pigment Red 175
(12) 12513
(13) KBr pellet

2215 $C_{29}H_{25}N_5O_5$



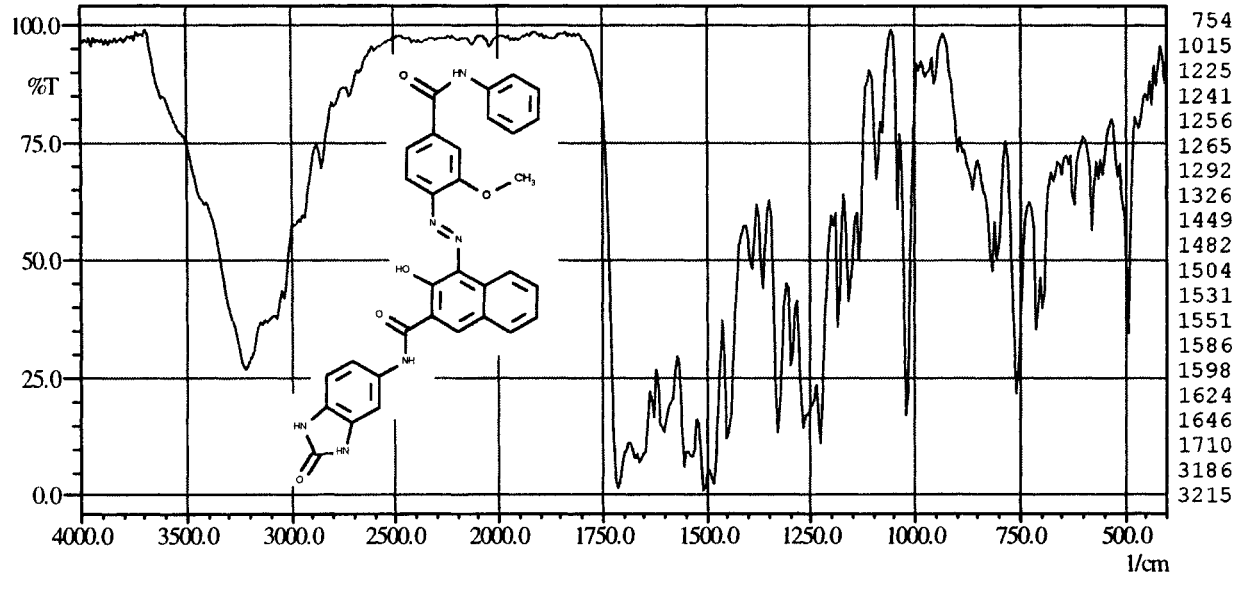
(1) **2-aminobenzoic butylester -> 2'-hydroxy-3'-naphthoyl-5-aminobenzimidazolone**
(2) Permanent Rot HF2B
(3) Hoechst
(4) 523.5 g mol^{-1}
(5) organic pigment
(6) red solid
(11) Pigment Red 208
(12) 12514
(13) KBr pellet

2215 $C_{25}H_{18}N_6O_6$



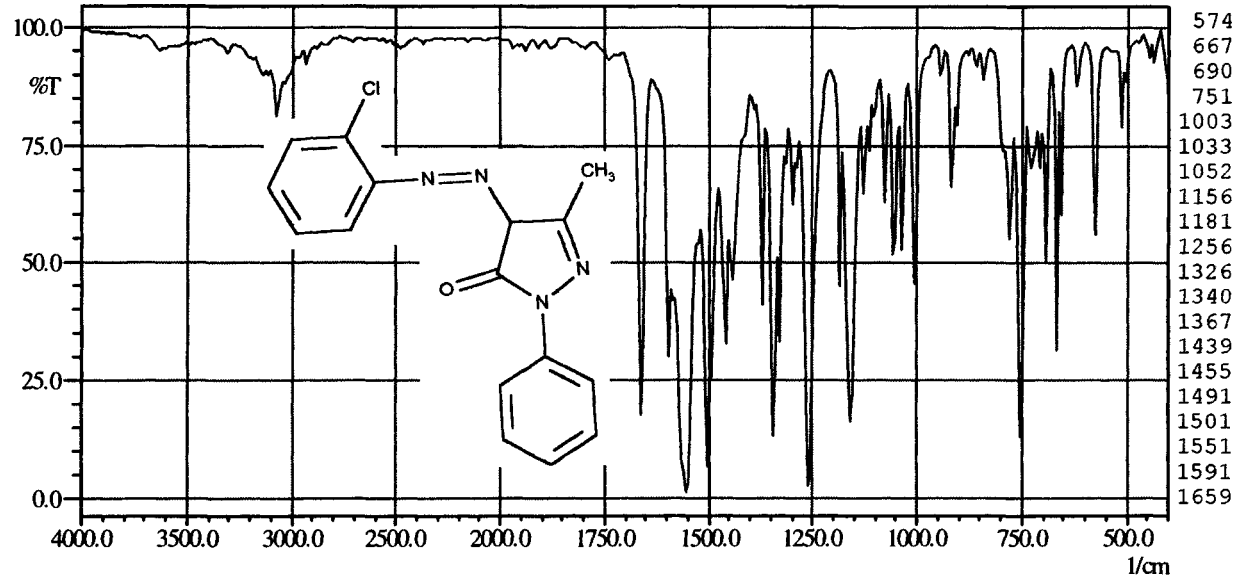
(1) **4-nitro-2-anisidine -> 2-hydroxynaphthoic arylide-N-(2-oxo-5-benzimidazoline)**
(2) Novoperm Marron HFM01
(3) Hoechst
(4) 498.5 g mol^{-1}
(5) organic pigment
(6) red-brown solid
(11) Pigment Red 171
(12) 12512
(13) KBr pellet

2215 $C_{32}H_{24}N_6O_5$



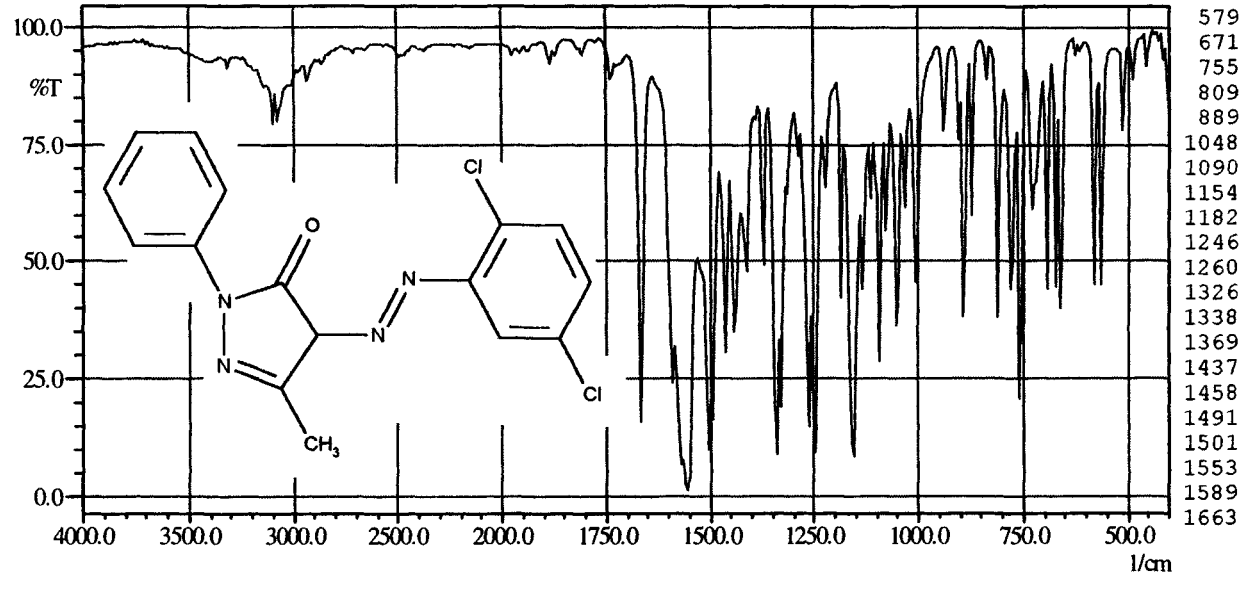
(1) **3-amino-4-methoxybenzanilide -> 2'-hydroxy-3'-naphthoyl-5-amino-benzimidazolone**
(2) Novoperm Carmin HF3C
(3) Hoechst
(4) 572.6 g mol^{-1}
(5) organic pigment
(6) dark-red solid
(11) Pigment Red 176
(12) 12515
(13) KBr pellet

2216 $C_{16}H_{13}ClN_4O$



(1) **2-chloroaniline -> 3-methyl-1-phenyl-5-pyrazolone**
(2) Permanent Gelb 4R
(3) Hoechst
(4) 312.7 g mol^{-1}
(5) organic pigment
(6) yellow solid
(11) Pigment Yellow 60
(12) 12705
(13) KBr pellet

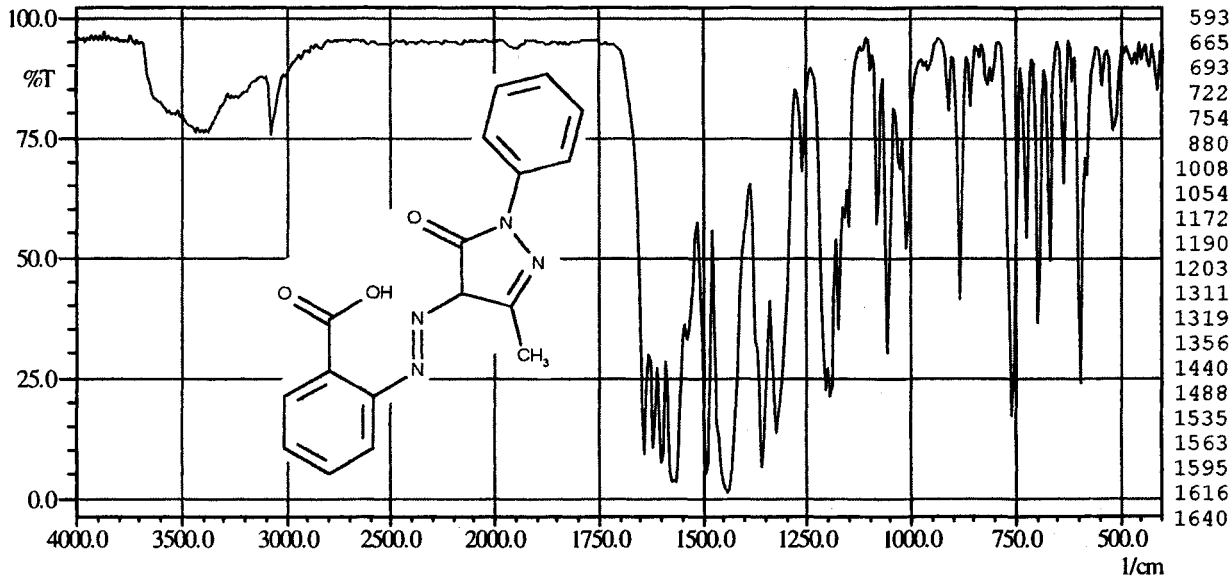
2216 $C_{16}H_{12}Cl_2N_4O$



(1) **2,5-dichloroaniline -> 3-methyl-1-phenyl-5-pyrazolone**
(2) Hansa Gelb R
(3) Hoechst
(4) 347.2 g mol^{-1}
(5) organic pigment
(6) yellow solid
(11) Pigment Yellow 10
(12) 12710
(13) KBr pellet

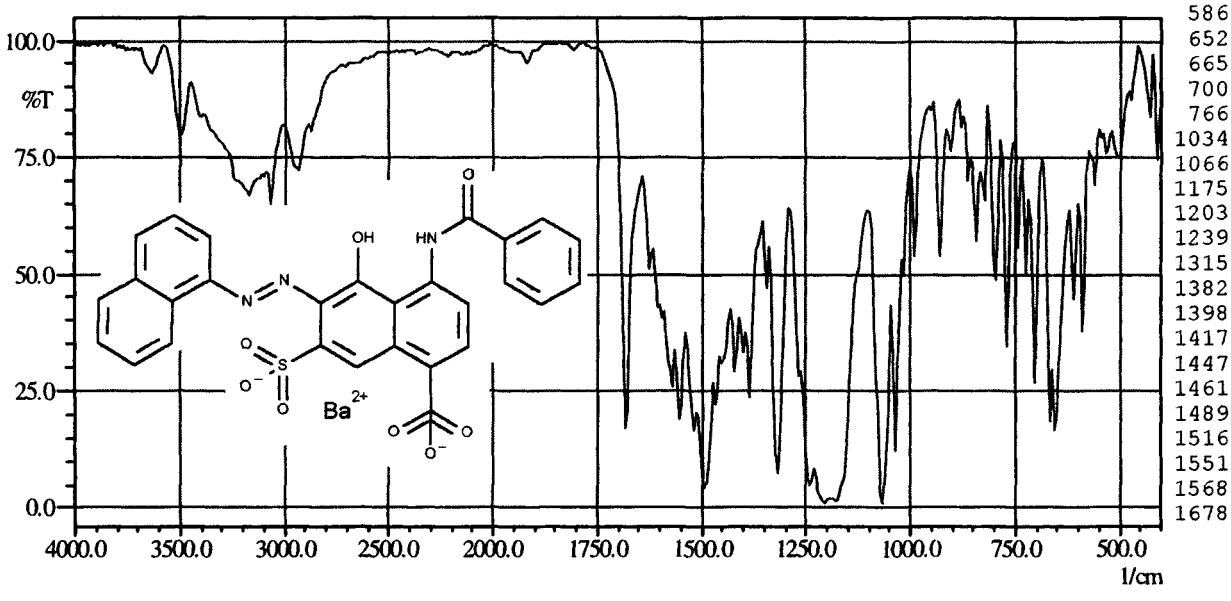
Next Page

2216 $C_{17}H_{14}N_4O_3$



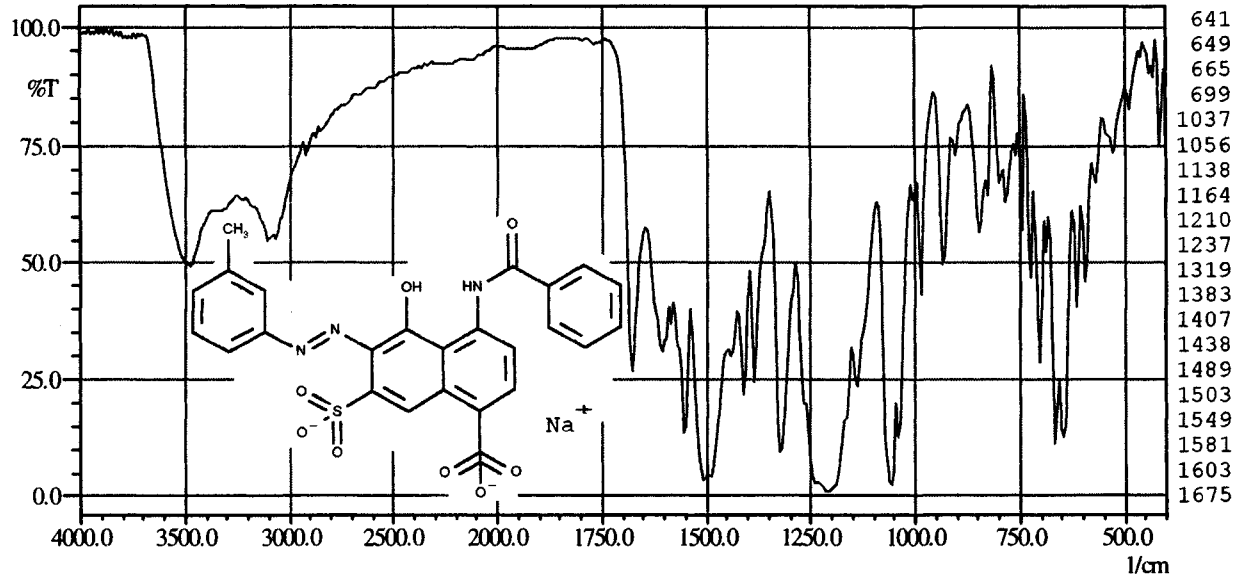
(1) **anthranilic acid -> 3-methyl-1-phenyl-5-pyrazolone**
(2) Filamid Yellow R
(3) Ciba-Geigy
(4) 322.3 g mol^{-1}
(5) organic pigment
(6) yellow solid
(11) Solvent Yellow 21
(12) 18690
(13) KBr pellet

2218 $C_{27}H_{17}N_3O_8S_2Ba$



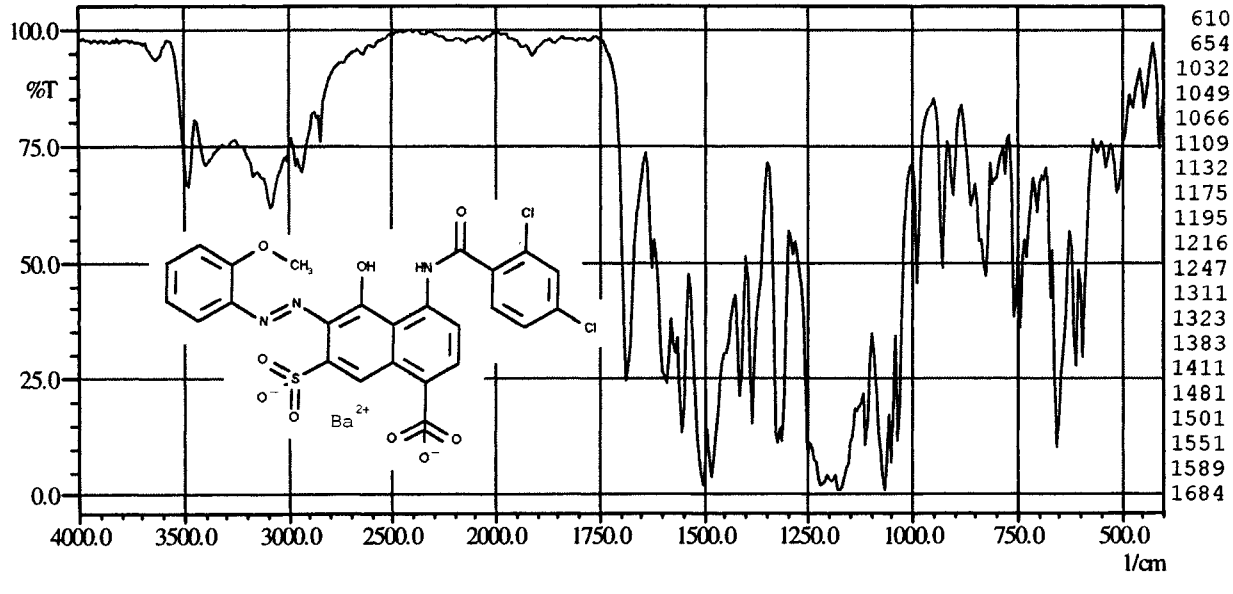
(1) **1-naphthylamine -> N-benzoyl-8-amino-1-naphthol-3,5-disulfonic acid, Ba-salt**
(2) Vulcanosinviolett BB
(3) Hoechst
(4) 712.9 g mol^{-1}
(5) organic pigment
(6) violet solid
(11) Pigment Violet 8
(12) 18005
(13) KBr pellet

2218 $C_{24}H_{17}N_3O_8S_2Na_2$



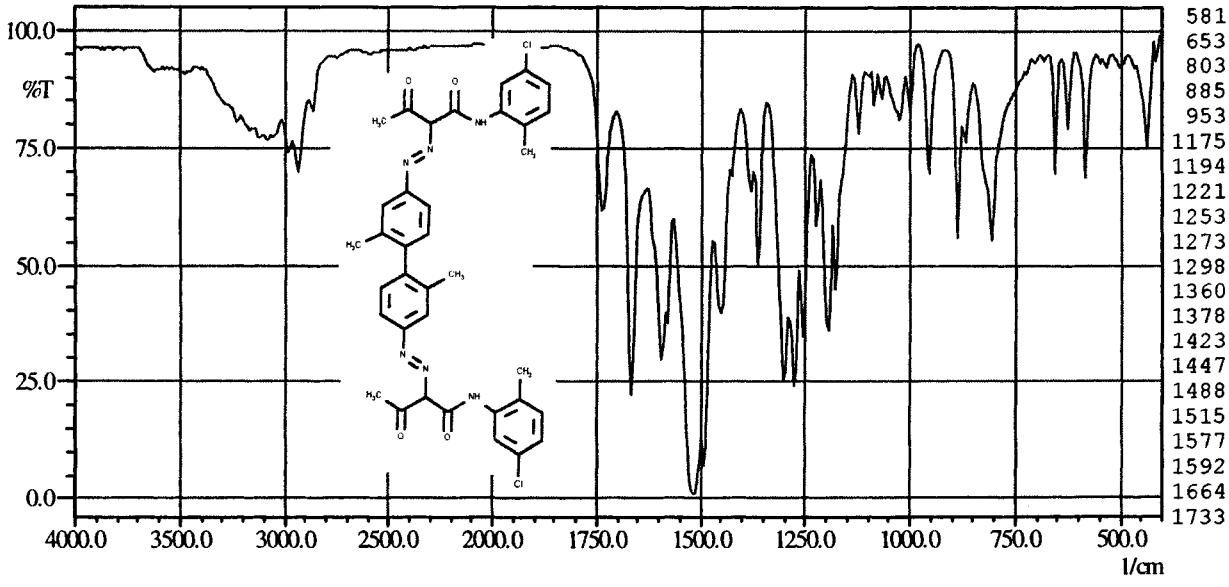
(1) **3-toluidine -> N-benzoyl-8-amino-1-naphthol-3,5-disulfonic acid, Na-salt**
(2) Anthosin 3B
(3) Hoechst
(4) 585.5 g mol^{-1}
(5) organic pigment
(6) red solid
(11) Pigment Red 66
(12) 18000
(13) KBr pellet

2218 $C_{24}H_{15}Cl_2N_3O_9S_2Ba$



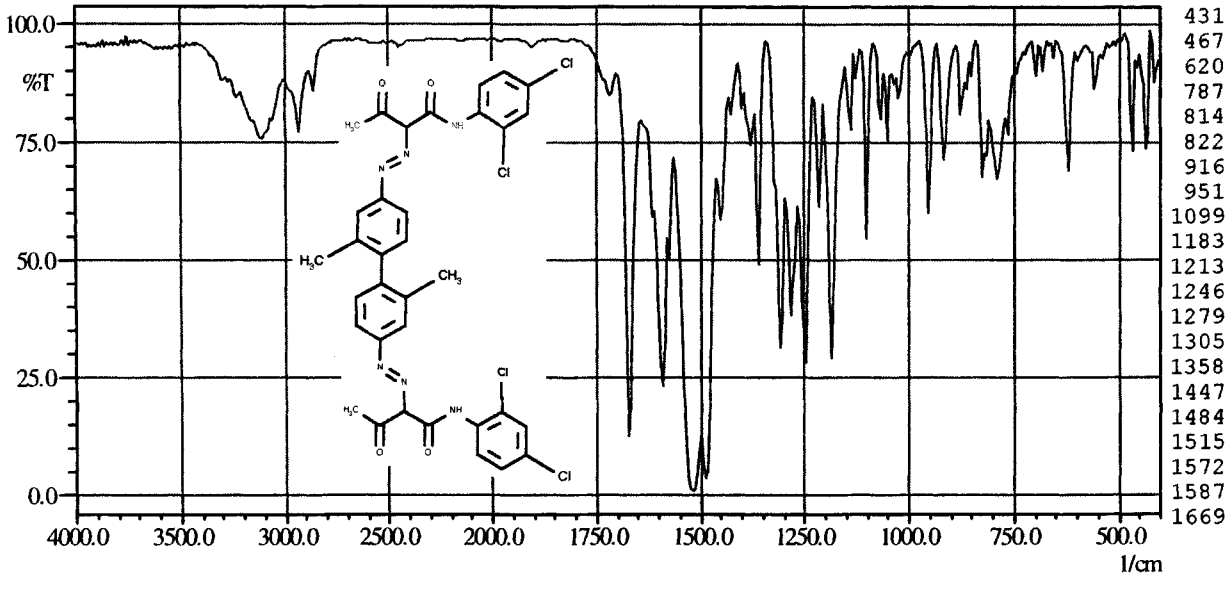
(1) **2-methoxyaniline -> N-(2',4'-dichlorobenzoyl)-8-amino-1-naphthol-3,5-disulfonic acid, Ba-salt**
(2) Vulkanosinrot 5B
(3) Hoechst
(4) 761.7 g mol^{-1}
(5) organic pigment
(6) red solid
(11) Pigment Red 67
(12) 18025
(13) KBr pellet

2221 $C_{36}H_{34}Cl_2N_6O_4$



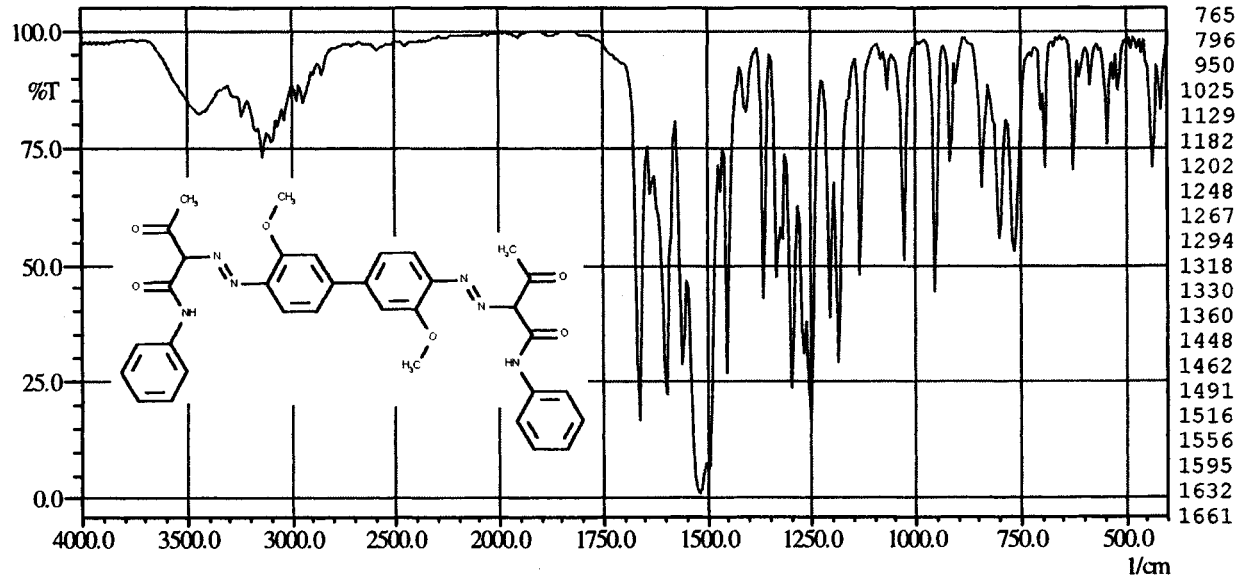
(1) **5-chloro-2-methylaniline -> N,N'-diacetoacetyl-3,3'-dimethylbenzidine**
(2) Helio Echtbrilliant Gelb GR
(3) Bayer
(4) 685.6 g mol^{-1}
(5) organic pigment
(6) yellow solid
(11) Pigment Yellow 77
(12) 20045
(13) KBr pellet

2221 $C_{34}H_{28}Cl_4N_6O_4$



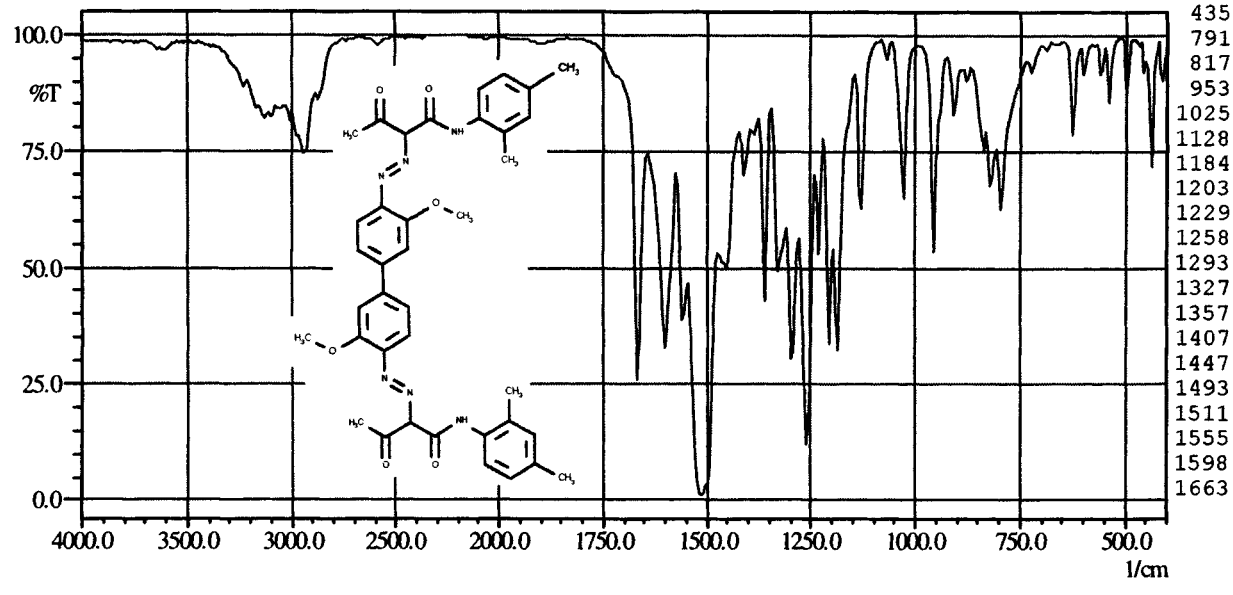
(1) **2,4-dichloroaniline -> N,N'-diacetoacetyl-3,3'-dimethylbenzidine**
(2) Permanent Gelb NCG
(3) Hoechst
(4) 726.4 g mol^{-1}
(5) organic pigment
(6) yellow solid
(11) Pigment Yellow 16
(12) 20040
(13) KBr pellet

2221 $C_{34}H_{32}N_6O_6$



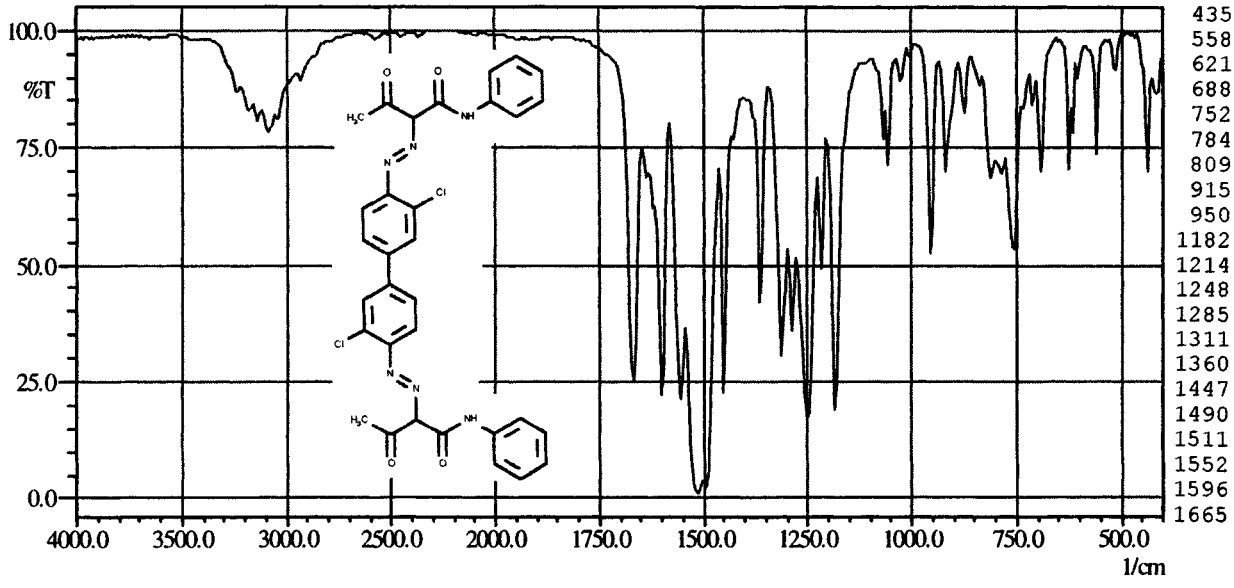
(1) **3,3'-dimethoxybenzidine->acetoacetic anilide**
(2) Symuler Fast Orange K
(3) DIC
(4) 620.7 g mol^{-1}
(5) organic pigment
(6) orange-coloured solid
(11) Pigment Orange 16
(12) 21160
(13) KBr pellet

2221 $C_{38}H_{40}N_6O_6$



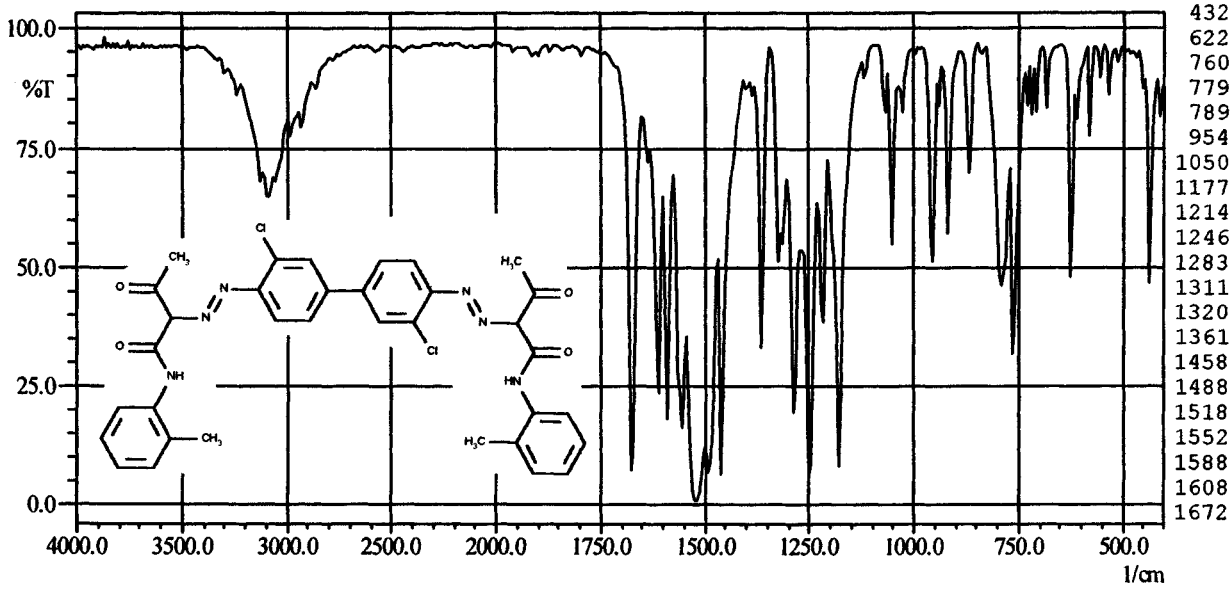
(1) **3,3'-dimethoxybenzidine -> acetoacetic arylide-2,4-dimethylanilide**
(2) Vulcan Echtorange GG
(3) Hoechst
(4) 676.7 g mol^{-1}
(5) organic pigment
(6) orange solid
(11) Pigment Orange 14
(12) 21165
(13) KBr pellet

2221 $C_{32}H_{26}Cl_2N_6O_4$



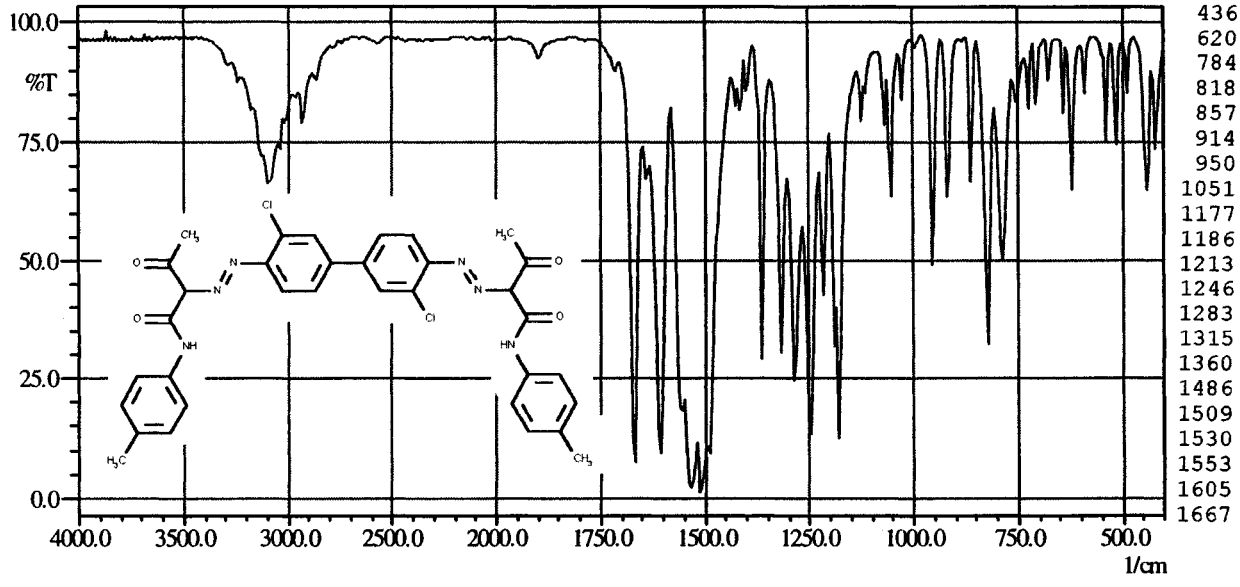
(1) **3,3'-dichlorobenzidine -> acetoacetic arylide-anilide**
(2) Permanent Gelb DHG
(3) Hoechst
(4) 629.5 g mol^{-1}
(5) organic pigment
(6) yellow solid
(11) Pigment Yellow 12
(12) 21090
(13) KBr pellet

2221 $C_{34}H_{30}Cl_2N_6O_4$



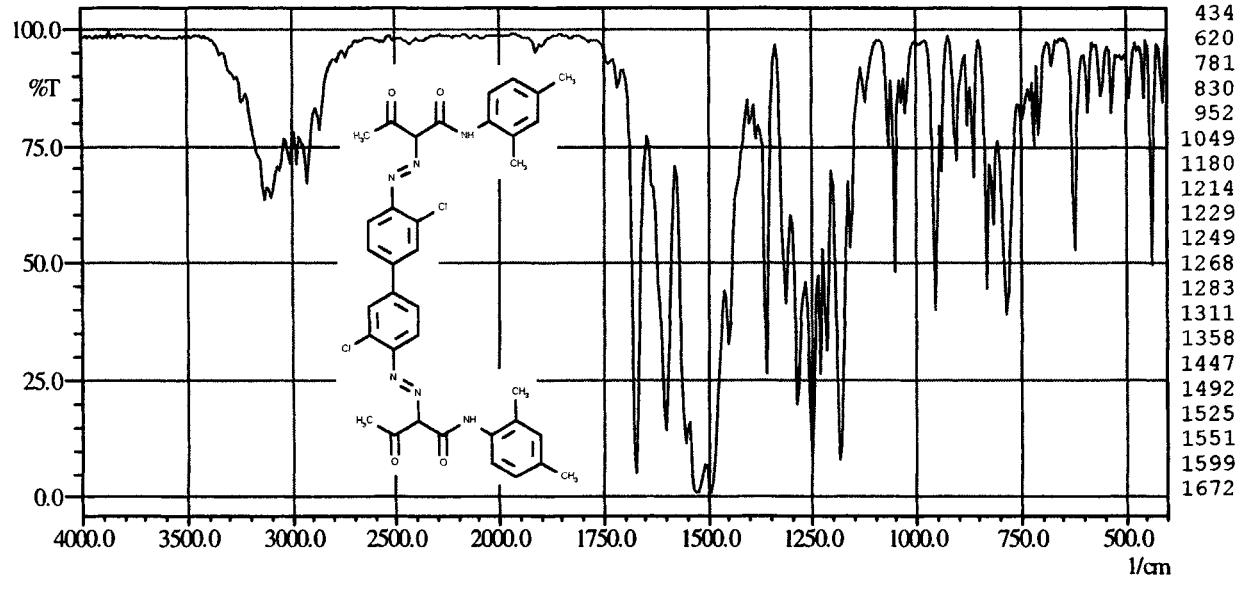
(1) **3,3'-dichlorobenzidine -> acetoacetic arylide-2-methylanilide**
(2) Irgalite Yellow BRM
(3) Ciba-Geigy
(4) 657.5 g mol^{-1}
(5) organic pigment
(6) yellow solid
(11) Pigment Yellow 14
(12) 21095
(13) KBr pellet

2221 $C_{34}H_{30}Cl_2N_6O_4$



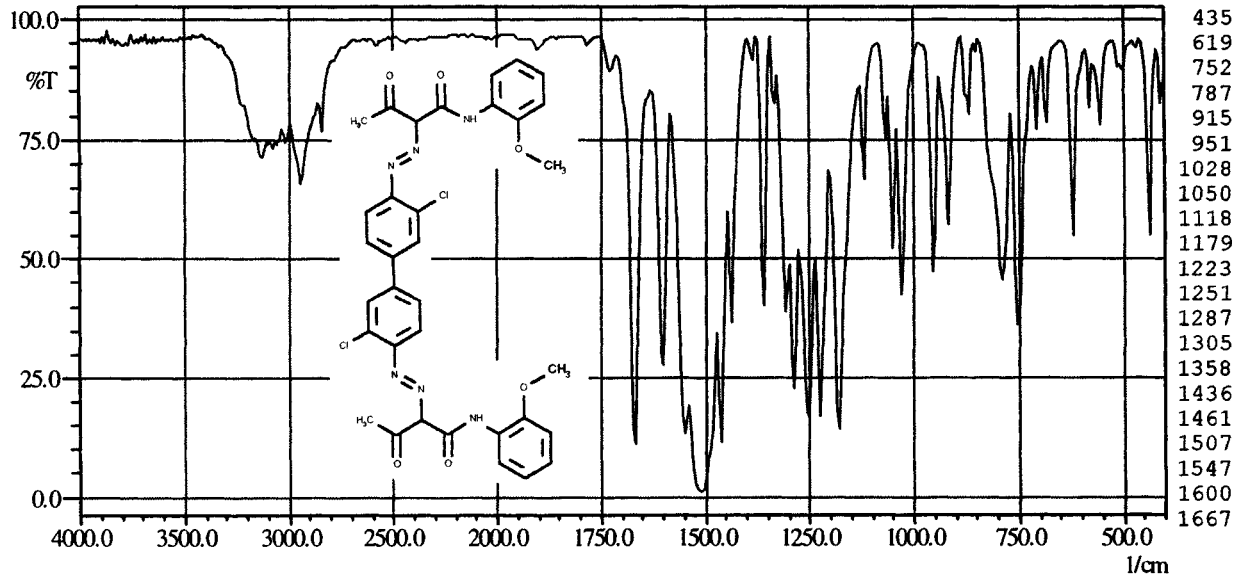
(1) **3,3'-dichlorobenzidine -> acetoacetic arylide-4-toluidide**
(2) Irgalite Yellow BAF
(3) Ciba-Geigy
(4) 657.5 g mol^{-1}
(5) organic pigment
(6) yellow solid
(11) Pigment Yellow 55
(12) 21096
(13) KBr pellet

2221 $C_{36}H_{34}Cl_2N_6O_4$



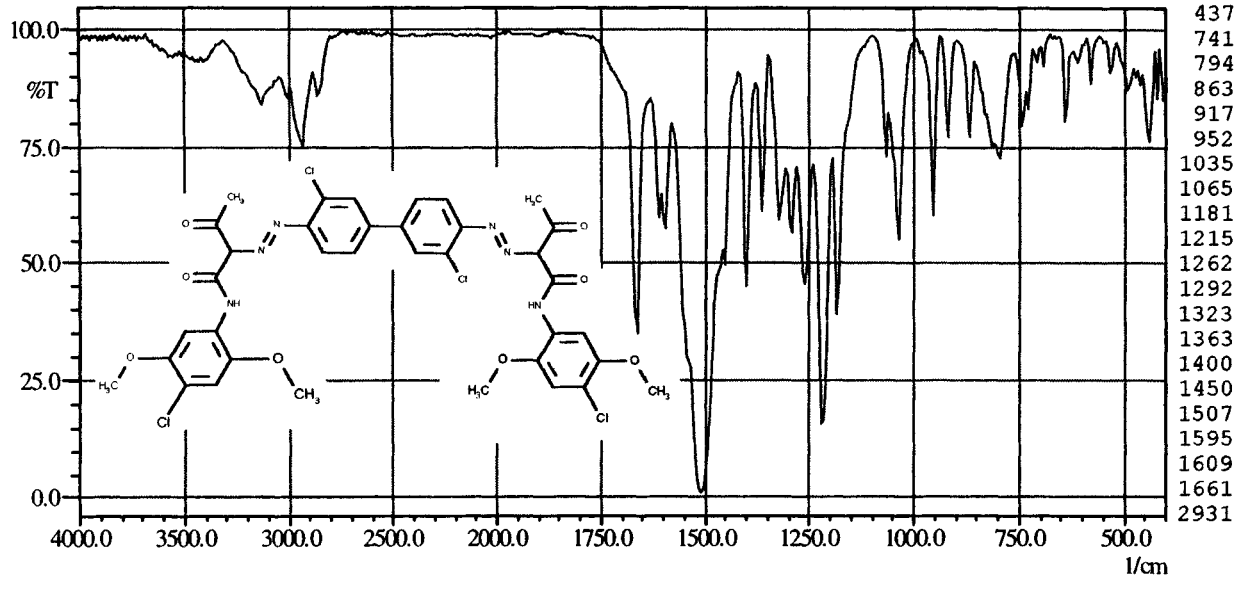
(1) **3,3'-dichlorobenzidine -> acetoacetic arylide-2,4-dimethylanilide**
(2) Irgalite Yellow BAWP
(3) Ciba-Geigy
(4) 685.6 g mol^{-1}
(5) organic pigment
(6) yellow solid
(11) Pigment Yellow 13
(12) 21100
(13) KBr pellet

2221 $C_{34}H_{26}Cl_2N_6O_6$



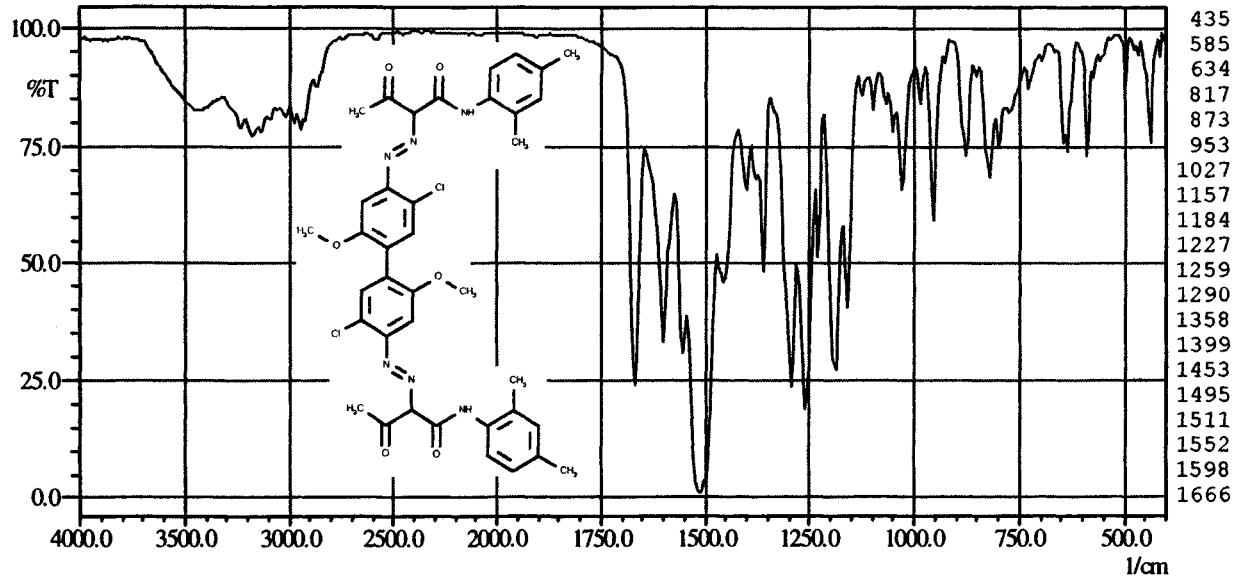
(1) **3,3'-dichlorobenzidine -> acetoacetic arylide-2-methoxyanilide**
(2) Irgalite Yellow 2GP
(3) Ciba-Geigy
(4) 685.5 g mol^{-1}
(5) organic pigment
(6) yellow solid
(11) Pigment Yellow 17
(12) 21105
(13) KBr pellet

2221 $C_{36}H_{32}Cl_4N_6O_8$



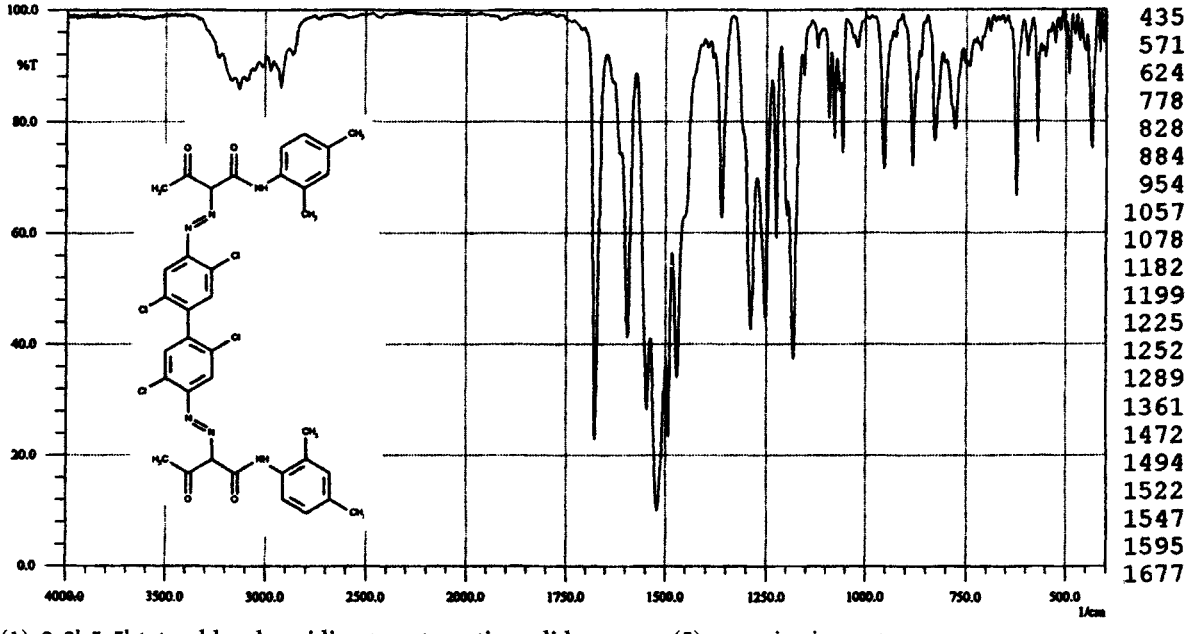
(1) **3,3'-dichlorobenzidine -> acetoacetic arylide-4-chloro-2,5-dimethoxyanilide**
(2) Diacetanil Yellow 3RH
(3) Capelle
(4) 818.5 g mol^{-1}
(5) organic pigment
(6) yellow solid
(11) Pigment Yellow 83
(12) 21108
(13) KBr pellet

2221 $C_{38}H_{38}Cl_2N_6O_6$



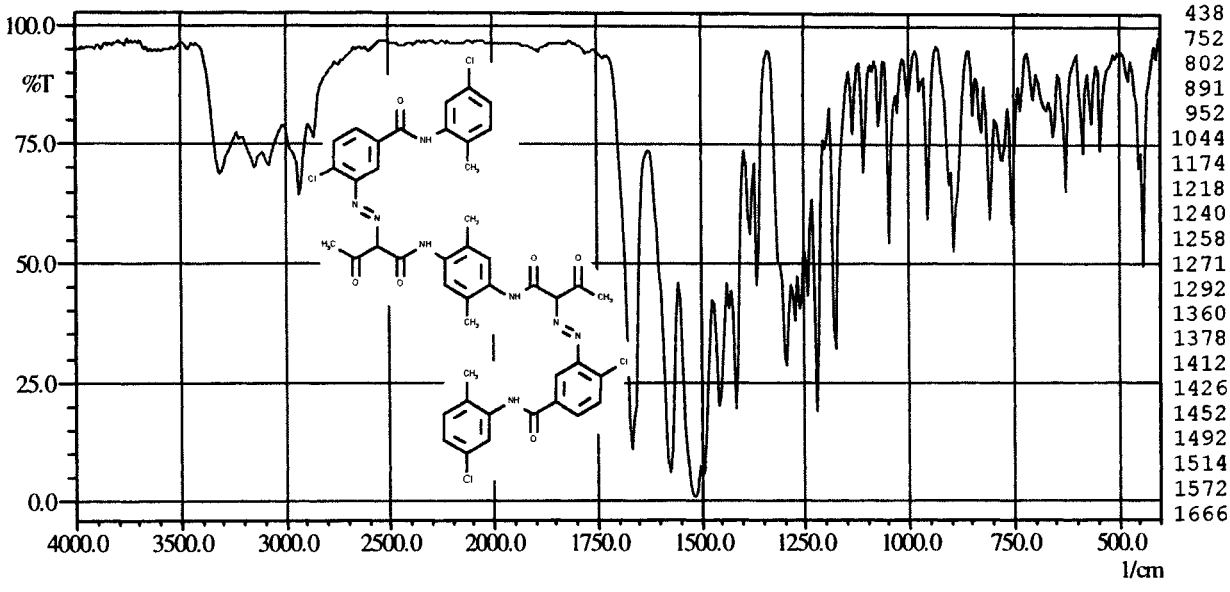
(1) **2,2'-dichloro-5,5'-dimethoxybenzidine -> acetoacetic arylide-2,4-dimethylanilide**
(2) Vulcan Echtgelb 5G
(3) Hoechst
(4) 745.7 g mol^{-1}
(5) organic pigment
(6) yellow solid
(11) Pigment Yellow 15
(12) 21220
(13) KBr pellet

2221 $C_{36}H_{32}Cl_4N_6O_4$



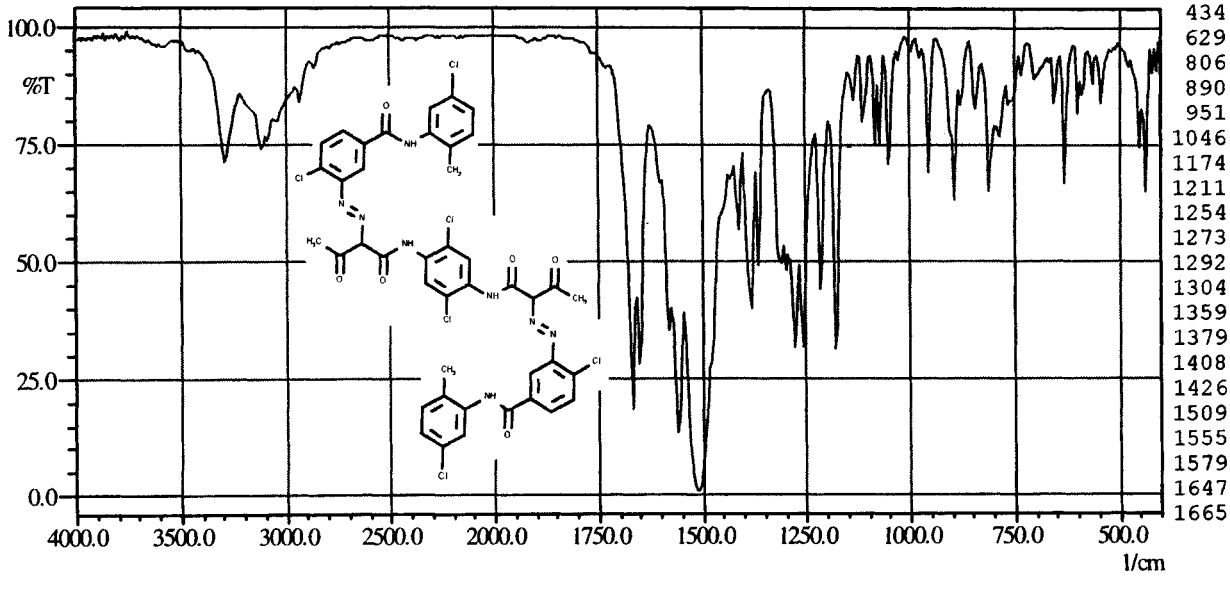
(1) **2, 2', 5, 5'-tetrachlorobenzidine->acetoacetic arylide-2, 4-dimethylanilide**
(2) Novoperm Gelb H10G
(3) Hoechst
(4) 754.5 g mol^{-1}
(5) organic pigment
(6) yellow solid
(11) Pigment Yellow 81
(12) 21127
(13) KBr pellet

2222 $C_{44}H_{38}Cl_4N_8O_6$



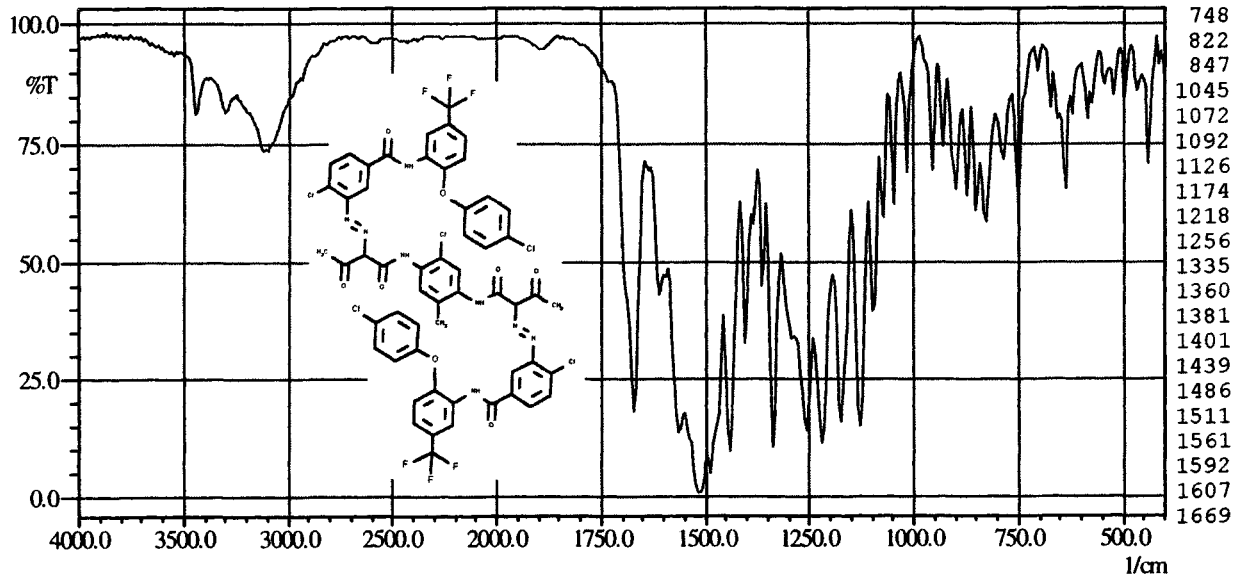
(1) **3-amino-4,5'-dichloro-2'-methylbenzanilide -> N,N'-(2,5-dimethyl-1,4-phenylene)-*bis*(acetoacetamide)**
(2) Cromophtal Gelb GR
(3) Ciba-Geigy
(4) 916.6 g mol^{-1}
(5) organic pigment
(6) yellow solid
(11) Pigment Yellow 95
(13) KBr pellet

2222 $C_{42}H_{32}Cl_6N_8O_6$



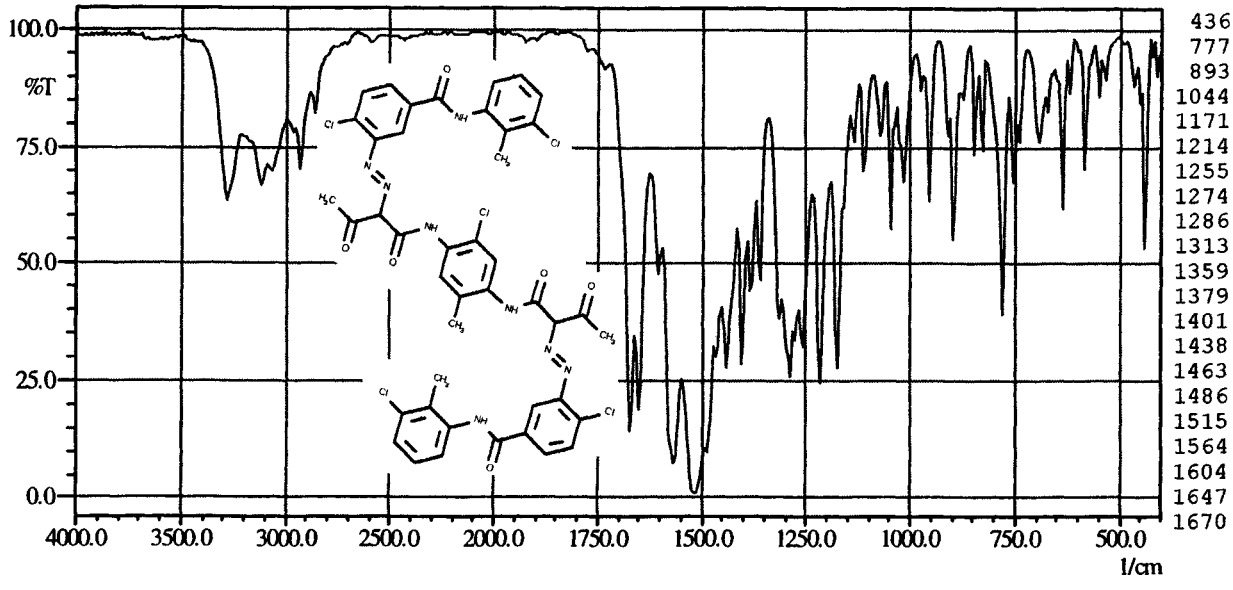
(1) **3-amino-4,5'-dichloro-2'-methylbenzanilide -> N,N'-(2,5-dichloro-1,4-phenylene)-*bis*(acetoacetamide)**
(2) Cromophtal Gelb 6G
(3) Ciba-Geigy
(4) 957.4 g mol^{-1}
(5) organic pigment
(6) yellow solid
(11) Pigment Yellow 94
(13) KBr pellet

2222 $C_{55}H_{37}F_6Cl_5N_8O_8$



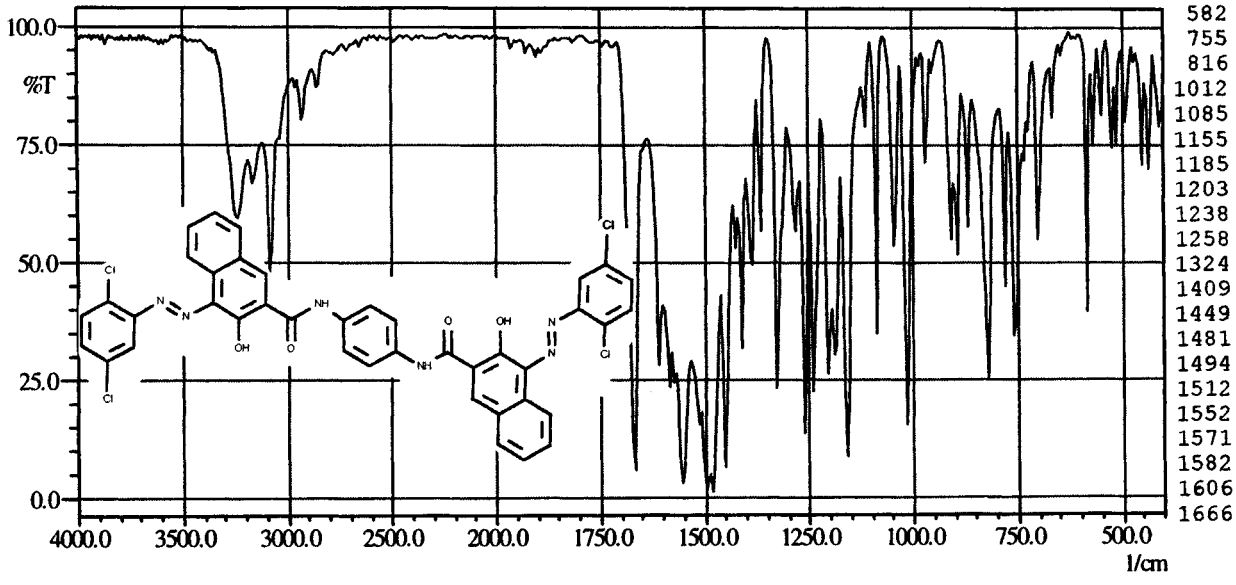
(1) **3-amino-4-chloro-2'-(4-chlorophenoxy)-5'-trifluoromethylbenzanilide -> N,N'-(2-chloro-5-methyl-1,4-phenylene)-*bis*(acetoacetamide)**
(2) Cromophtal Gelb 8G
(3) Ciba-Geigy
(4) 1229 g mol^{-1}
(5) organic pigment
(6) yellow solid
(11) Pigment Yellow 128
(12) 20037
(13) KBr pellet

2222 $C_{43}H_{35}Cl_5N_8O_6$



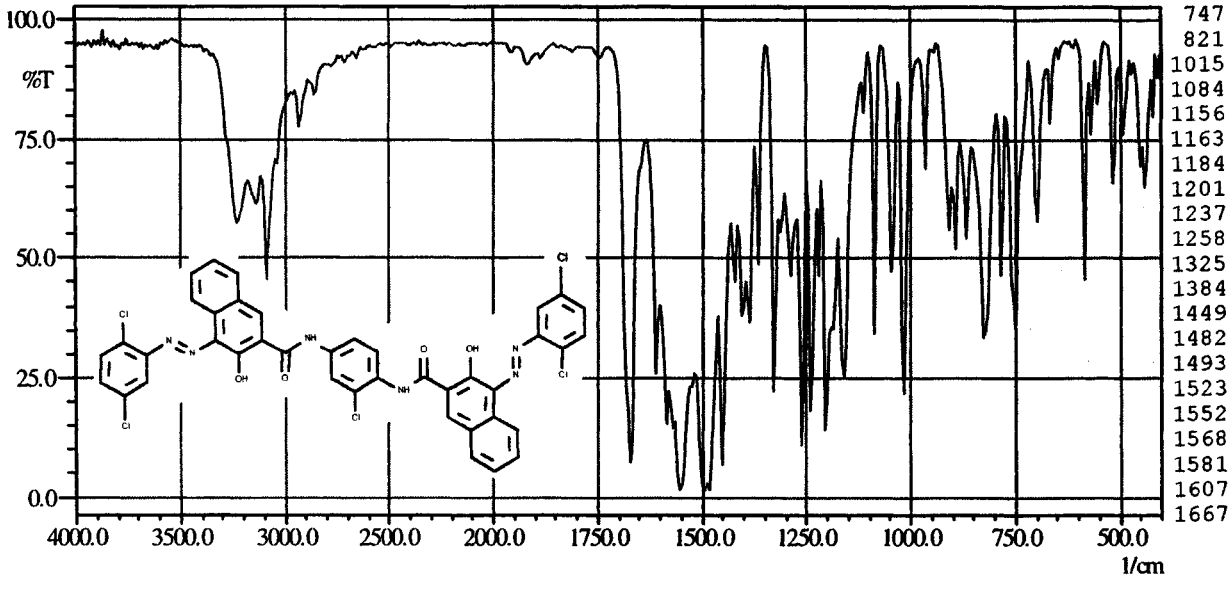
(1) **3-amino-3,4'-dichloro-2'-methylbenzanilide-> 3-ketobutyrylchloride condensed with 2-chloro-5-methyl-*p*-phenylenediamine**
(2) Cromophtal Gelb 3G
(3) Ciba-Geigy
(4) 937.0 g mol^{-1}
(5) organic pigment
(6) yellow solid
(11) Pigment Yellow 93
(13) KBr pellet

2223 $C_{40}H_{24}Cl_4N_6O_4$



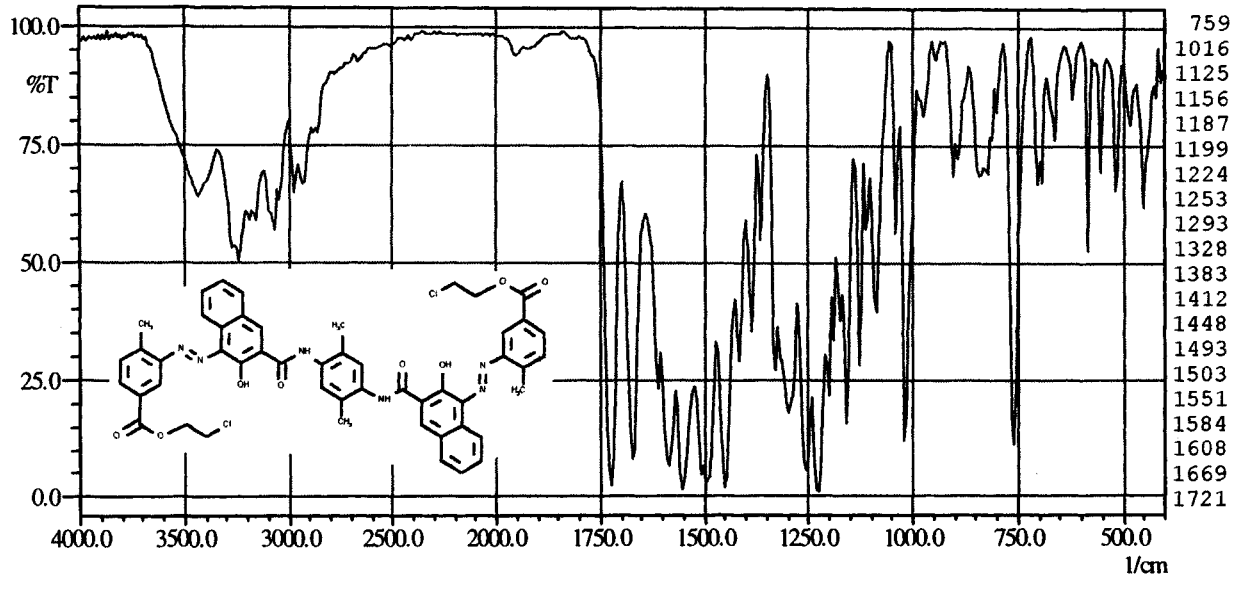
(1) **2,5-dichloroaniline -> N,N'-1,4-phenylene-*bis*(3-hydroxy-2-naphthamide)**
(2) Cromophtal Scharlach RN
(3) Ciba-Geigy
(4) 794.4 g mol^{-1}
(5) organic pigment
(6) scarlet solid
(11) Pigment Red 166
(12) 20035
(13) KBr pellet

2223 $C_{40}H_{23}Cl_5N_6O_4$



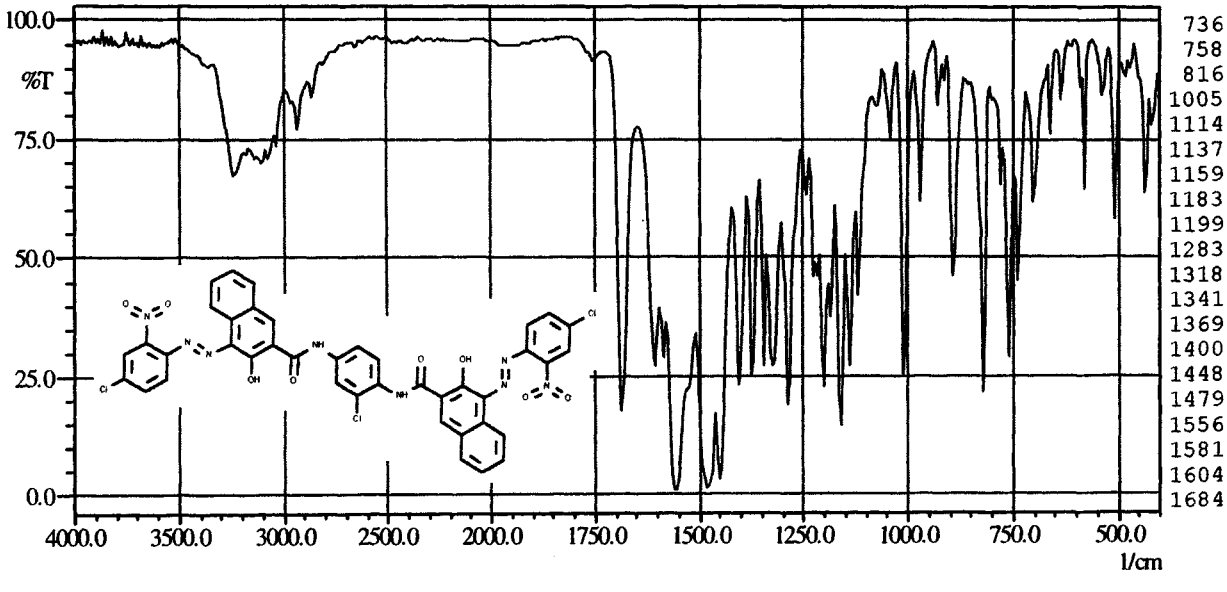
(1) **2,5-dichloroaniline-N,N'-(2-chloro-1,4-phenylene)-*bis*(3-hydroxy-2-naphthamide)**
(2) Cromophtal Rot BRN
(3) Ciba-Geigy
(4) 828.9 g mol^{-1}
(5) organic pigment
(6) red solid
(11) Pigment Red 144
(13) KBr pellet

2223 $C_{50}H_{42}Cl_2N_6O_8$



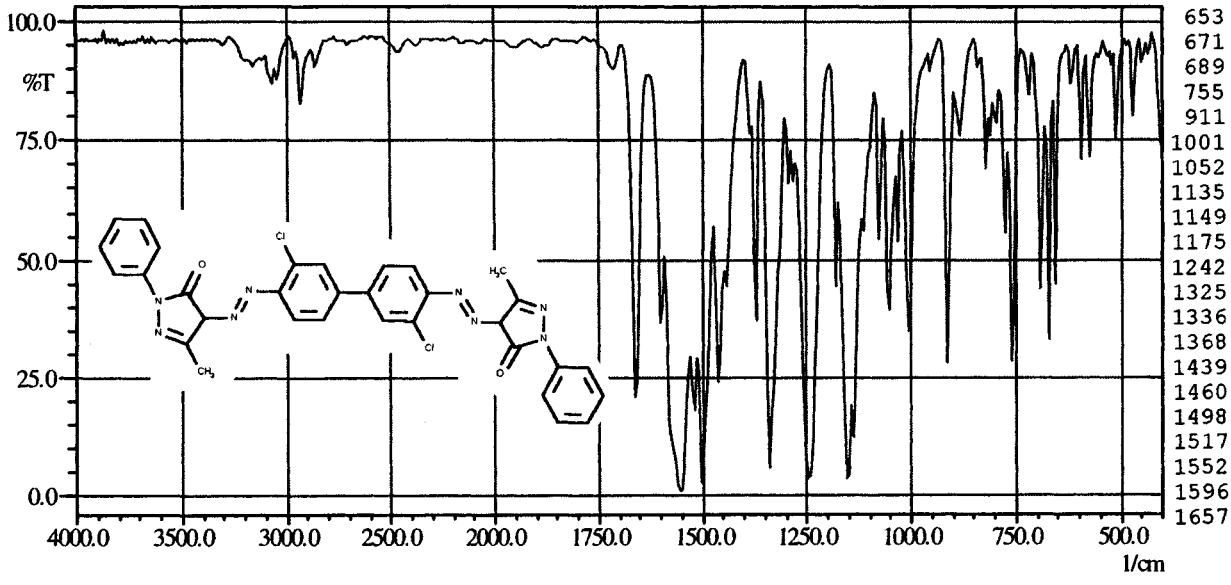
(1) **3-amino-*p*-toluic acid 2-chloroethyl ester -> N,N'-(2,5-dimethyl-1,4-phenylene)-*bis*(3-hydroxy-2-naphthamide)**
(2) Cromophtal Rot G
(3) Ciba-Geigy
(4) 925.8 g mol^{-1}
(5) organic pigment
(6) red solid
(11) Pigment Red 22
(13) KBr pellet

2223 $C_{40}H_{25}Cl_2N_7O_6$



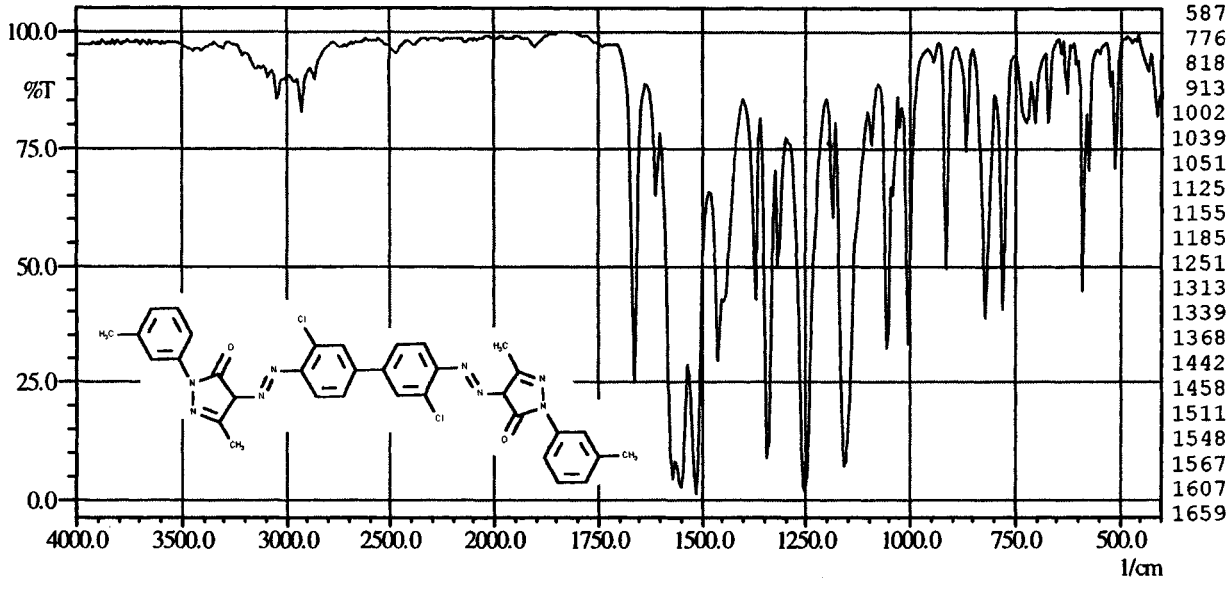
(1) **4-chloro-2-nitroaniline -> N,N'-(2-chloro-1,4-phenylene)-*bis*(3-hydroxy-2-naphthamide)**
(2) Cromophtal Braun 5R
(3) Ciba-Geigy
(4) 770.5 g mol^{-1}
(5) organic pigment
(6) brown solid
(11) Pigment Brown 23
(13) KBr pellet

2224 $C_{32}H_{24}Cl_2N_8O_2$



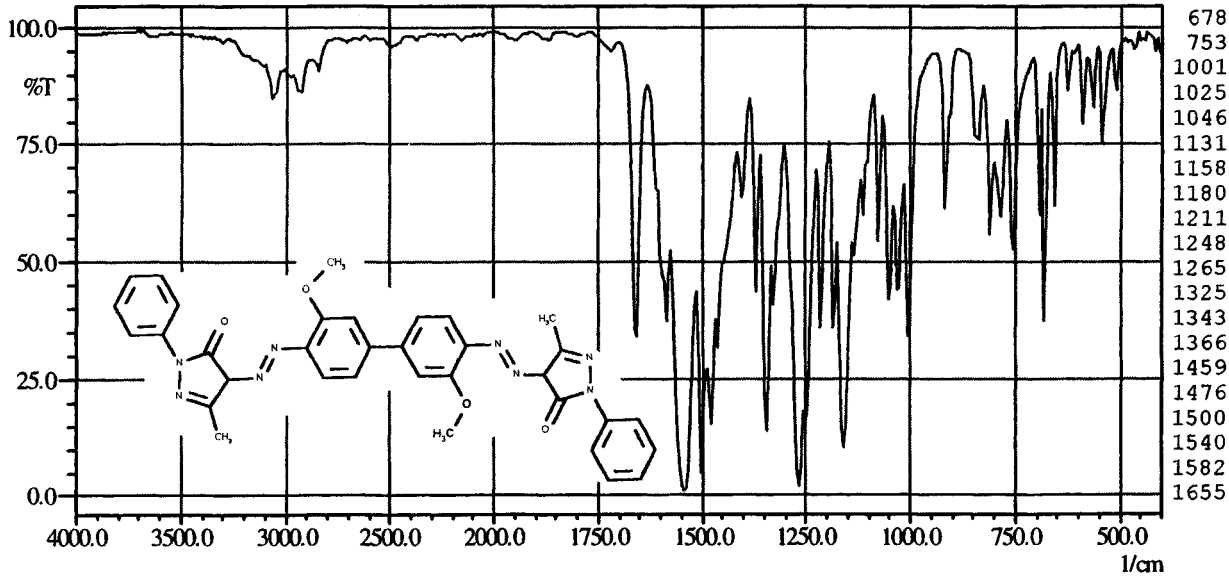
(1) **3,3'-dichlorobenzidine -> 3-methyl-1-phenyl-5-pyrazolone**
(2) Irgalite Orange P
(3) Ciba-Geigy
(4) 623.5 g mol^{-1}
(5) organic pigment
(6) orange solid
(11) Pigment Orange 13
(12) 21110
(13) KBr pellet

2224 $C_{34}H_{28}Cl_2N_8O_2$



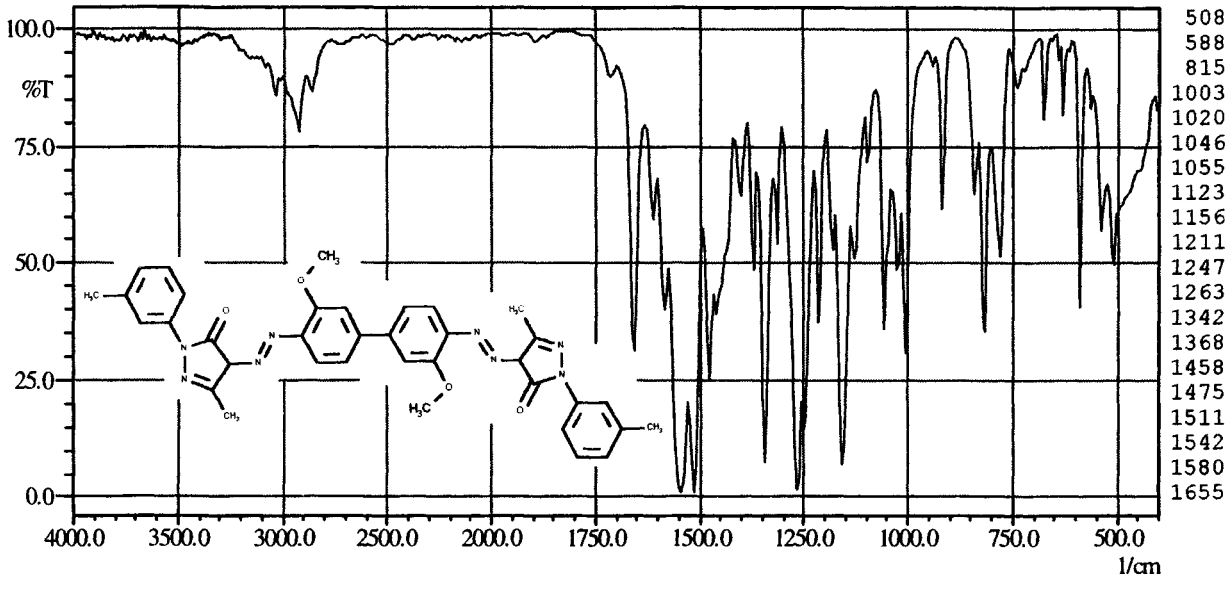
(1) **3,3'-dichlorobenzidine -> 3-methyl-1-(3'-tolyl)-5-pyrazolone**
(2) Permanent Orange RL 70
(3) Hoechst
(4) 651.6 g mol^{-1}
(5) organic pigment
(6) orange solid
(11) Pigment Orange 34
(12) 21115
(13) KBr pellet

2224 $C_{34}H_{30}N_8O_4$



(1) **2,2'-dianisidine -> 3-methyl-1-phenyl-5-pyrazolone**
(2) Elektra Red
(3) commercial
(4) 614.7 g mol^{-1}
(5) organic pigment
(6) red solid
(11) Pigment Red 41
(12) 21200
(13) KBr pellet

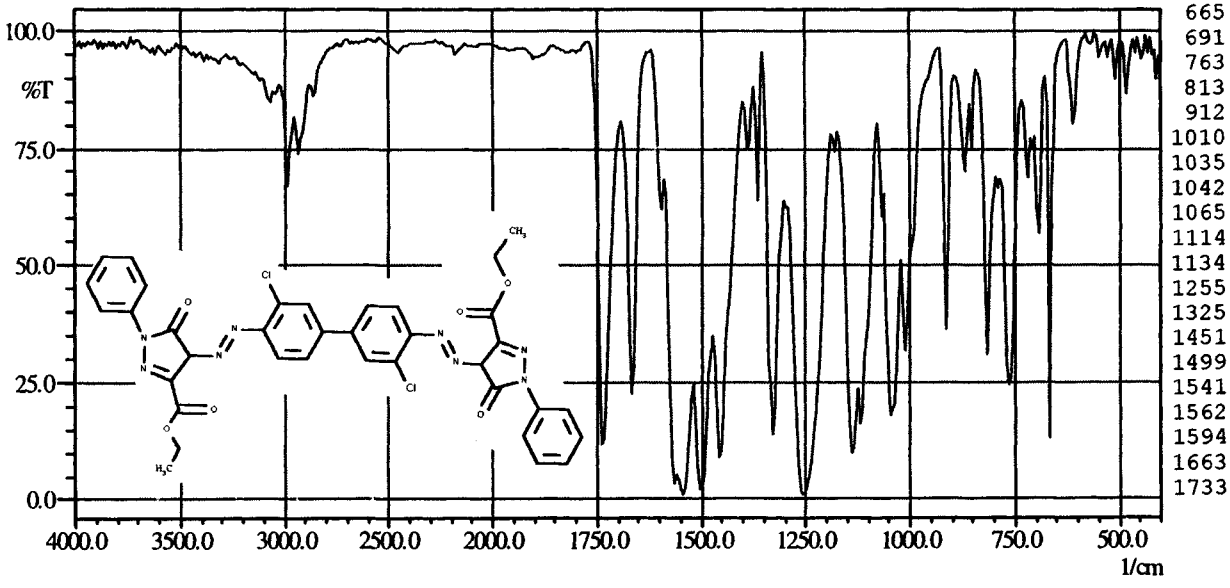
2224 $C_{34}H_{30}N_8O_4$



(1) **3,3'-dimethoxybenzidine -> 3-methyl-1,4'-tolyl-5-pyrazolone**
(2) PV-Rot G 1
(3) Hoechst
(4) 614.6 g mol^{-1}
(5) organic pigment
(6) red solid
(11) Pigment Red 37
(12) 21205
(13) KBr pellet

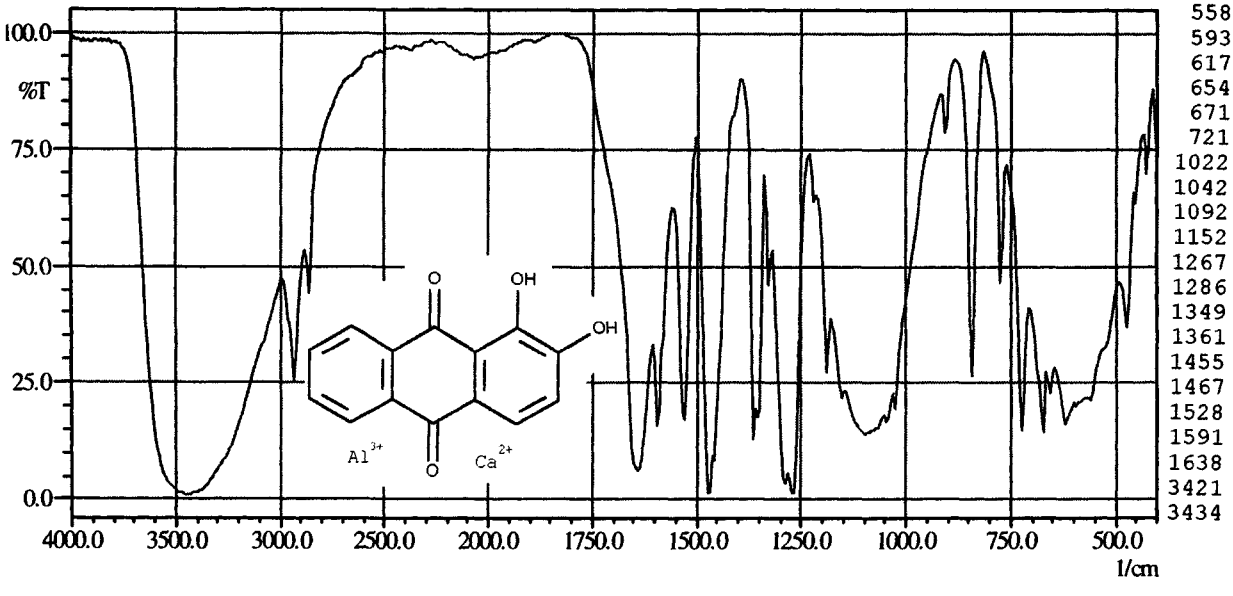
Previous Page

2224 $C_{36}H_{28}Cl_2N_8O_6$



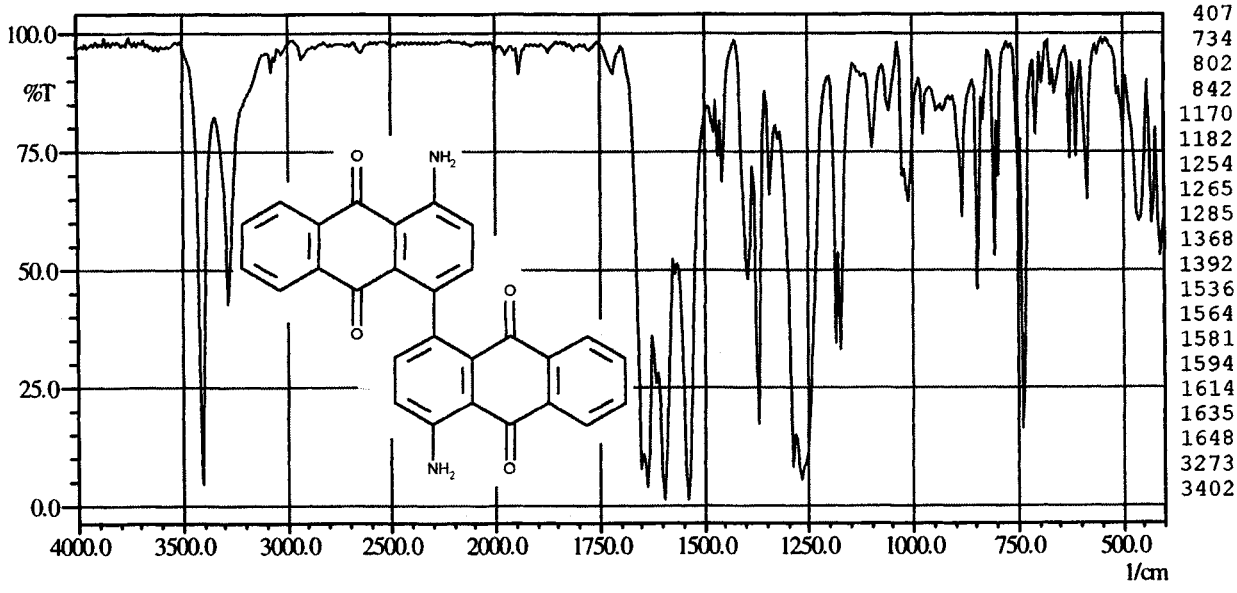
(1) **3,3'-dichlorobenzidine -> ethoxycarbonyl-1-phenyl-5-pyrazolone**
(2) Sicoplast V Rot
(3) BASF
(4) 739.6 g mol^{-1}
(5) organic pigment
(6) red solid
(13) KBr pellet

22311 $C_{14}H_8O_4AlCa$



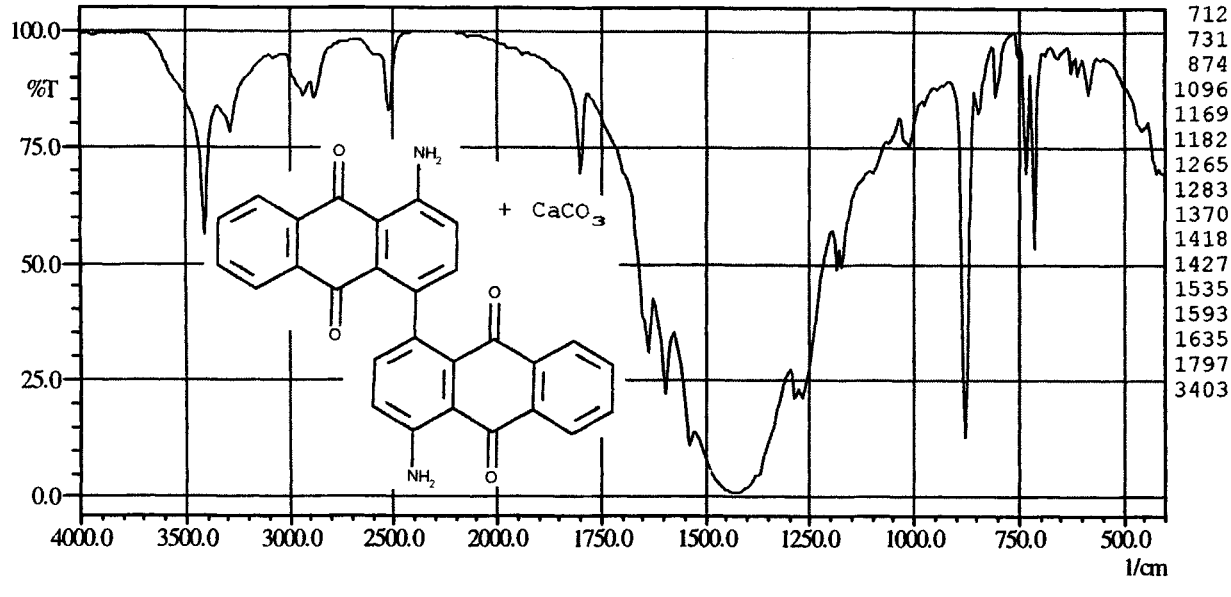
(1) **1,2-dihydroxy-9,10-anthraquinone (alizarin), Al-Ca lake**
(2) Krapplack C
(3) Rubia tinctorum
(4) 240.2 g mol^{-1}
(5) organic pigment
(6) red solid
(11) Pigment Red 83
(12) 58000
(13) KBr pellet

22311 $C_{28}H_{16}N_2O_4$



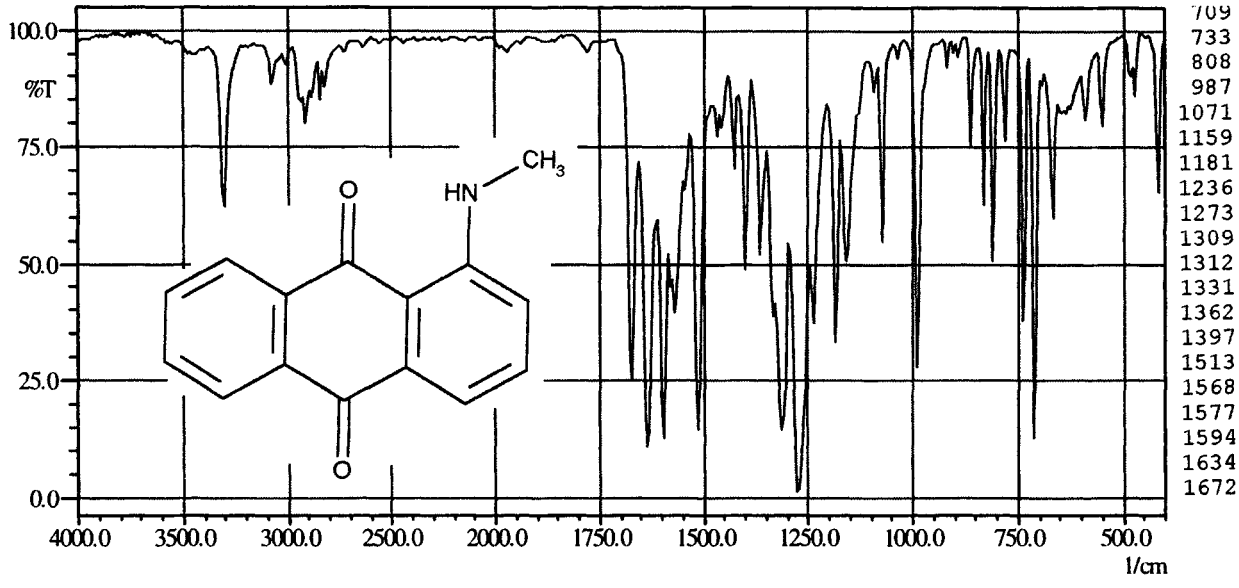
(1) **4,4'-*bis*(1-amino-9,10-anthraquinone)**
(2) Indofast Red R6340
(3) Bayer
(4) 444.4 g mol^{-1}
(5) organic pigment
(6) red solid
(11) Pigment Red 177
(12) 65300
(13) KBr pellet

22311 $C_{28}H_{16}N_2O_4 + CaCO_3$



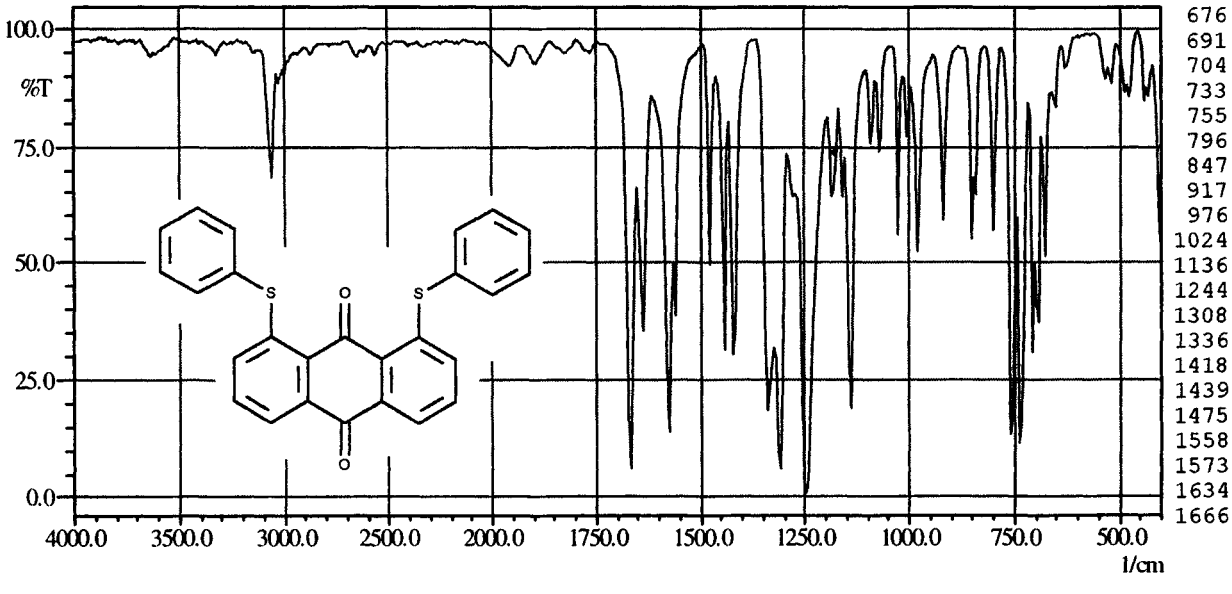
(1) **4,4-*bis*(1-amino-9,10-anthraquinonediyl) on $CaCO_3$**
(2) Cromophtal Rot C20
(3) Ciba
(4) 444.4 g mol^{-1}
(5) dispersed organic pigment
(6) red solid
(13) KBr pellet

22311 $C_{15}H_{11}NO_2$



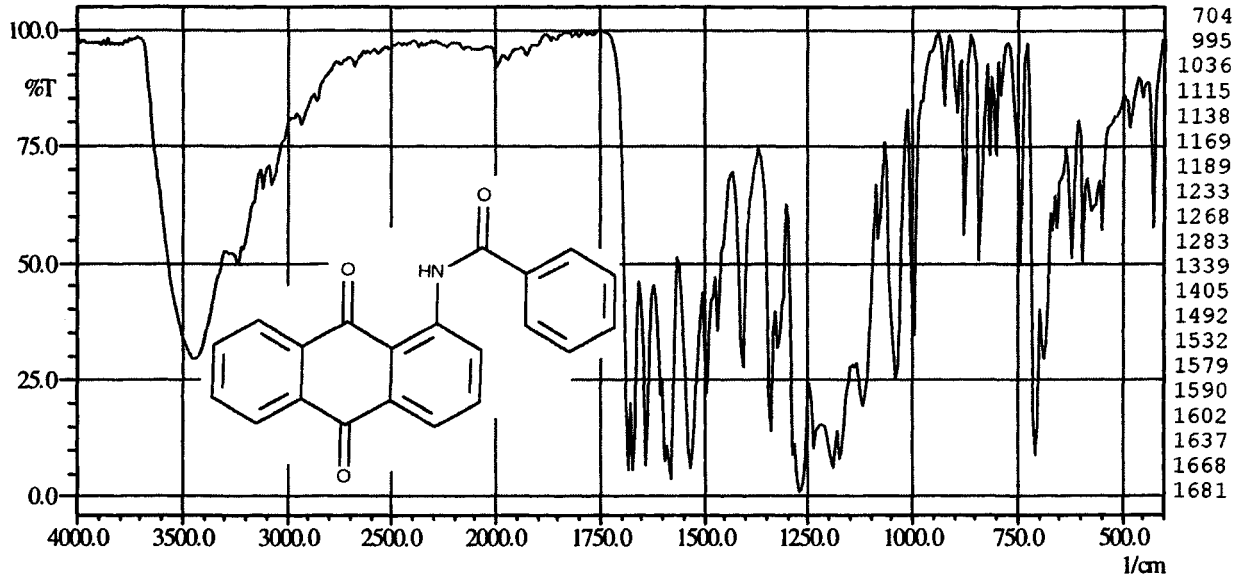
(1) **1-methylamino-9,10-anthraquinone**
(2) Oracet Red G
(3) Ciba-Geigy
(4) 237.3 g mol^{-1}
(5) organic pigment
(6) red solid
(11) Solvent Red 111
(12) 60505

22311 $C_{26}H_{16}O_2S_2$



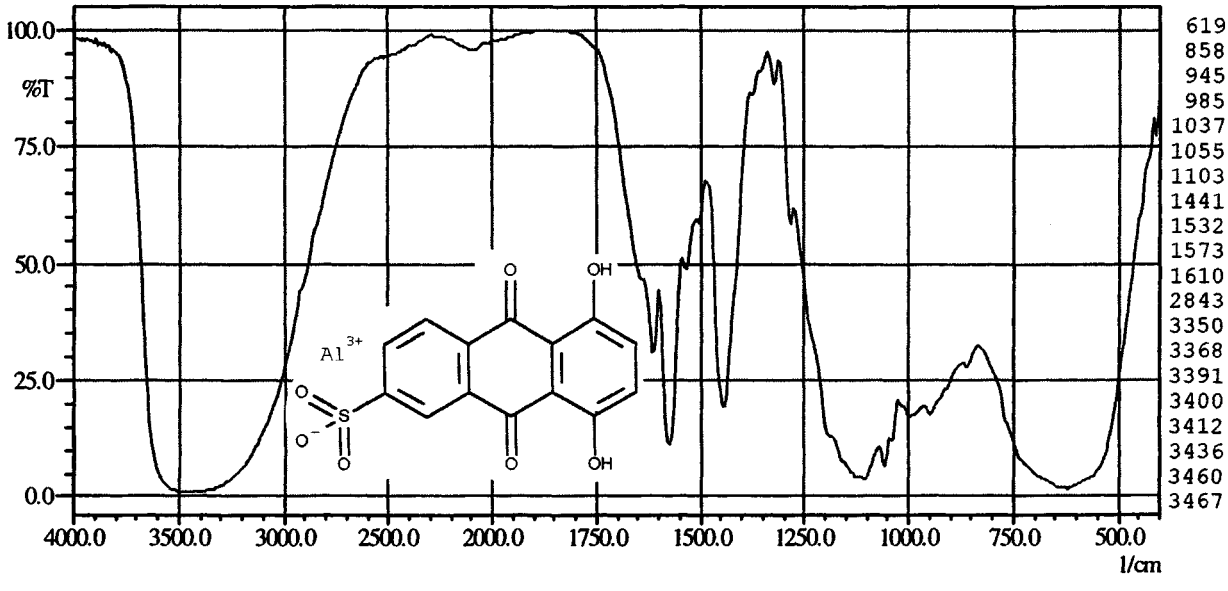
(1) **1,8-*bis*(thiophenyl)-9,10-anthraquinone**
(2) Oracet Yellow GHS
(3) Ciba-Geigy
(4) 424.5 g mol^{-1}
(5) organic pigment
(6) yellow solid
(11) Solvent Yellow 163
(12) 58840
(13) KBr pellet

22311 $C_{21}H_{13}NO$



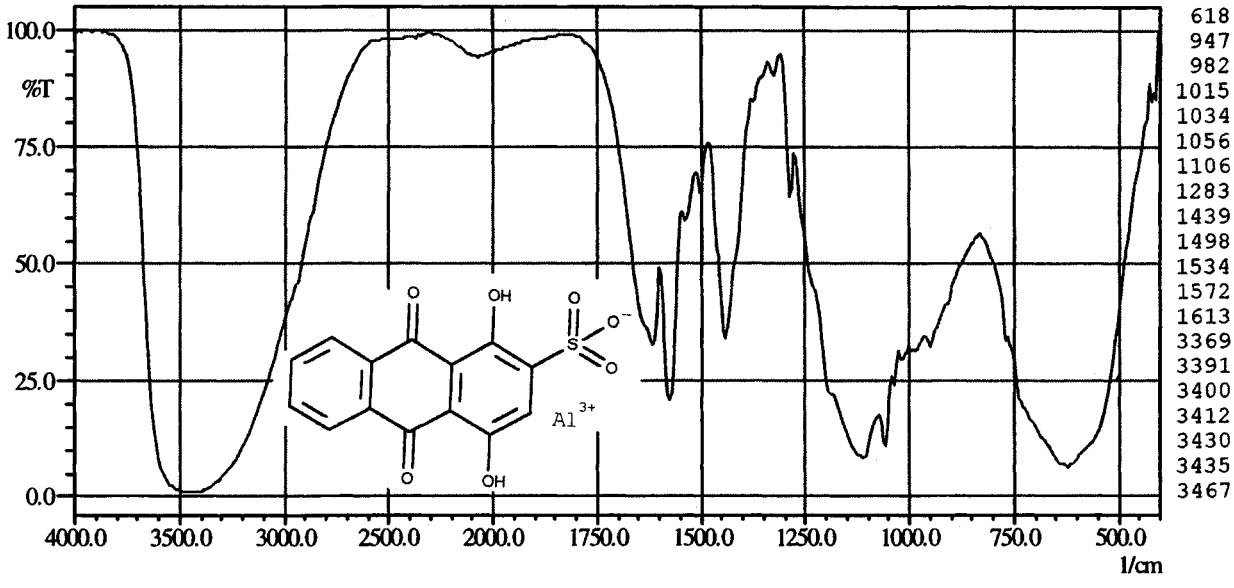
(1) **1-aminoanthraquinonebenzamide**
(2) Pigmosolgelb G
(3) commercial
(4) 295.3 g mol^{-1}
(5) organic pigment
(6) yellow solid
(13) KBr pellet

22311 $C_{14}H_7O_7SAl$



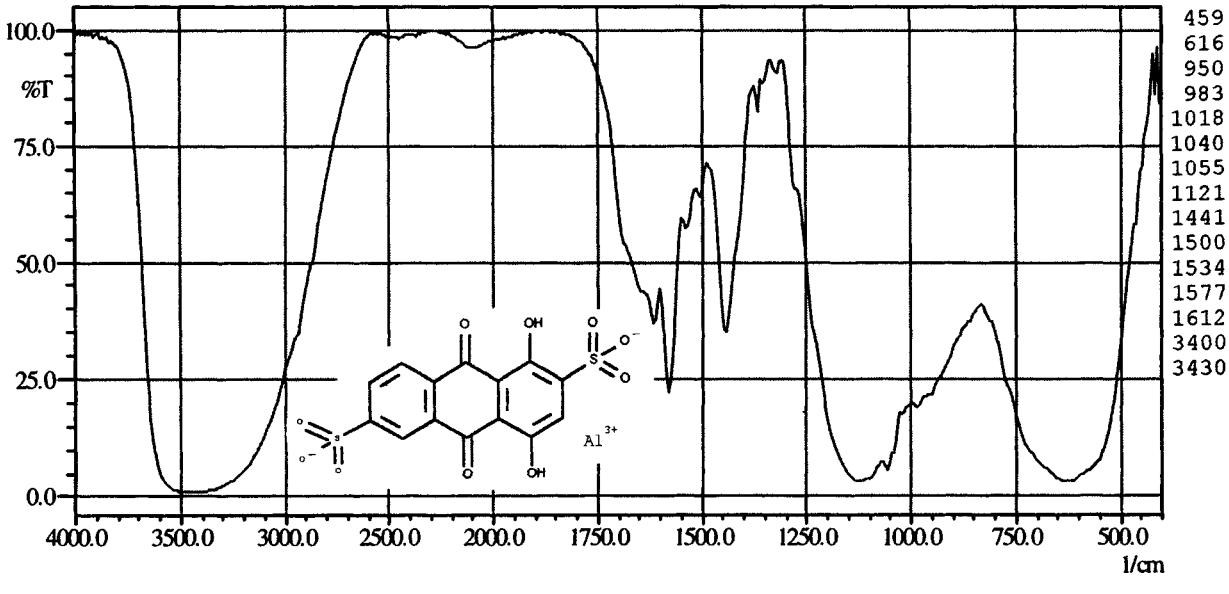
(1) **quinizarin-2-sulfonic acid, Al-salt**
(2) Violett 31372
(3) commercial
(4) 346.3 g mol^{-1}
(5) organic pigment
(6) violet solid
(11) Pigment Violet 5
(12) 58055
(13) KBr pellet

22311 $C_{14}H_7O_7SAl$



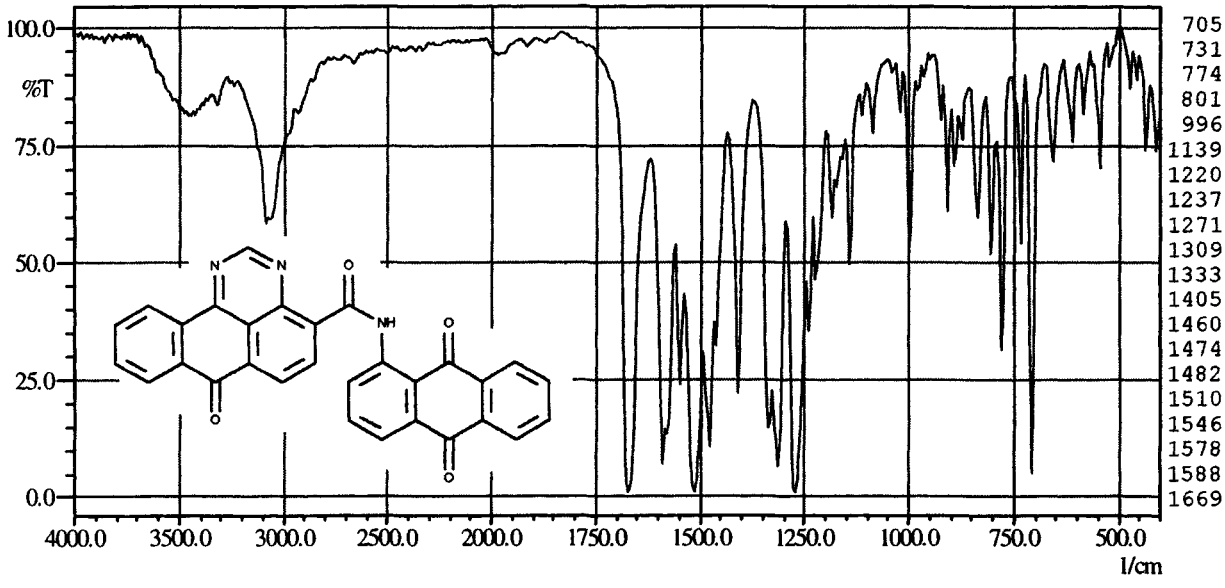
(1) **quinizarin-6-sulfonic acid, Al-lake**
(2) Violett 31372 R
(3) commercial
(4) 346.3 g mol^{-1}
(5) organic pigment
(6) violet solid
(11) Pigment Violet 6
(12) 58060
(13) KBr pellet

22311 $C_{14}H_6O_{10}S_2Al$



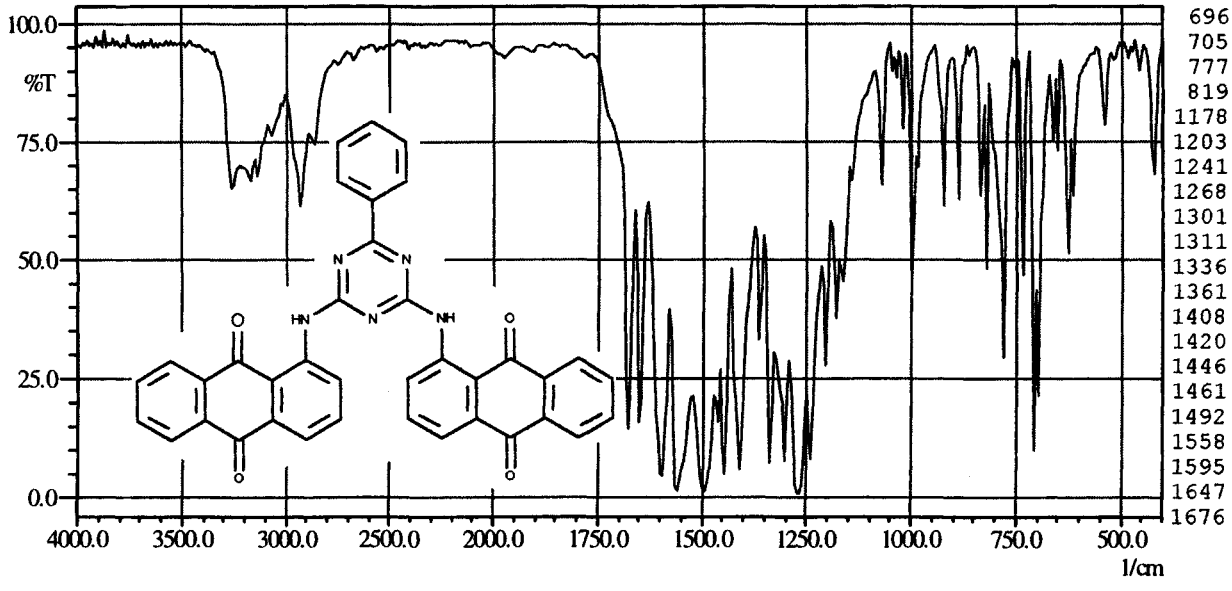
(1) **quinizarin-2,6-disulfonic acid Al-salt**
(2) Violett 31372 B
(3) commercial
(4) 425.3 g mol^{-1}
(5) organic pigment
(6) violet solid
(11) Pigment Violet 7
(12) 58065
(13) KBr pellet

22311 $C_{30}H_{15}N_3O_4$



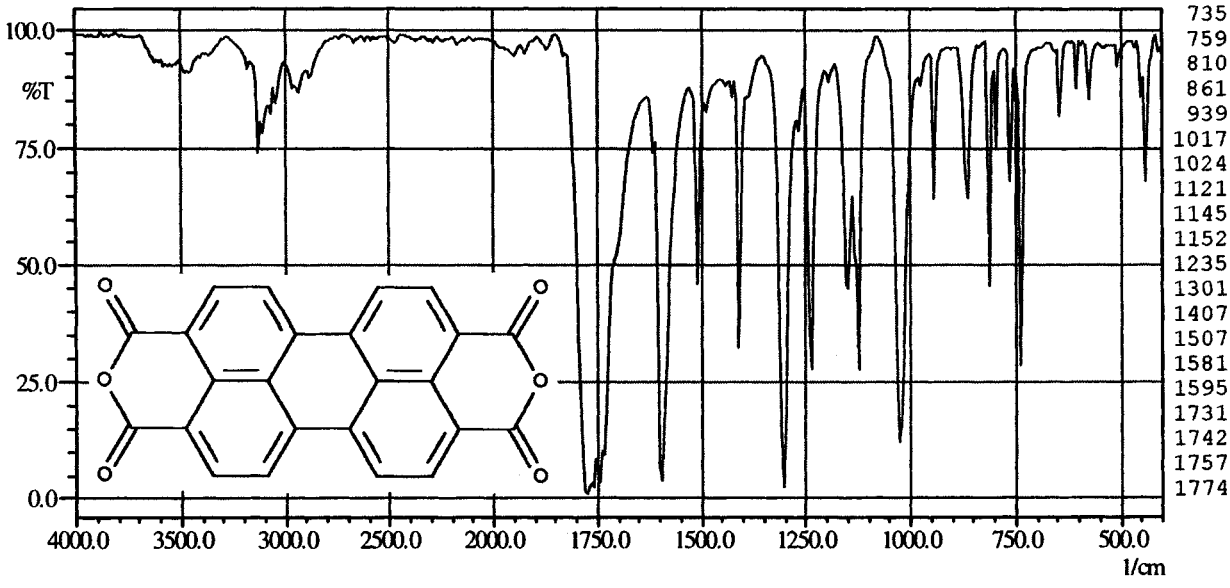
(1) **N-1-anthraquinone-anthrapyrimidine-4-carboxylic amide**
(2) Paliogen Gelb 1560
(3) BASF
(4) 481.5 g mol^{-1}
(5) organic pigment
(6) yellow solid
(11) Pigment Yellow 108
(12) 68420
(13) KBr pellet

22311 $C_{37}H_{21}N_5O_4$



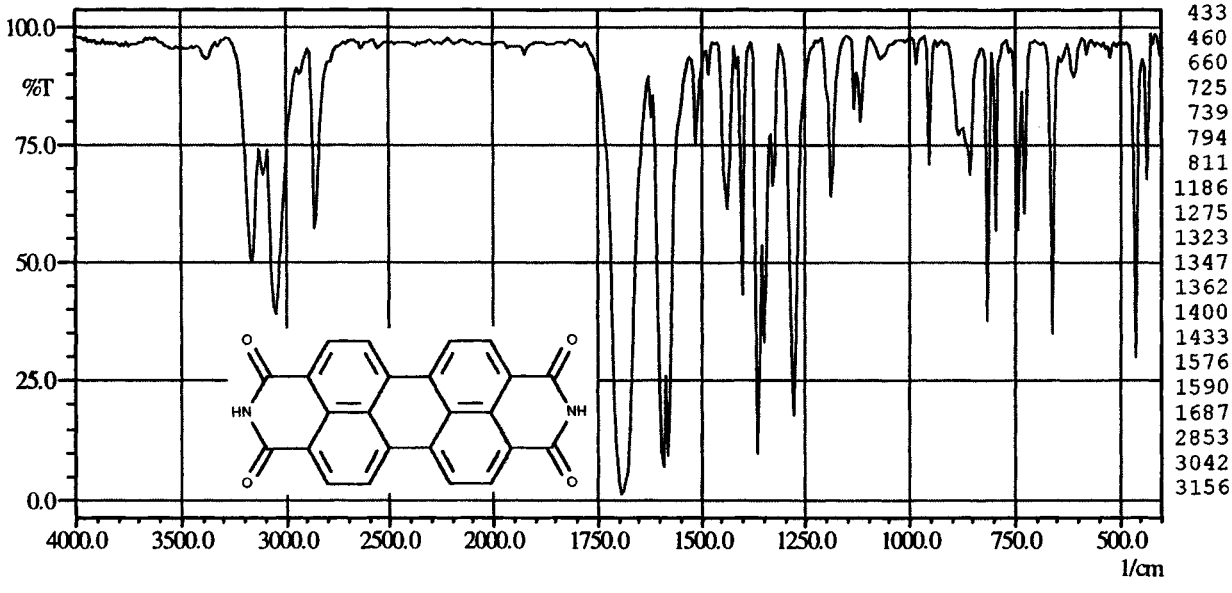
(1) **N,N'-(5-phenyl-1,3-triazine)-*bis*(1-amino-9, 10-anthraquinone)**
(2) Cromophtal Gelb AGR
(3) Ciba-Geigy
(4) 599.6 g mol^{-1}
(5) organic pigment
(6) yellow solid
(11) Pigment Yellow 147
(13) KBr pellet

22312 $C_{24}H_8O_6$



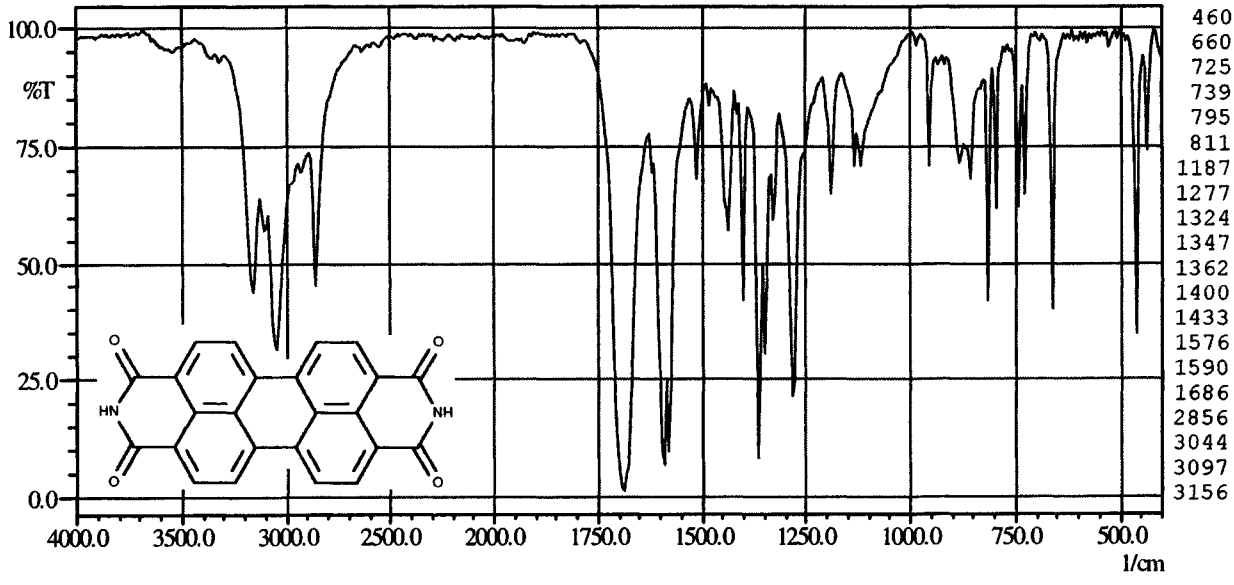
(1) **perylene-3,4,9,10-tetracarboxylic acid anhydride**
(2) Irgazin Rot BPT
(3) Ciba-Geigy
(4) 392.3 g mol^{-1}
(5) organic pigment
(6) red solid
(11) Pigment Red 224
(12) 71127
(13) KBr pellet

22312 $C_{24}H_{10}N_2O_4$



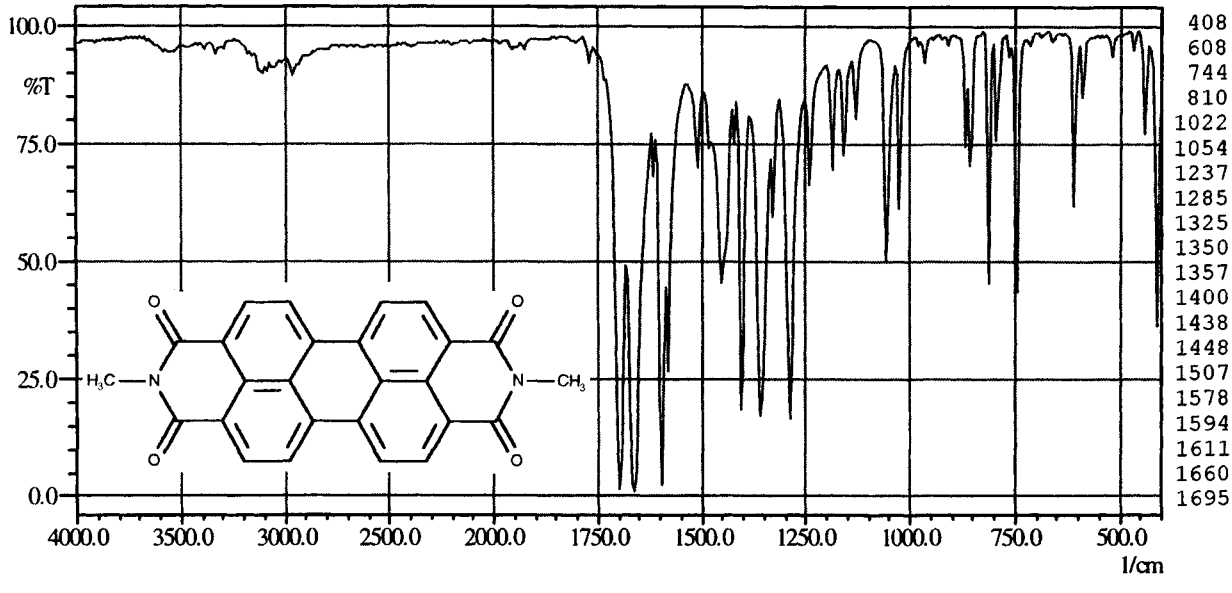
(1) **perylene-3,4,9,10-tetracarboxylic acid diimide**
(2) Perindo Violet V4047
(3) Harmon
(4) 390.3 g mol^{-1}
(5) organic pigment
(6) violet solid
(11) Pigment Violet 29
(12) 71129
(13) KBr pellet

22312 $C_{24}H_{10}N_2O_4$



(1) **perylene-3,4,9,1-tetracarboxylic acid diimide**
(2) PV-Echtbordo B
(3) Hoechst
(4) 390.3 g mol^{-1}
(5) organic pigment
(6) dark-red solid
(11) Pigment Brown 26
(12) 71129
(13) KBr pellet

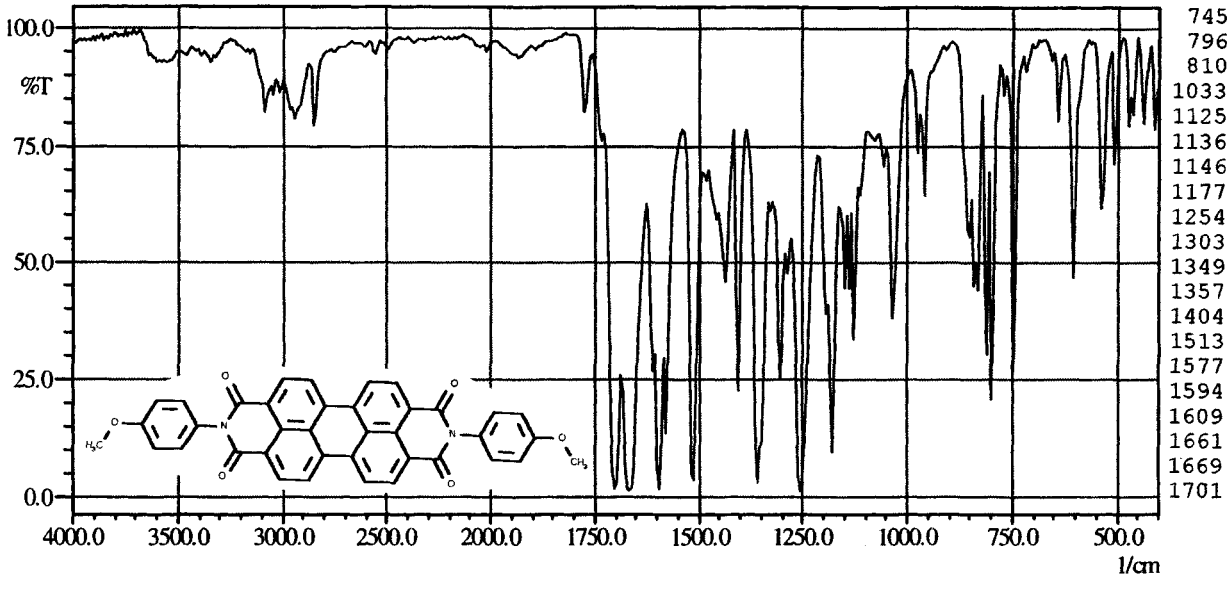
22312 $C_{26}H_{14}N_2O_4$



(1) **N,N'-dimethylperylene-3,4,9,10-tetracarboxylic acid diimide**
(2) Paliogen Red L 4120
(3) BASF
(4) 418.4 g mol^{-1}
(5) organic pigment
(6) red solid
(11) Pigment Red 179
(12) 71130
(13) KBr pellet

22312

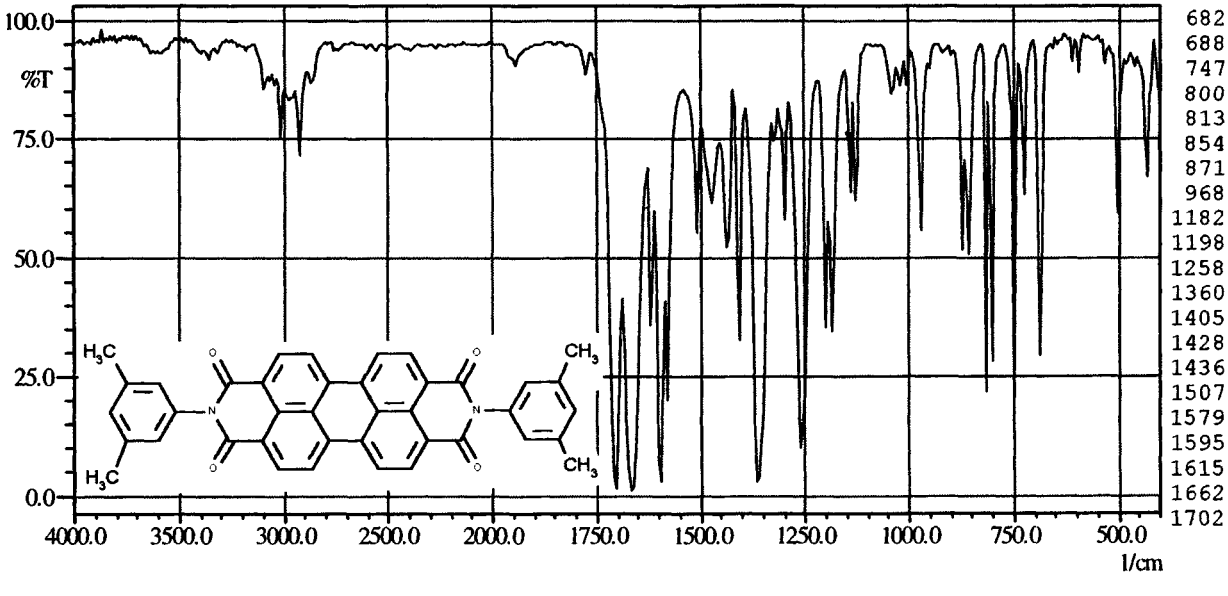
$C_{38}H_{22}N_2O_6$



(1) **N,N'-di-4'-anisylperylene-3,4,9,10-tetracarboxylic acid diimide**
(2) Indofast Brilliant Scarlet R-6500
(3) Harmon
(4) 602.6 g mol^{-1}
(5) organic pigment
(6) scarlet solid
(11) Pigment Red 190
(12) 71140
(13) KBr pellet

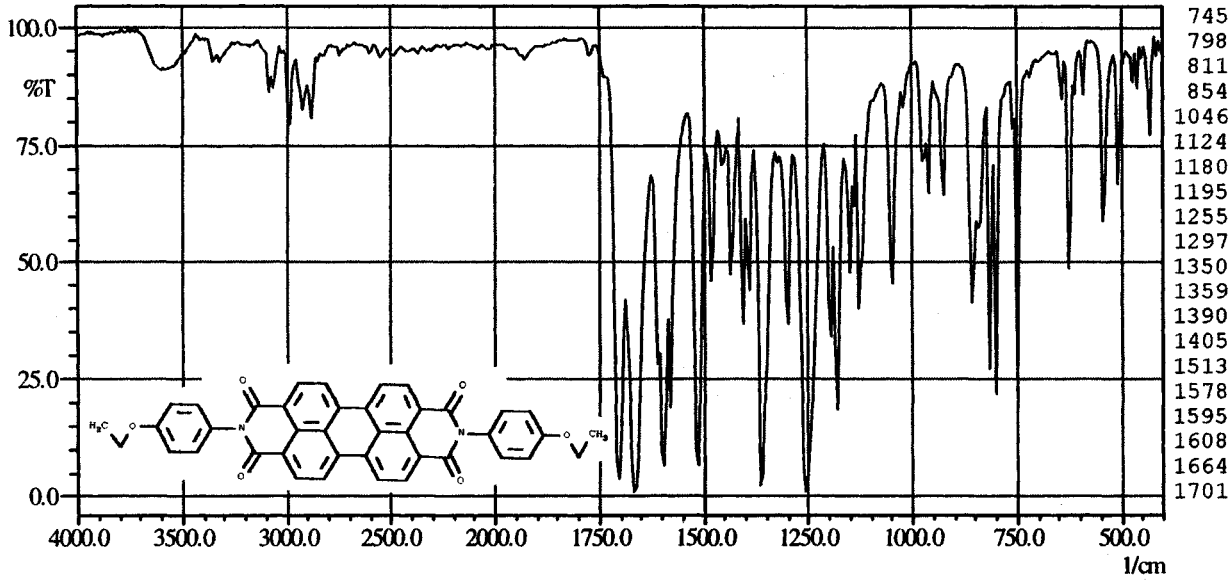
22312

$C_{40}H_{26}N_2O_4$



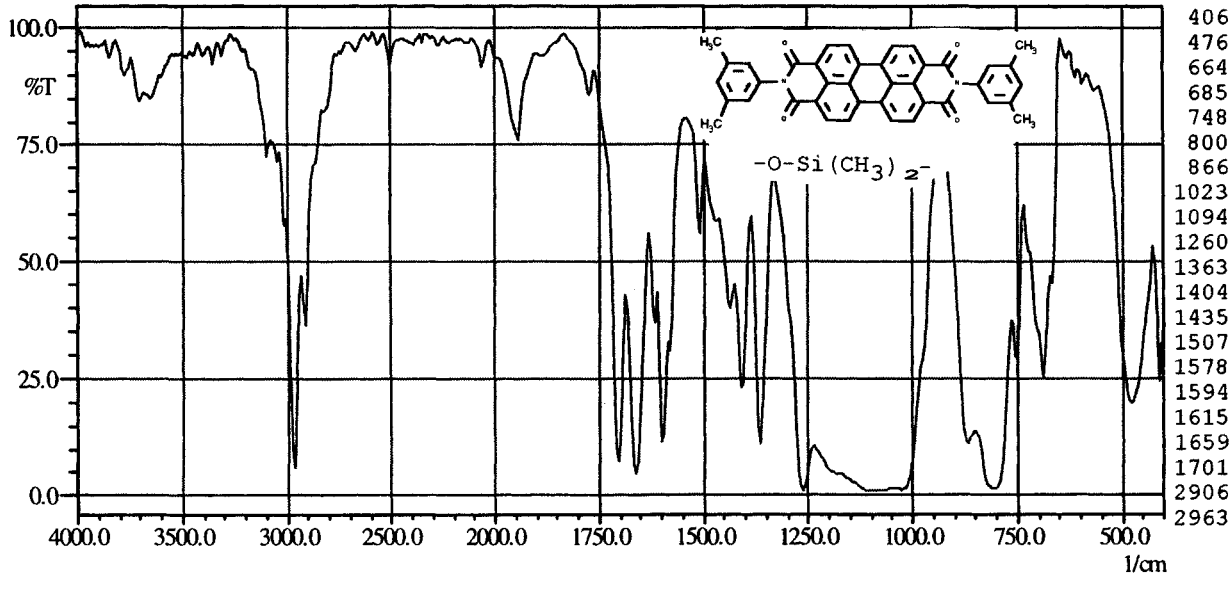
(1) **N,N'-di-3',5'-xylylperylene-3,4,9,10-tetracarboxylic acid diimide**
(2) Paliogen Rot K3580
(3) BASF
(4) 598.7 g mol^{-1}
(5) organic pigment
(6) red solid
(11) Pigment Red 149
(12) 71137
(13) KBr pellet

22312 $C_{40}H_{26}N_2O_6$



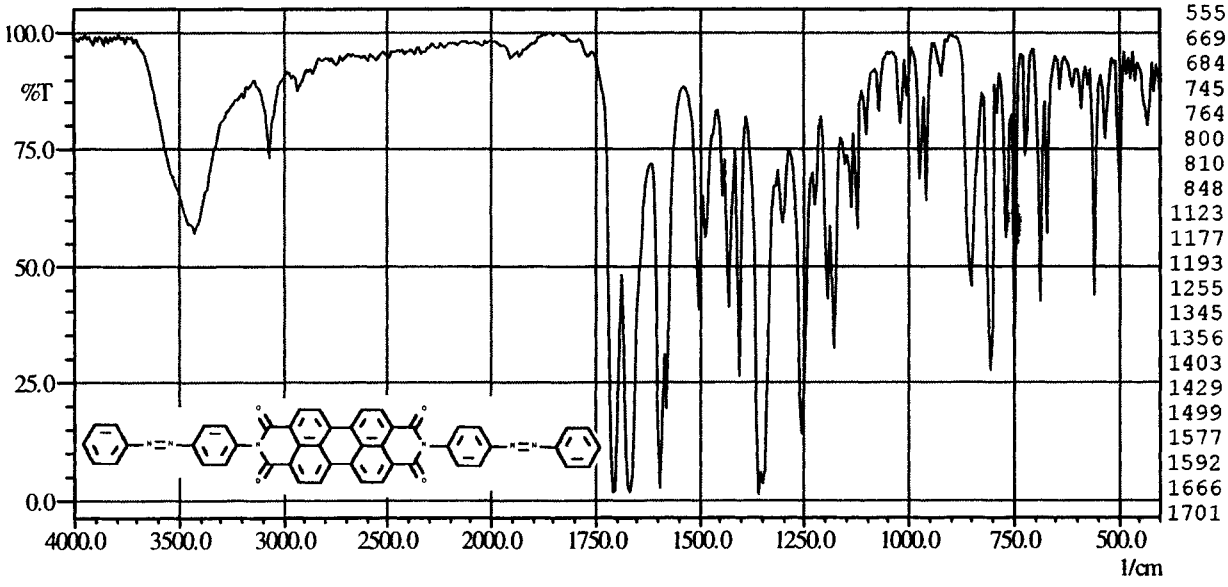
(1) **perylene derivative**
(2) Indofast Brilliant Scarlet-Toner R-6300
(3) Harmon
(4) 630.6 g mol^{-1}
(5) organic pigment
(6) scarlet solid
(11) Pigment Red 126
(13) KBr pellet

22312 $C_{40}H_{26}N_2O_4$



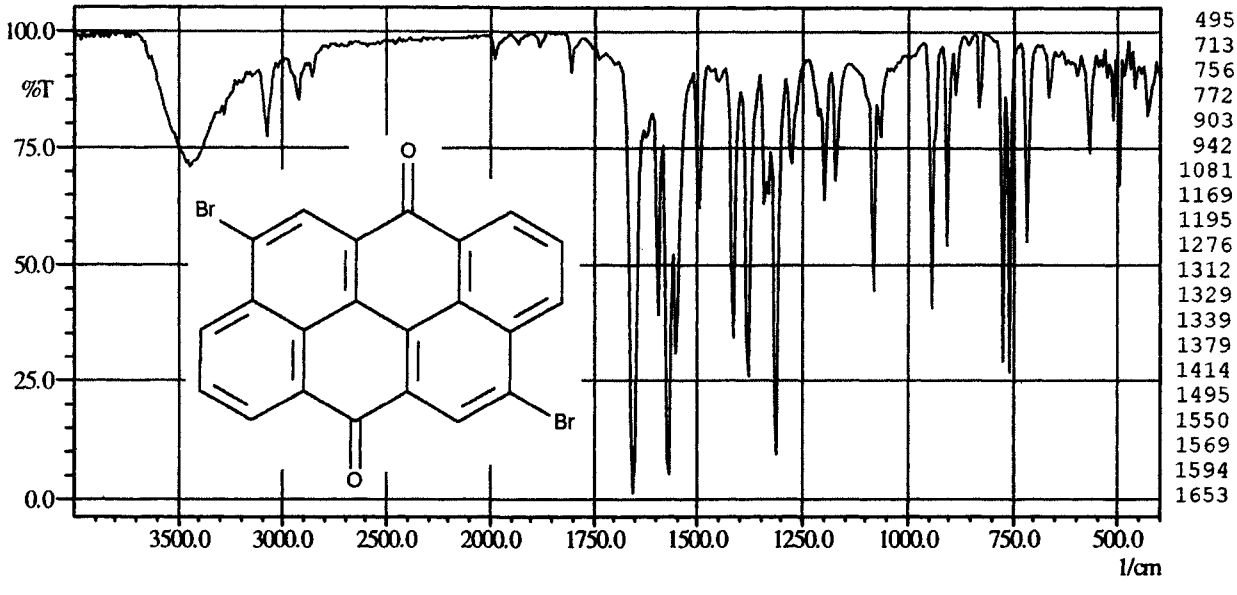
(1) **N,N'-di-3',5'-xylylperylene-3,4,9,10-tetracarboxylic acid diimide with poly(dimethylsiloxane)**
(2) Wacker HTV-Farbpaste
(3) Wacker
(4) 598.7 g mol^{-1}
(5) dispersed organic pigment
(6) red paste
(13) layer on KBr

22312 $C_{48}H_{26}N_6O_4$



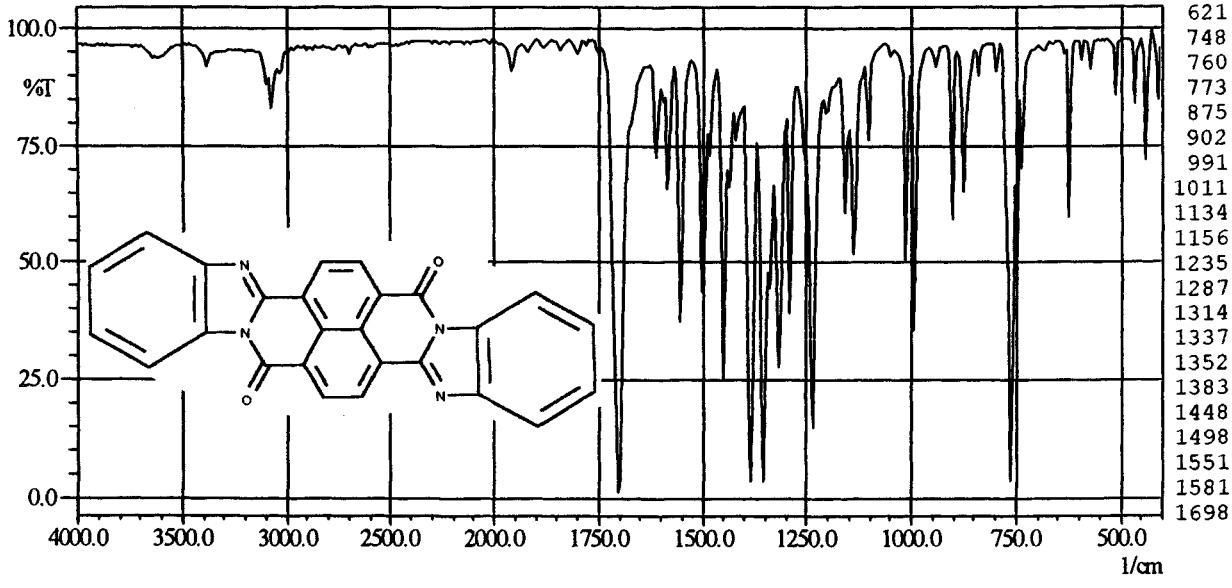
(1) **diimide of 3,4,9,10-perylenetetracarboxylic acid with 4-phenylazoaniline**
(2) Paliogen Rot L3910 HD
(3) Hoechst
(4) 750.8 g mol^{-1}
(5) organic pigment
(6) red solid
(11) Pigment Red 178
(12) 71155
(13) KBr pellet

22313 $C_{22}H_8Br_2O_2$



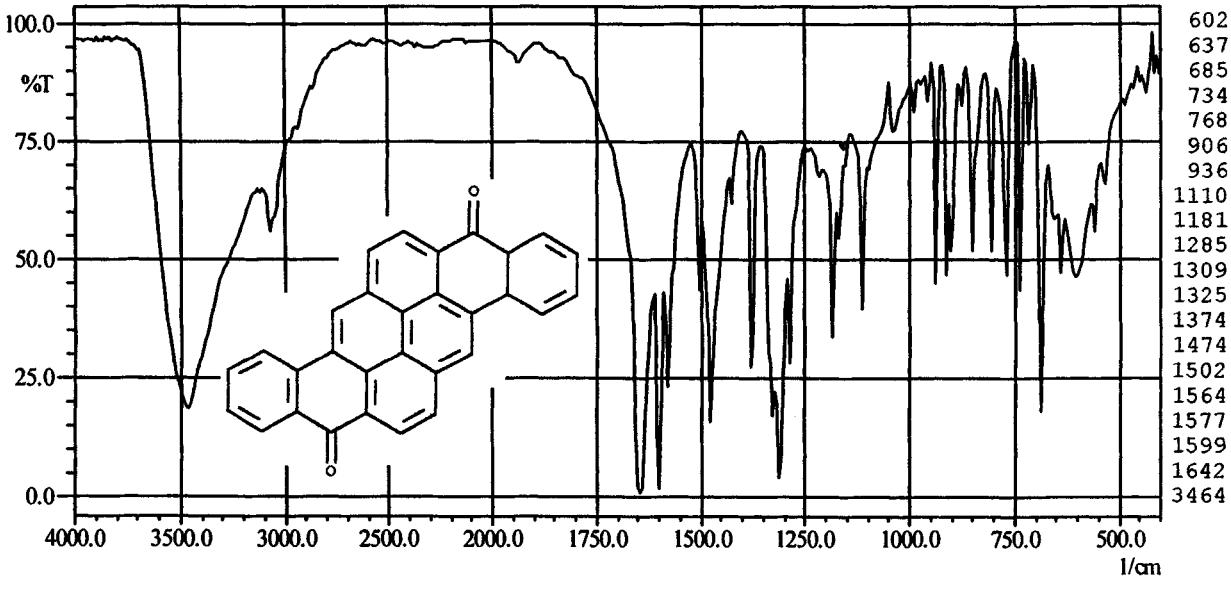
(1) **2,7-dibromoanthanthrone**
(2) Monolite Red Y
(3) ICI
(4) 464.1 g mol^{-1}
(5) organic pigment
(6) light-red solid
(11) Pigment red 168

22314 $C_{26}H_{12}N_4O_2$



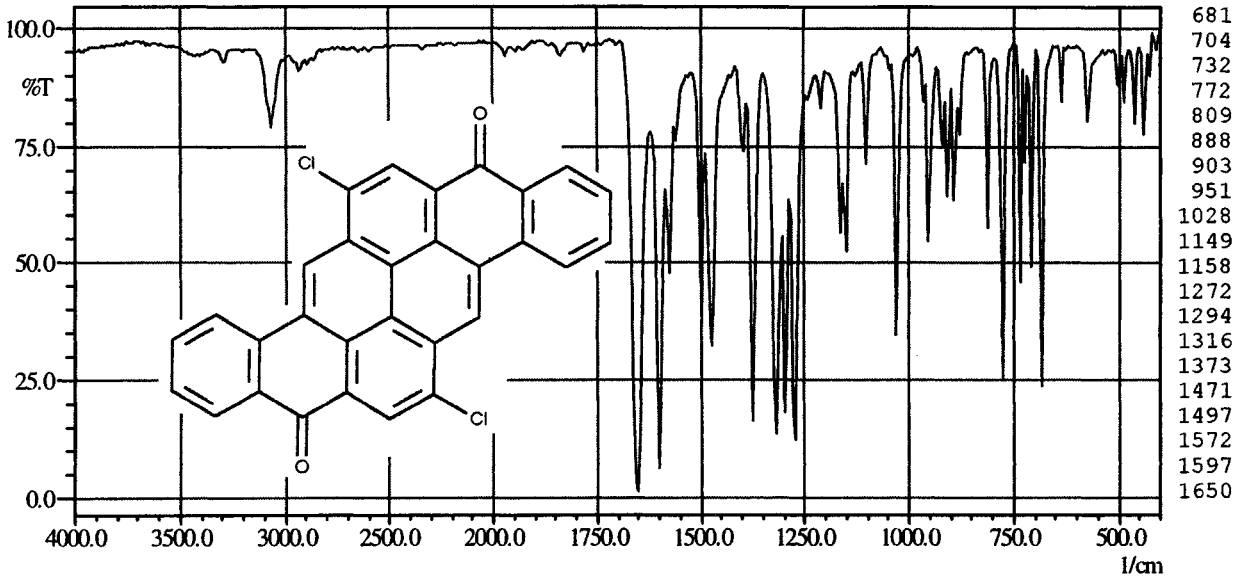
(1) **dibenzimidazolo(1,2-e,1',2'-m)-4,9-diaza-3,8-pyrenequinone**
(2) PV-Echtorange GRL
(3) Hoechst
(4) 412.4 g mol^{-1}
(5) organic pigment
(6) orange solid
(11) Pigment Orange 43
(12) 71105
(13) KBr pellet

22315 $C_{30}H_{14}O_2$



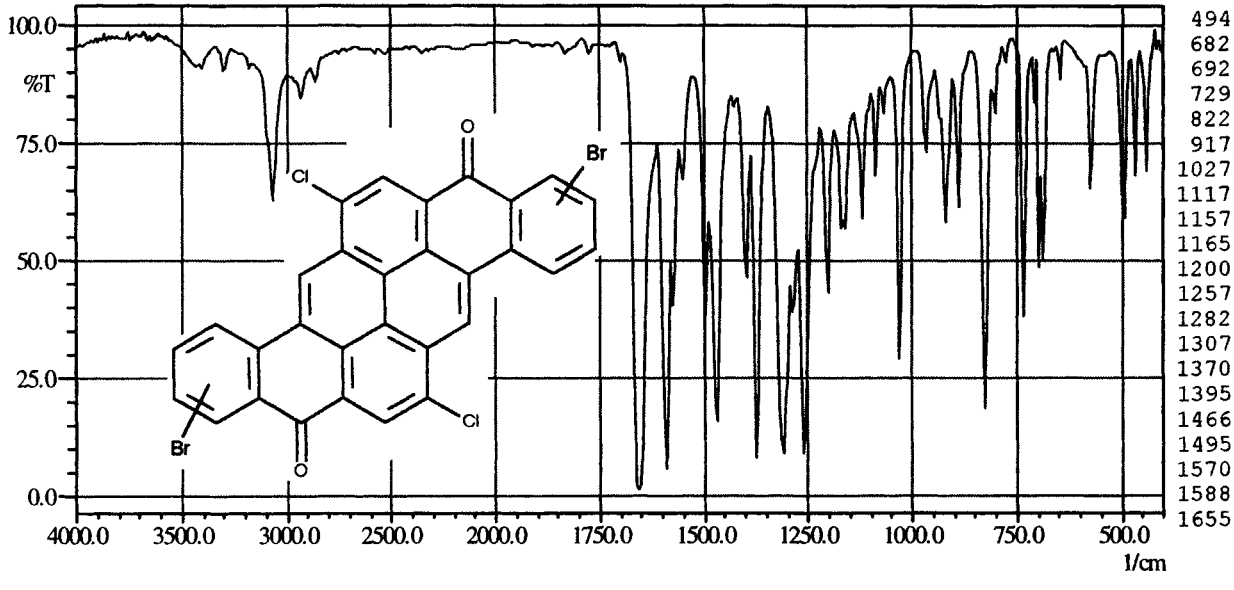
(1) **pyranthrone**
(2) Indanthren Goldorange G
(3) Hoechst
(4) 406.4 g mol^{-1}
(5) organic pigment
(6) orange solid
(11) Pigment Orange 40
(12) 59700
(13) KBr pellet

22315 $C_{30}H_{12}Cl_2O_2$



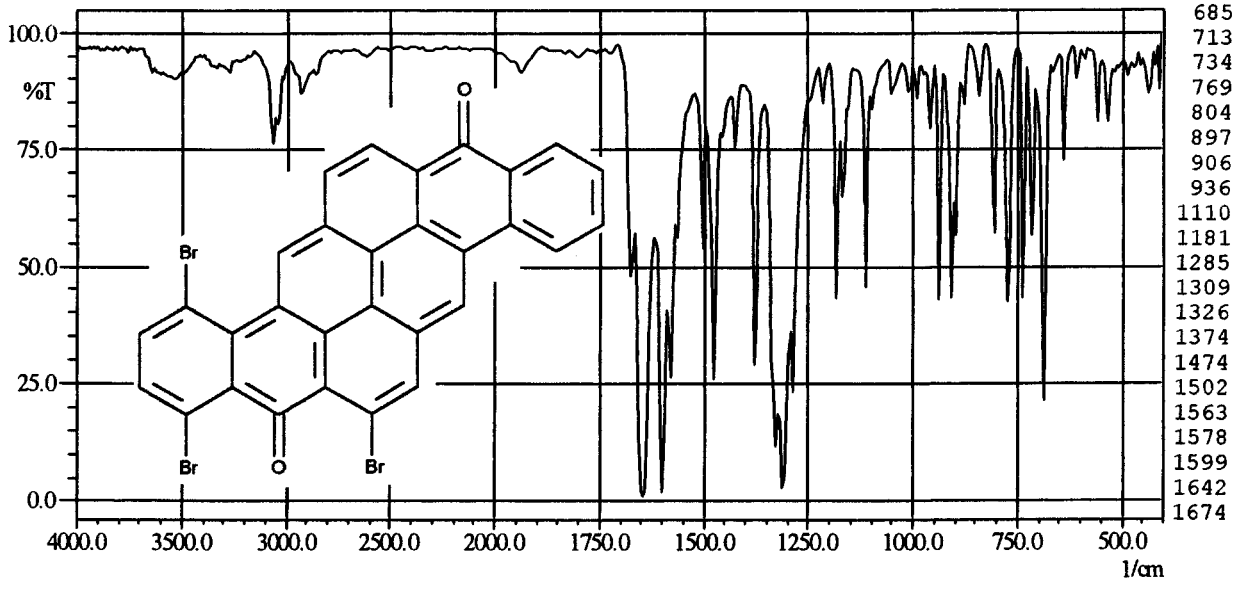
(1) **6,14-dichloropyranthrone**
(2) Paliogen Orange L 2640
(3) BASF
(4) 475.3 g mol^{-1}
(5) organic pigment
(6) orange solid
(11) Pigment Orange 51
(13) KBr pellet

22315 $C_{30}H_{10}Cl_2Br_2O_2$



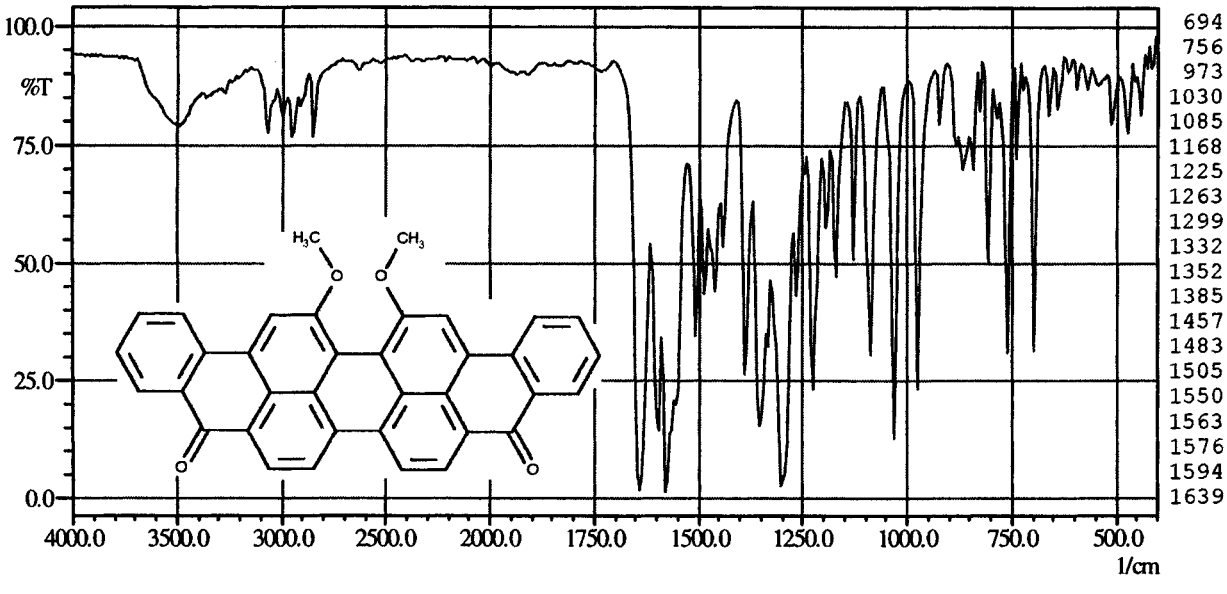
(1) **6,14-dichloro-1,9-dibromopyranthrone**
(2) Paliogen Rot L 3340
(3) BASF
(4) 633.1 g mol^{-1}
(5) organic pigment
(6) red solid
(11) Pigment Red 226
(13) KBr pellet

22315 $C_{30}H_{11}Br_3O_2$



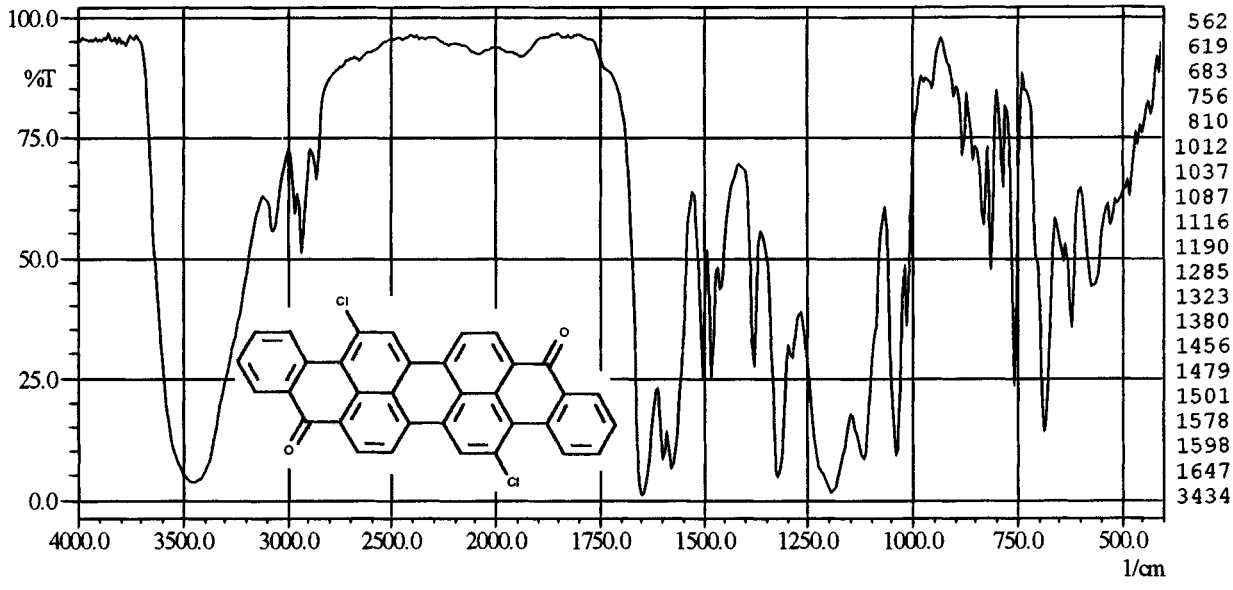
(1) **7,9,12-tribromopyranthrone**
(2) Paliogen Orange 3GT
(3) BASF
(4) 643.1 g mol^{-1}
(5) organic pigment
(6) orange solid
(11) Pigment Red 216
(12) 59710
(13) KBr pellet

22316 $C_{34}H_{20}O_4$



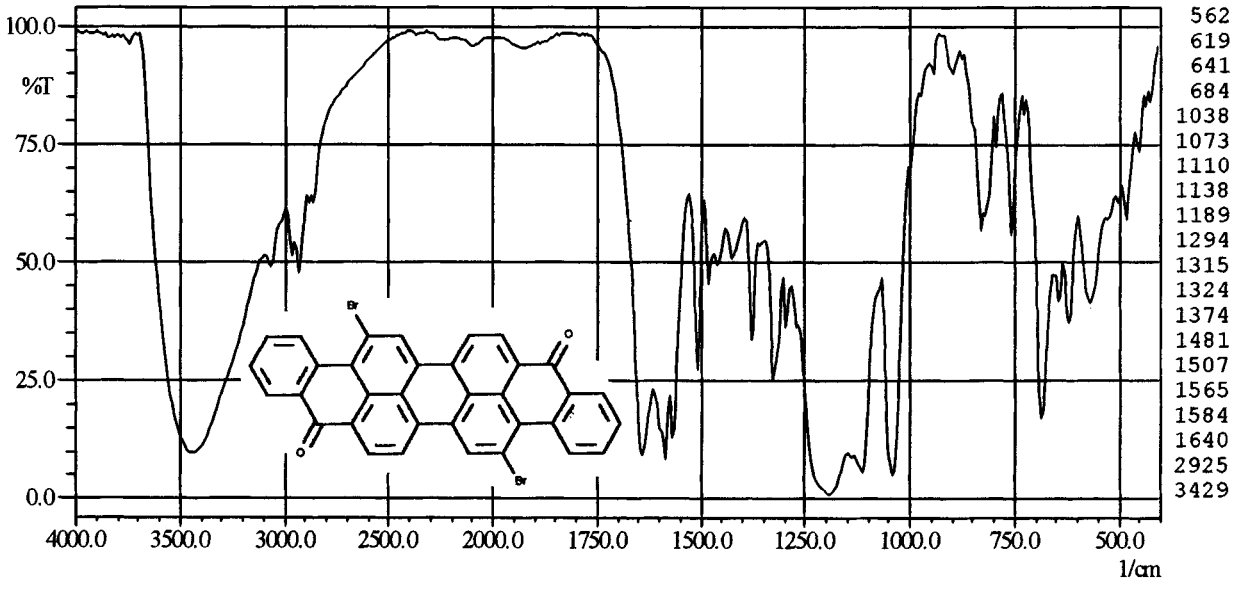
(1) **16,17-dimethoxyviolanthrone**
(2) Indanthren Brilliant Gruen FFB
(3) Hoechst
(4) 492.5 g mol^{-1}
(5) organic pigment
(6) green solid
(11) VAT Green 1
(12) 59825
(13) KBr pellet

22316 $C_{34}H_{14}Cl_2O_2$



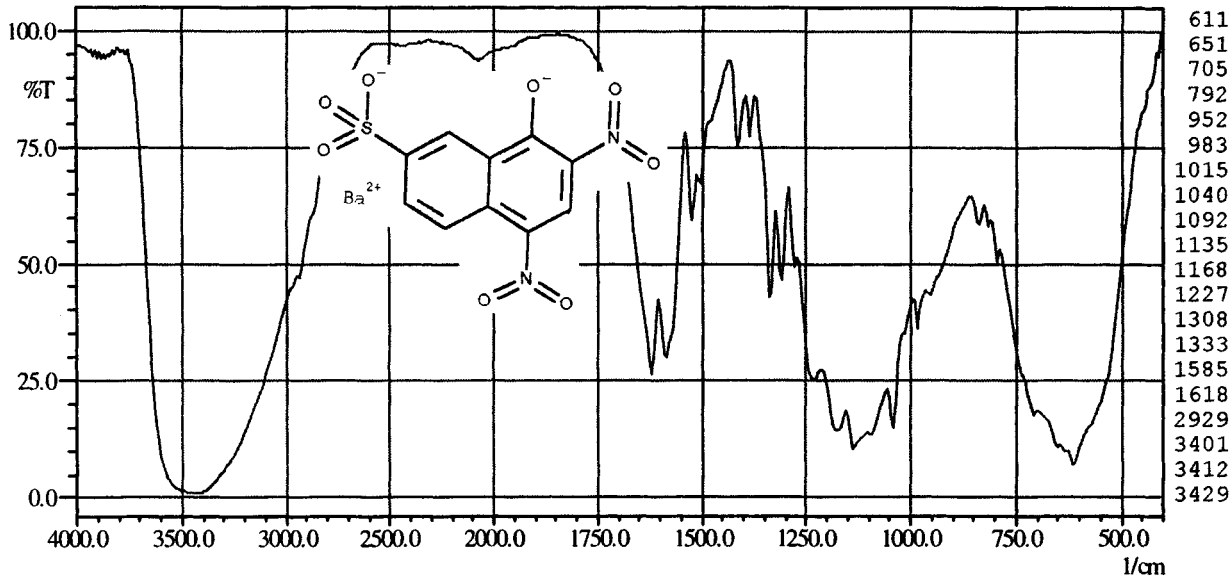
(1) **5,14-dichloroisoviolanthrone**
(2) Indanthren Brilliant Violett RR
(3) Hoechst
(4) 525.4 g mol^{-1}
(5) organic pigment
(6) violet solid
(11) VAT Violet 1
(12) 60010
(13) KBr pellet
(14) partially converted into quinhydrone derivative

22316 $C_{34}H_{14}Br_2O_2$



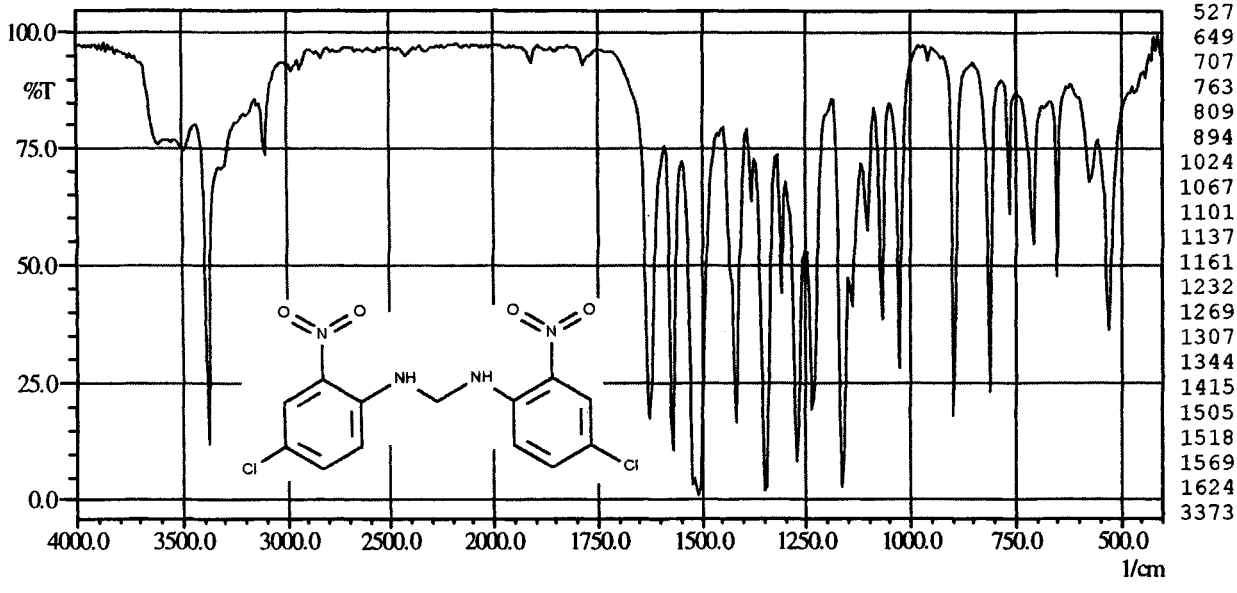
(1) **5,14-dibromoisoviolanthrone**
(2) Indanthren Brilliant Violett 3B
(3) Hoechst
(4) 614.3 g mol^{-1}
(5) organic pigment
(6) violet solid
(11) VAT Violet 9
(12) 60005
(13) KBr pellet
(14) partially converted into quinhydrone derivative

22317 $C_{10}H_4N_2O_7SBa$



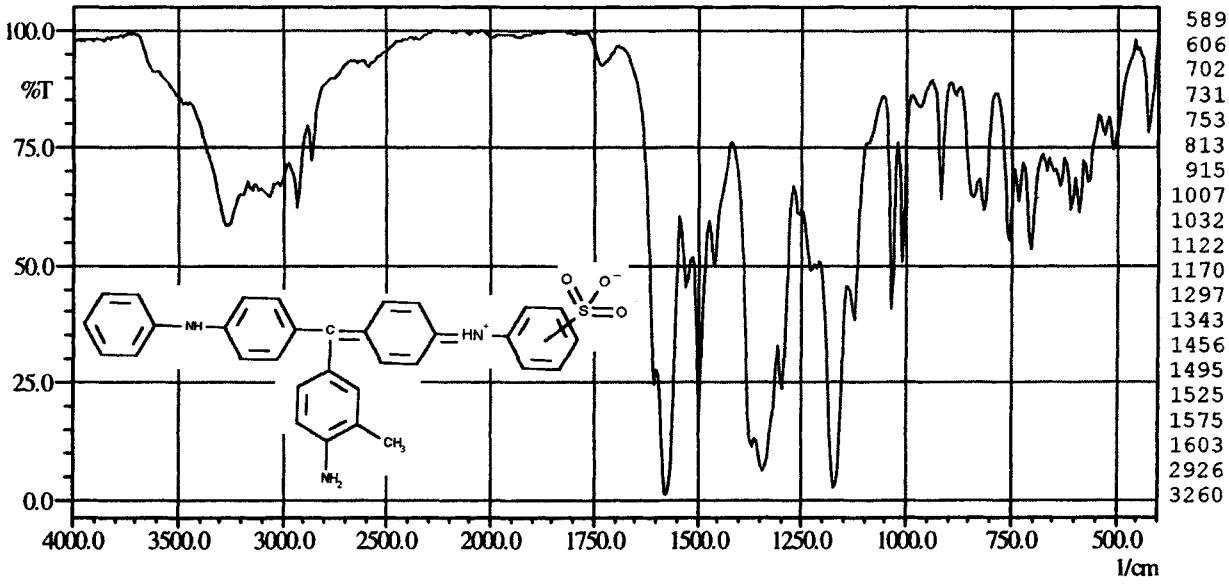
(1) **2,4-dinitro-1-naphthol-7-sulfonic acid, Ba-lake on blanc fixe**
(2) Hellgelber Lack 1
(3) commercial
(4) 433.5 g mol^{-1}
(5) organic pigment
(6) yellow solid
(11) Acid Yellow 1
(12) 10316
(13) KBr pellet

22318 $C_{13}H_8Cl_2N_4O_4$



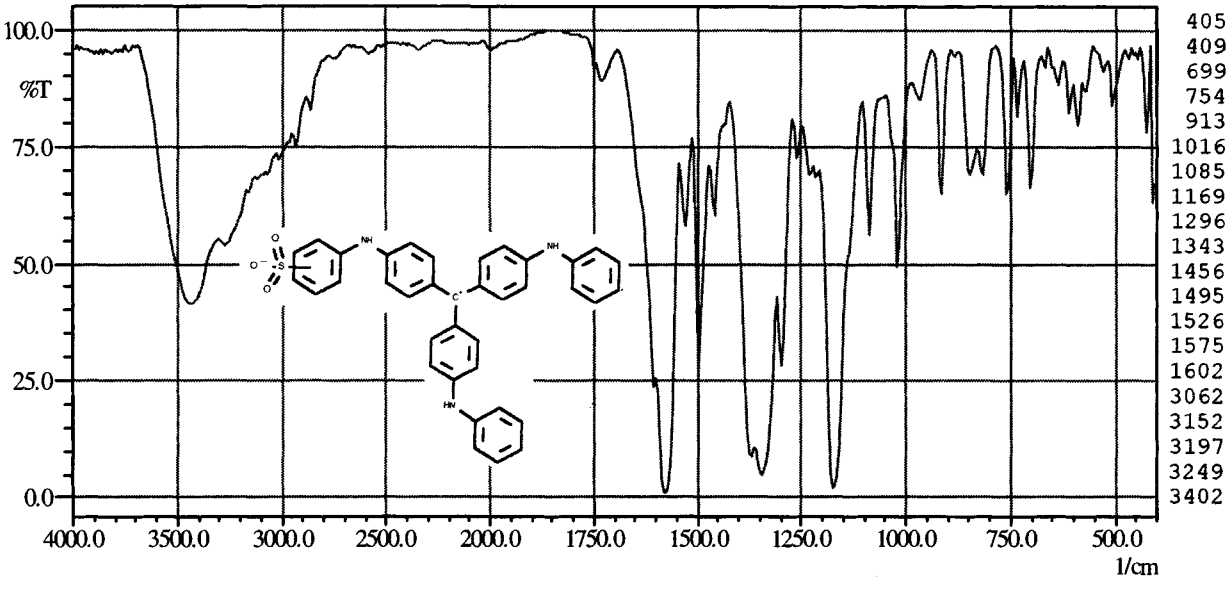
(1) **N,N'-di-4-chloro-2-nitrophenylmethylendiamine, methylen-bis(4-chloro-2-nitrophenylamin)**
(2) Lithol Echtgelb GG
(3) BASF
(4) 355.1 g mol^{-1}
(5) organic pigment
(6) yellow solid
(11) Pigment Yellow 11
(12) 13205
(13) KBr pellet

22318 $C_{31}H_{27}N_3O_3S$



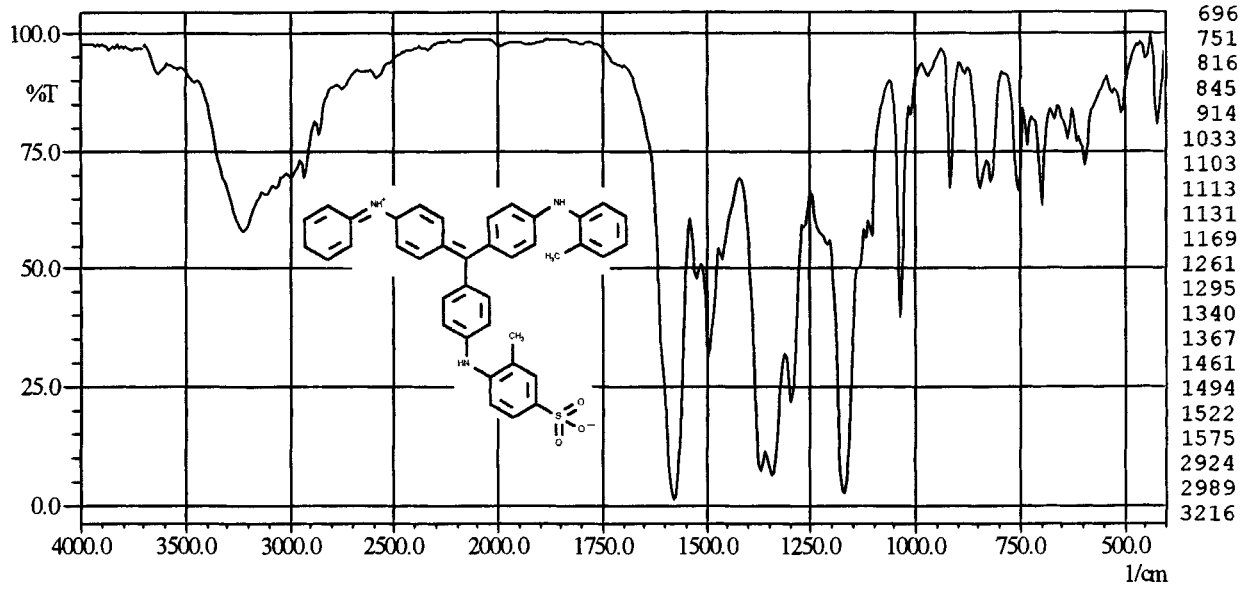
(1) **4-(amino-3-tolyl)-4'-N-phenylaminophenyl-4"-N-sulfophenylaminophenylmethane, free acid**
(2) Arionblau 1
(3) Siegle
(4) 521.6 g mol^{-1}
(5) organic pigment
(6) blue solid
(11) ACID Blue 110
(12) 42750
(13) KBr pellet

22318 $C_{37}H_{29}N_3O_3S$



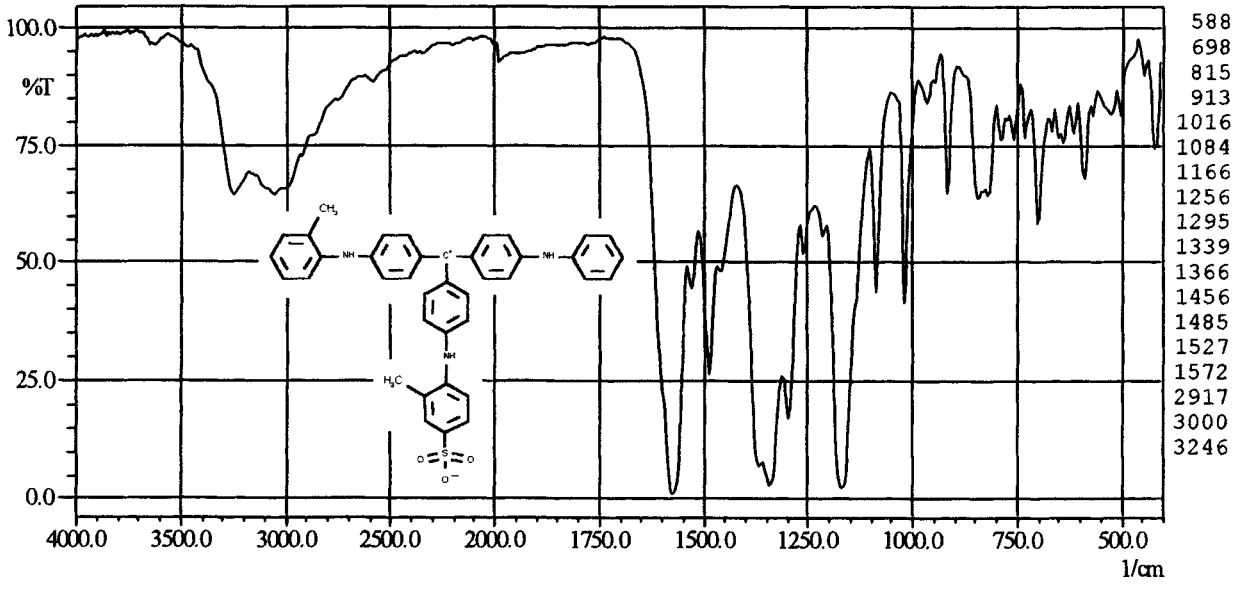
(1) ***bis*(4-N-phenylaminophenyl)-4-N"-sulfophenylaminophenylmethane**
(2) Reflex Blau R51
(3) Hoechst
(4) 595.7 g mol^{-1}
(5) organic pigment
(6) blue solid
(11) Pigment Blue 61:1
(12) 42765
(13) KBr pellet

22318 $C_{38}H_{33}N_3O_3S$



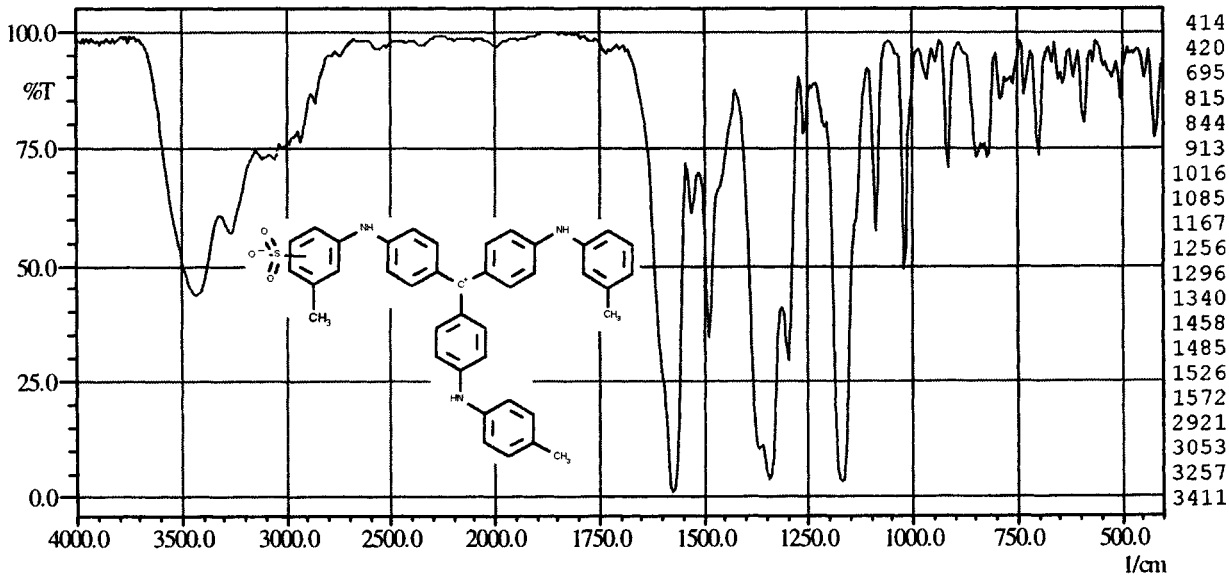
(1) **4-N-phenylaminophenyl-4'-N-(2"-tolylaminophenyl)-4"'-N-(4""-sulfo-2""-tolylaminophenyl)methane**
(2) Reflex Blau RB
(3) Hoechst
(4) 611.7 g mol^{-1}
(5) organic pigment
(6) blue solid
(11) Pigment Blue 57
(12) 42795
(13) KBr pellet

22318 $C_{39}H_{33}N_3O_3S$



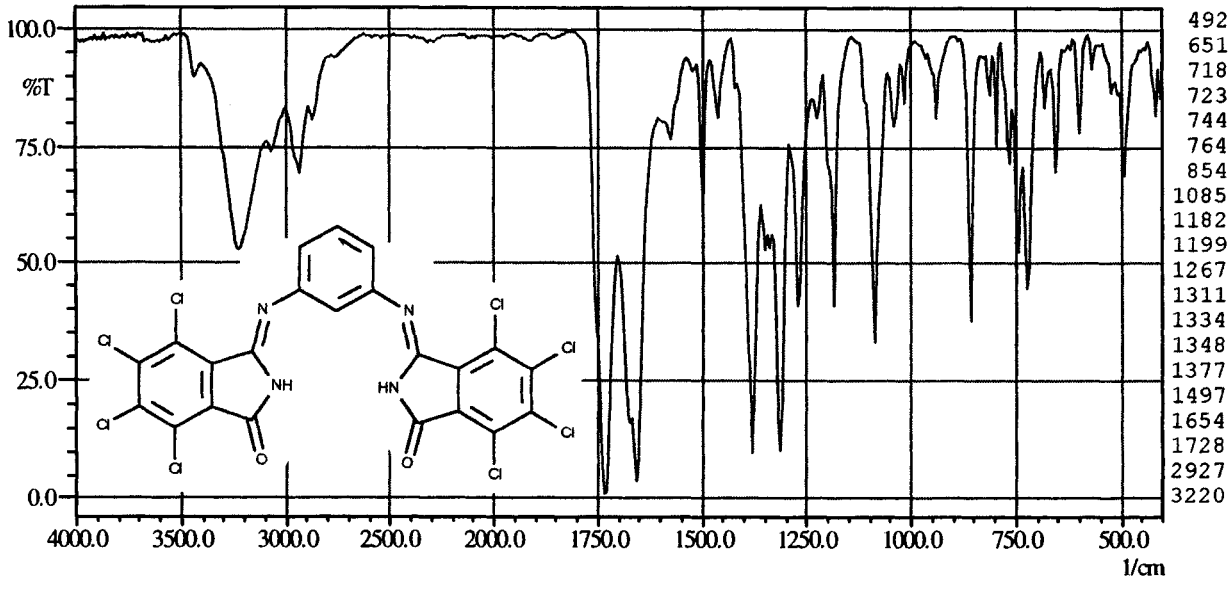
(1) ***bis*(4-N-3'-tolylaminophenyl)-4"-N-(4"'-sulfo-3"'-tolylaminophenyl)methane**
(2) Reflex Blau 2G
(3) Hoechst
(4) 623.8 g mol^{-1}
(5) organic pigment
(6) blue solid
(11) Pigment Blue 56
(12) 42800
(13) KBr pellet

22318 $C_{40}H_{35}N_3O_3S$



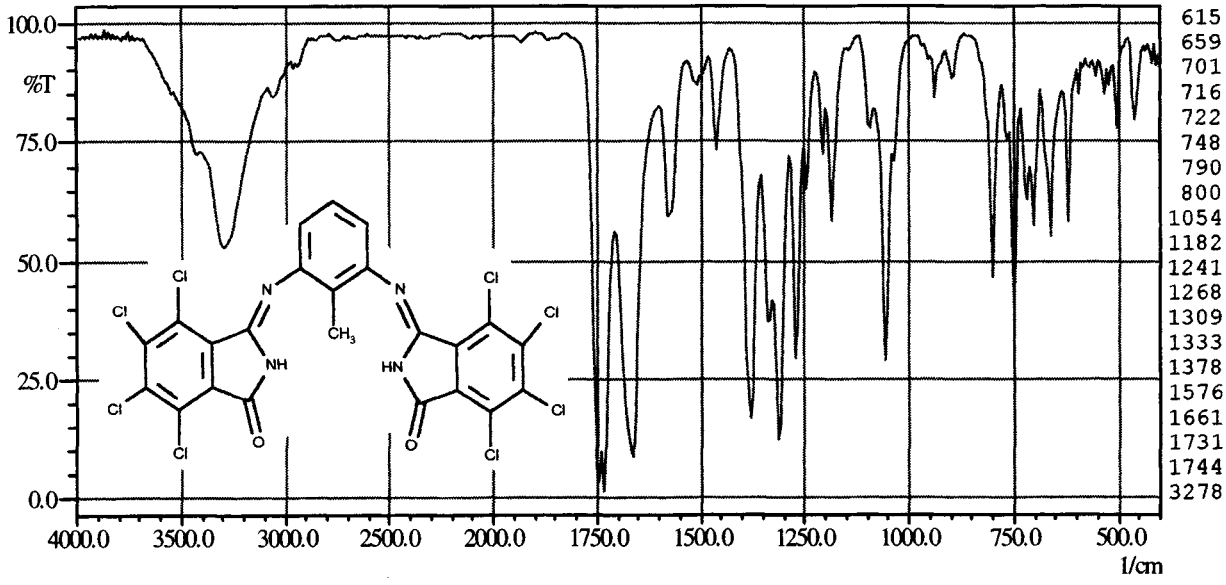
(1) ***bis*(4-N-3'-tolylaminophenyl)-4"-N-(4"'-sulfo-3"'-tolylaminophenyl)methane**
(2) Reflex Blau 3G 51
(3) Hoechst
(4) 637.8 g mol^{-1}
(5) organic pigment
(6) blue solid
(11) Pigment Blue 56
(12) 42800
(13) KBr pellet

22321 $C_{22}H_6Cl_8N_4O_2$



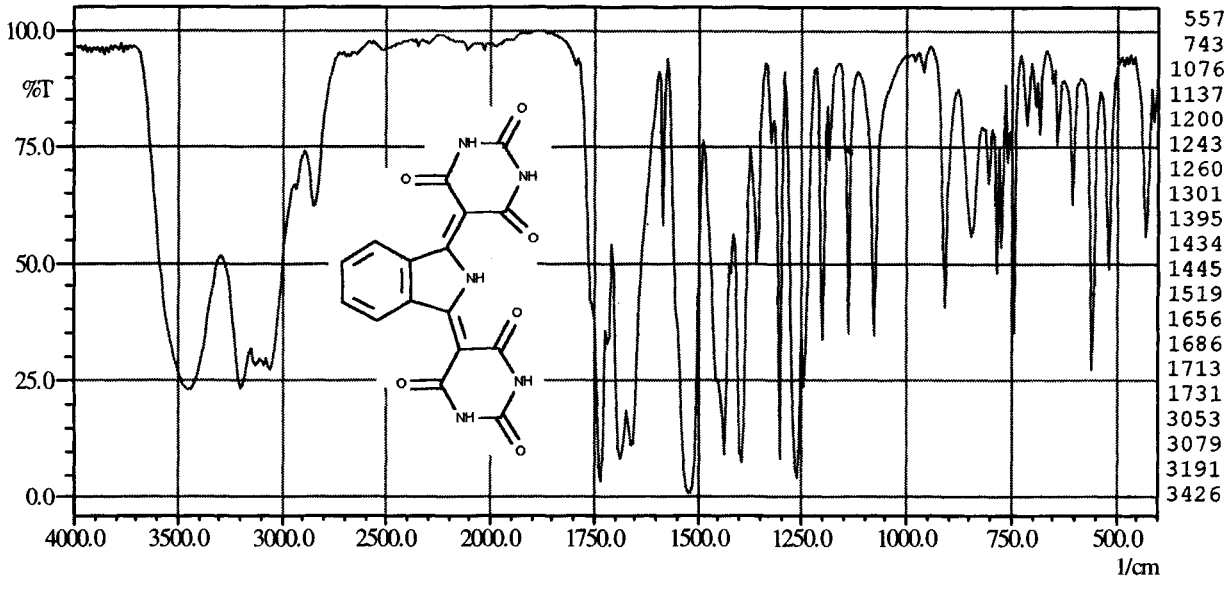
(1) **N,N'-1,3-phenylene-*bis*(3-iminotetrachloroisoindolin-1-one)**
(2) Cromophtal Gelb 2RLTS
(3) Ciba-Geigy
(4) 641.9 g mol^{-1}
(5) organic pigment
(6) yellow solid
(11) Pigment Yellow 110
(12) 56280
(13) KBr pellet

22321 $C_{23}H_8Cl_8N_4O_2$



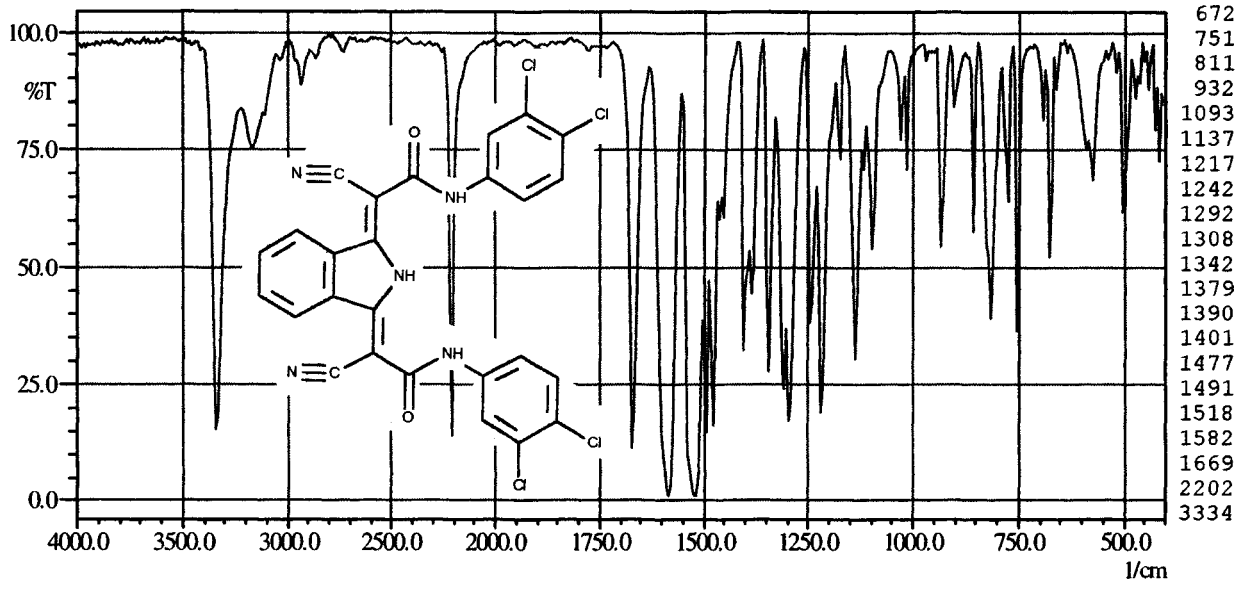
(1) **N,N'-(2,6-toluenediyl)-*bis*(3-iminotetrachloroisoindolin-1-one), azomethine-type**
(2) Irgazin Gelb 2GLTN
(3) Ciba-Geigy
(4) 655.9 g mol^{-1}
(5) organic pigment
(6) yellow solid
(11) Pigment Yellow 109
(12) 56284
(13) KBr pellet

22321 $C_{16}H_9N_5O_6$



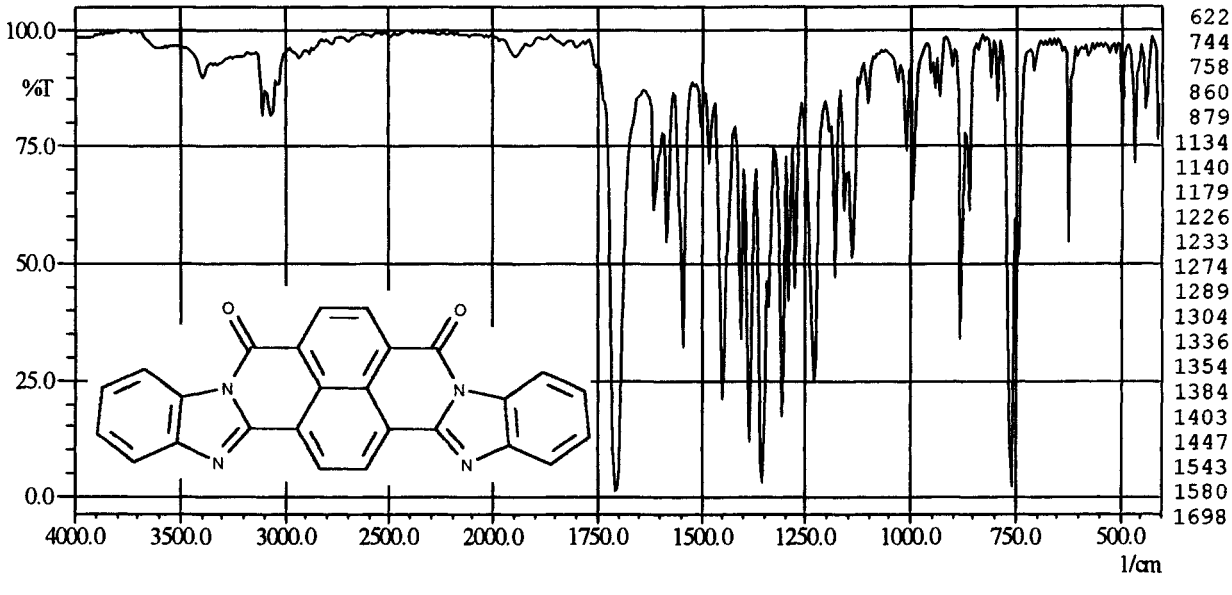
(1) **isoindoline derivative**
(2) Fanchon Fast Yellow Y-5700
(3) Harmon
(4) 367.2 g mol^{-1}
(5) organic pigment
(6) yellow solid
(11) Pigment Yellow 139
(13) KBr pellet

22321 $C_{26}H_{13}Cl_4N_5O_2$



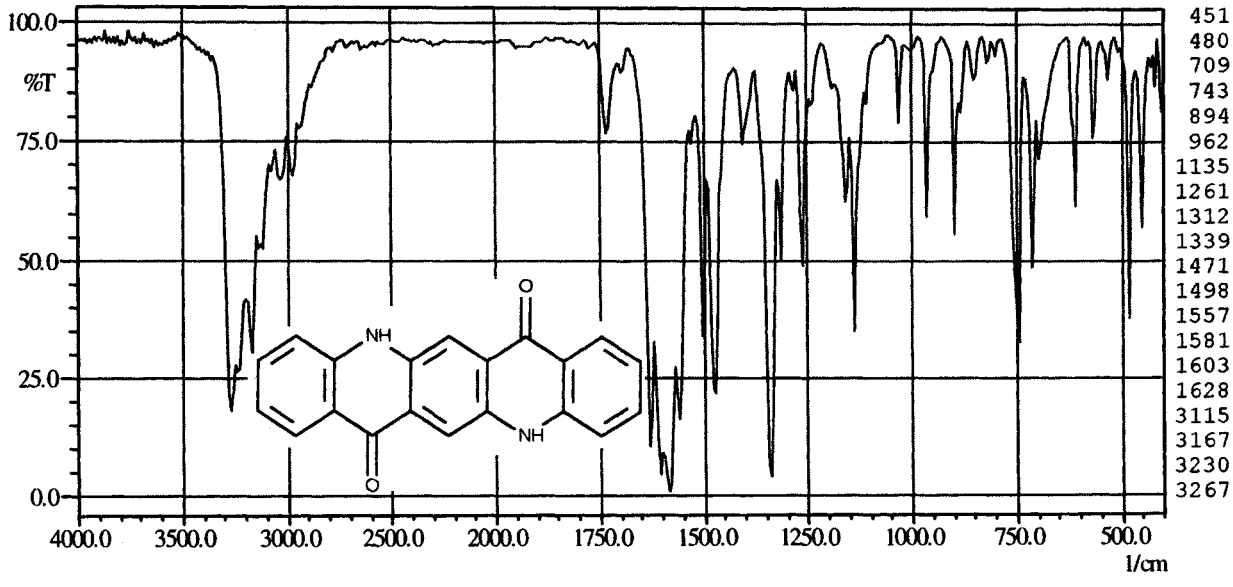
(1) **isoindolinone derivative, azomethine-type**
(2) Irgazin Orange 3GL
(3) Ciba-Geigy
(4) 569.2 g mol^{-1}
(5) organic pigment
(6) orange solid
(11) Pigment Orange 66
(13) KBr pellet

22321 $C_{26}H_{12}N_4O_2$



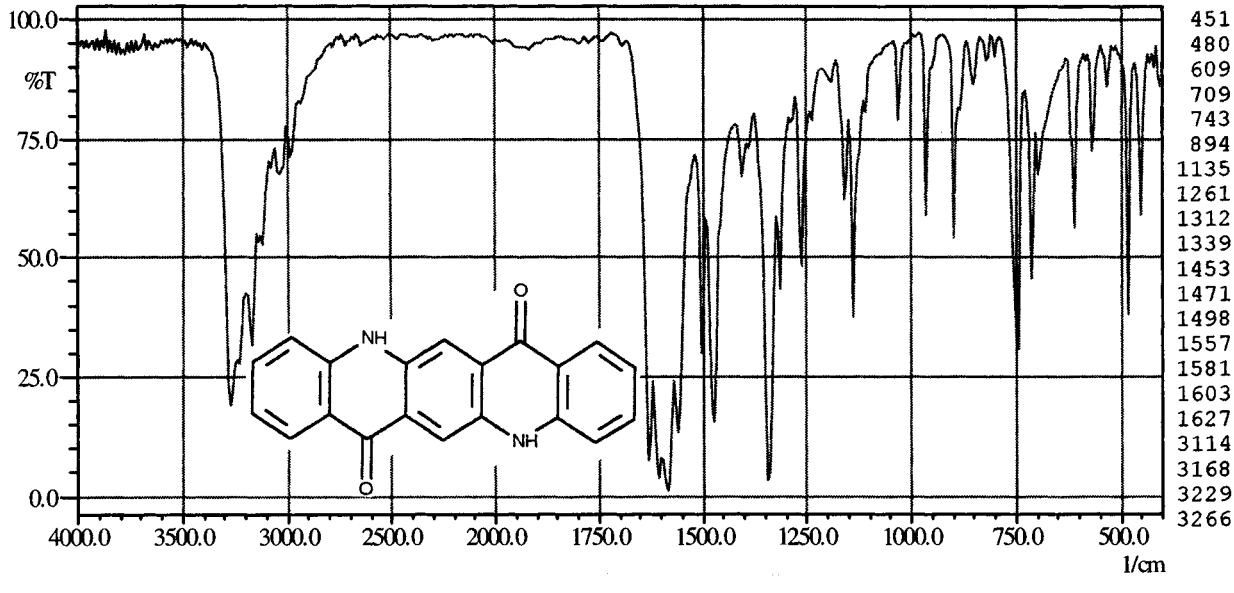
(1) **dibenzimidazolo(1,2-e,2',1'-l)-4,9-diaza-3, 10-pyrene-quinone**
(2) Permanent Rot TG
(3) Hoechst
(4) 412.4 g mol^{-1}
(5) organic pigment
(6) red solid
(11) Pigment Red 194
(12) 71100
(13) KBr pellet

22322 $C_{20}H_{12}N_2O_2$



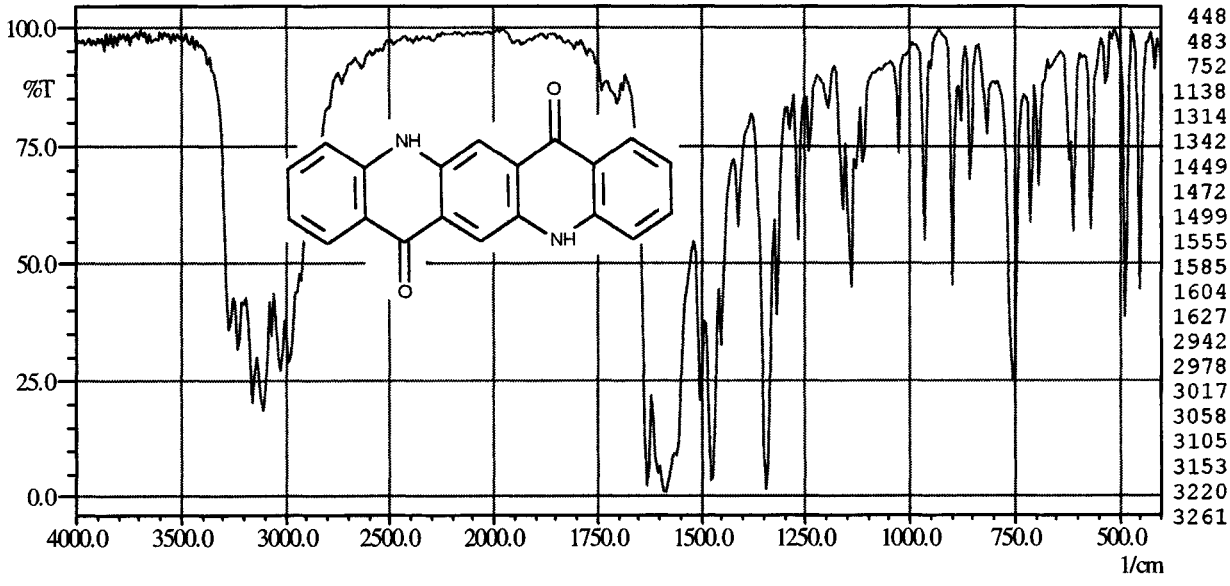
(1) **7,14-dioxo-5,7,12,14-tetrahydroquinolino-[2,3-b]-acridine, β-form**
(2) Cinquasia Violet R RT-891-D
(3) DuPont
(4) 312.3 g mol^{-1}
(5) organic pigment
(6) violet solid
(11) Pigment Violet 19
(12) 46500
(13) KBr pellet

22322 $C_{20}H_{14}N_2O_2$



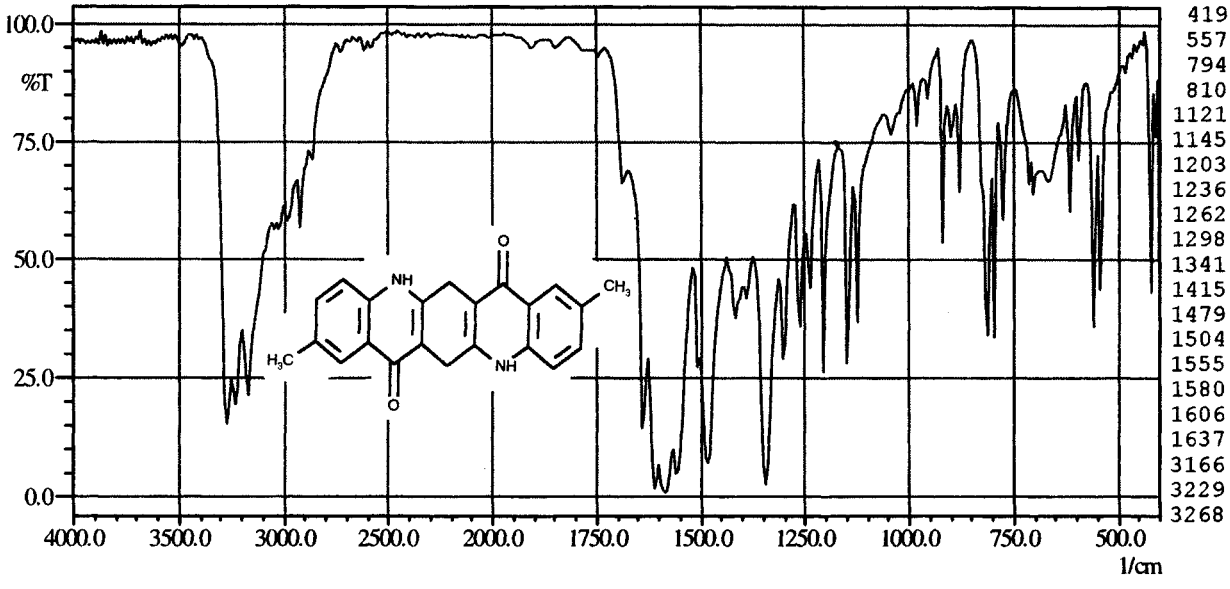
(1) **7,14-dioxo-5,7,12,14-tetrahydroquinolino(2,3-b)acridine, β-form**
(2) Hostaperm Rotviolett ER02
(3) Hoechst
(4) 312.3 g mol^{-1}
(5) organic pigment
(6) red-violet solid
(11) Pigment Violet 19
(12) 465
(13) KBr pellet

22322 $C_{20}H_{12}N_2O_2$



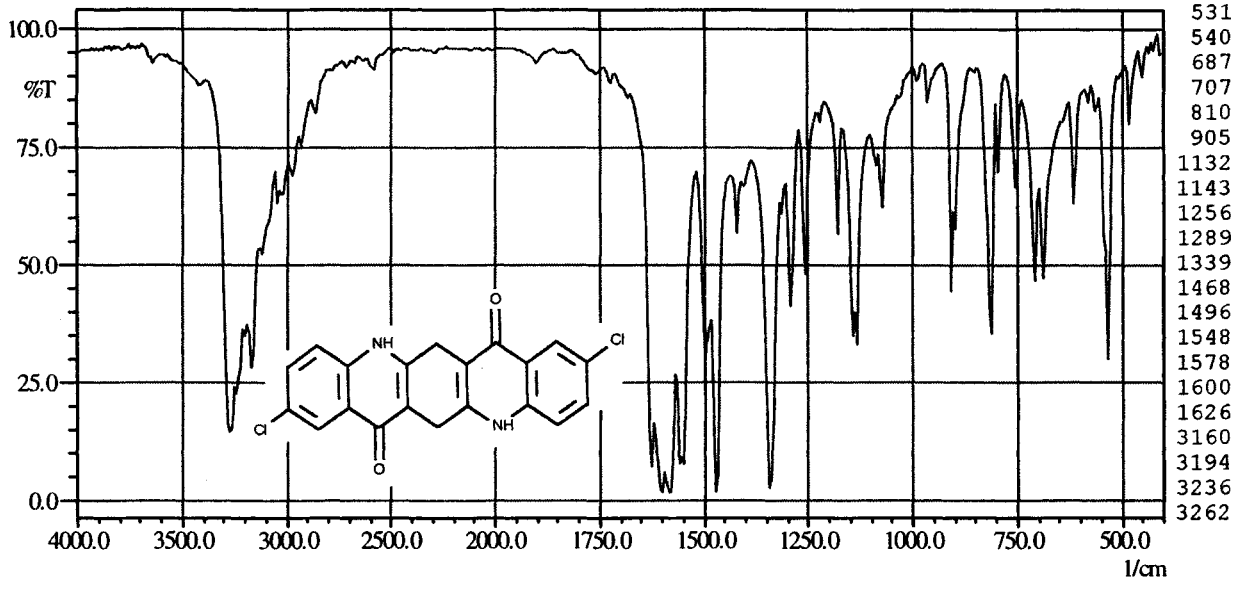
(1) **7,14-dioxo-5,7,12,14-tetrahydroquinolino-[2,3-b]acridine, γ-form**
(2) Hostaperm Rot E2B 70
(3) Hoechst
(4) 312.3 g mol^{-1}
(5) organic pigment
(6) red solid
(11) Pigment Violet 19
(12) 46500
(13) KBr pellet

22322 $C_{22}H_{18}N_2O_2$



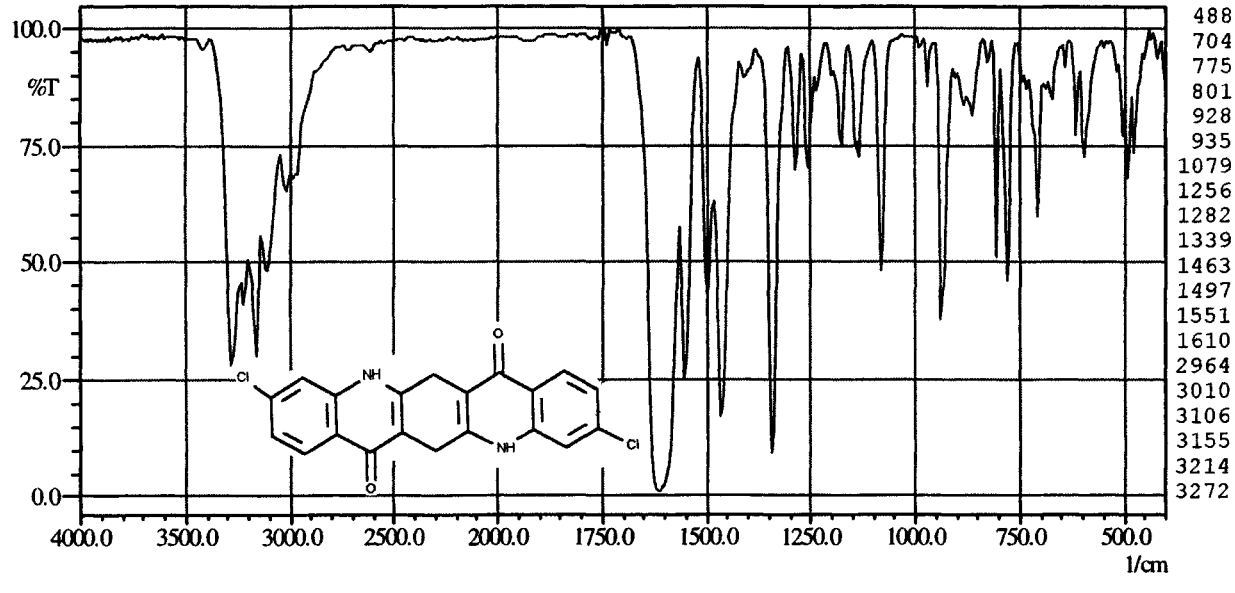
(1) **2,9-dimethyl-7,14-dioxo-5,7,12,14, tetrahydroquinolino[2,3-b]acridine**
(2) Hostaperm Rosa E Transparent
(3) Hoechst
(4) 342.4 g mol^{-1}
(5) organic pigment
(6) pink solid
(11) Pigment Red 122
(12) 73915
(13) KBr pellet

22322 $C_{20}H_{12}Cl_2O_2$



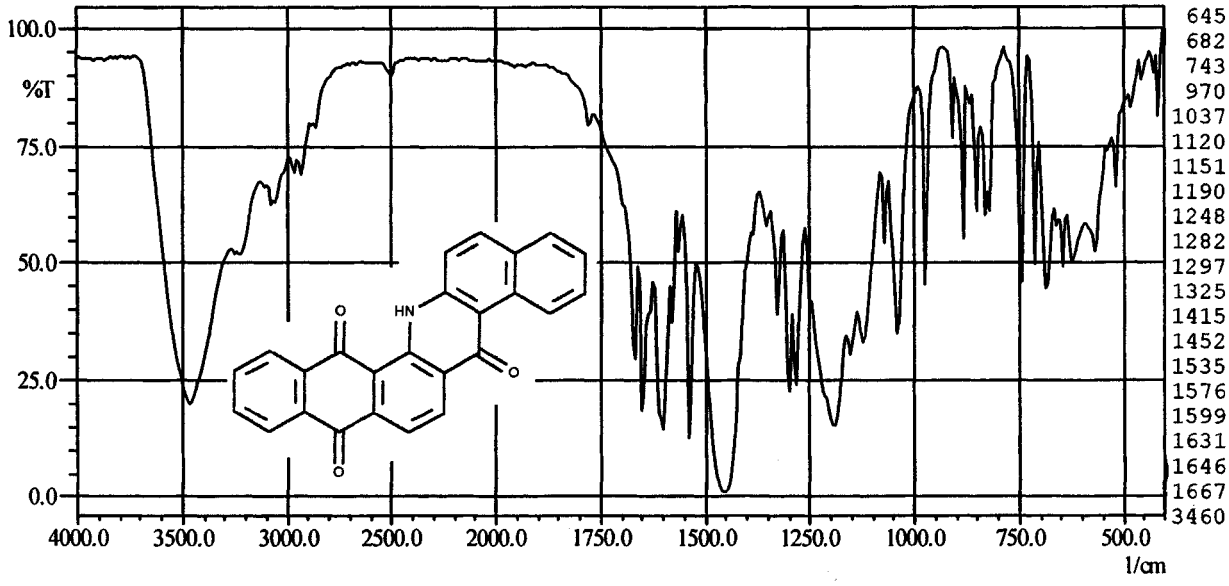
(1) **2,9-dichloro-7,14-dioxo-5,7,12,14-tetrahydroquinolino[2,3-b]acridine**
(2) Quindo Magenta RV 6843
(3) Harmon
(4) 355.2 g mol^{-1}
(5) organic pigment
(6) solid
(11) Pigment Red 202
(12) 73905
(13) KBr pellet

22322 $C_{20}H_{12}Cl_2N_2O_2$



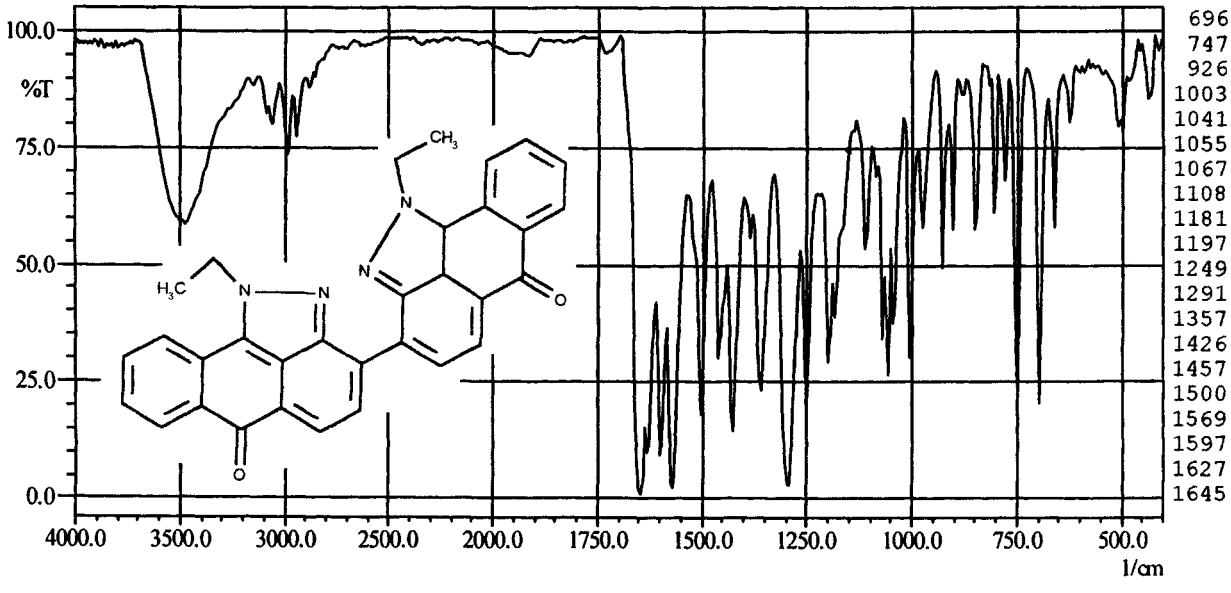
(1) **3,10-dichloro-7,14-dioxo-5,7,12,14-tetrahydroquinolino[2,3-b]acridine**
(2) Hostaperm Rot EG Transparent
(3) Hoechst
(4) 383.2 g mol^{-1}
(5) organic pigment
(6) red solid
(11) Pigment Red 209
(12) 73905
(13) KBr pellet

22322 $C_{25}H_{13}NO_3$



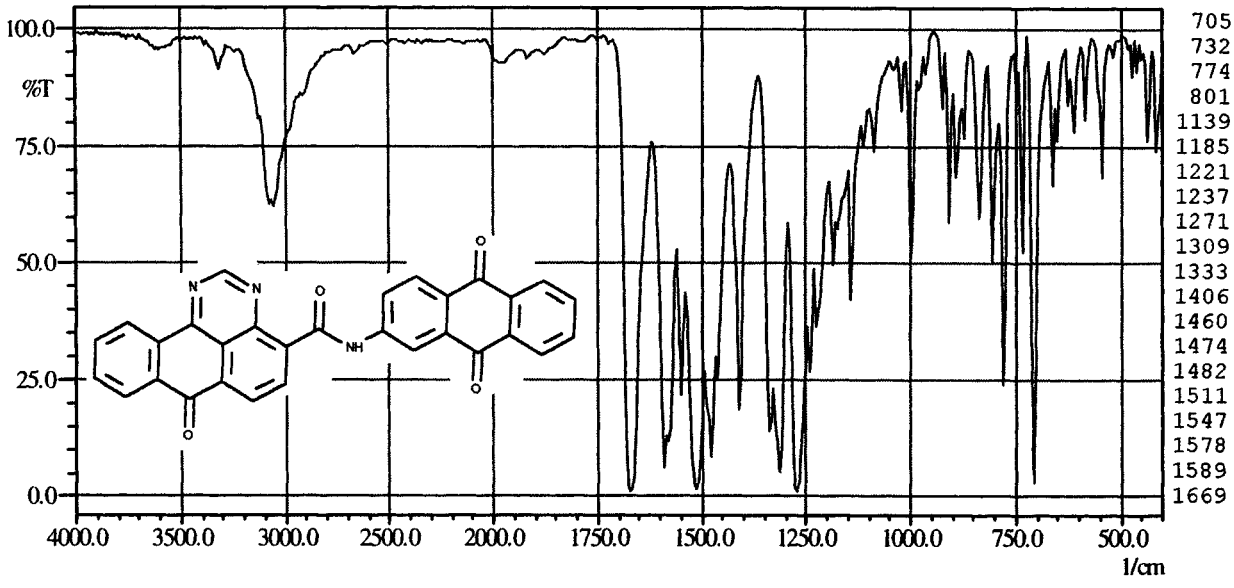
(1) **3,8,16-trioxo-3,8,9,16-tetrahydronaphthalinobenzo-[a]naphth-[2,3-H]acridine-5,8,13(14H)trione**
(2) Indanthren Rot RK
(3) Hoechst
(4) 375.4 g mol^{-1}
(5) organic pigment
(6) red solid
(11) VAT Red 35
(12) 68000
(13) KBr pellet

22323 $C_{32}H_{22}N_4O_2$



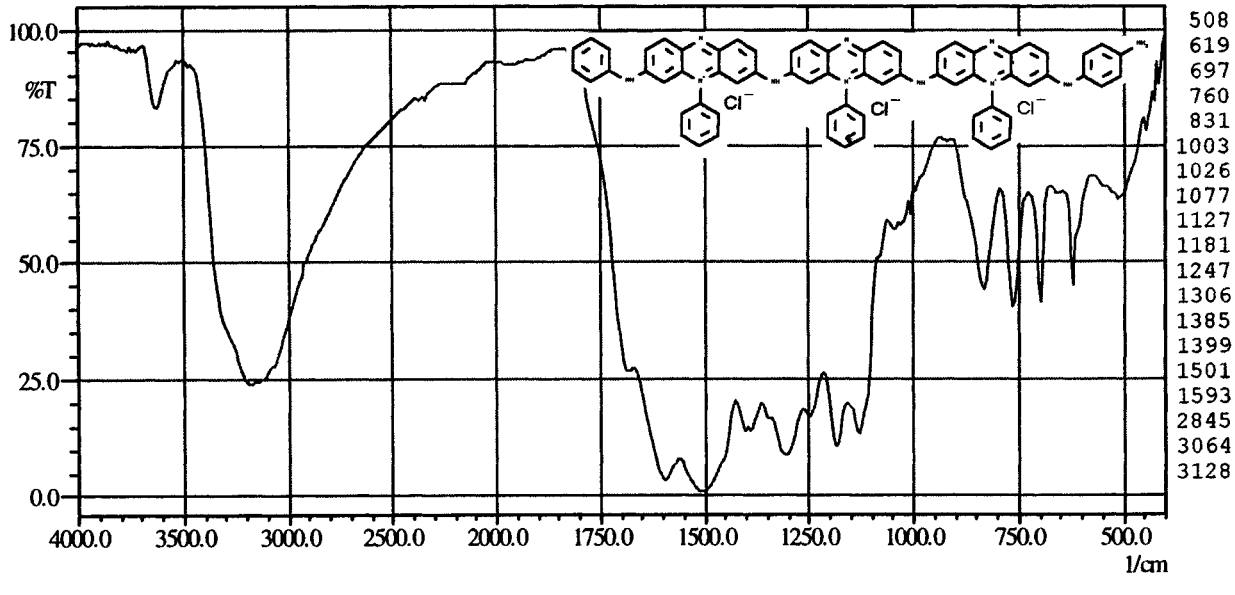
(1) **N,N'-diethyldipyrazoleanthronyl**
(2) Indanthren Rubin R
(3) commercial
(4) 494.6 g mol^{-1}
(5) organic pigment
(6) ruby solid
(11) VAT Red 13
(12) 70320
(13) KBr pellet

22324 $C_{30}H_{15}N_3O_4$



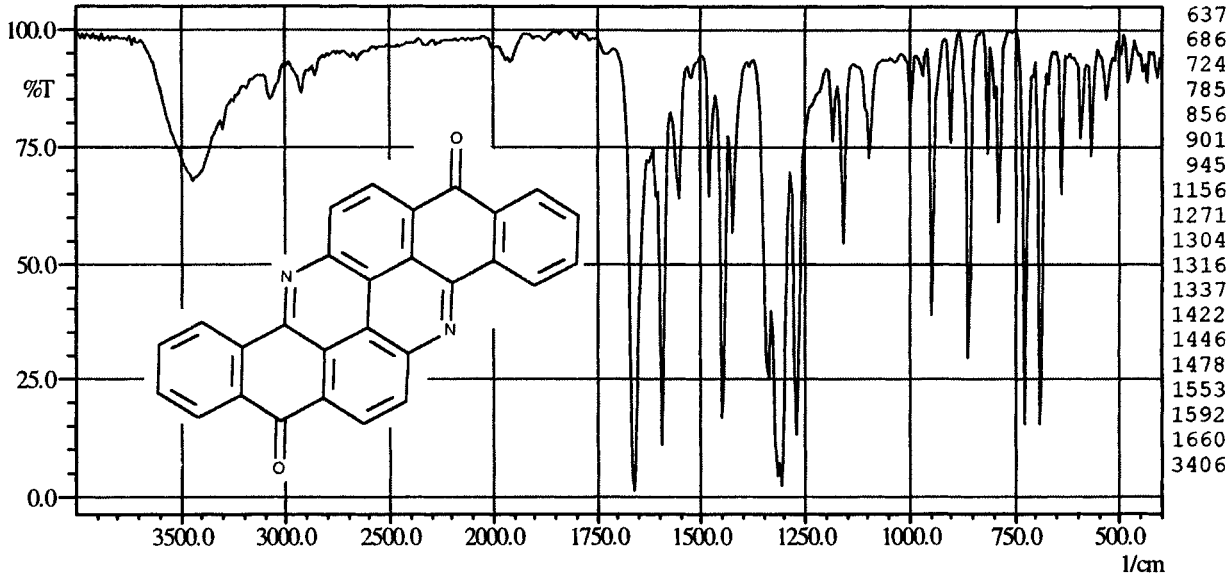
(1) **anthrapyrimidine derivative**
(2) Indanthren Yellow 20
(3) Hoechst
(4) 481.5 g mol^{-1}
(5) organic pigment
(6) yellow solid
(11) VAT Yellow 20
(12) 68420
(13) KBr pellet

22325 $C_{66}H_{48}Cl_3N_{11}$



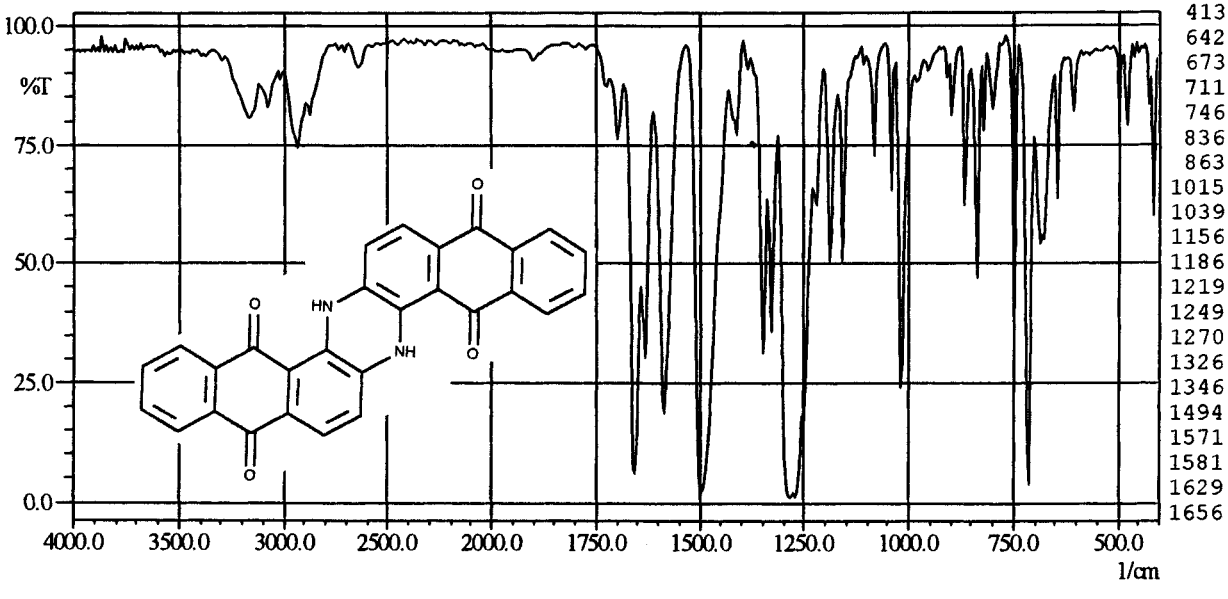
(1) **N-phenyl-2-aminophenazoniumchloride derivative**
(2) Pigmentschwarz 1
(3) commercial
(4) 1102 g mol^{-1}
(5) organic pigment
(6) black solid
(11) Pigment Black 1
(12) 50440
(13) KBr pellet

22326 $C_{28}H_{12}N_2O_2$



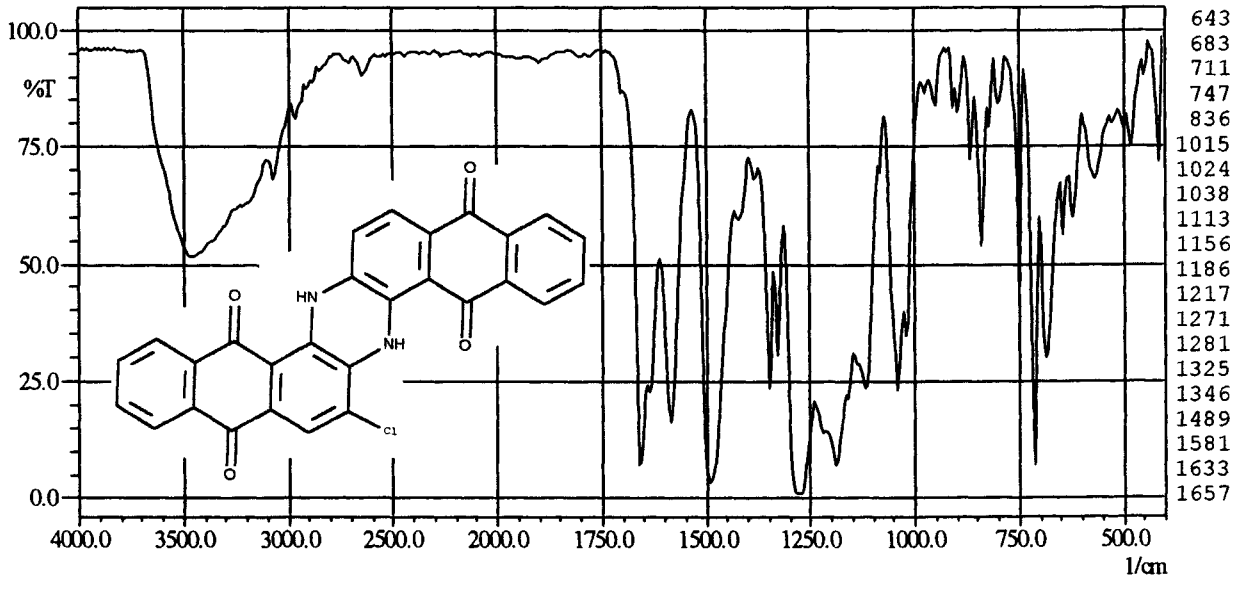
(1) **flavanthrone**
(2) Monolite Yellow FR
(3) ICI
(4) 408.4 g mol^{-1}
(5) organic pigment
(6) orange solid
(11) Pigment yellow 24

22327 $C_{28}H_{14}N_2O_4$



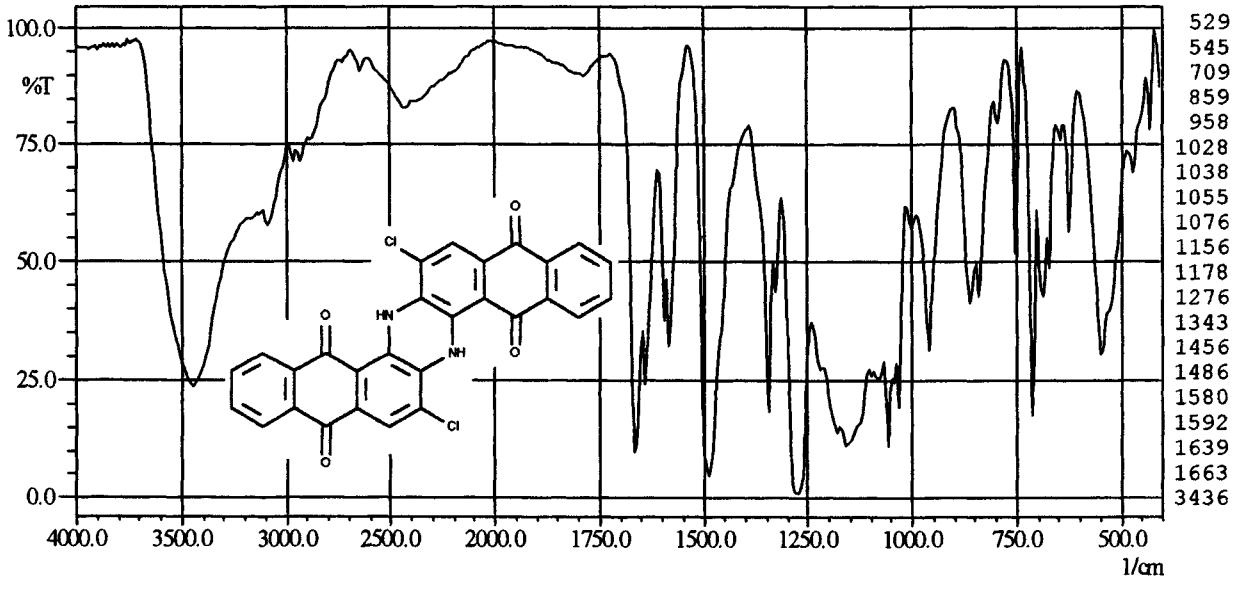
(1) **indanthrone**
(2) Cromophtal Blau A3R
(3) Ciba-Geigy
(4) 442.4 g mol^{-1}
(5) organic pigment
(6) blue solid
(11) Pigment Blue 60
(12) 69800
(13) KBr pellet

22327 $C_{28}H_{13}ClN_2O_2$



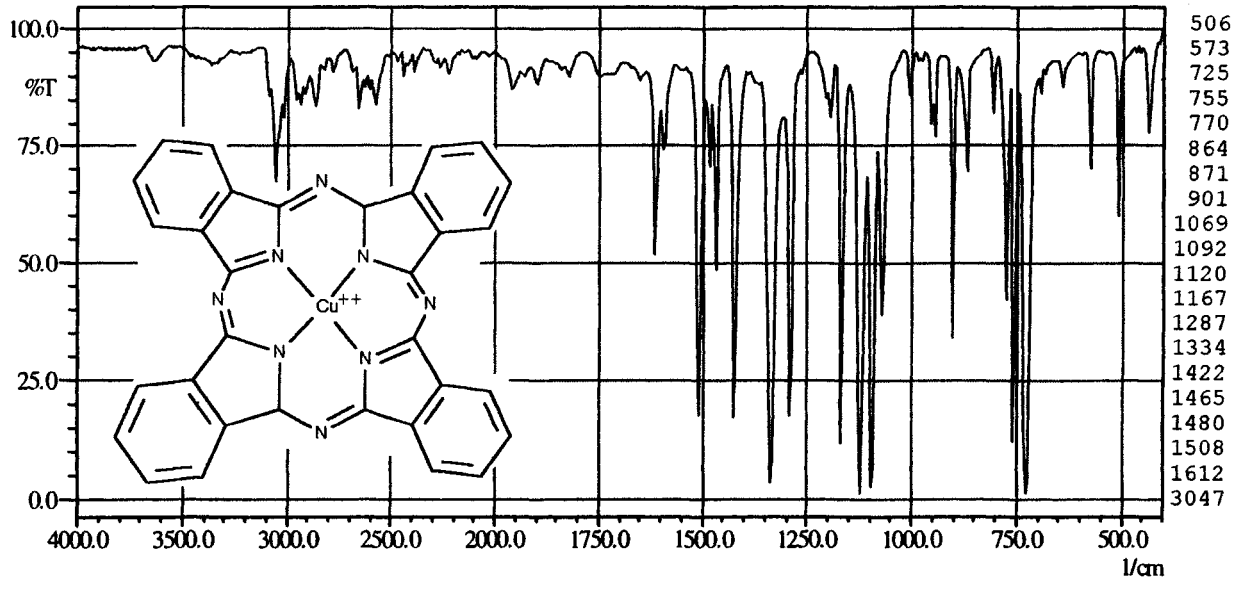
(1) **7-chloroindanthrone**
(2) Indanthren Blau GCD
(3) Hoechst
(4) 476.9 g mol^{-1}
(5) organic pigment
(6) blue solid
(11) Pigment Blue 22
(12) 69810
(13) KBr pellet

22327 $C_{28}H_{12}Cl_2N_2O_4$



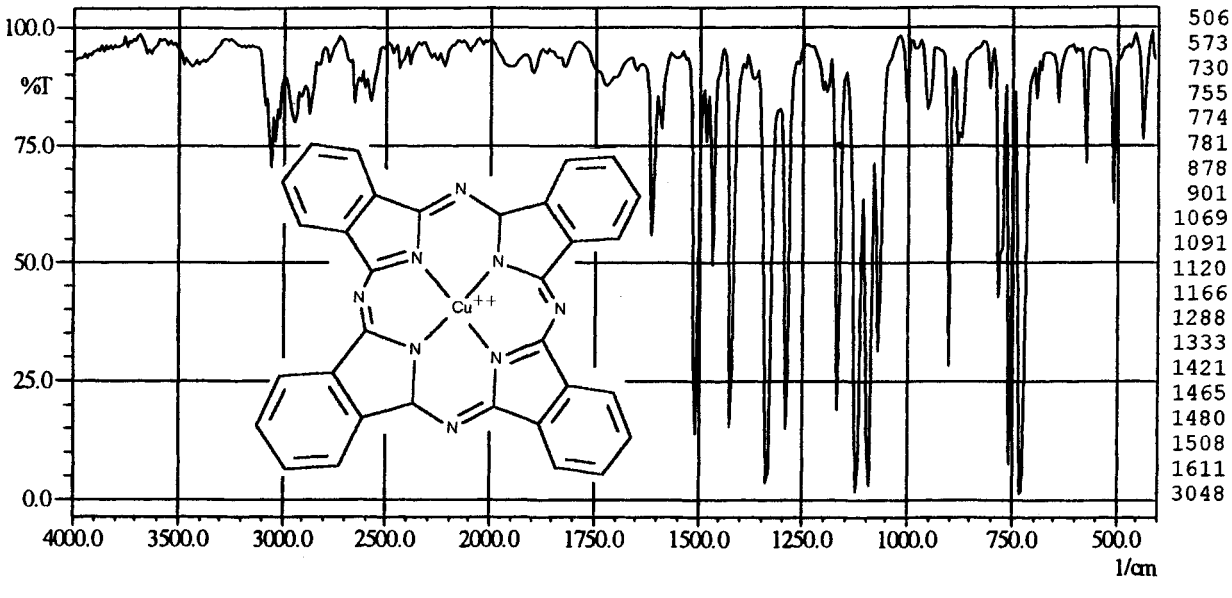
(1) **7,16-dichloroindanthrone**
(2) Indanthren Blau BC
(3) Hoechst
(4) 511.3 g mol^{-1}
(5) organic pigment
(6) blue solid
(11) Pigment Blue 64
(12) 69825
(13) KBr pellet
(14) partially converted into quinhydrone derivative

22328 $C_{32}H_{16}N_8Cu$



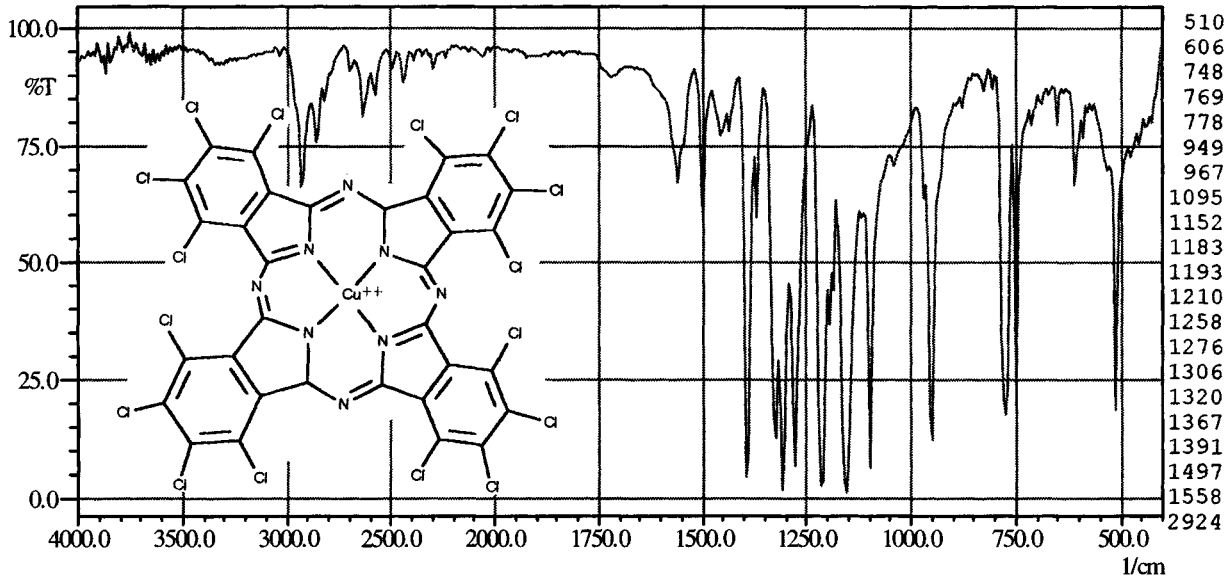
(1) **Cu-phthalocyanine, α-form**
(2) Irgalite Blue BLR/P
(3) Ciba-Geigy
(4) 576.1 g mol^{-1}
(5) organic pigment
(6) blue solid
(11) Pigment Blue 15
(12) 74160
(13) KBr pellet
(14) not stabilized

22328 $C_{32}H_{16}N_8Cu$



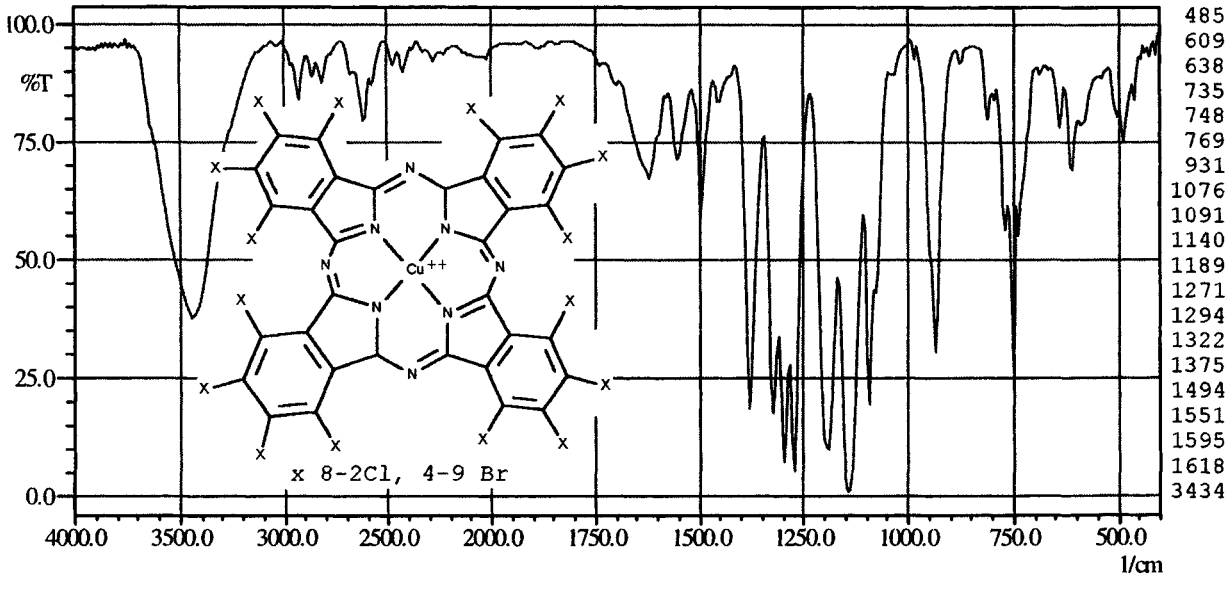
(1) **Cu-phthalocyanine, β-form**
(2) Cromophtal Blau 4GNP
(3) Ciba-Geigy
(4) 576.1 g mol^{-1}
(5) organic pigment
(6) blue solid
(11) Pigment Blue 15:3
(12) 74160:3
(13) KBr pellet

22328 $C_{32}Cl_{16}N_8Cu$



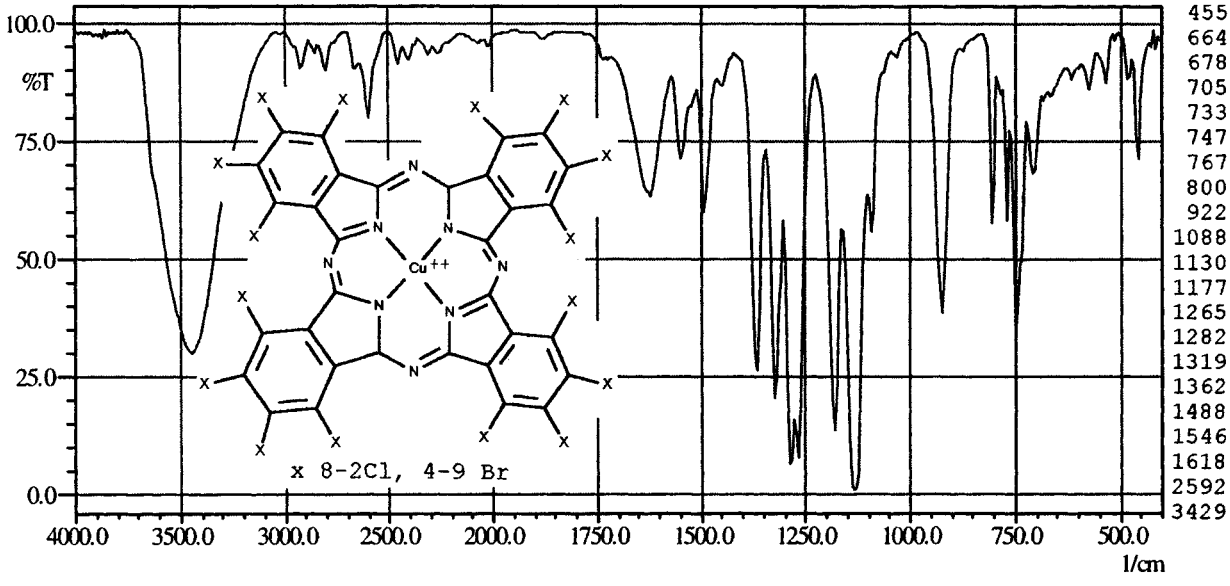
(1) **Cu-hexadecachlorophthalocyanine**
(2) Bayplast Gruen HG
(3) Bayer
(4) 1127 g mol^{-1}
(5) organic pigment
(6) green solid
(11) Pigment Green 7
(12) 74260
(13) KBr pellet

22328 $C_{32}Cl_{10}Br_6N_8Cu$



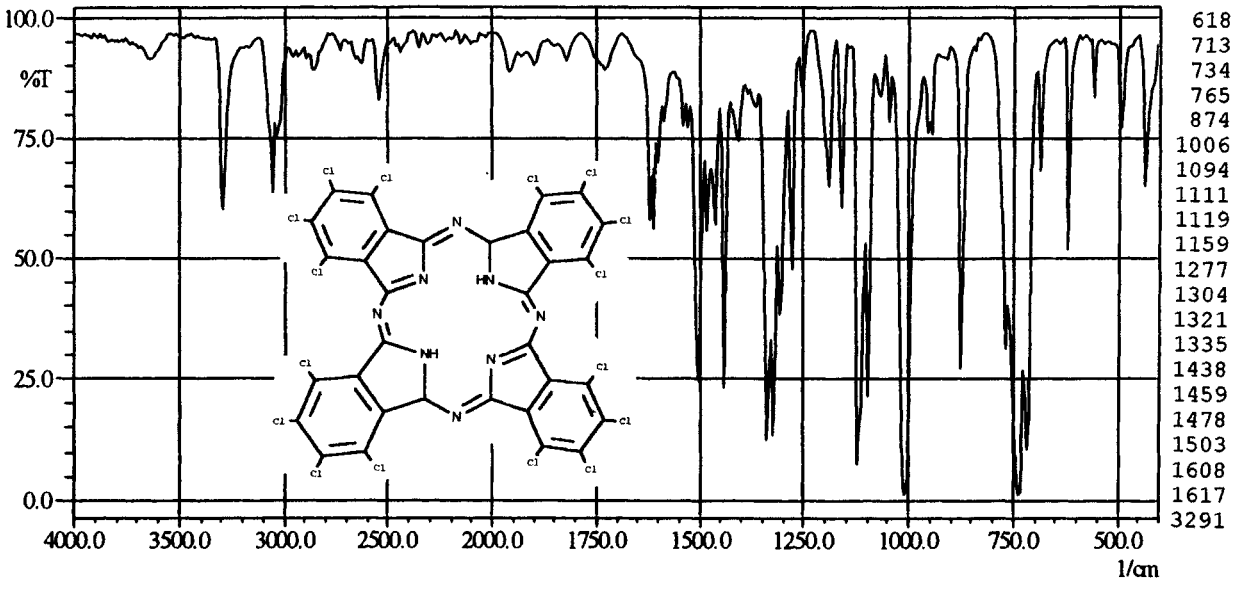
(1) **Cu-hexabromodecachlorophthalocyanine**
(2) Bayplast Gruen 8HG
(3) Bayer
(4) 1394 g mol^{-1}
(5) organic pigment
(6) green solid
(11) Pigment Green 36
(12) 74265
(13) KBr pellet (contains H_2O)
(14) substitution uncertain

22328 $C_{32}Cl_{10}Br_6N_8Cu$



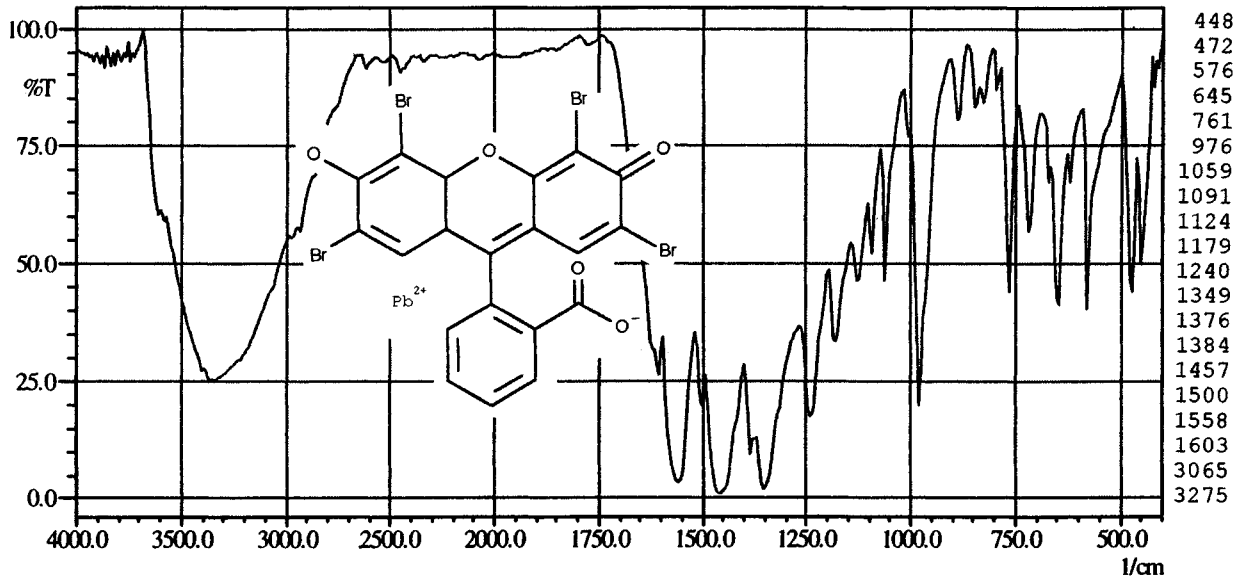
(1) **Cu-hexabromodecachlorophthalocyanine**
(2) Bayplast Gruen 8GN
(3) Bayer
(4) 1394 g mol^{-1}
(5) organic pigment
(6) green solid
(11) Pigment Green 36
(12) 74265
(13) KBr pellet (contains H_2O)
(14) substitution uncertain

22328 $C_{32}H_2Cl_{16}N_8$



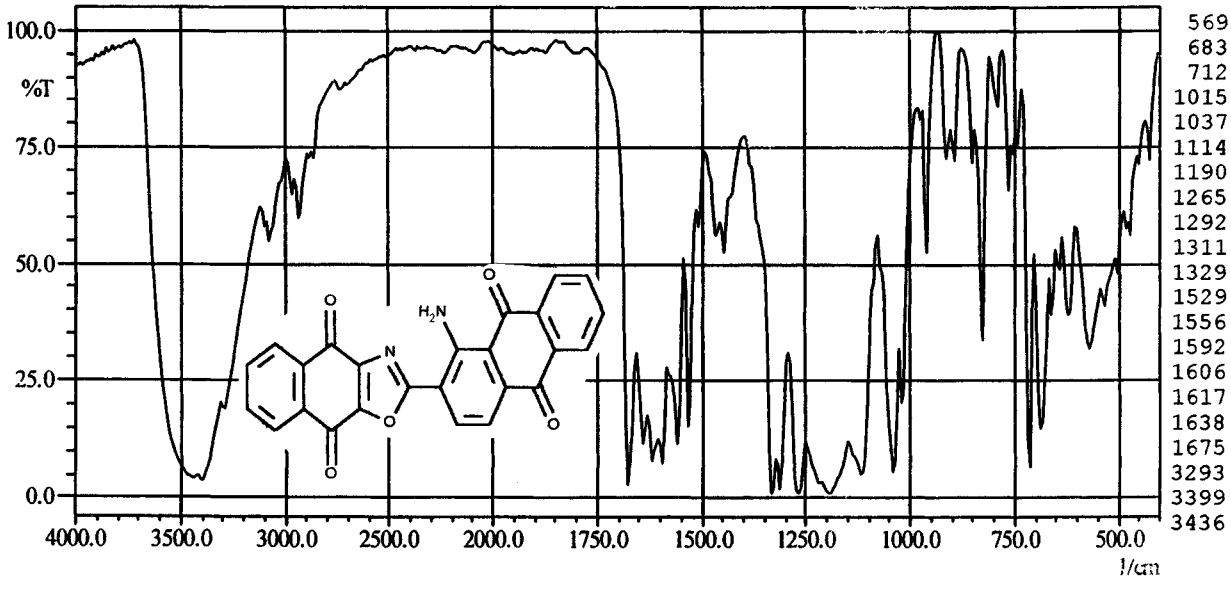
(1) **phthalocyanine, halogenated, metalfree**
(2) Heliogen Blau LG
(3) Hoechst
(4) 1065 g mol^{-1}
(5) organic pigment
(6) blue solid
(11) Pigment Blue 16
(12) 74100
(13) KBr pellet

2233 $C_{20}H_6Br_4O_5Pb$



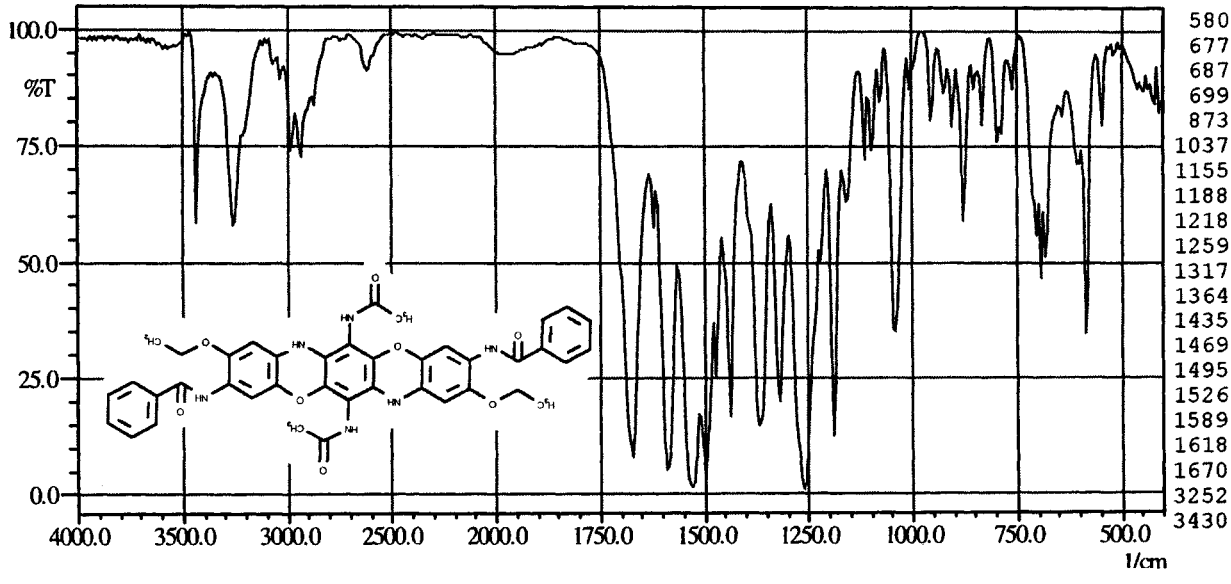
(1) **2,4,5,7-tetrabromofluorescein, Pb-salt**
(2) Eosin A salzfrei
(3) commercial
(4) 853.1 g mol^{-1}
(5) organic pigment
(6) red solid
(11) Pigment Red 90
(12) 45380
(13) KBr pellet

2233 $C_{25}H_{12}N_2O_5$



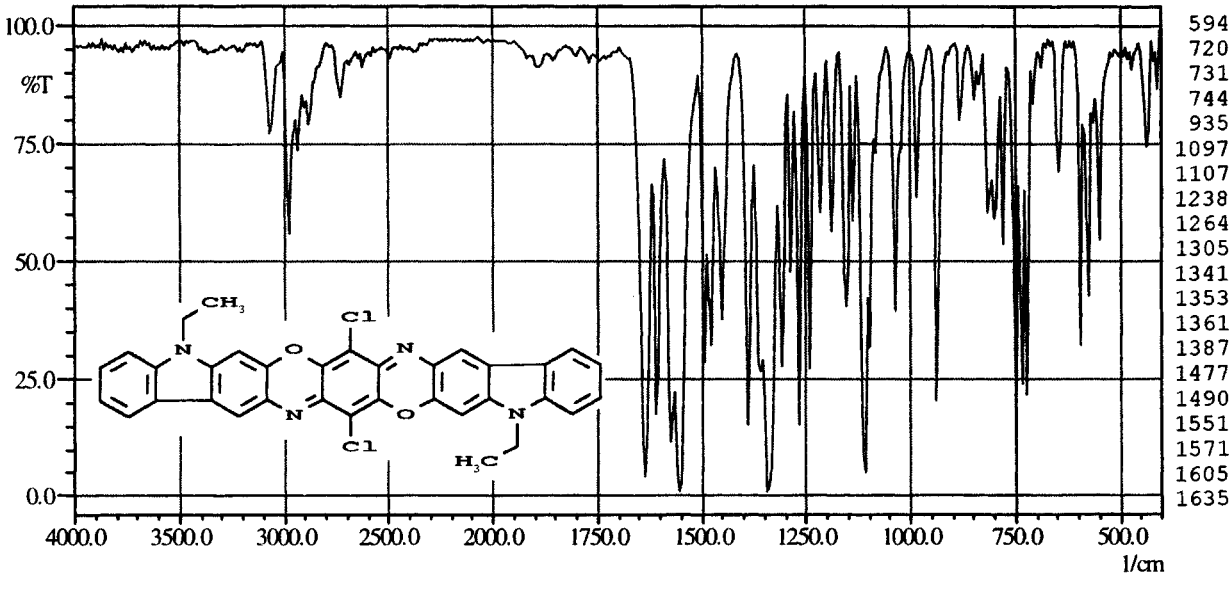
(1) **oxazoloanthraquinone pigment**
(2) Indanthren Rot FBB
(3) Hoechst
(4) 420.4 g mol^{-1}
(5) organic pigment
(6) red solid
(11) VAT Red 20
(12) 67000
(13) KBr pellet

2233 $C_{40}H_{36}N_6O_6$



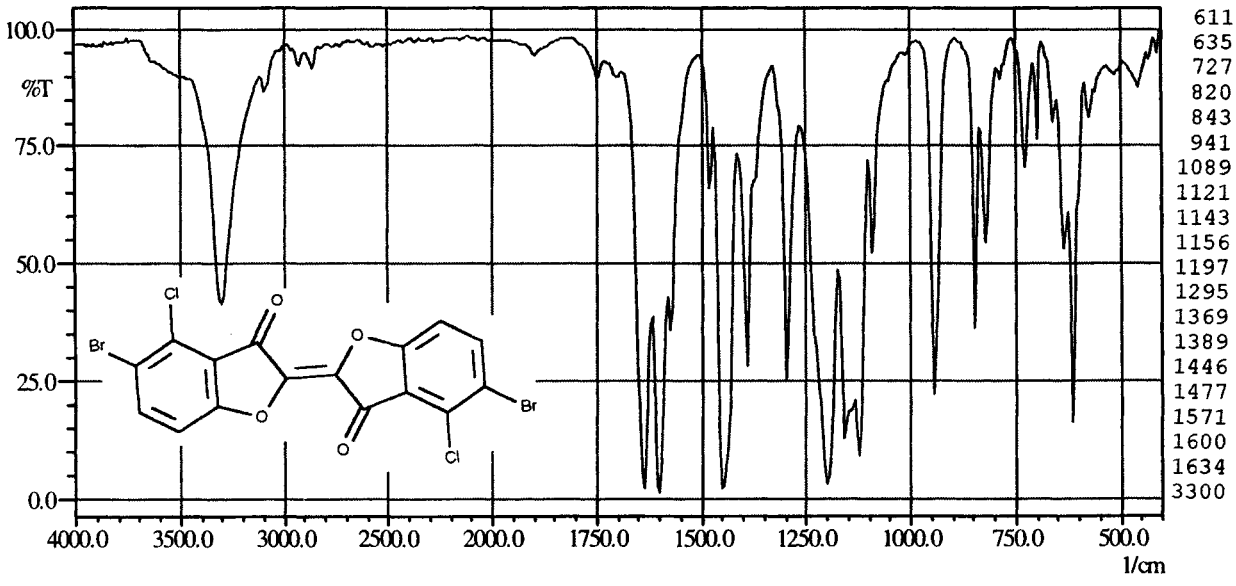
(1) **2,6-dibenzamido-9,10-diacetamido-3,7-diethoxytriphendioxazine**
(2) Cromophtal Violett B
(3) Ciba-Geigy
(4) 696.7 g mol^{-1}
(5) organic pigment
(6) violet solid
(11) Pigment Violet 37
(13) KBr pellet

2233 $C_{34}H_{22}Cl_2N_4O_2$



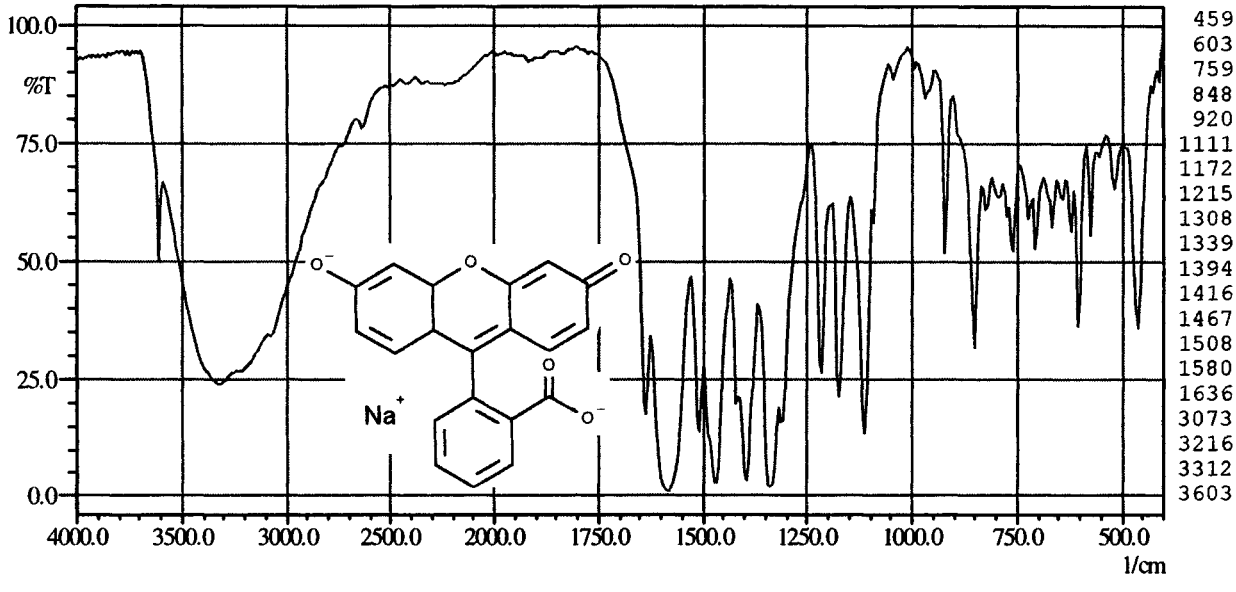
(1) **phenoxazine derivative**
(2) Hostaperm Violett RL Spezial
(3) Hoechst
(4) 589.5 g mol^{-1}
(5) organic pigment
(6) violet solid
(11) Pigment Violet 23
(12) 51319
(13) KBr pellet

2233 $C_{16}H_4Cl_2Br_2O_4$



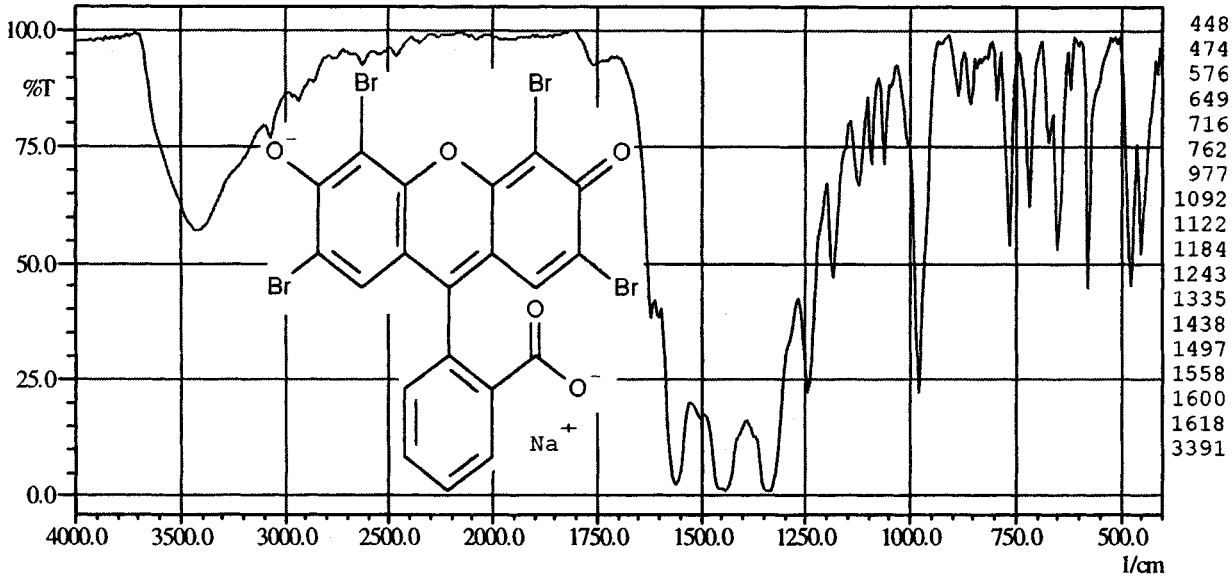
(1) **5,5'-dibromo-4,4'-dichloroindigo**
(2) Brilliant Indigo 4G
(3) commercial
(4) 490.9 g mol^{-1}
(5) organic pigment
(6) blue solid
(11) VAT Blue 2
(12) 73045
(13) KBr pellet

2233 $C_{20}H_{10}O_5Na_2$



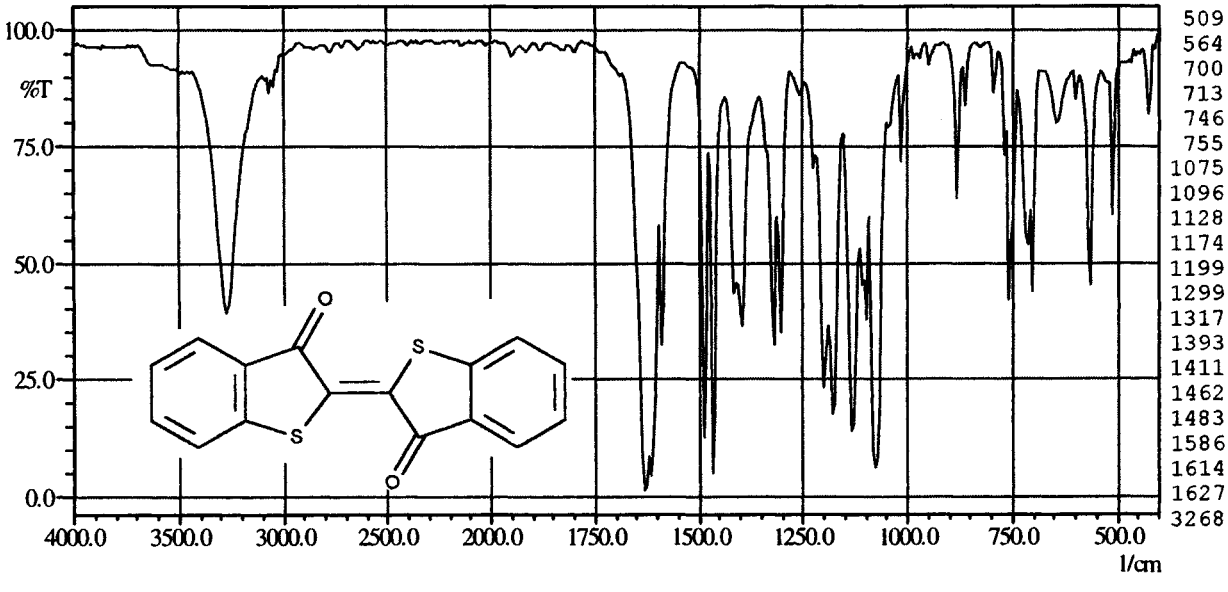
(1) **di-Na fluorescein**
(2) Uranin A extra
(3) commercial
(4) 376.3 g mol^{-1}
(5) organic pigment
(6) dark-red solid
(11) Acid Yellow 73
(12) 45350
(13) KBr pellet

2233 $C_{20}H_6Br_4O_5Na_2$



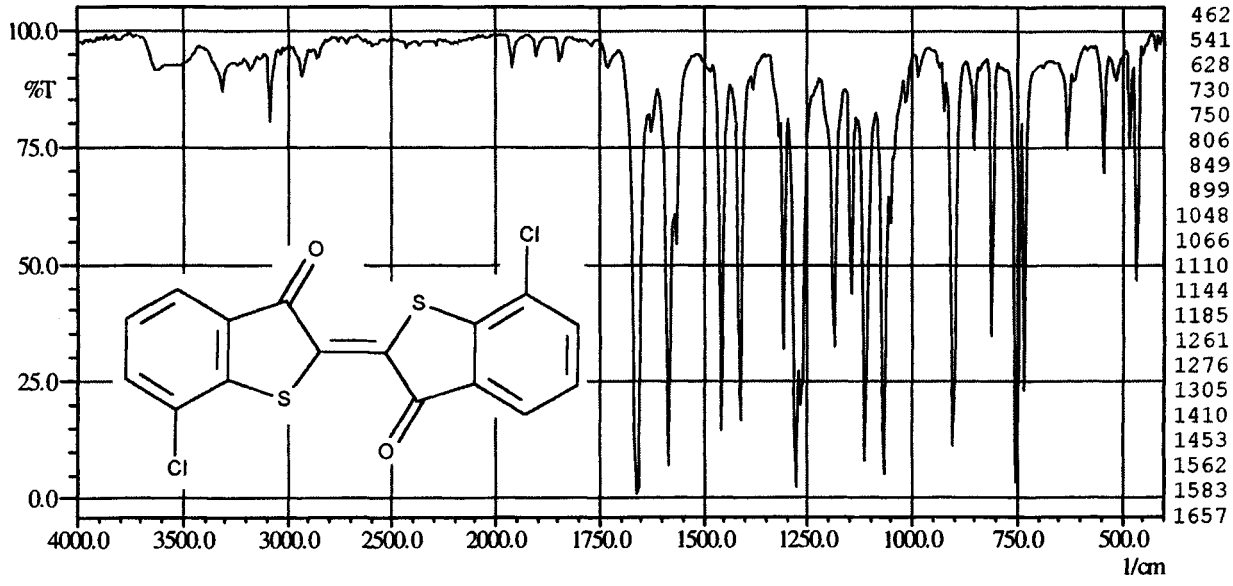
(1) **2,4,5,7-tetrabromofluorescein, Na-salt**
(2) Phloxinlack 1
(3) commercial
(4) 691.9 g mol^{-1}
(5) organic pigment
(6) red solid
(11) Pigment Red 90A
(12) 45380
(13) KBr pellet

2234 $C_{16}H_8O_2S_2$



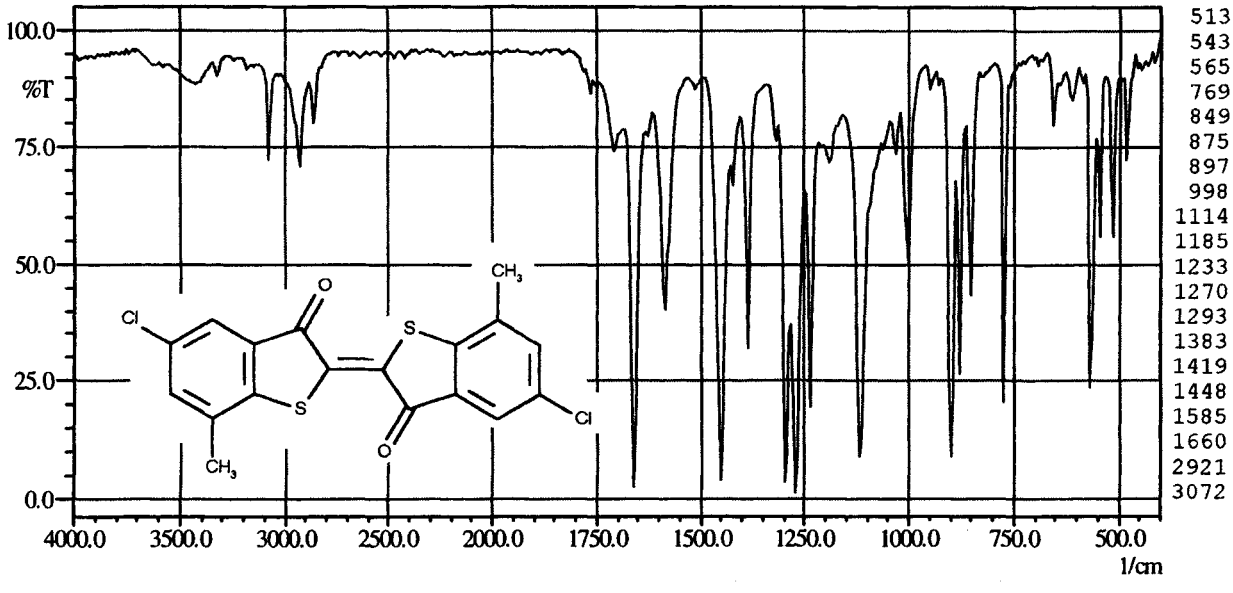
(1) **thioindigo**
(2) Indigo
(3) commercial
(4) 296.4 g mol^{-1}
(5) organic pigment
(6) blue solid
(7) 392 °C
(11) VAT Blue 1
(12) 73000
(13) KBr pellet

2234 $C_{16}H_6Cl_2O_2S_2$



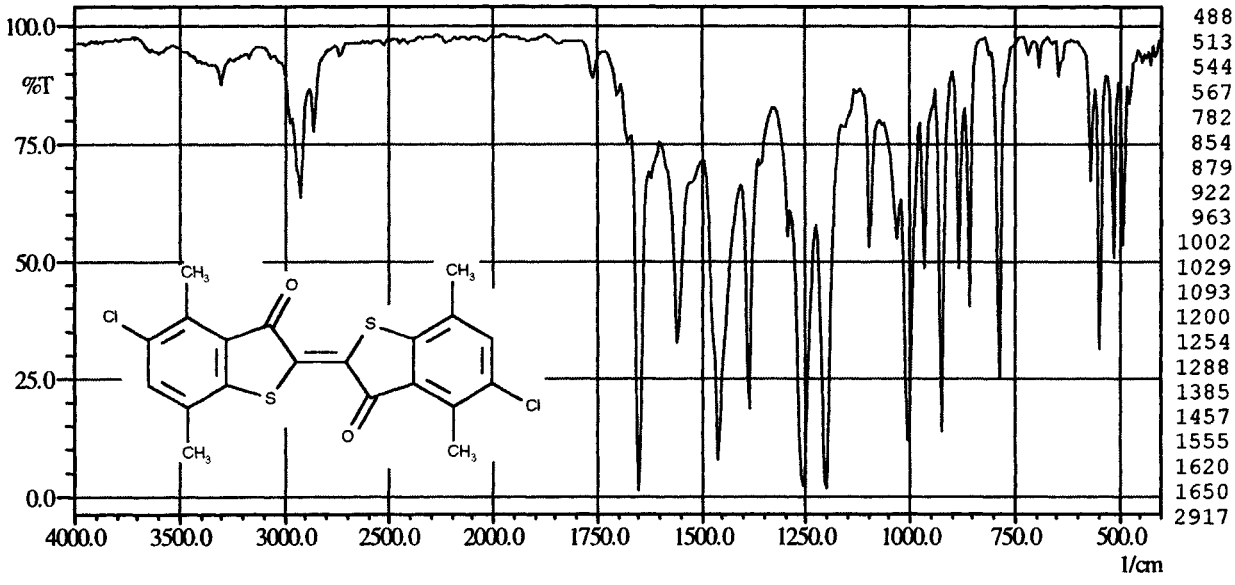
(1) **7,7'-dichlorothioindigo**
(2) Indo Red MV-6632
(3) Harmon
(4) 365.3 g mol^{-1}
(5) organic pigment
(6) red solid
(11) Pigment Red 87
(12) 73310
(13) KBr pellet

2234 $C_{18}H_{10}Cl_2O_2S_2$



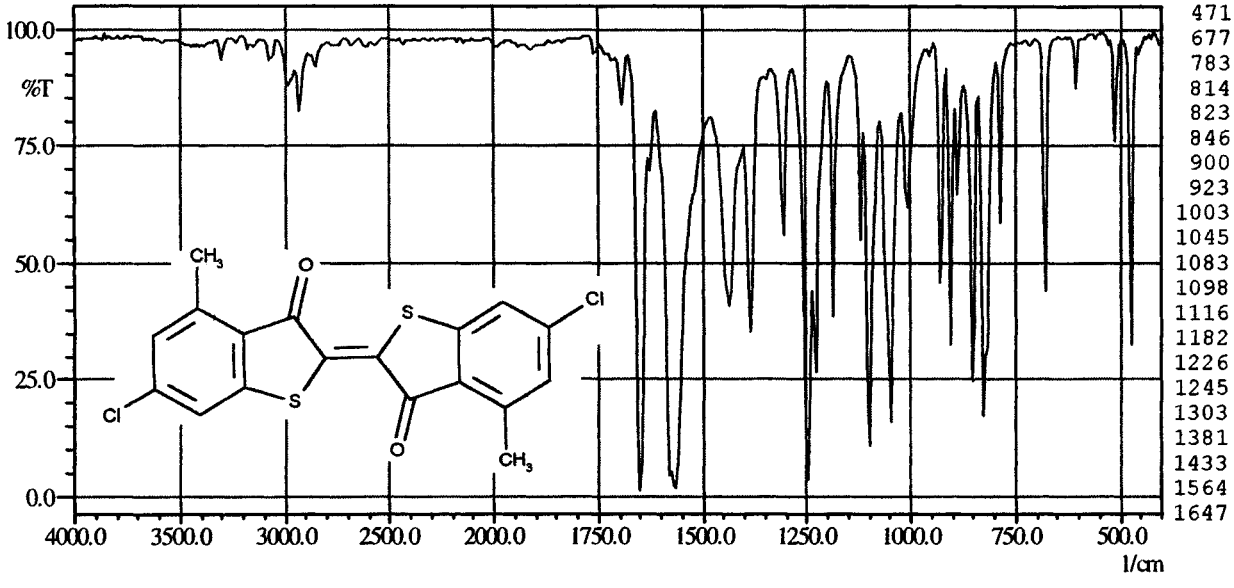
(1) **5,5'-dichloro-7,7'-dimethylthioindigo**
(2) Indanthren Rotviolett RH
(3) Hoechst
(4) 393.3 g mol^{-1}
(5) organic pigment
(6) violet solid
(11) Pigment Violet 36
(12) 73385
(13) KBr pellet

2234 $C_{20}H_{14}Cl_2O_2S_2$



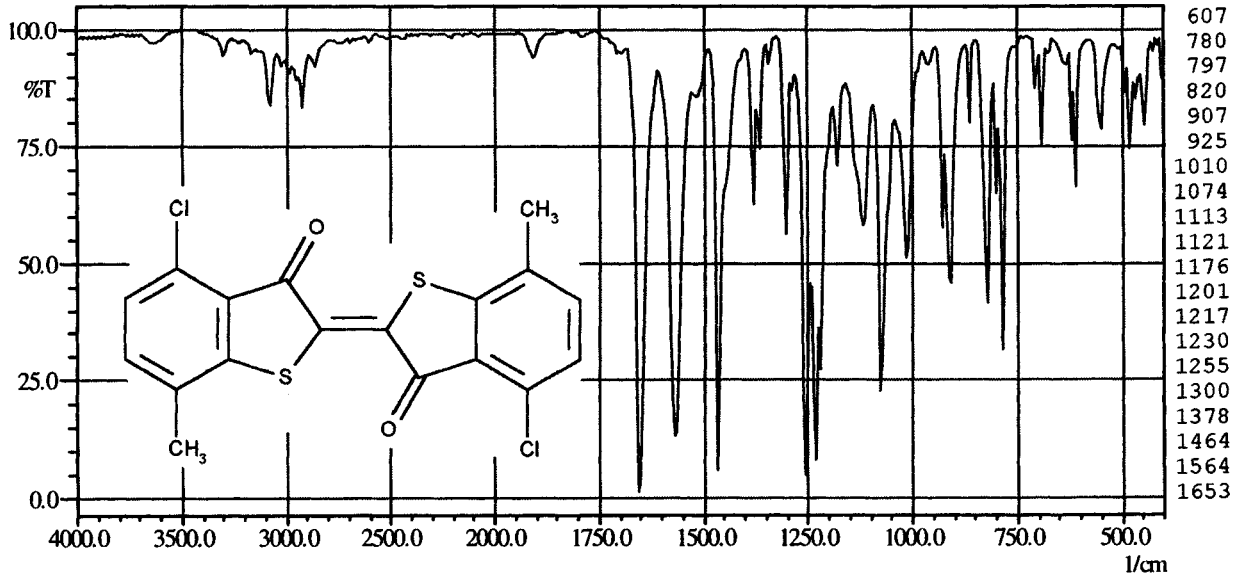
(1) **5,5'-dichloro-4,4',7,7'-tetramethylthioindigo**
(2) Indanthren Brilliant Bordo RRL
(3) Hoechst
(4) 421.4 g mol^{-1}
(5) organic pigment
(6) dark-red solid
(11) Pigment Violet 38
(12) 73395
(13) KBr pellet

2234 $C_{18}H_{10}Cl_2O_2S_2$



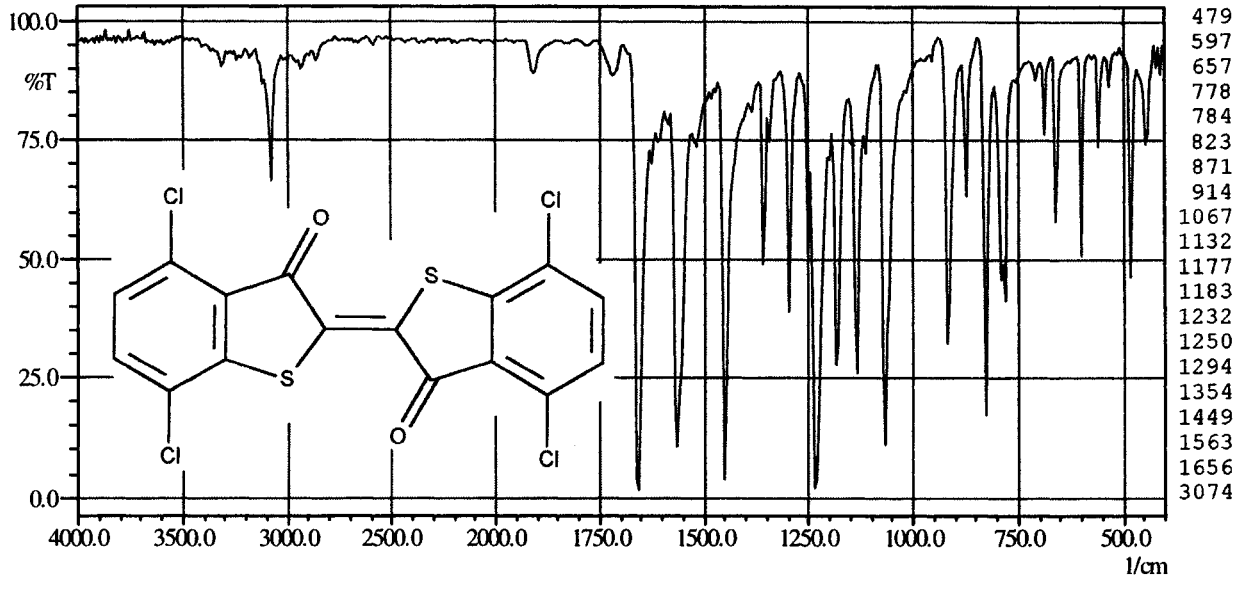
(1) **6,6'-dichloro-4,4'-dimethylthioindigo**
(2) Oracet Pink RF
(3) Ciba-Geigy
(4) 393.3 g mol^{-1}
(5) organic pigment
(6) pink solid
(11) Vat Red 1
(12) 73360
(13) KBr pellet

2234 $C_{18}H_{10}Cl_2O_2S_2$



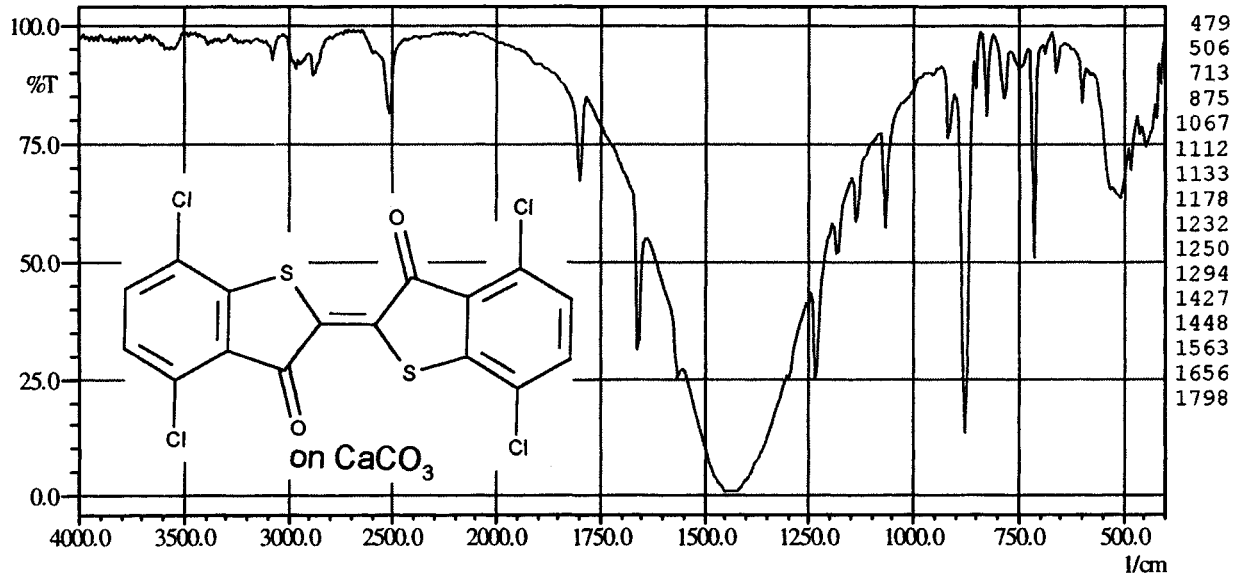
(1) **4,4'-dichloro-7,7'-dimethylthioindigo**
(2) Thiosa Fast Red MV-6604
(3) Harmon
(4) 393.3 g mol^{-1}
(5) organic pigment
(6) red solid
(11) Pigment Red 198
(12) 73390
(13) KBr pellet

2234 $C_{16}H_4Cl_4O_2S_2$



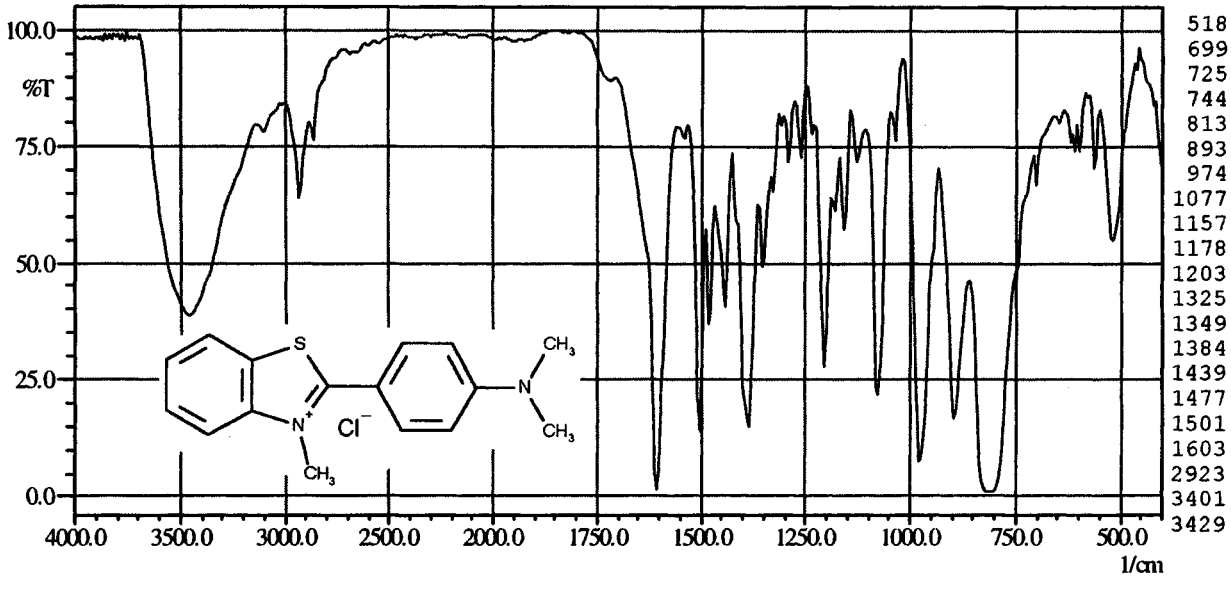
(1) **4,4',7,7'-tetrachlorothioindigo**
(2) Novoperm Rotviolett MRS
(3) Hoechst
(4) 434.1 g mol^{-1}
(5) organic pigment
(6) red-violet solid
(11) Pigment Red 88
(12) 73312
(13) KBr pellet

2234 $C_{16}H_4Cl_4O_2S_2$



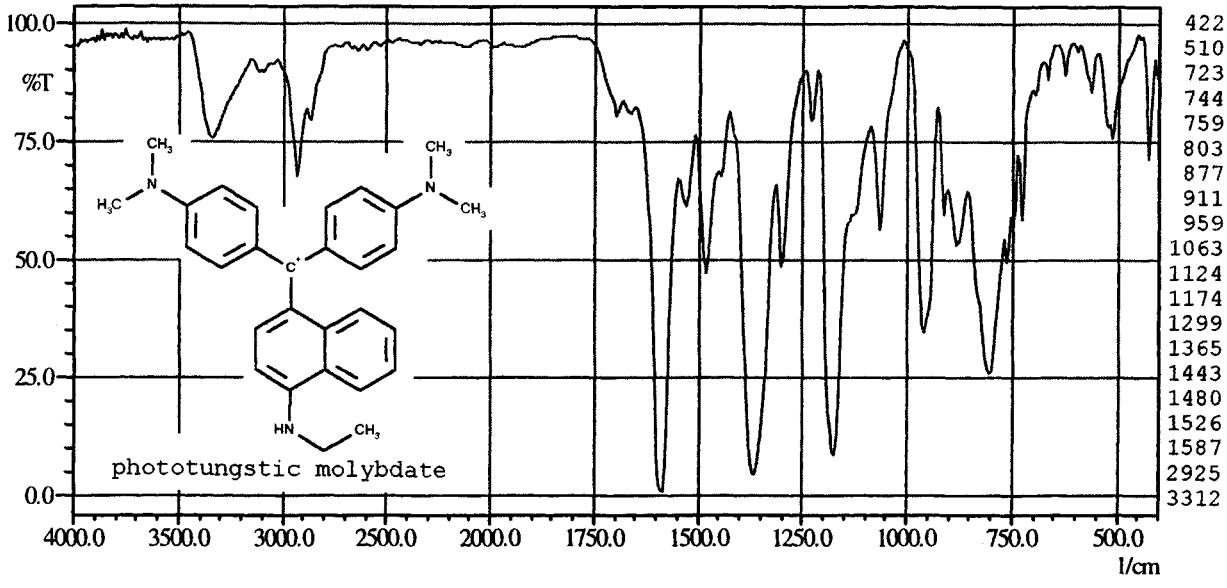
(1) **4,4',7,7'-tetrachlorothioindigo on $CaCO_3$**
(2) Cromophtal Bordo RN
(3) Ciba-Geigy
(4) 434.1 g mol^{-1}
(5) organic pigment
(6) dark-red solid
(11) Pigment Red 88
(12) 73312
(13) KBr pellet

2236 $C_{16}H_{17}ClN_2S$



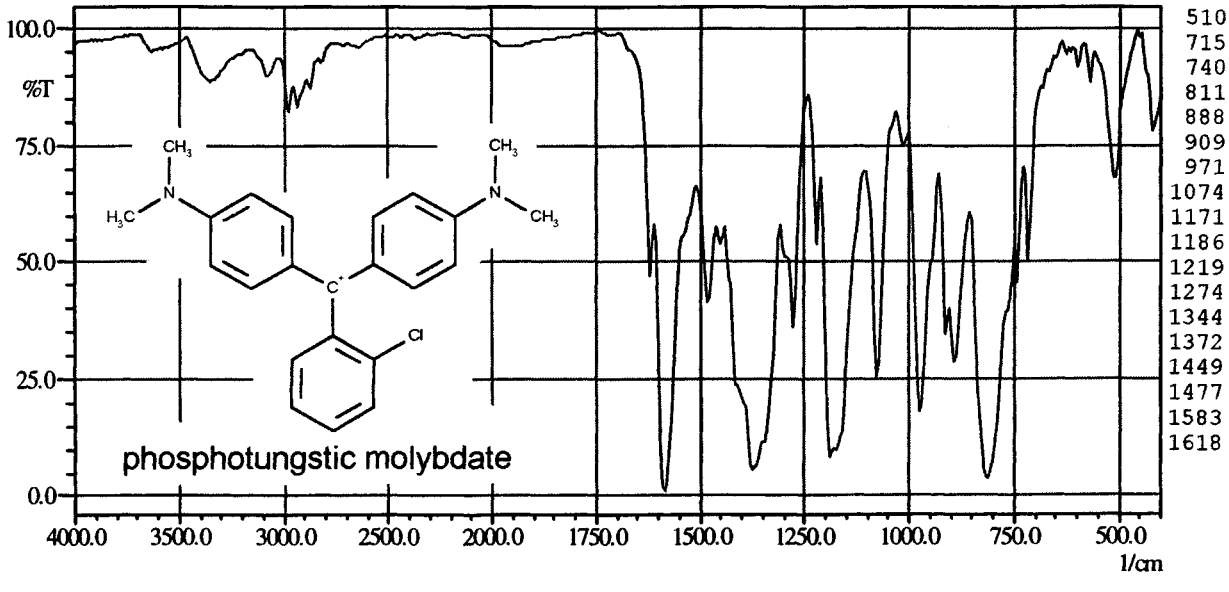
(1) **2(4'-N,N-dimethylaminophenyl)-3,6-dimethylthiazolinium chloride**
(2) Fanalgelb G supra
(3) Siegle
(4) 304.8 g mol^{-1}
(5) organic pigment
(6) yellow solid
(11) Pigment Yellow 18
(12) 49005
(13) KBr pellet

2237



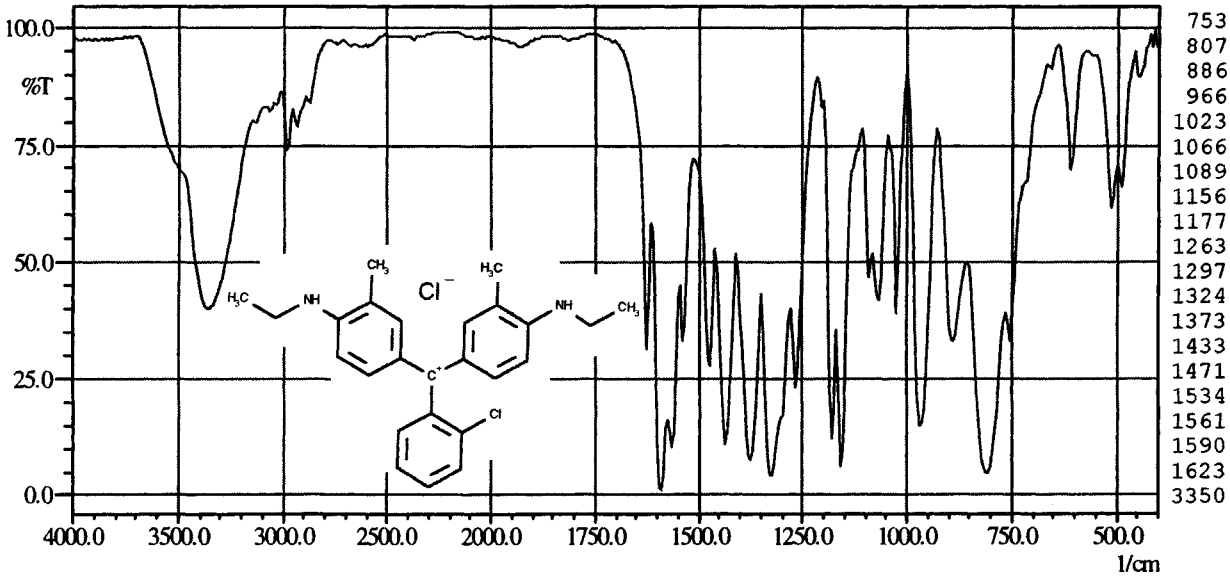
(1) **PW-molybdato-complex of bis(4-N,N-diethyl-aminophenyl)-4'-N-ethylaminonaphthalenemethane**
(2) Lumiere Blue (like Victoria Blue BO)
(3) Capelle
(5) organic pigment
(6) blue solid
(11) Pigment Blue 1
(12) 42595:2
(13) KBr pellet
(14) only the organic structure is shown

2237



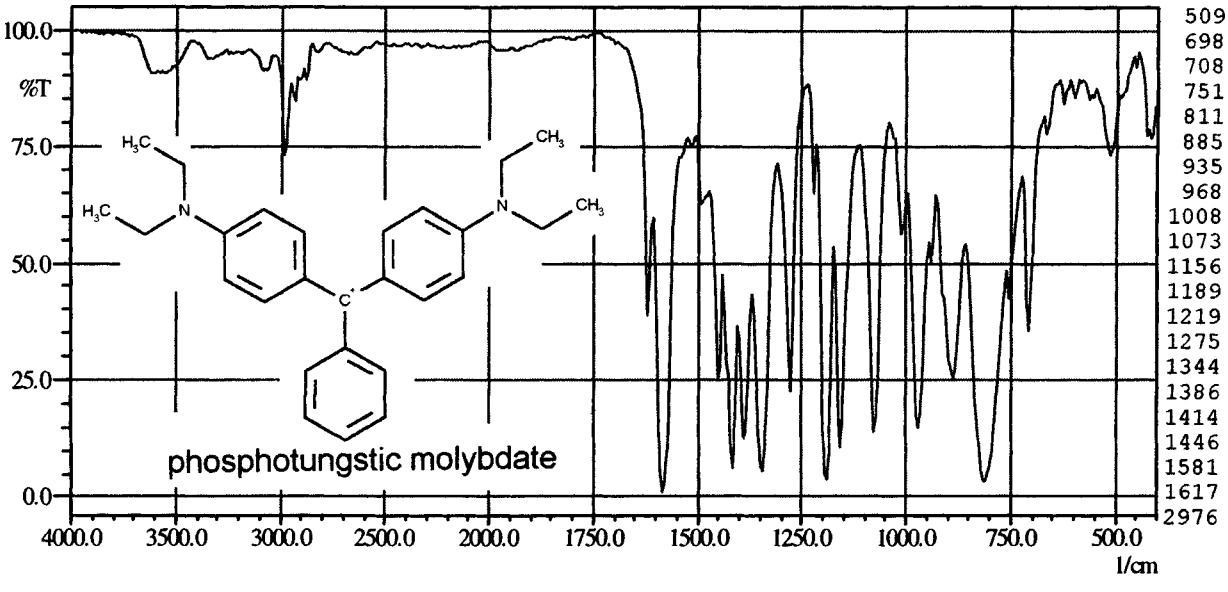
(1) **PW-molybdato complex of bis(4-N-dimethylamino-phenyl)-2''-chlorophenylmethane**
(2) Siegleblau-Extrakt D 449
(3) Siegle
(5) organic pigment
(6) blue solid
(11) Pigment Blue 9
(12) 42025:1
(13) KBr pellet
(14) only the organic structure is shown

2237 $C_{19}H_{28}Cl_2N_2$



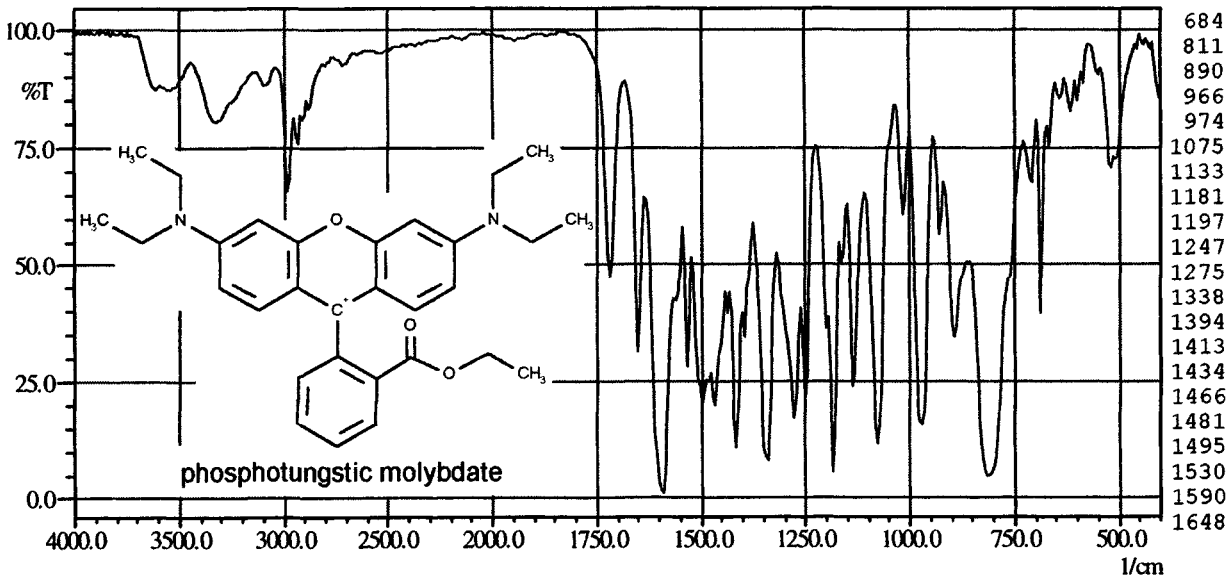
(1) **PW-molybdato complex of bis(4-N-ethylamino-3-methylphenyl)-2"-chlorophenylmethane**
(2) Fanalbremer Blau B Supra
(3) Siegle
(4) 355.4 g mol^{-1}
(5) organic pigment
(6) blue solid
(11) Pigment Blue 3
(12) 42140
(13) KBr pellet
(14) only the organic structure is shown

2237



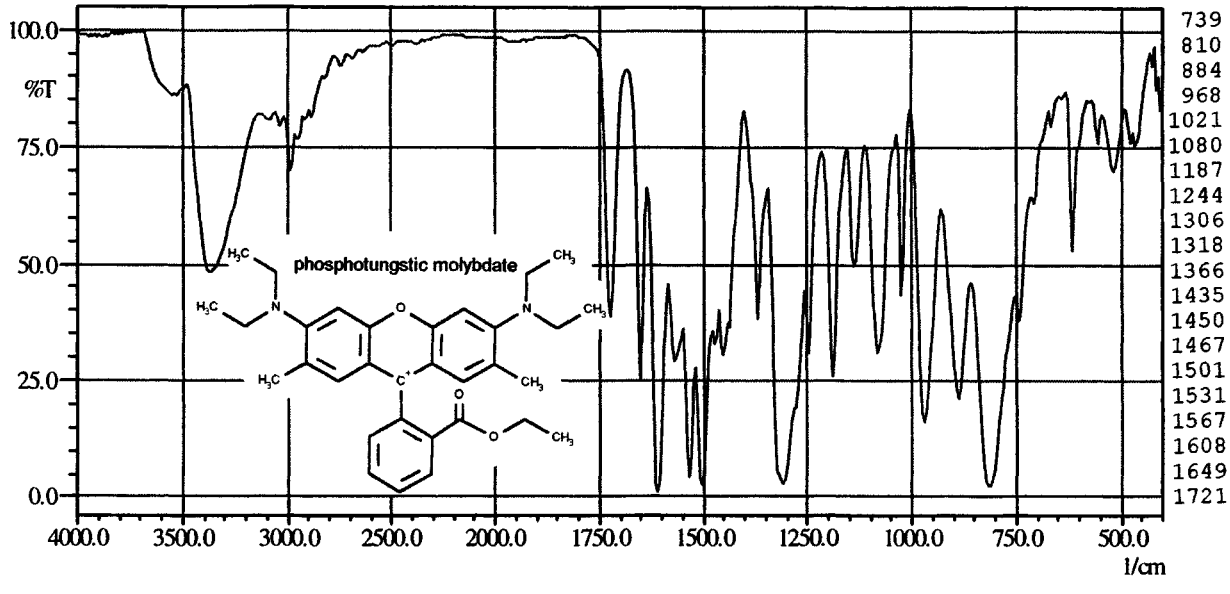
(1) **PW-molybdato complex of *bis*(4-N-diethylaminophenyl)-phenylmethane**
(2) Sieglegruen-Extrakt D 454
(3) Siegle
(5) organic pigment
(6) green solid
(11) Pigment Green 1
(12) 42040:1
(13) KBr pellet
(14) only the organic structure is shown

2237



(1) **complex of Rhodamine 3 B**
(2) Fanalrot 6B supra
(3) Siegle
(5) organic pigment
(6) red solid
(11) Pigment Violet 2
(12) 45175:1
(13) KBr pellet
(14) structure of the organic residue only

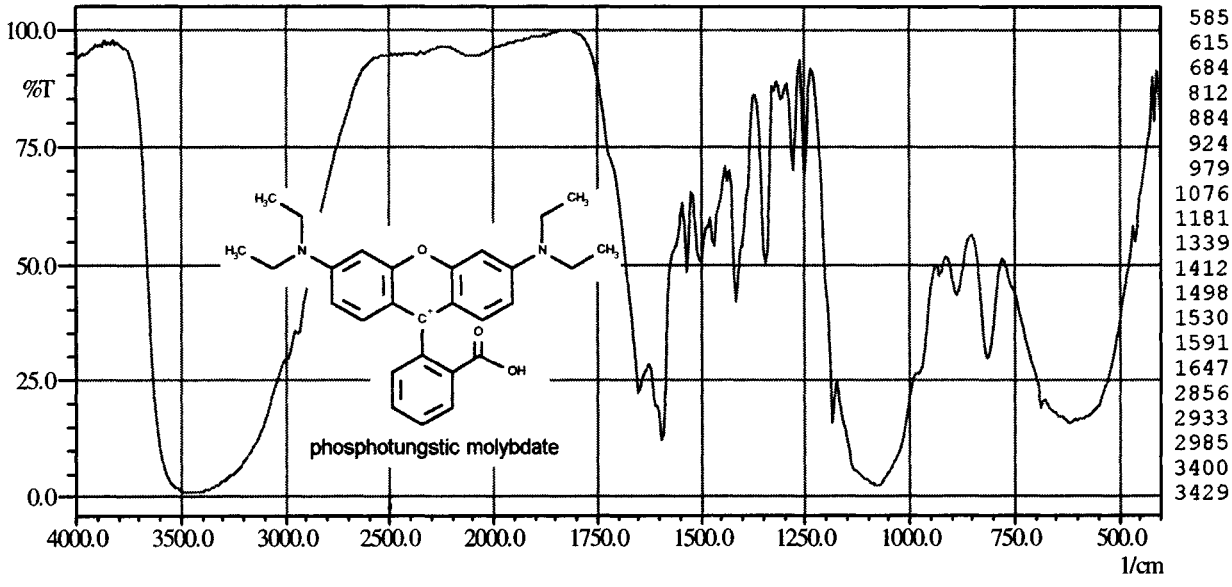
2237



(1) **PW-molybdato-complex of Rhodamine 6 G**
(2) Sieglerosa Extrakt D 443
(3) Siegle
(5) organic pigment
(6) pink solid
(11) Pigment Red 81:1
(12) 45160:1
(13) KBr pellet
(14) structure of the organic residue only

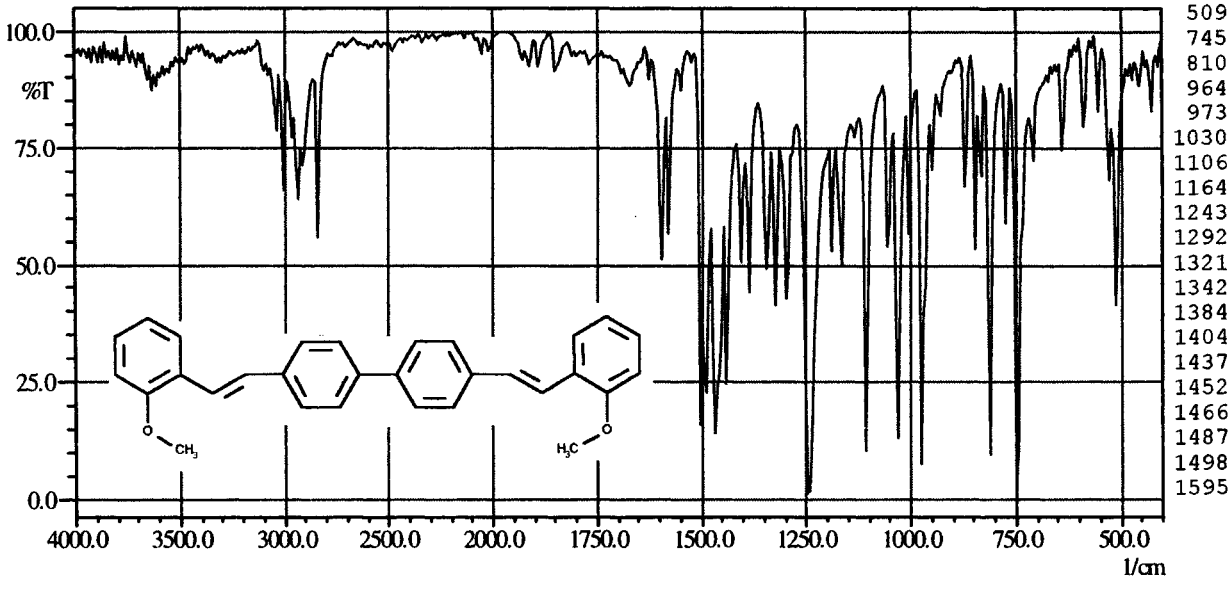
Previous Page

2237



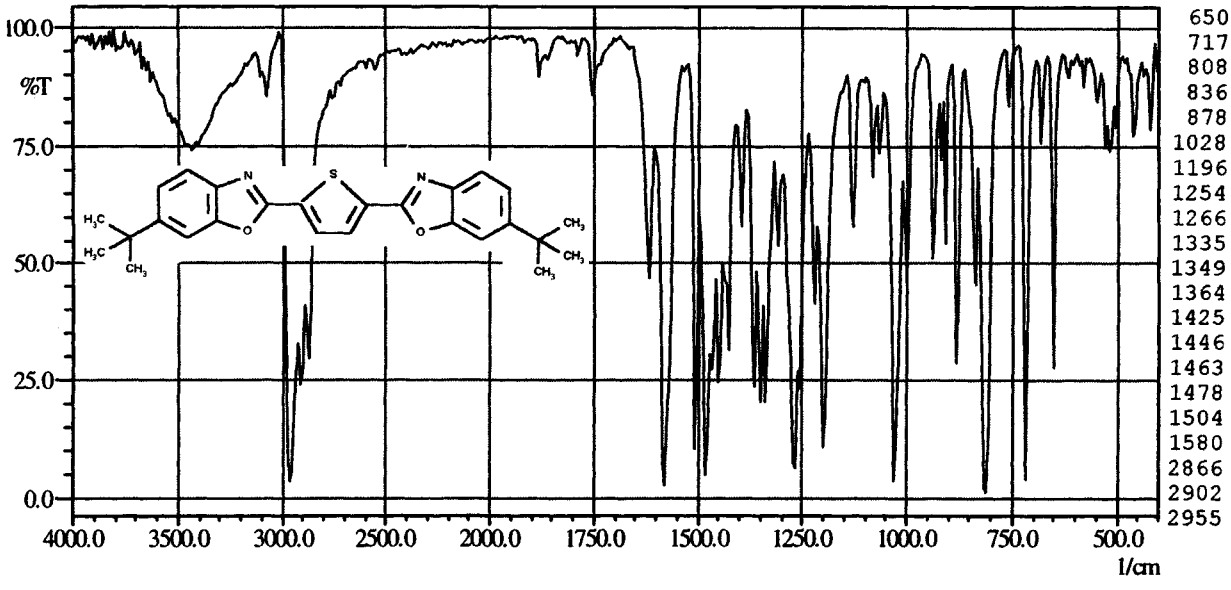
(1) **PW-molybdato-complex of Rhodamine B**
(2) Sieglerotviolett D 445
(3) Siegle
(5) organic pigment
(6) violet solid
(11) Pigment Violet 1
(12) 45170:2
(13) KBr pellet
(14) structure of the organic residue only

241 $C_{30}H_{26}O_3$



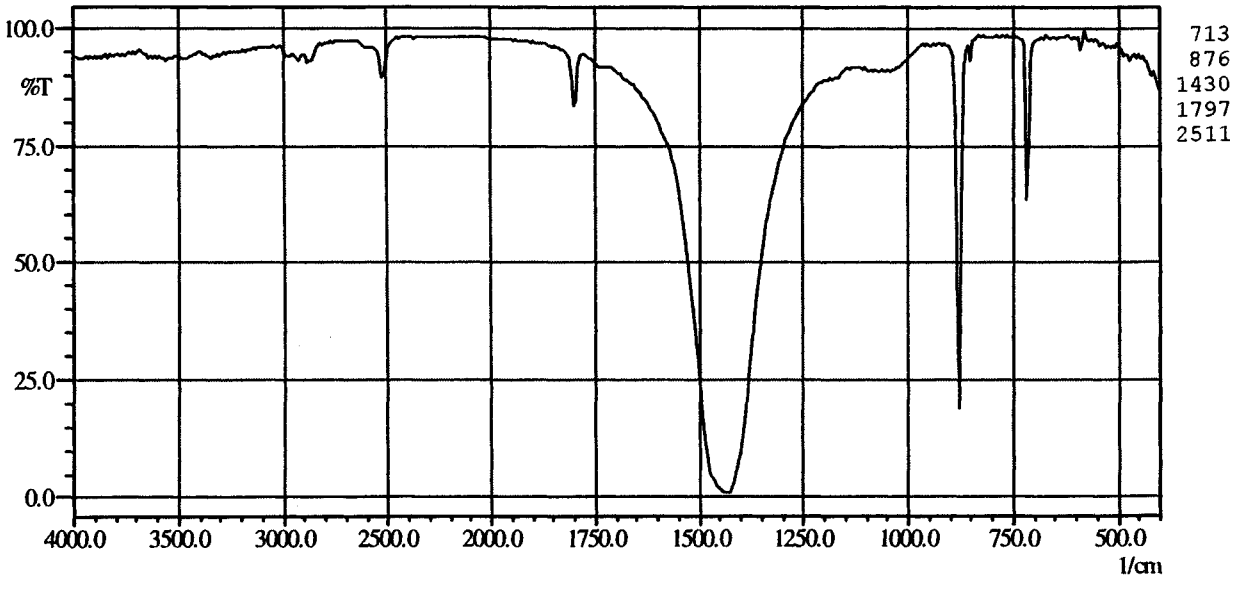
(1) **4,4'-bis(2-methoxy)stilbene**
(2) Uvitex FP
(3) Ciba-Geigy
(4) 418.5 g mol^{-1}
(5) fluorescent brightening agent
(6) yellowish-green solid
(8) 219 °C
(9) 1.23 g cm^{-3}
(13) KBr pellet, surface roughed

245 $C_{26}H_{26}N_2O_2S$



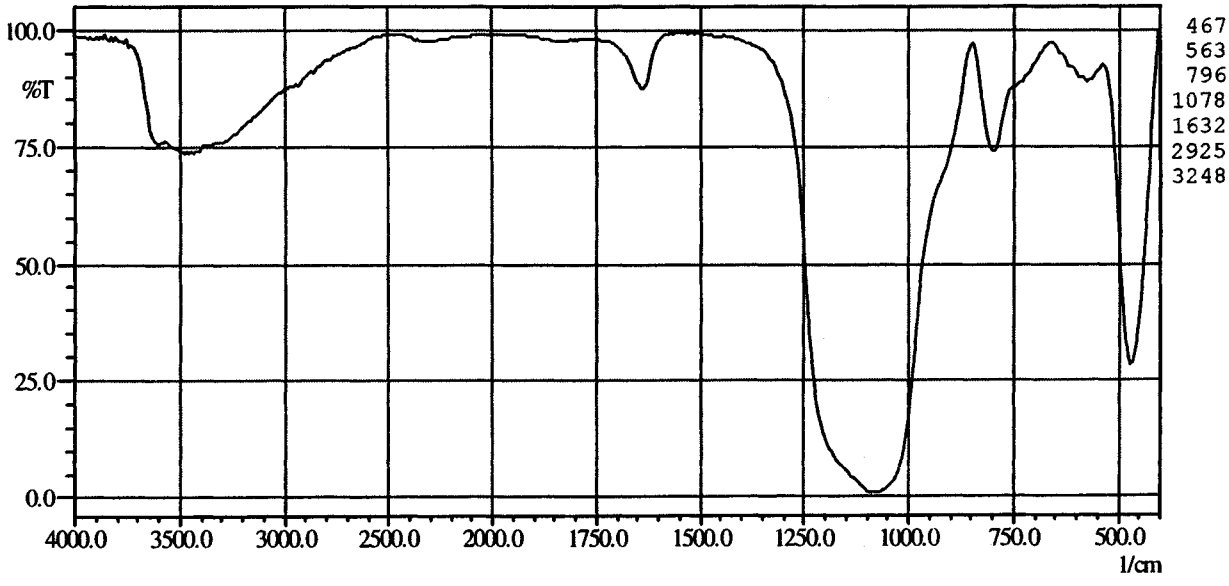
(1) **2,2'-(2,5-thiophenediyl)-bis(5-t-butylbenzoxazole)**
(2) Uvitex OB
(3) Ciba-Geigy
(4) 430.6 g mol^{-1}
(5) fluorescent whitening agent
(6) yellowish solid
(7) 200 °C
(9) 1.03 g cm^{-3}
(13) KBr pellet

25112 $CaCO_3$



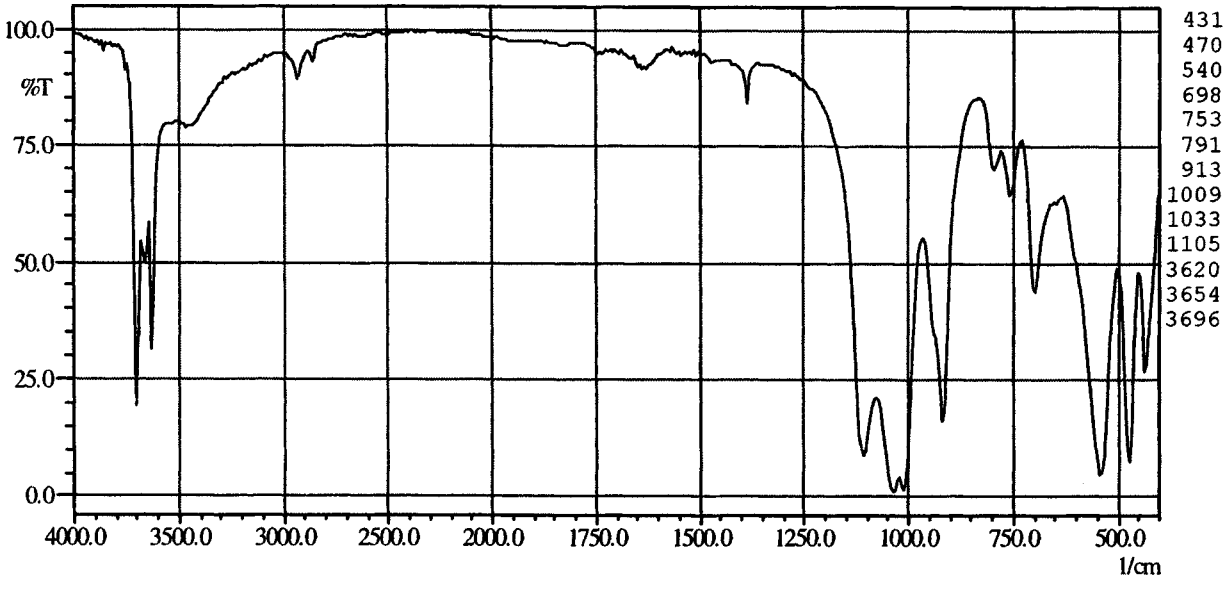
(1) **Ca carbonate**
(2) Omya BSH
(3) Omya
(4) 100.1 g mol^{-1}
(5) filler
(6) colourless solid
(13) KBr pellet
(14) calcite

25114



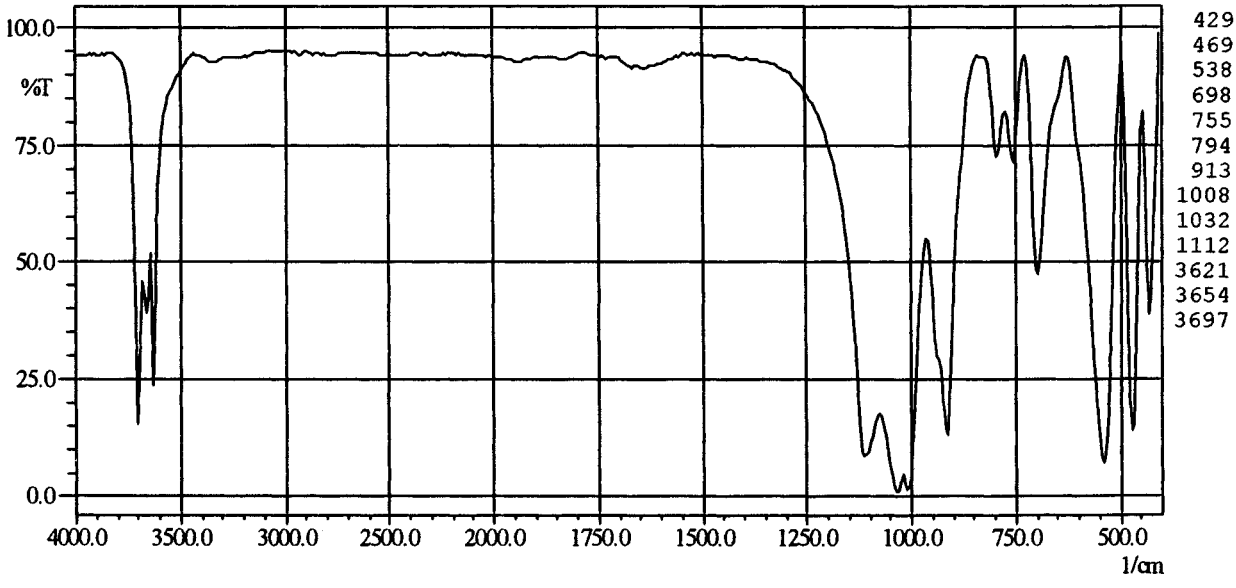
(1) **Na-Al silicate**
(2) Vulkasil A 1
(3) Bayer
(5) filler
(6) colourless solid
(9) 2 g cm^{-3}
(13) KBr pellet

25114 $Al_4(OH)_8Si_4O_{10}$



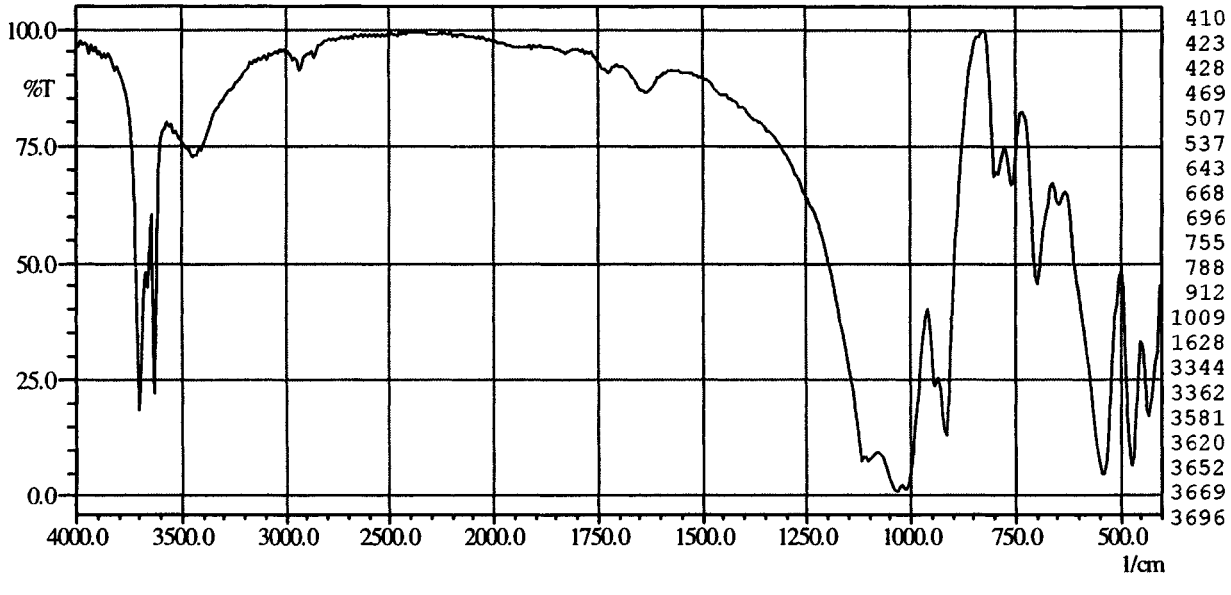
(1) **Al hydroxysilicate**
(2) Kaolin Argirex
(3) Kaolin
(4) 516.3 g mol^{-1}
(5) filler
(6) light-grey solid
(13) KBr pellet

25114 $Al_2(SiO_3)_2$



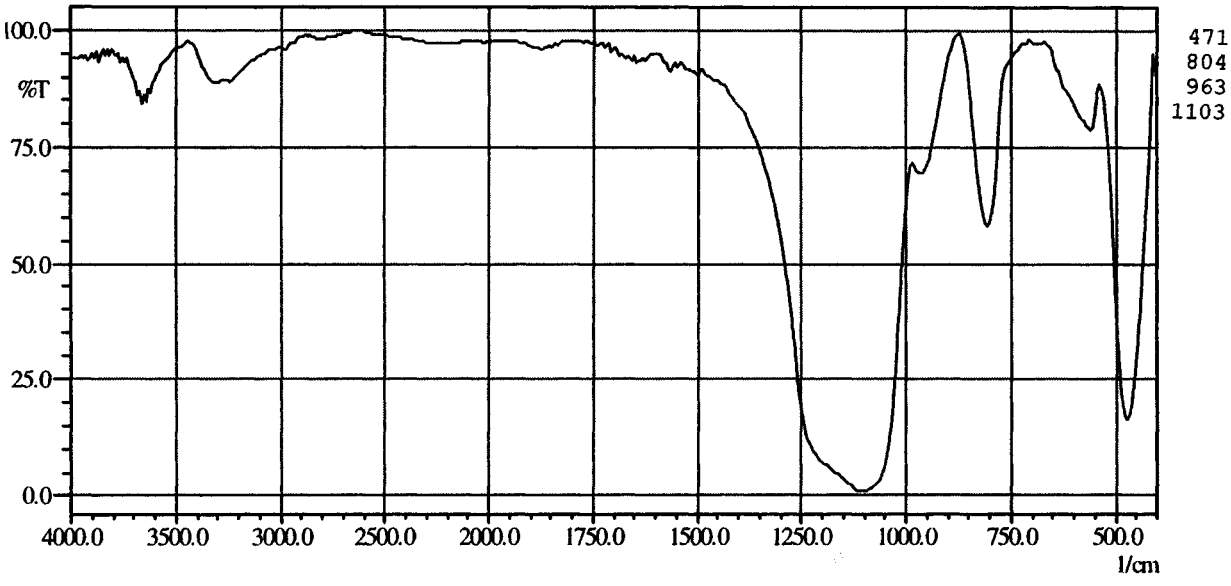
(1) **calcinated Al silicate**
(2) Argirex B24
(3) Blancs MinÈraux
(5) inorganic pigment, filler
(6) greyish solid
(13) KBr pellet

25114 $Al_4(OH)_8Si_4O_{10}$



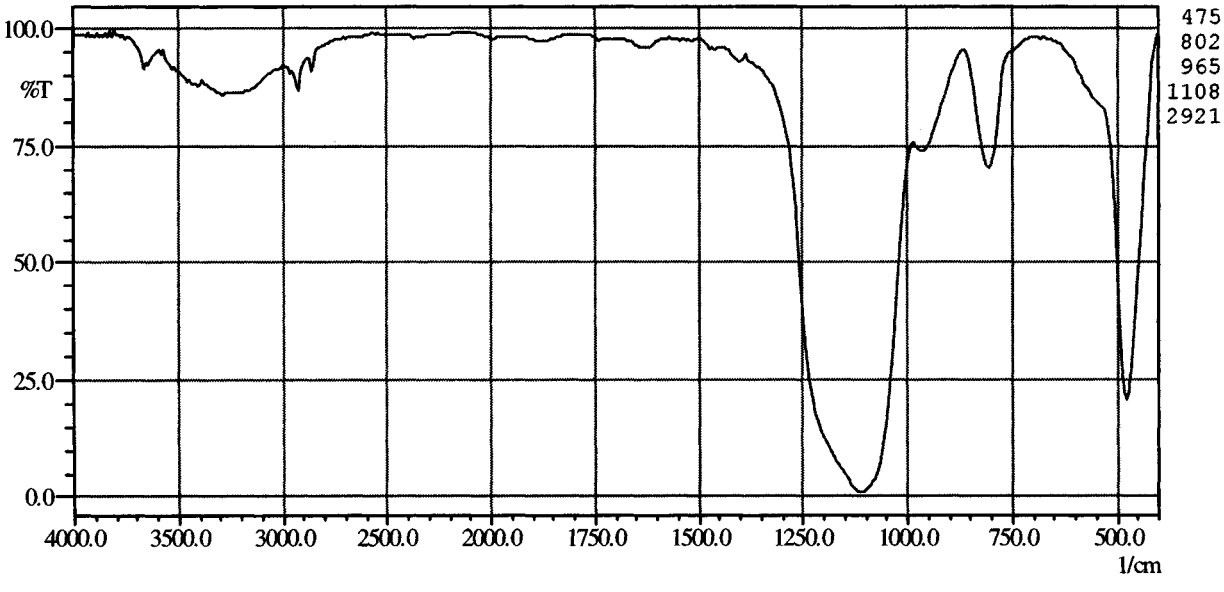
(1) **Al hydroxysilicate**
(2) China Clay Polewhite LM
(3) Freudenberg (Brunne collection)
(4) 516.3 g mol^{-1}
(5) filler
(6) colourless solid
(13) KBr pellet

2514 SiO_2



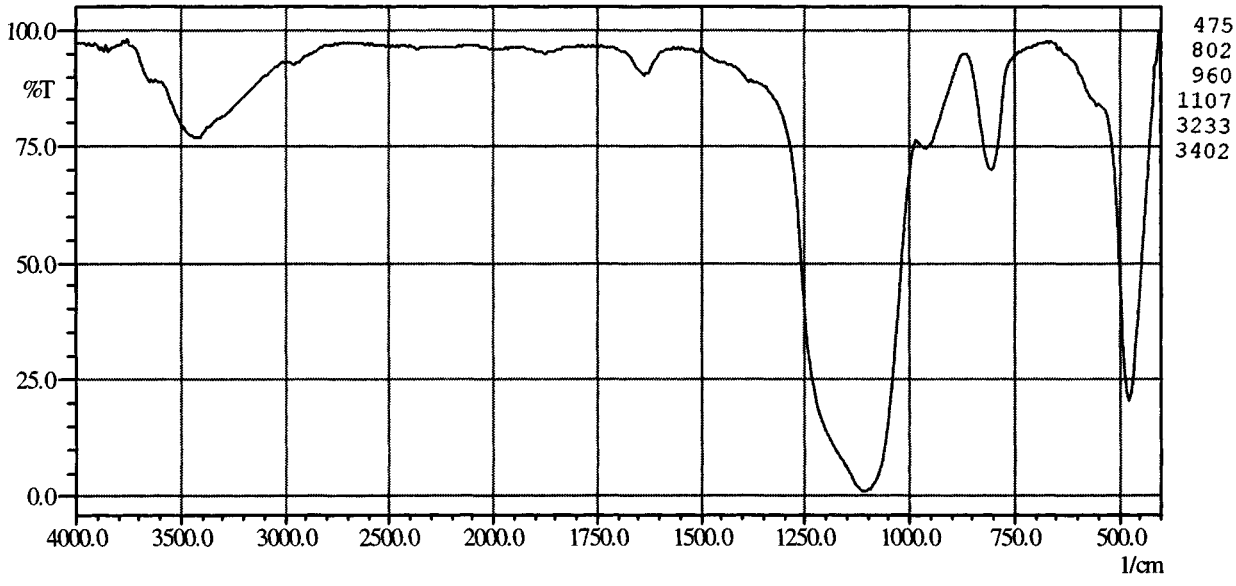
(1) **amorphous SiO_2**
(2) Perkasil KS 404
(3) Akzo Chemie
(5) filler
(6) colourless solid
(13) KBr pellet

2514 SiO_2



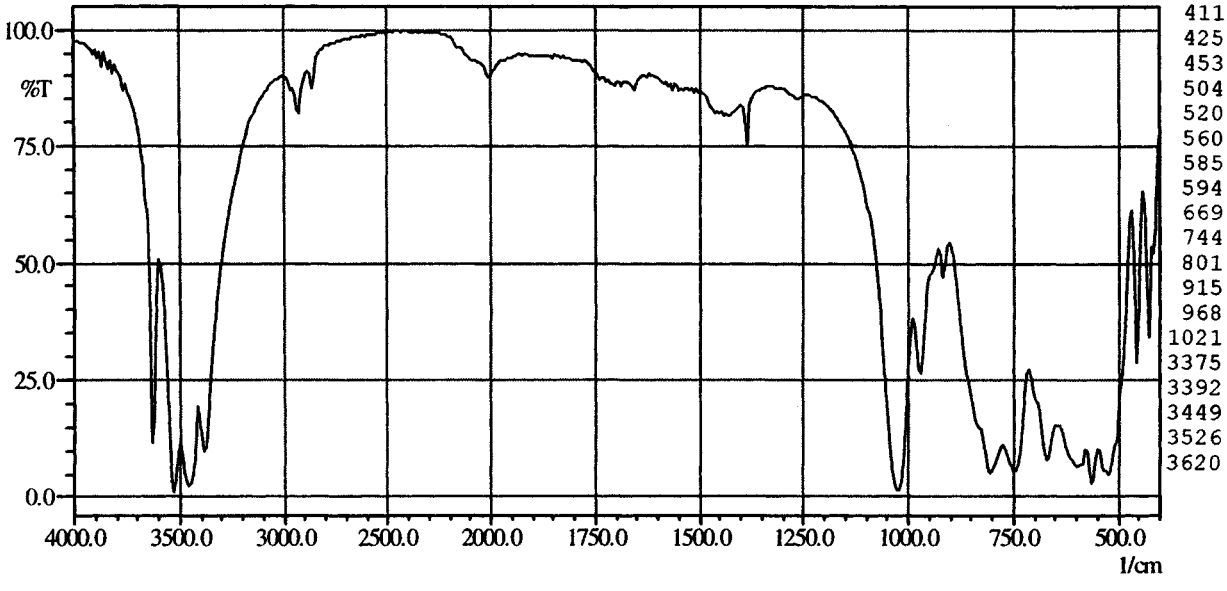
(1) **active SiO_2**
(2) Vulkasil N
(3) Bayer
(4) 60.07 g mol^{-1}
(5) filler
(6) colourless solid
(9) 2 g cm^{-3}
(13) KBr pellet

2514+25114



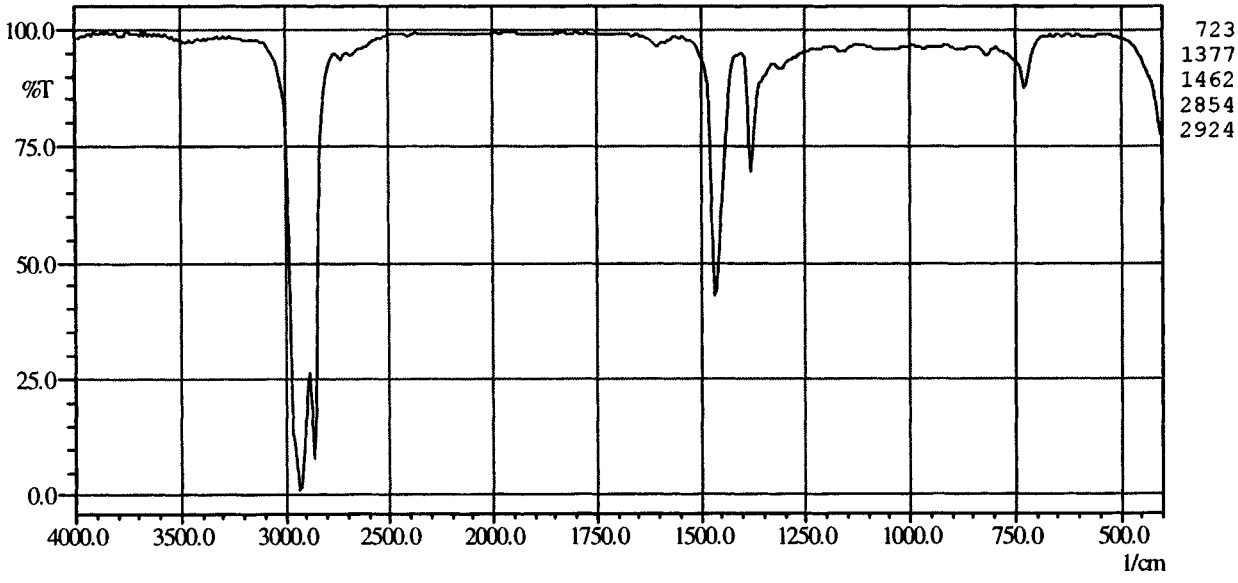
(1) **SiO_2 with Ca silicate**
(2) Vulkasil C
(3) Bayer
(5) filler
(6) colourless solid
(9) 2 g cm^{-3}
(13) KBr pellet

2514 **$Al(OH)_3$**



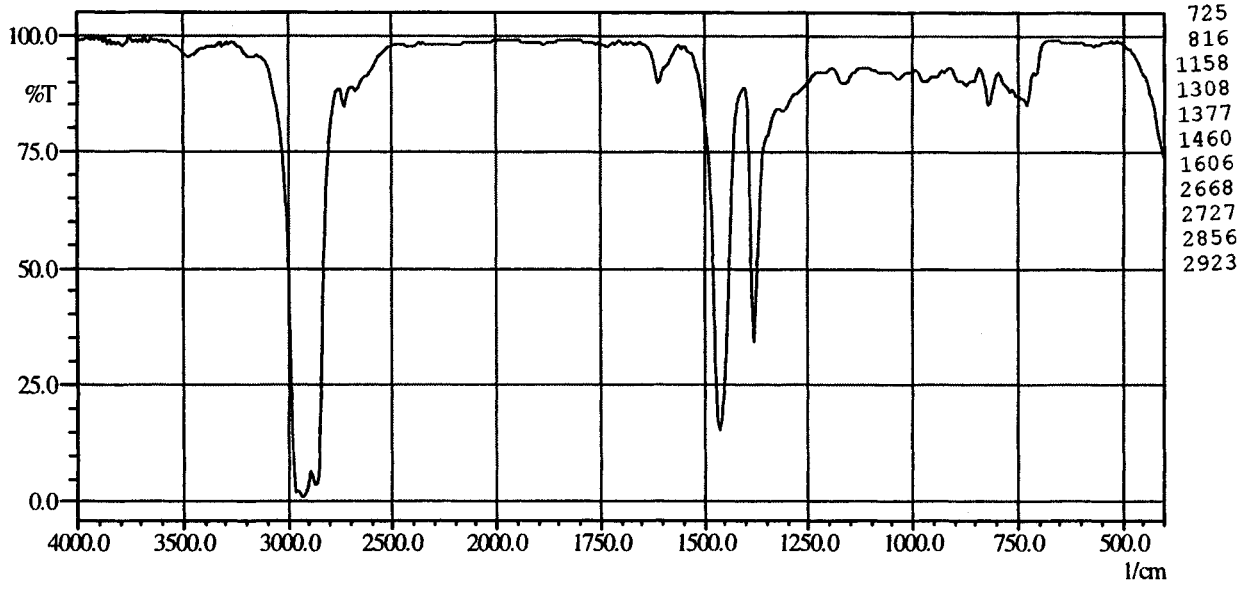
(1) **Al hydroxide**
(2) Apyral B 40 E
(3) Bayer
(4) 78.00 g mol^{-1}
(5) filler, flame retardant
(6) colourless solid
(9) 2.4 g cm^{-3}
(13) KBr pellet

311



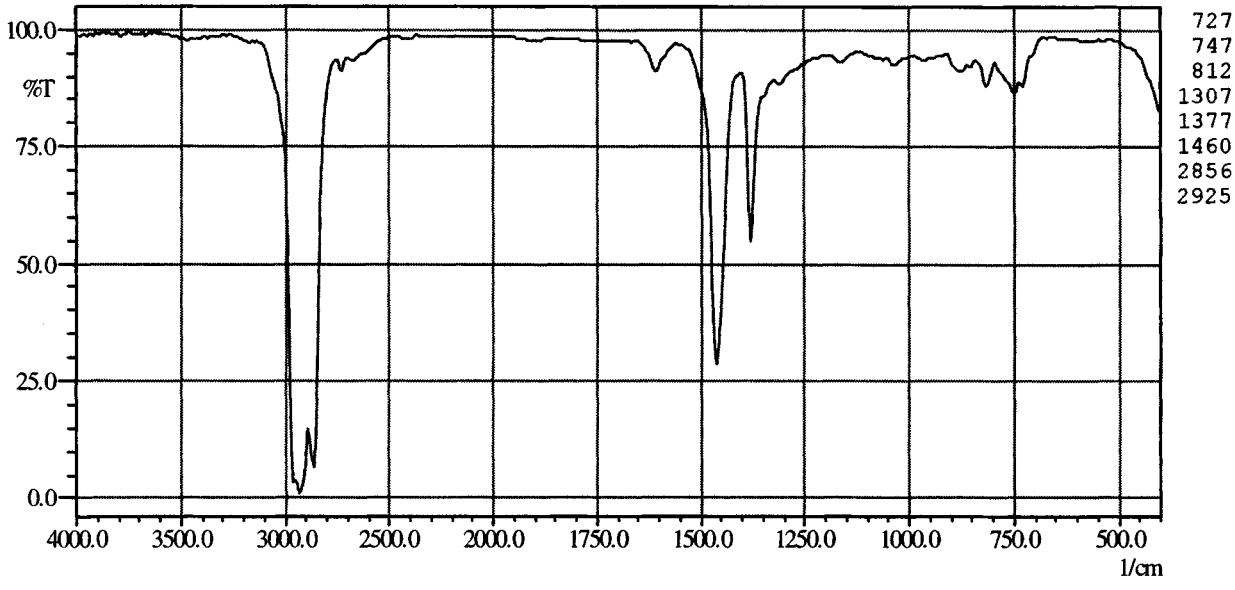
(1) **paraffinic mineral oil**
(2) Naftolen P 613 K
(3) Chemetall
(5) rubber plasticiser
(6) brown liquid
(13) layer btw KBr

312



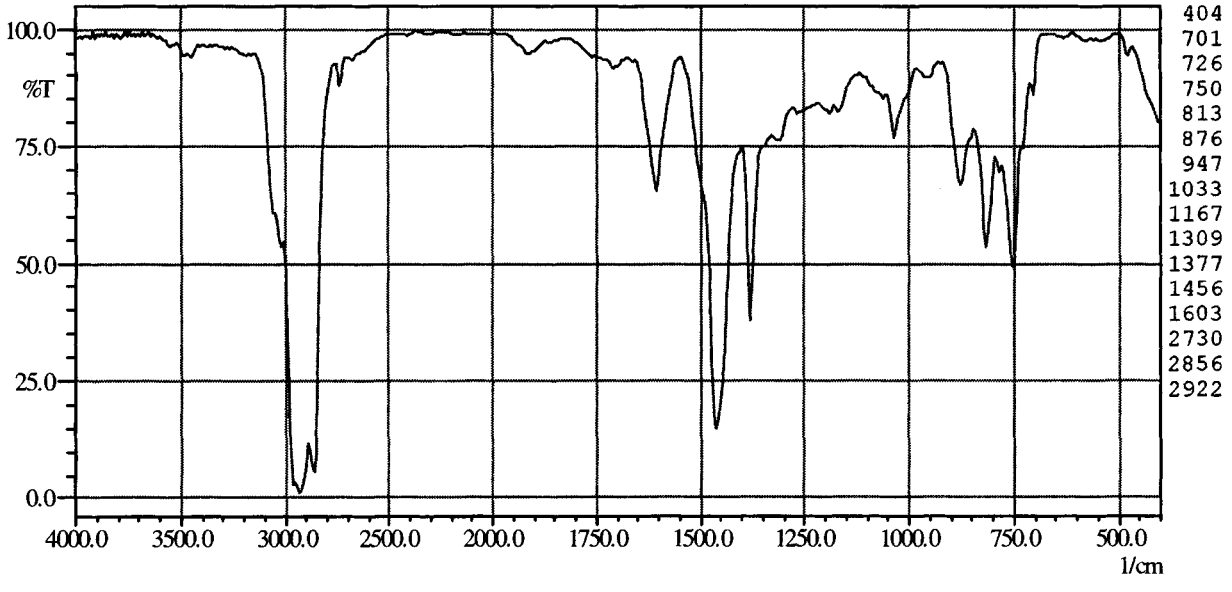
(1) **mixture of predominantly aliphatic hydrocarbons**
(2) Naftolen V 4057
(3) Chemetall
(5) rubber plasticiser
(6) brown liquid
(13) layer btw KBr

312



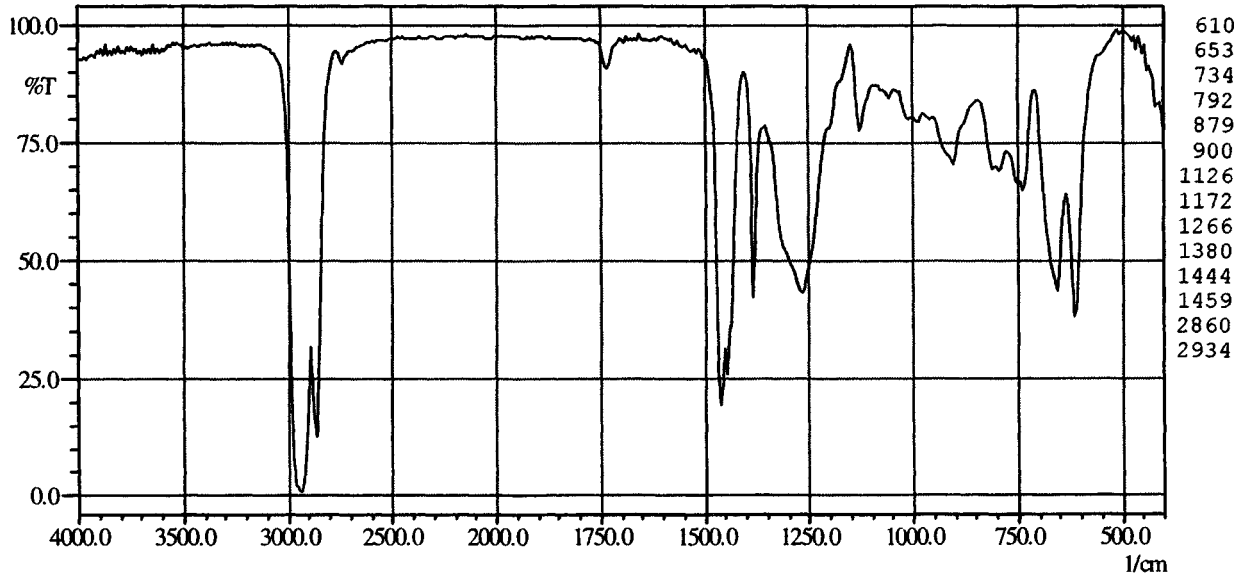
(1) **naphthenic mineral oil**
(2) Naftolen N 400
(3) Chemetall
(4) 315 g mol^{-1}
(5) rubber plasticiser
(6) brown liquid
(9) 0.907 g cm^{-3}
(10) 1.503
(13) layer btw KBr

313



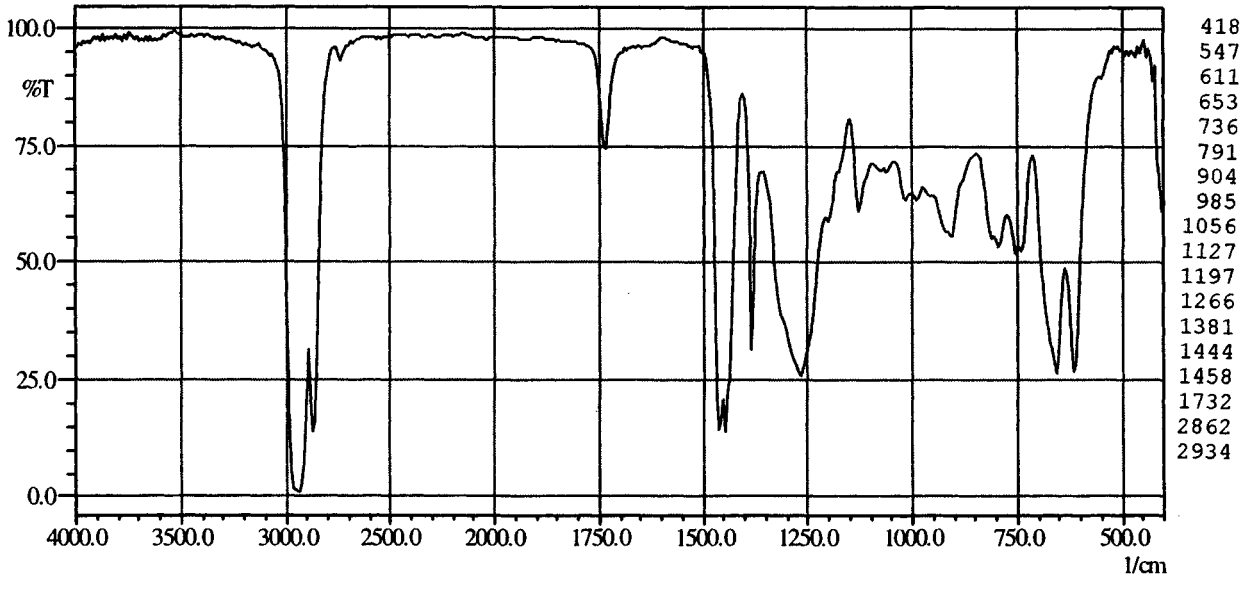
(1) **aromatic mineral oil**
(2) Naftolen NV
(3) Chemetall
(5) rubber plasticiser
(6) black liquid
(13) layer btw KBr

314



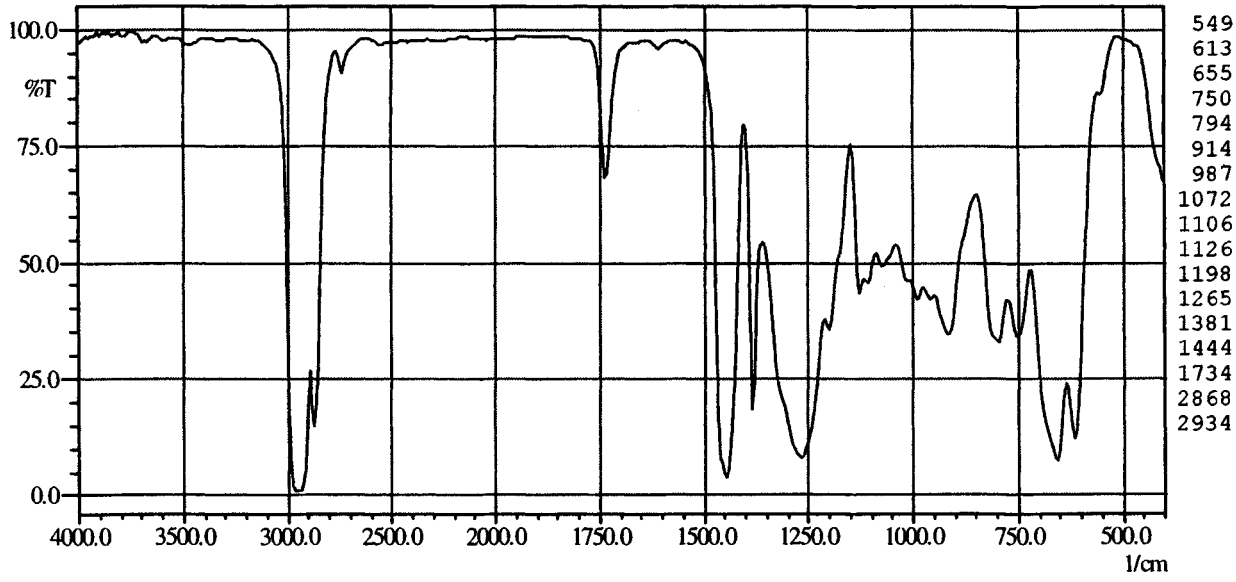
(1) **aliphatic C_{15},C_{16} chloroparaffin**
(2) Chlorparaffin Huels 40G
(3) Huels
(5) plasticiser
(6) colourless, clear liquid
(9) 1.09 g cm^{-3}
(10) 1.487
(13) layer btw KBr

314



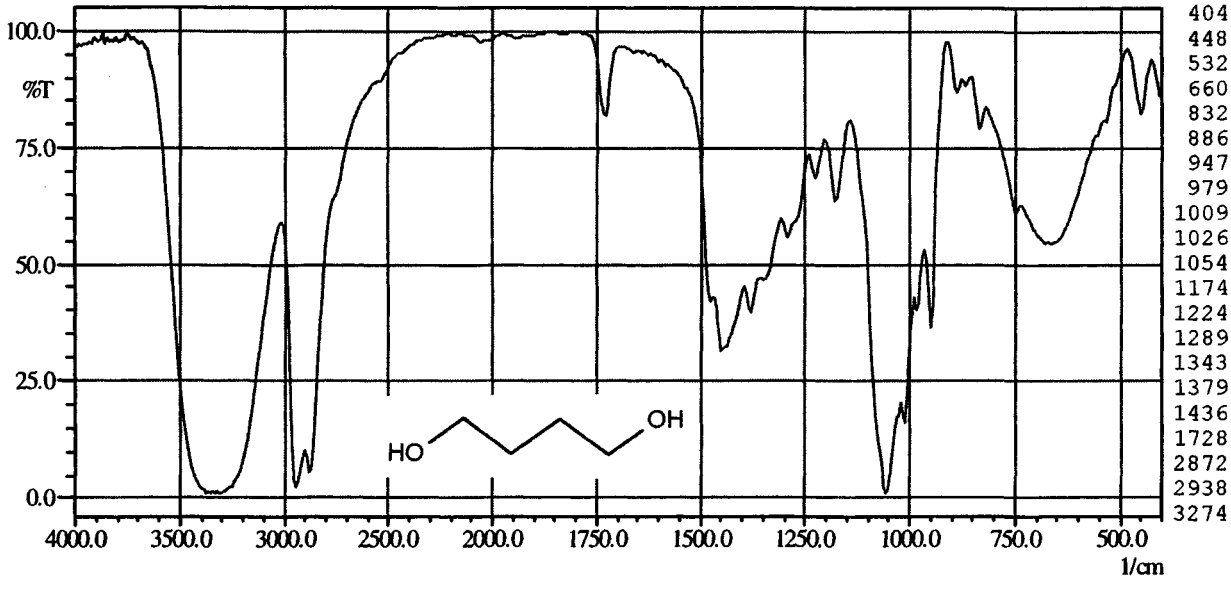
(1) **aliphatic C_{15},C_{16} chloroparaffin (40...56 % Cl)**
(2) Chlorparaffin Huels 45G
(3) Huels
(5) plasticiser
(6) colourless, clear liquid
(9) 1.14 g cm^{-3}
(10) 1.495
(13) layer btw KBr

314



(1) **aliphatic C_{15},C_{16}-chloroparaffin**
(2) Chlorparaffin Huels 52G
(3) Huels
(5) plasticiser
(6) colourless, clear liquid
(9) 1.24 g cm^{-3}
(10) 1.511
(13) layer btw KBr

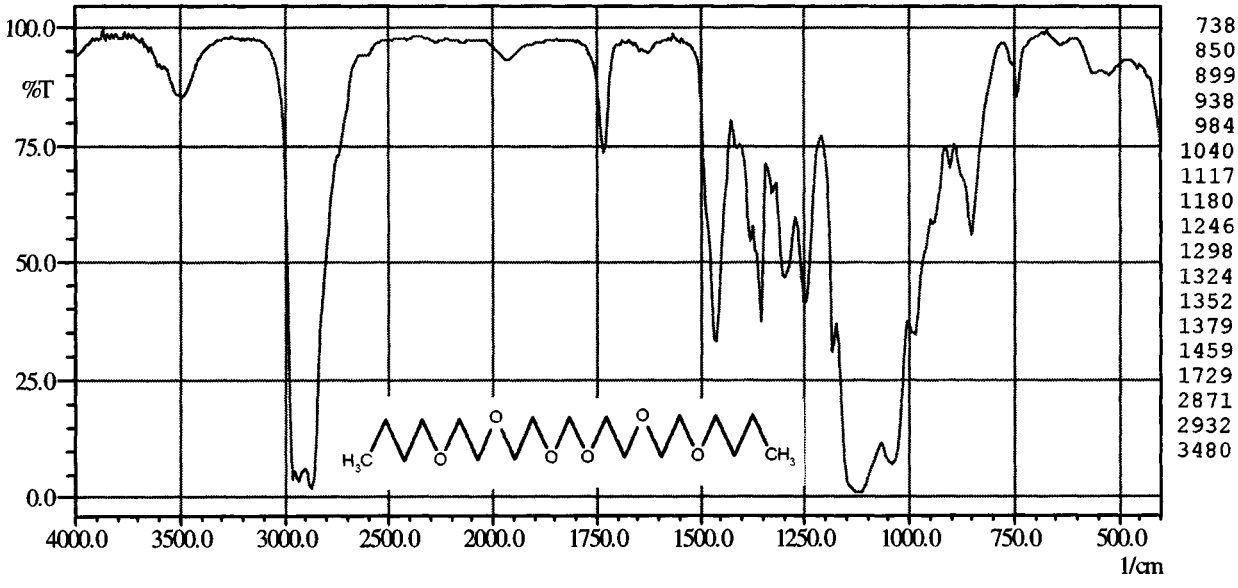
322 $C_4H_{10}O_2$



(1) **1,4-butanediol**
(2) 1,4-Butandiol
(3) Huels
(4) 90.12 g mol^{-1}
(5) plasticiser, educt
(6) colourless, clear liquid
(7) 16 °C
(8) 230 °C
(9) 1.017 g cm^{-3}
(10) 1.445v
(13) layer btw KBr
(14) with ester impurity

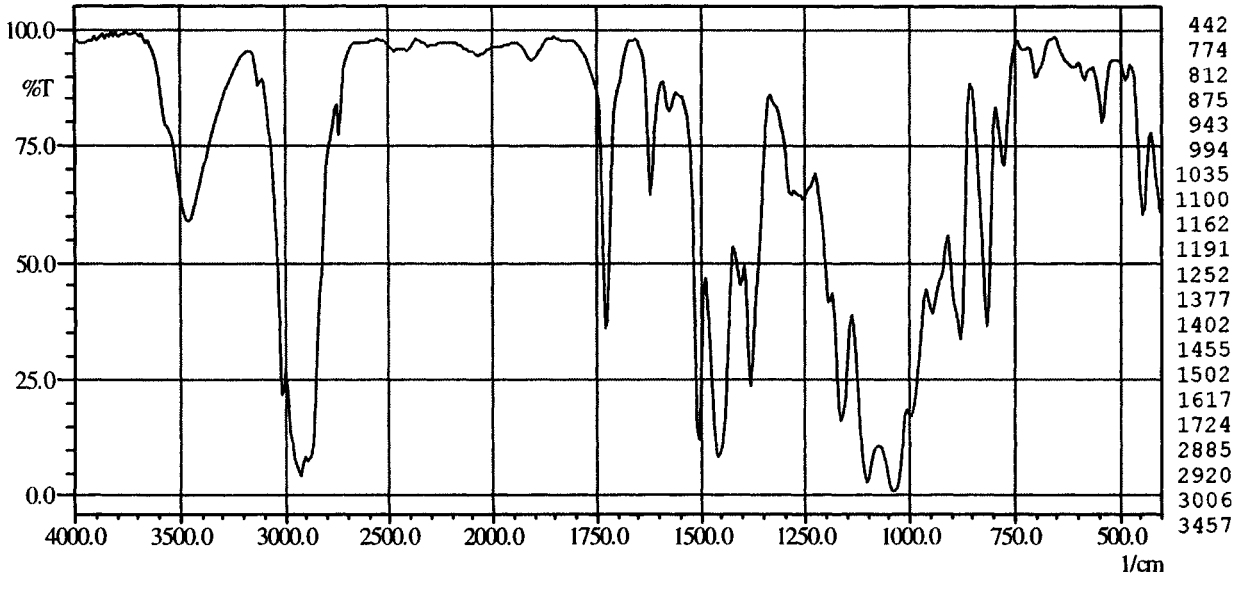
Next Page

323 $C_{17}H_{36}O_6$



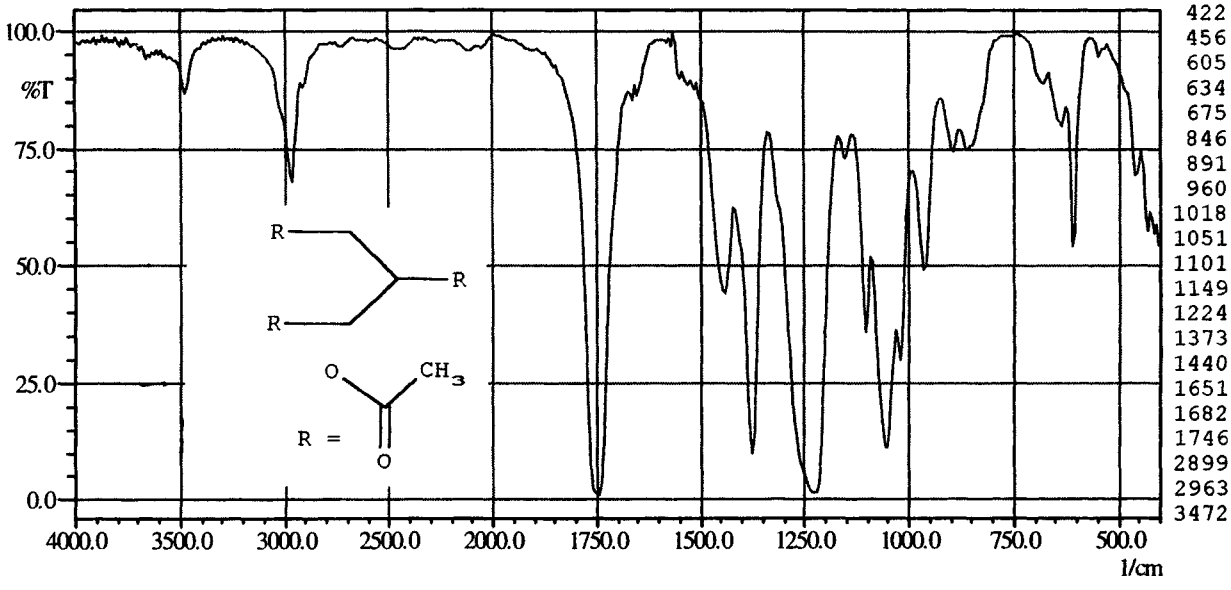
(1) **di-butoxyethoxyethyl formal**
(2) Reomol BCF
(3) Ciba-Geigy
(4) 336.5 g mol^{-1}
(5) plasticiser
(6) colourless, clear liquid
(9) 0.964 g cm^{-3}
(10) 1.435
(13) layer btw KBr

326



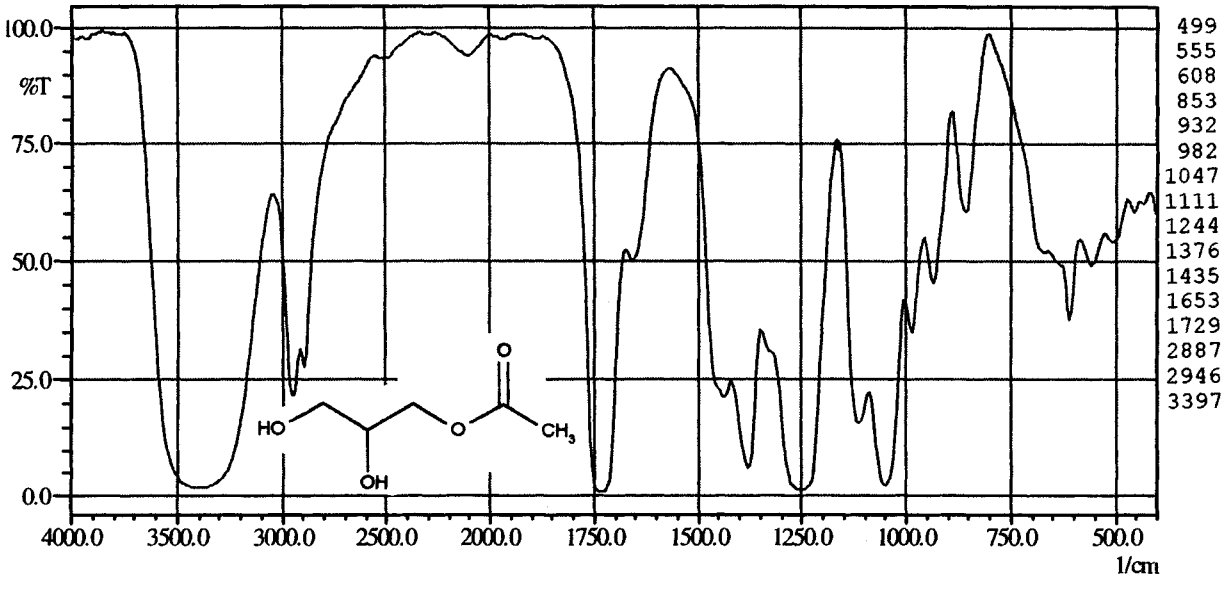
(1) **polyether with ester and alcoholic groups**
(2) Vulkanol FH
(3) Bayer
(5) plasticiser
(6) colourless, clear liquid
(9) 1.06 g cm^{-3}
(10) 1.57
(13) layer btw KBr

3311 $C_9H_{14}O_6$



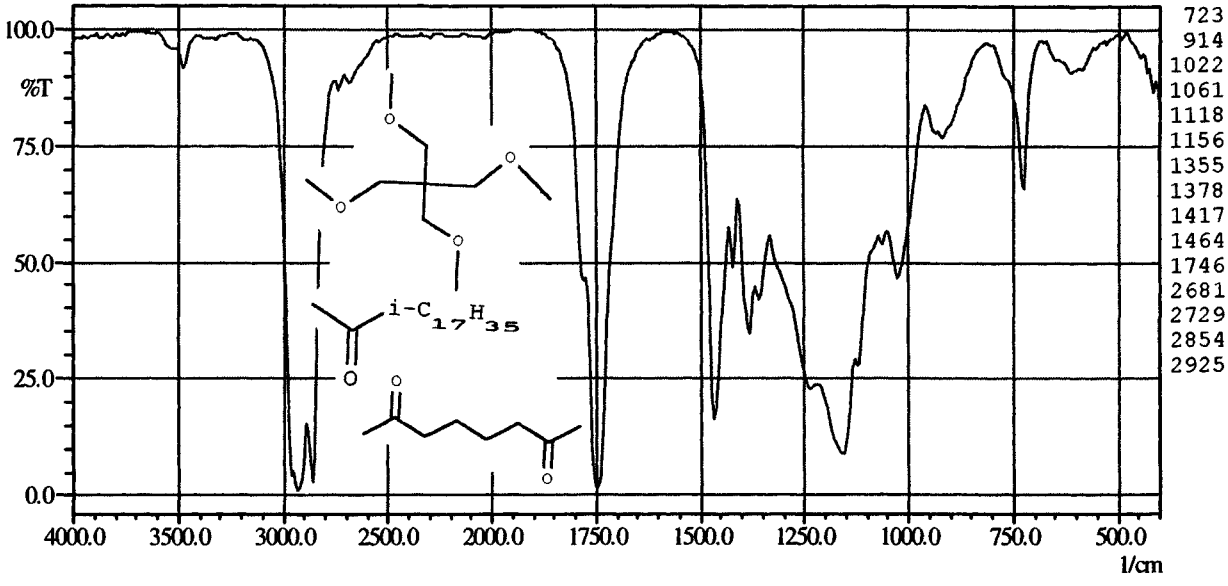
(1) **glyceroltriacetate**
(2) Triacetin
(3) Bayer
(4) 218.2 g mol^{-1}
(5) plasticiser
(6) colourless, clear liquid
(7) 3 °C
(8) 258 °C
(9) 1.155 g cm^{-3}
(10) 1.431
(13) layer btw KBr

3311 $C_5H_{10}O_4$



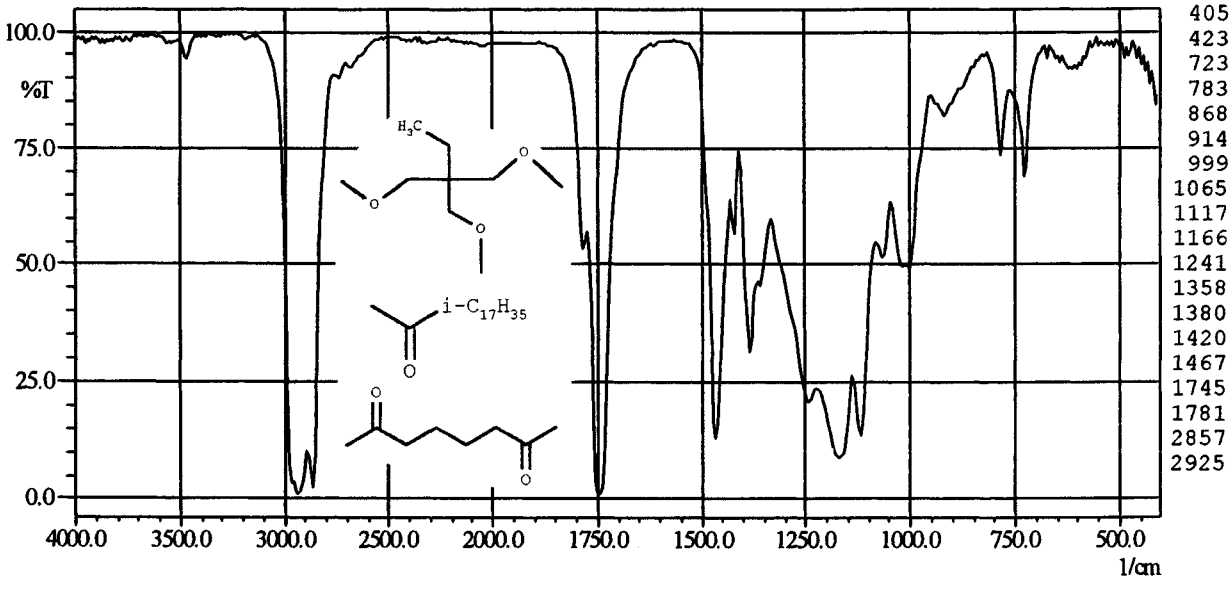
(1) **glycerol monoacetate**
(2) Hallco C-918
(3) C.P. Hall, Krahn-Chemie
(4) 134.1 g mol^{-1}
(5) plasticiser
(6) colourless, clear liquid
(7) −40 °C
(9) 1.209 g cm^{-3}
(10) 1.451
(13) layer btw KBr

3312



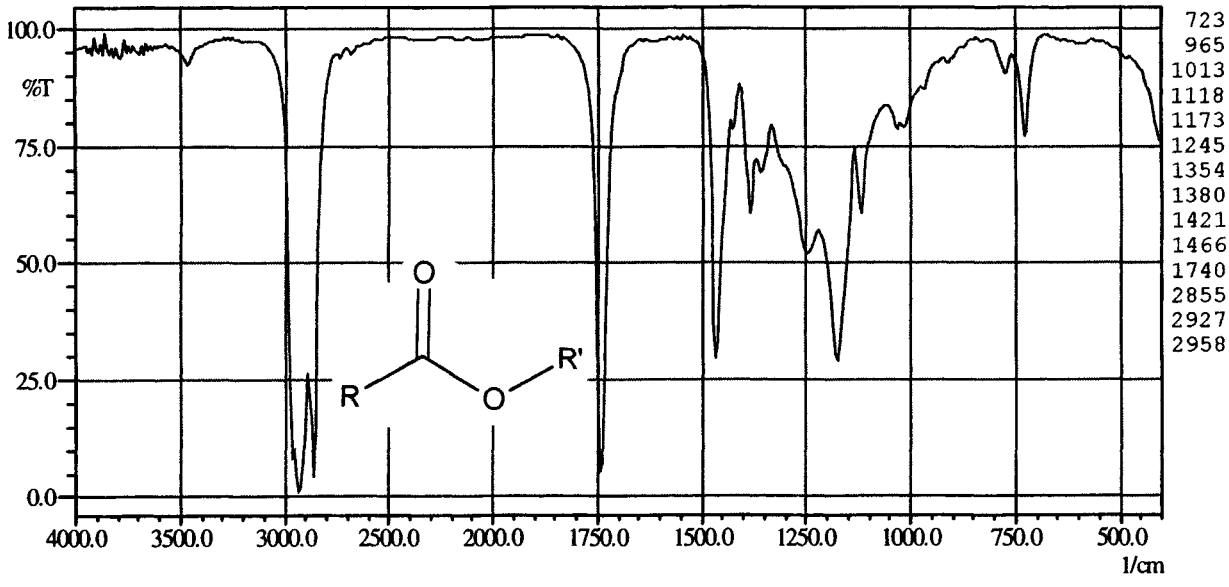
(1) **pentaerythritol(isostearate adipate)**
(2) Ester KE-23
(3) Freudenberg (Brunne collection)
(5) plasticiser
(6) colourless, viscous liquid
(13) layer on KBr

3312



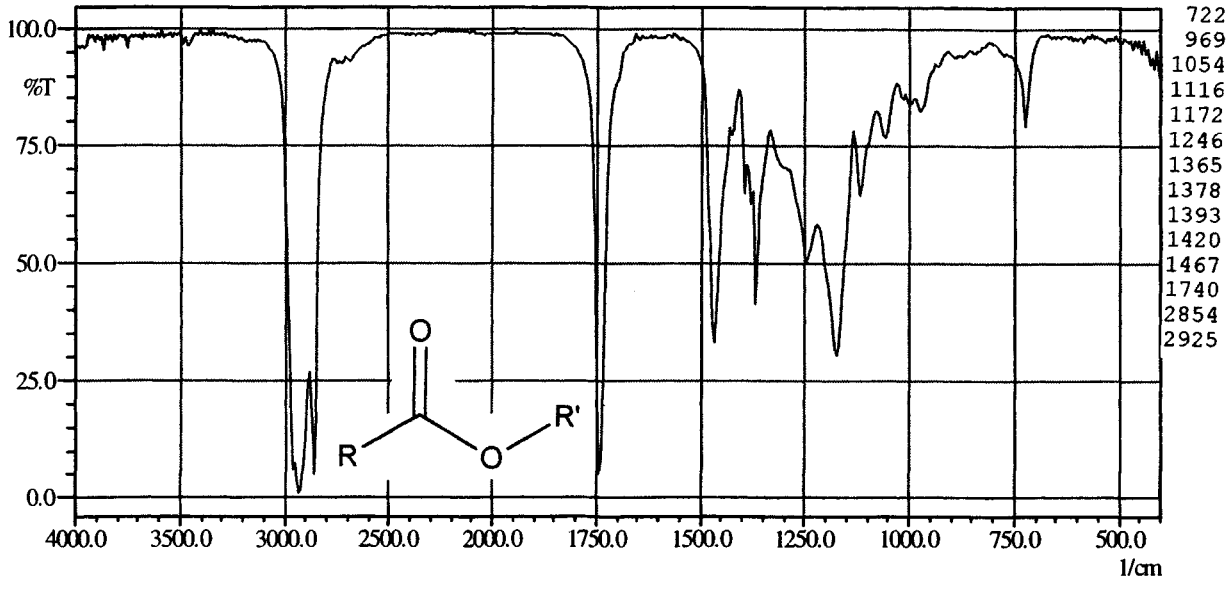
(1) **trimethylolpropane(isostearate adipate)**
(2) Ester KE-25
(3) Freudenberg (Brunne collection)
(5) plasticiser
(6) colourless, viscous liquid
(13) layer on KBr

3312



(1) **aliphatic monocarboxylic acid ester**
(2) Edenol 192
(3) Henkel
(5) plasticiser
(6) colourless, clear liquid
(9) 1.45 g cm^{-3}
(10) 0.858
(13) layer btw KBr

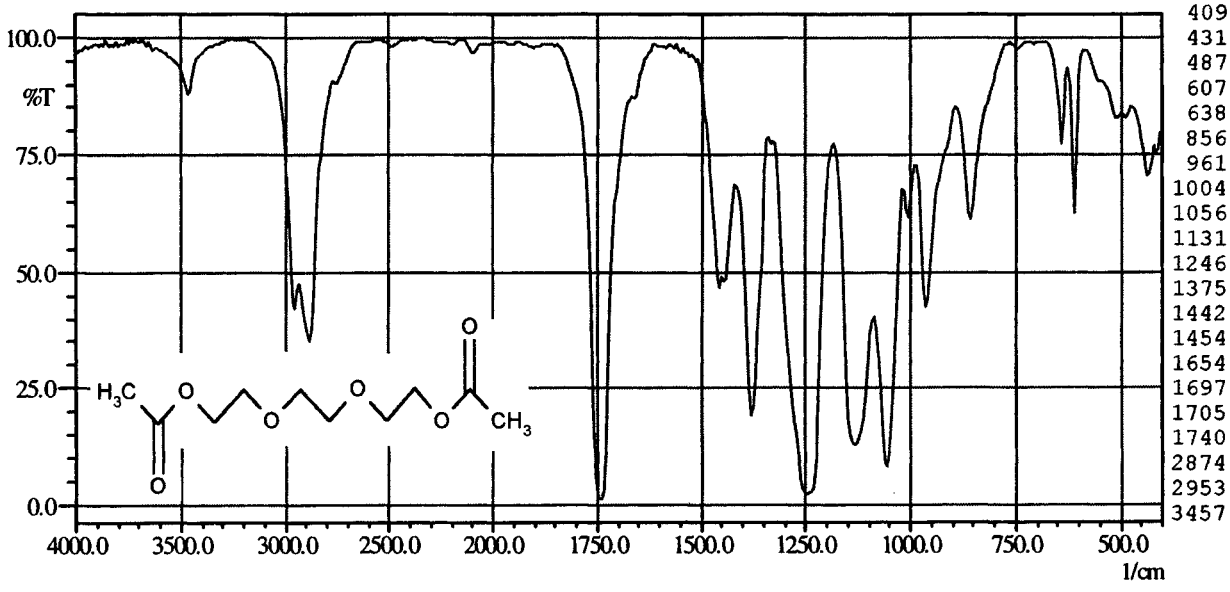
3312



(1) **aliphatic carboxylic acid ester**
(2) Edenol 194
(3) Henkel
(5) plasticiser
(6) colourless, clear liquid
(9) 0.86 g cm^{-3}
(13) layer btw KBr

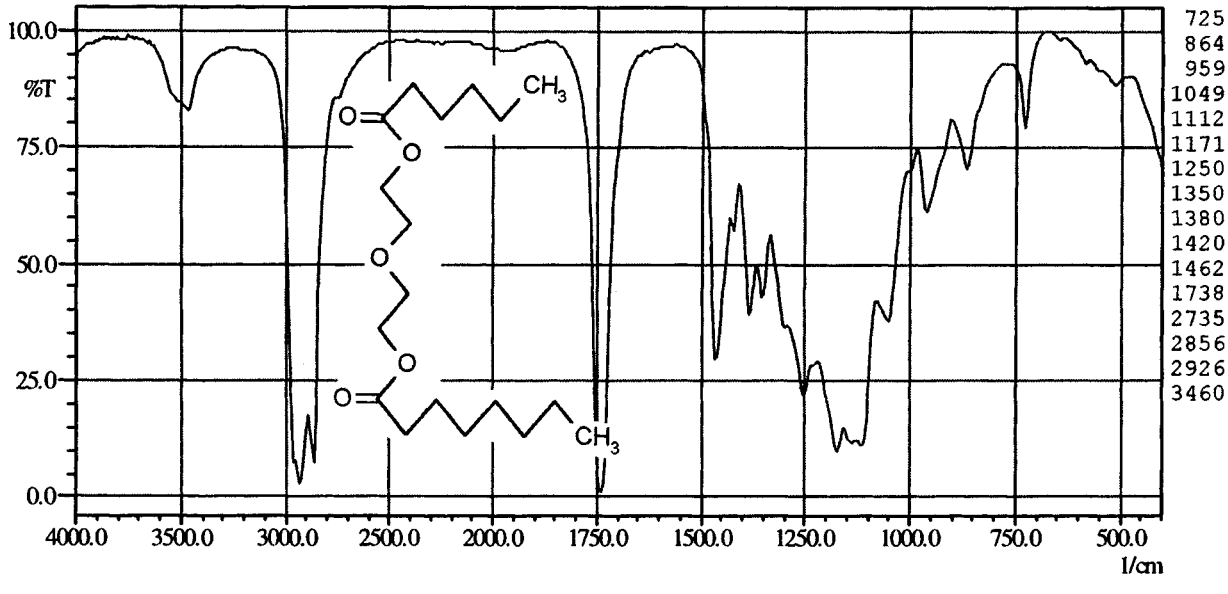
3313

$C_{10}H_{18}O_6$



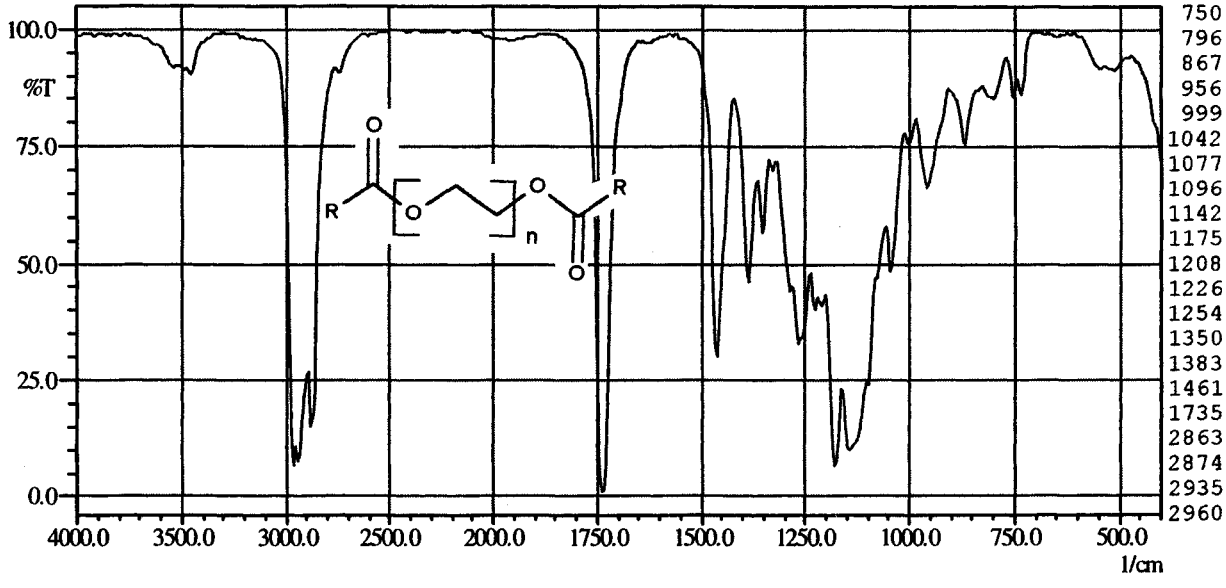
(1) **tri(ethyleneglycol)diacetate**
(2) Tegda
(3) Bayer
(4) 234.2 g mol^{-1}
(5) plasticiser
(6) colourless, clear liquid
(13) layer btw KBr

3313



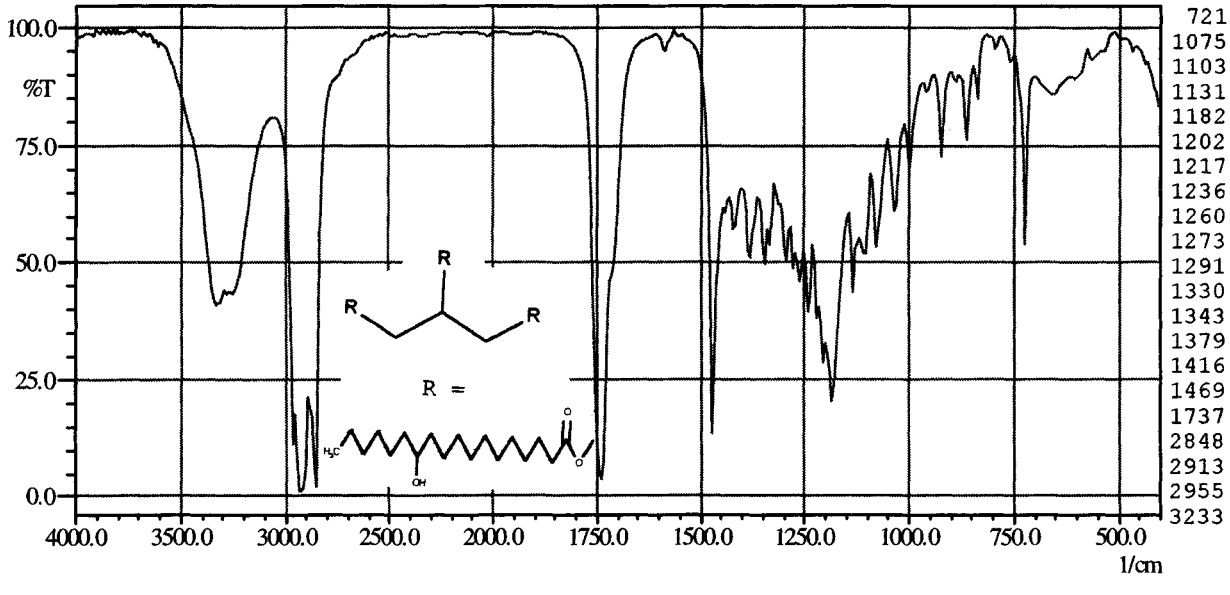
(1) **triethyleneglycol caprate-caprylate**
(2) Plasthall 4141
(3) C.P. Hall, Krahn-Chemie
(4) 430 g mol^{-1}
(5) plasticiser
(6) colourless, clear liquid
(7) -5 °C
(9) 0.968 g cm^{-3}
(10) 1.446
(13) layer btw KBr

3313



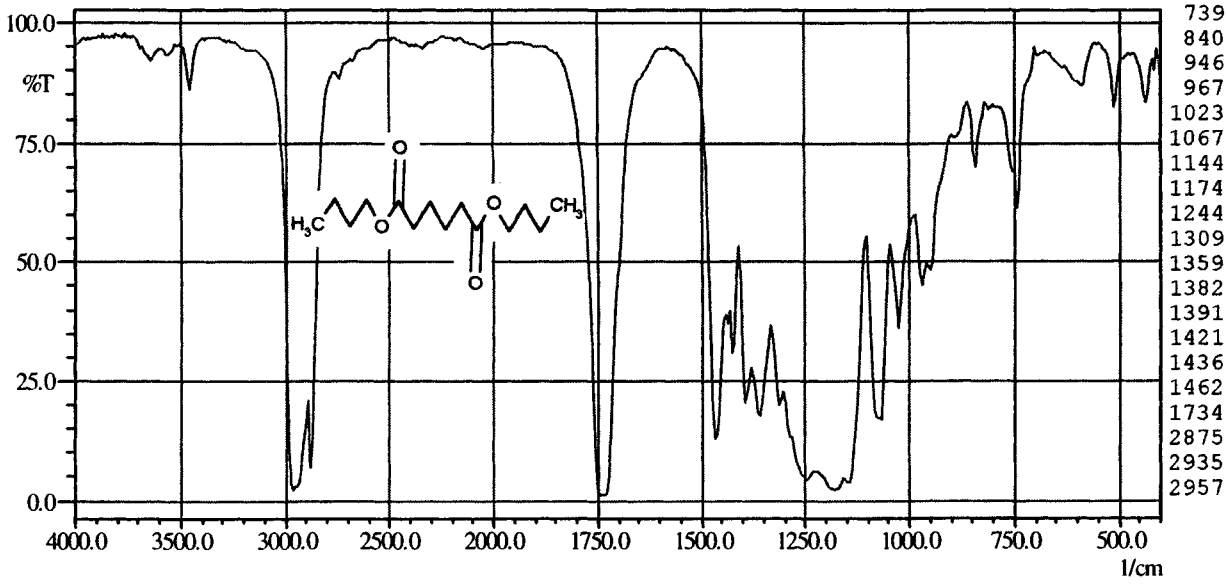
(1) **polyglycol ester of fatty acids**
(2) Witamol 460
(3) Huels
(5) plasticiser
(6) colourless, clear liquid
(13) layer btw KBr

3314



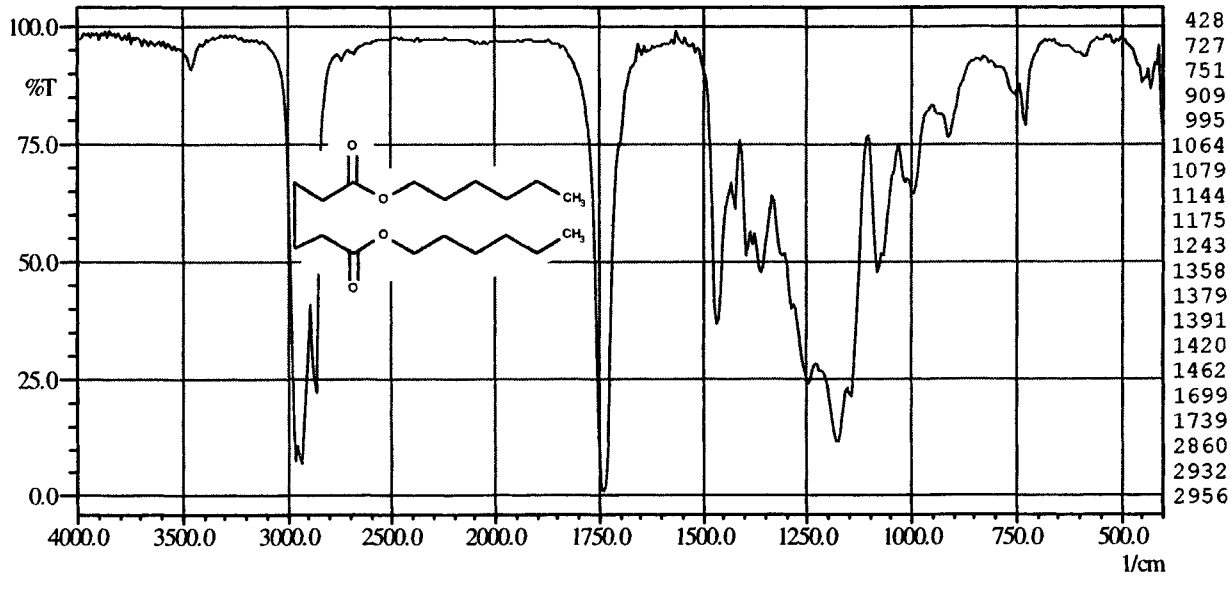
(1) **hydrogenated castor oil**
(2) Loxiol EP 15
(3) Henkel
(5) lubricant
(6) colourless solid
(7) 87 °C
(9) 0.895 g cm^{-3}
(13) recrystallised film from melt

3321 $C_{14}H_{26}O_4$



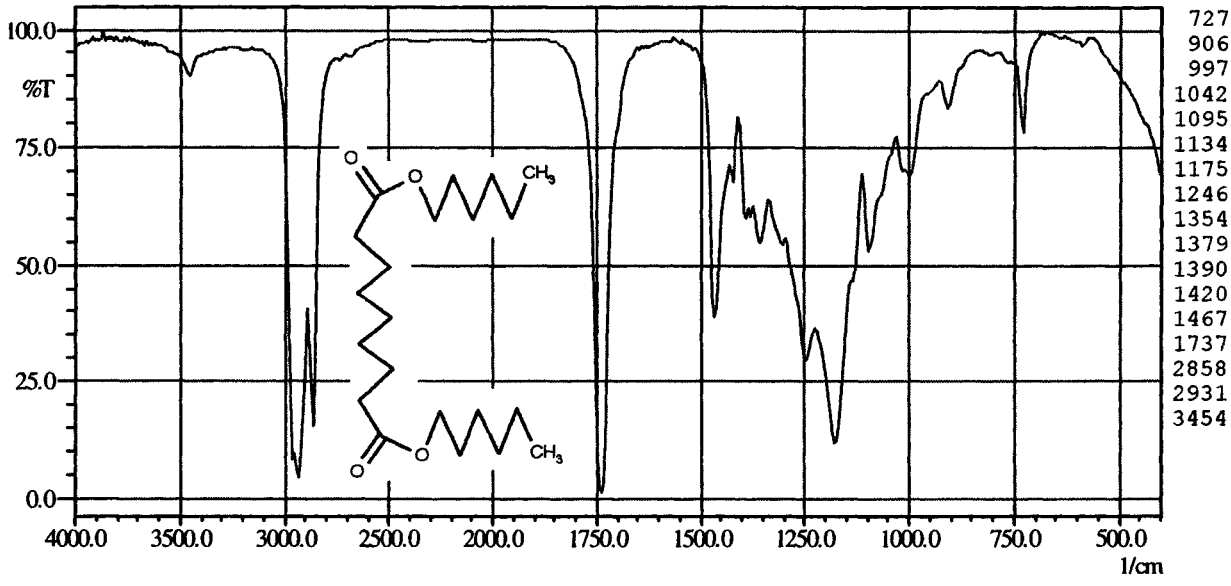
(1) **dibutyladipate**
(2) Adimoll DB
(3) Bayer
(4) 258.4 g mol^{-1}
(5) plasticiser
(6) colourless, clear liquid
(8) 305 °C
(9) 0.962 g cm^{-3}
(10) 1.436
(13) layer btw KBr

3321 $C_{18}H_{34}O_4$



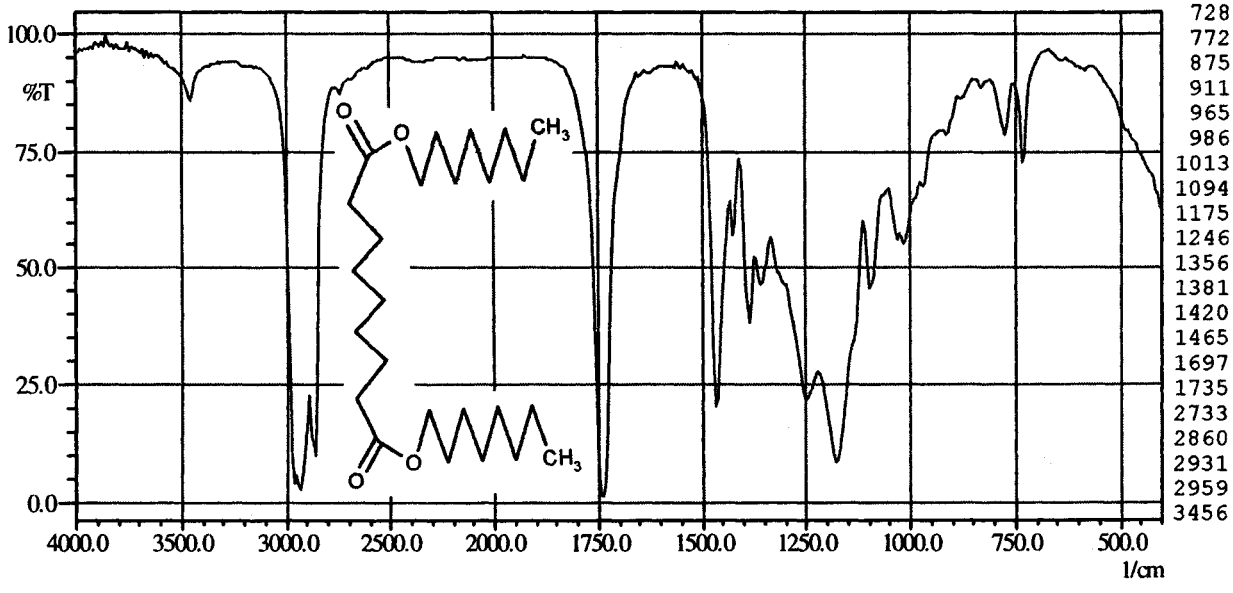
(1) **dihexyladipate**
(2) Adimoll PH
(3) Bayer
(4) 314.5 g mol^{-1}
(5) plasticiser
(6) colourless, clear liquid
(13) layer btw KBr

3321 $C_{21}H_{40}O_4$



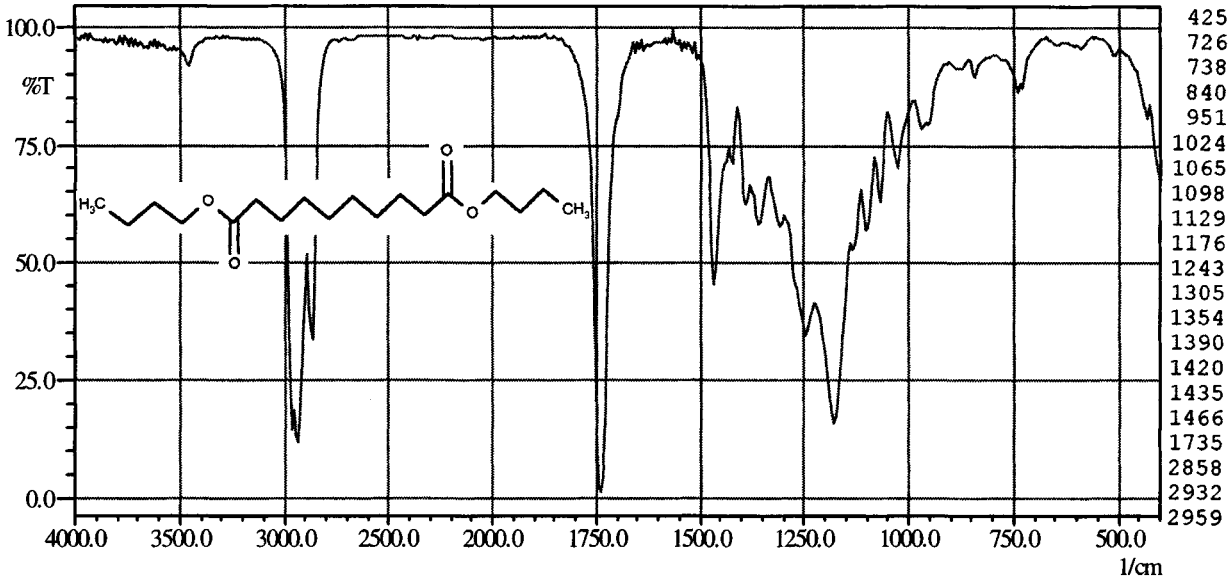
(1) **dihexylazelate**
(2) Priplast 3013 DNHZ
(3) Unichema Chemie
(4) 356.6 g mol^{-1}
(5) plasticiser
(6) pale-yellow liquid
(13) layer btw KBr
(14) 1,9-nonanedioic dihexylester

3321 $C_{25}H_{48}O_4$



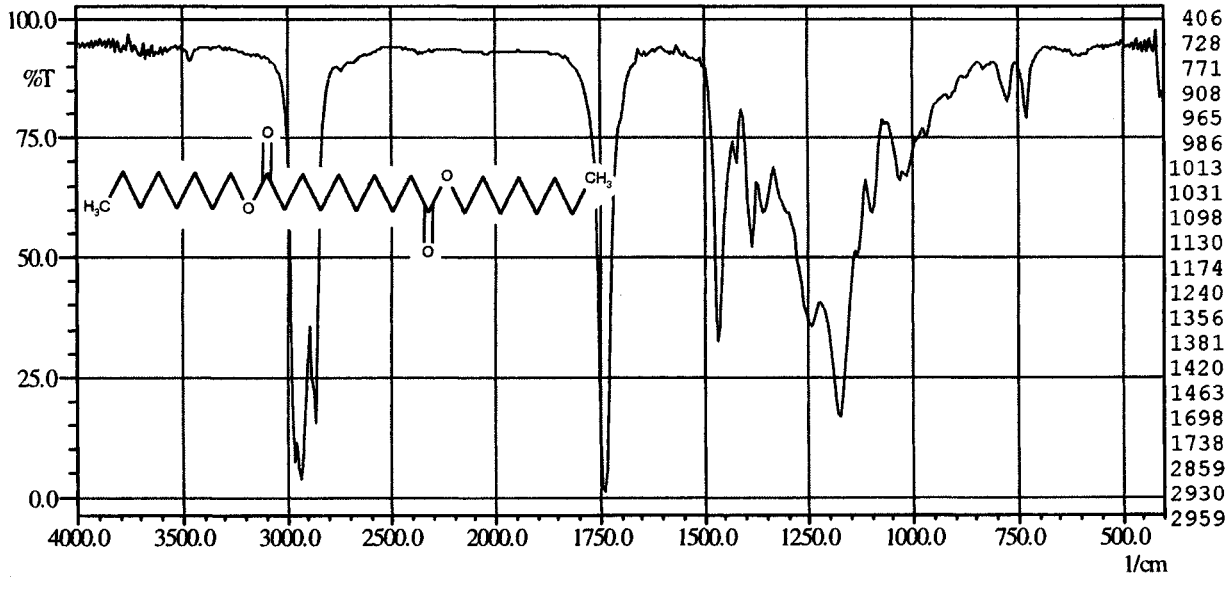
(1) **dioctylazelate**
(2) Priplast 3018 DOZ
(3) Unichema Chemie
(4) 412.7 g mol^{-1}
(5) plasticiser
(6) pale-yellow liquid
(13) layer btw KBr
(14) 1,9-nonanedioic dioctylester

3321 $C_{18}H_{34}O_4$



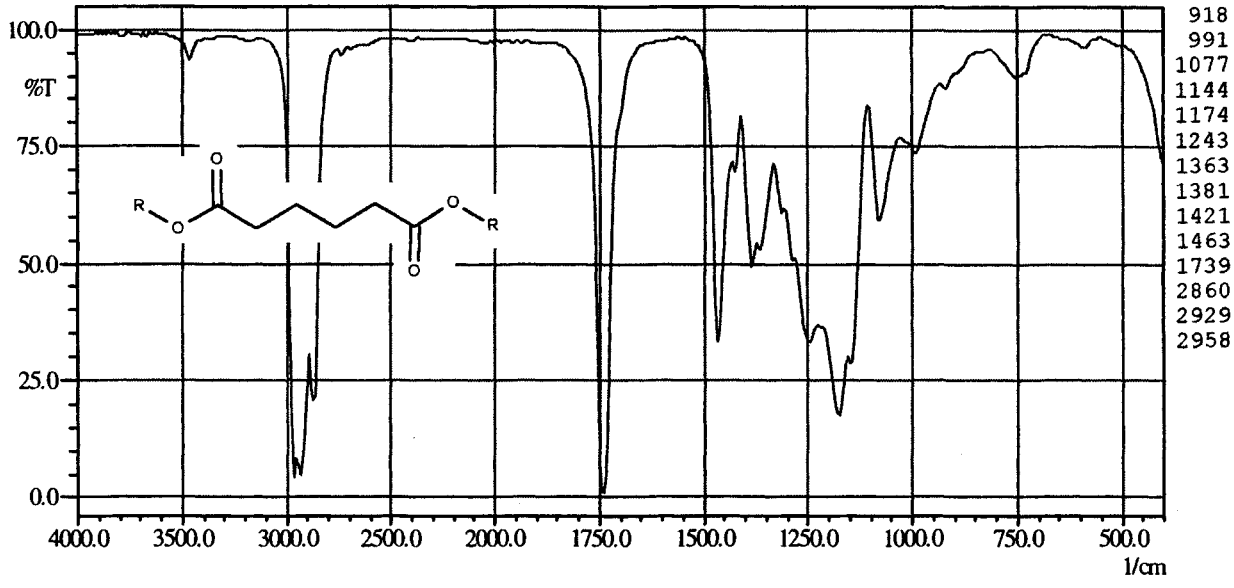
(1) **dibutylsebacate**
(2) Edenol DBS
(3) Henkel
(4) 314.5 g mol^{-1}
(5) plasticiser
(6) colourless, clear liquid
(9) 0.934 g cm^{-3}
(10) 1.442
(13) layer btw KBr

3321 $C_{26}H_{50}O_4$



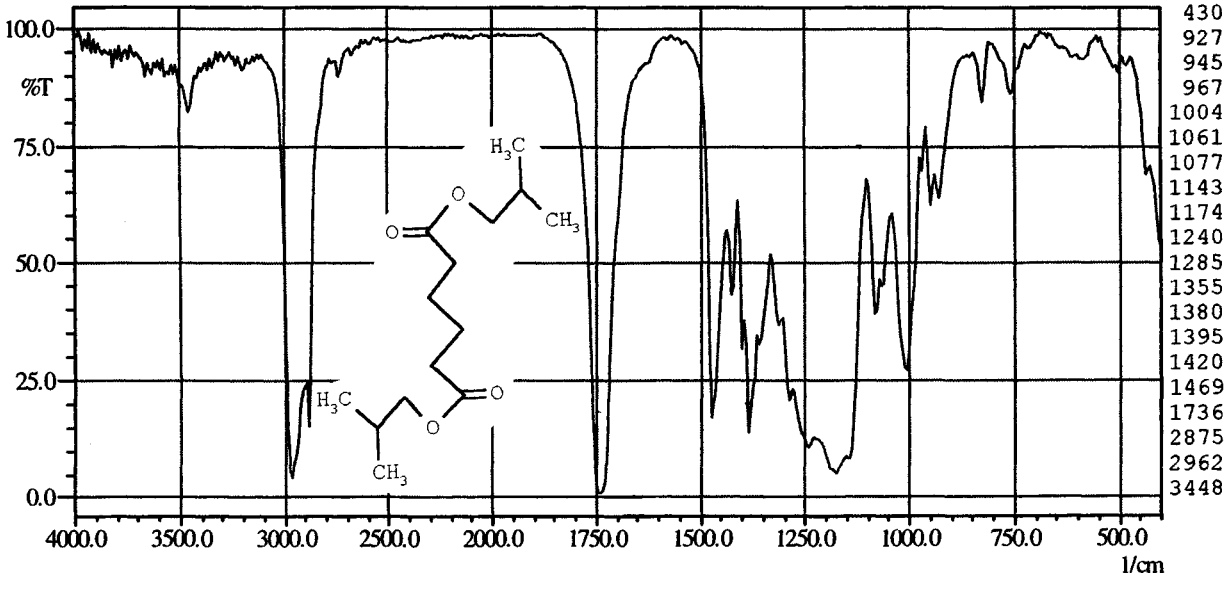
(1) **dioctylsebacate**
(2) Edenol 888
(3) Henkel
(4) 426.7 g mol^{-1}
(5) plasticiser
(6) colourless, clear liquid
(9) 0.913 g cm^{-3}
(10) 1.45
(13) layer btw KBr

3321



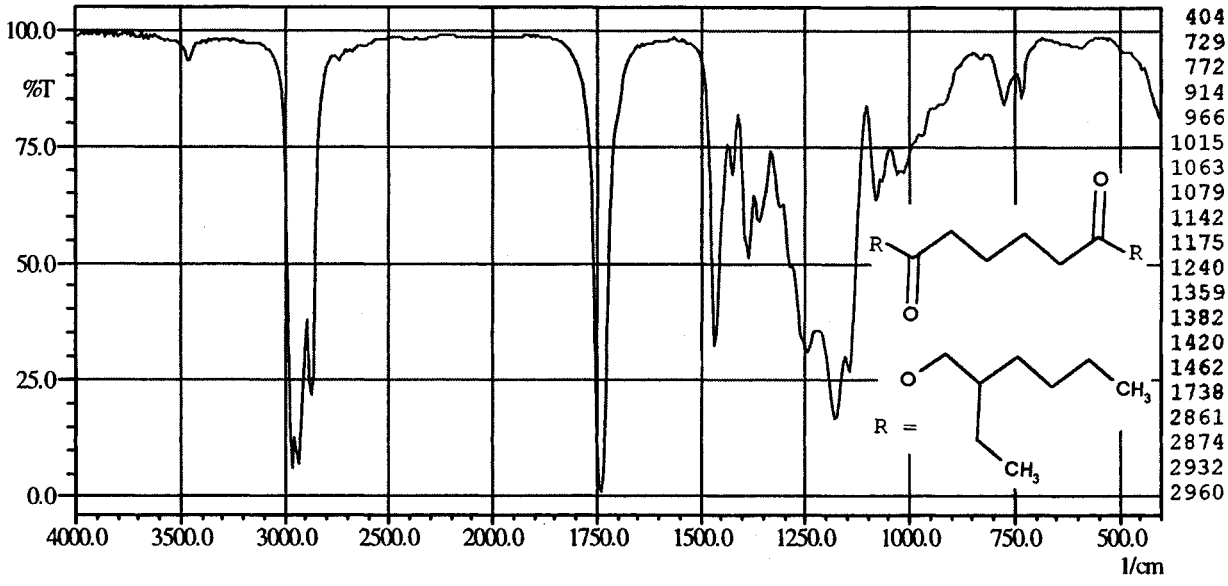
(1) **di(C_8...C_{10}-alkyl)adipate**
(2) Linplast 810 XA
(3) Condea
(5) plasticiser
(6) colourless, clear liquid
(7) −33 °C
(9) 0.918 g cm^{-3}
(13) layer btw KBr

3322 $C_{14}H_{26}O_4$



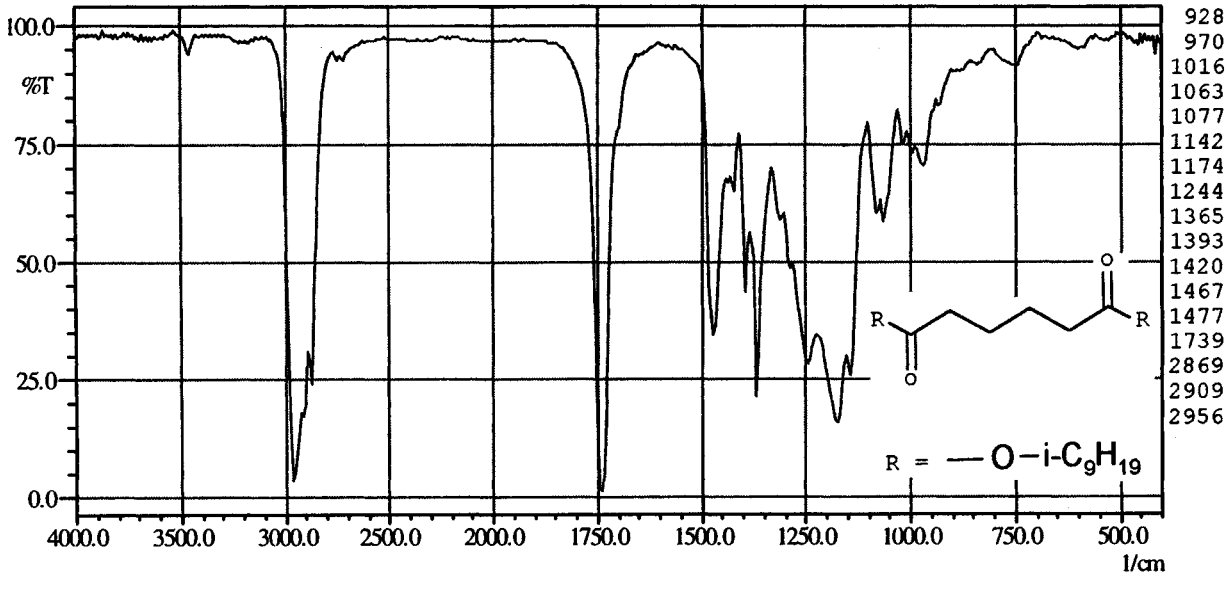
(1) **di-*i*-butyladipate**
(3) Freudenberg (Brunne collection)
(4) 258.4 g mol^{-1}
(5) plasticiser
(6) colourless, clear liquid
(13) layer btw KBr

3322 $C_{22}H_{42}O_4$



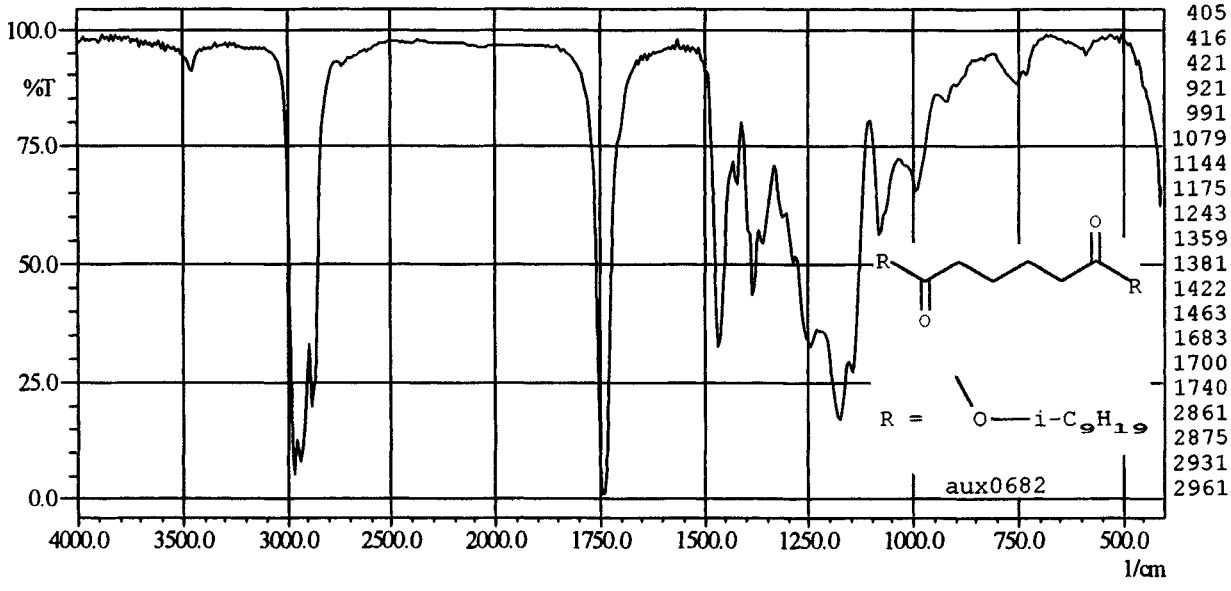
(1) **di(2-ethylhexyl)adipate**
(2) Hexaplas DOA
(3) ICI
(4) 370.6 g mol^{-1}
(5) plasticiser
(6) colourless, clear liquid
(9) 0.929 g cm^{-3}
(10) 1.447
(13) layer btw KBr

3322 $C_{24}H_{46}O_4$



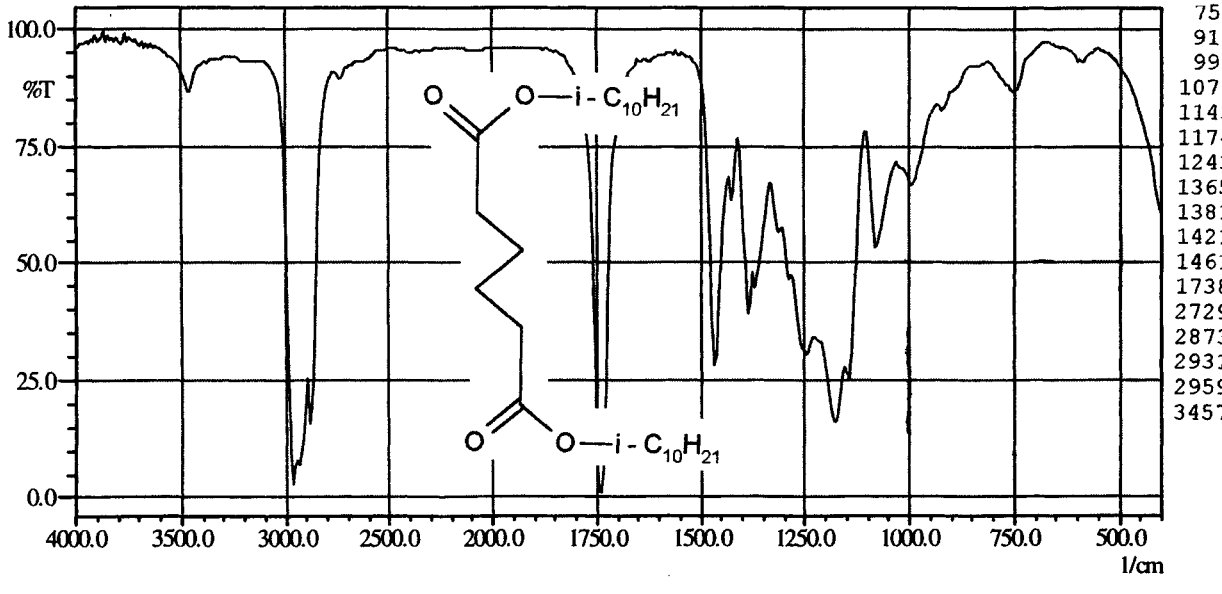
(1) **di-*i*-nonyladipate**
(2) Adimoll DN
(3) Bayer
(4) 398.6 g mol^{-1}
(5) plasticiser
(6) colourless, clear liquid
(8) 255 °C / 1300 Pa
(9) 0.915 g cm^{-3}
(10) 1.448
(13) layer btw KBr
(14) structure of *i*-nonyl is undefined

3322 $C_{24}H_{46}O_4$



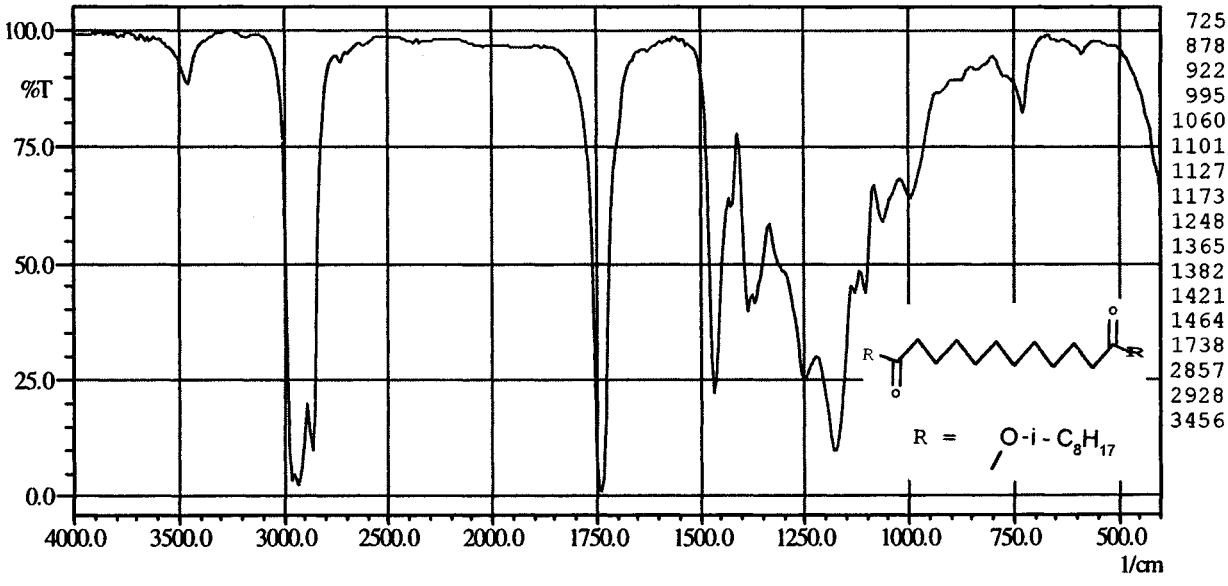
(1) **di-*i*-nonyladipate, mixture of isomers with high amount of linear chains**
(2) Plastomoll DNA
(3) BASF
(4) 398.6 g mol^{-1}
(5) PVC plasticiser
(6) colourless, clear liquid
(9) 0.923 g cm^{-3}
(10) 1.451
(13) layer between KBr

3322 $C_{24}H_{30}O_4$



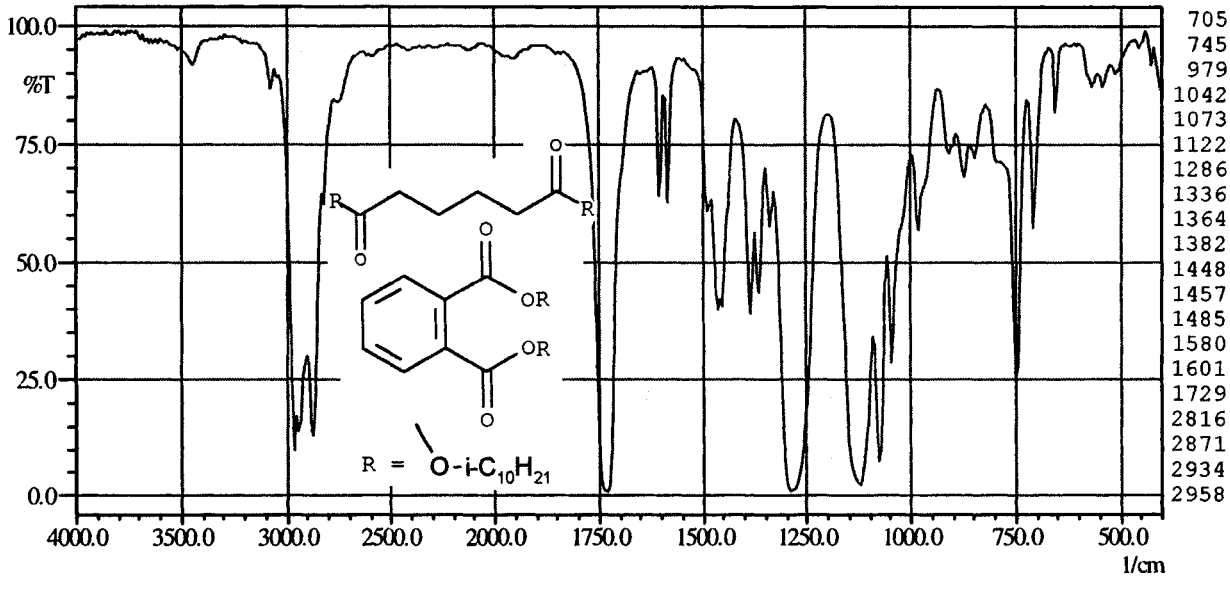
(1) **di-*i*-decyladipate**
(2) Jayflex DIDA
(3) Exxon Chemical
(4) 382.5 g mol^{-1}
(5) plasticiser
(6) colourless, clear liquid
(7) −60 °C
(9) 0.919 g cm^{-3}
(10) 1.453
(13) layer btw KBr

3322 $C_{28}H_{54}O_4$



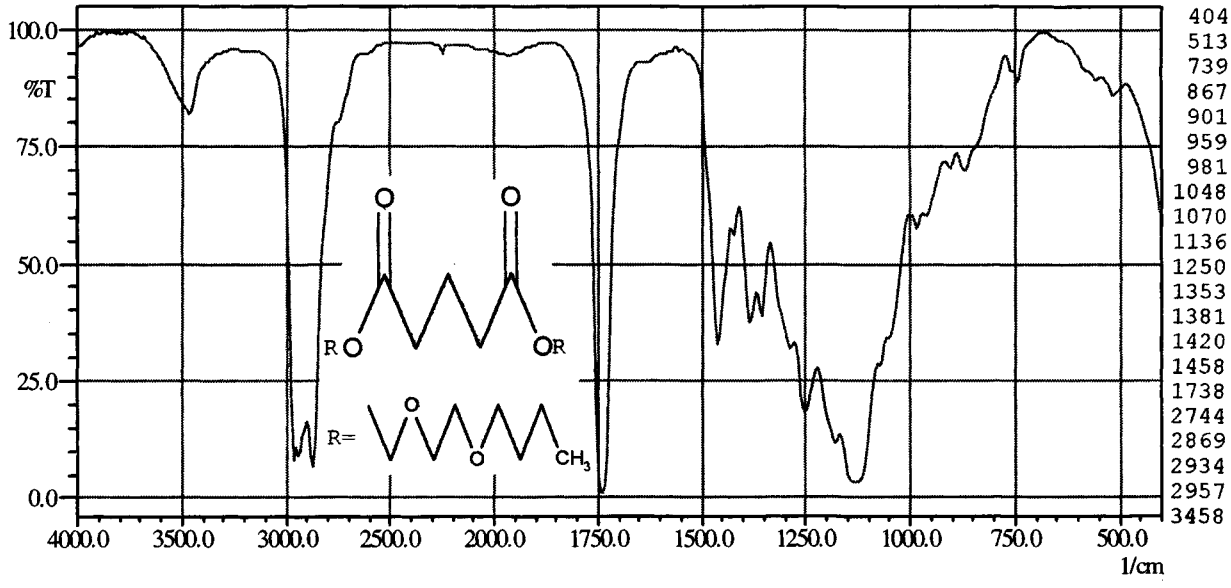
(1) **di(*i*-octyl)dodecanedioate**
(2) Plasthall DIODD
(3) C.P. Hall, Krahn-Chemie
(4) 454.7 g mol^{-1}
(5) plasticiser
(6) colourless, clear liquid
(7) –70 °C
(9) 0.909 g cm^{-3}
(10) 1.45
(13) layer btw KBr

3322+3422



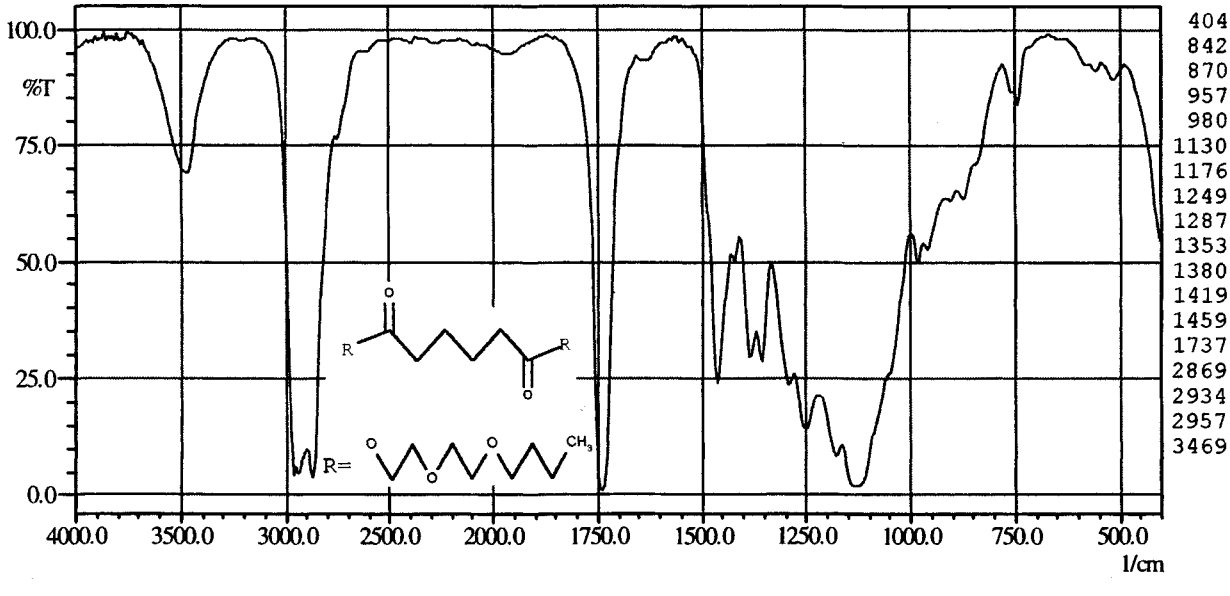
(1) **mixture of di-*i*-decyladipate and di-*i*-decylphthalate**
(2) Palatinol CE
(3) BASF
(5) plasticiser
(6) colourless, clear liquid
(13) layer btw KBr

3323 $C_{21}H_{40}O_8$



(1) **di(butoxyethoxyethyl)glutarate**
(2) Plasthall DBEEG
(3) C.P. Hall, Krahn-Chemie
(4) 420.6 g mol^{-1}
(5) plasticiser
(6) colourless, clear liquid
(7) -60 °C
(9) 1.016 g cm^{-3}
(10) 1.444
(13) layer btw KBr

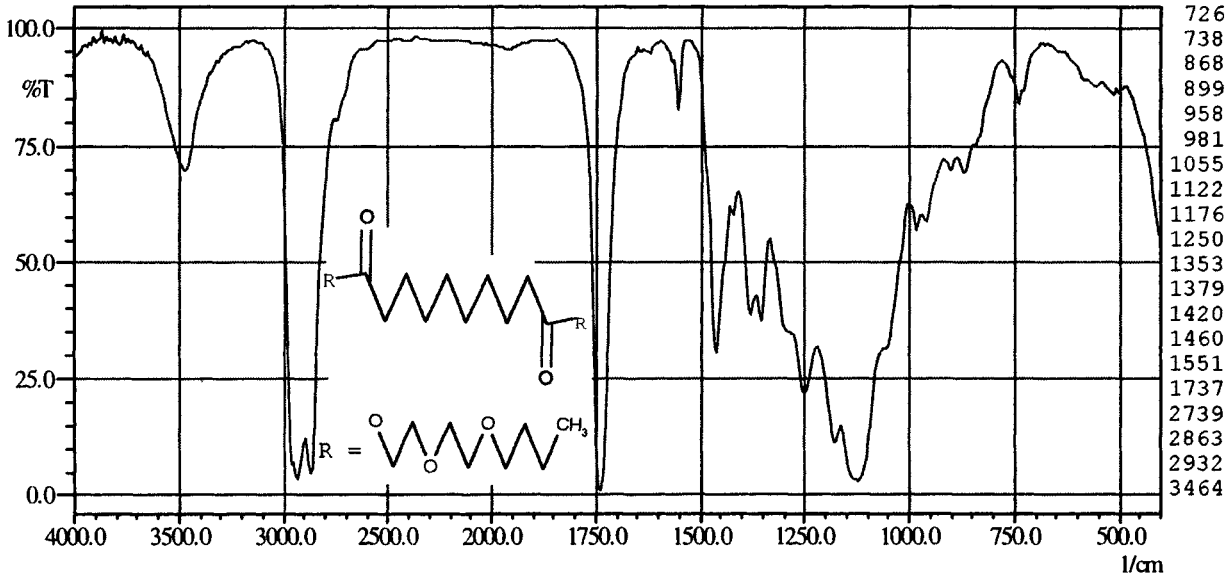
3323 $C_{22}H_{42}O_8$



(1) **di(butoxyethoxyethyl)adipate**
(2) Plasthall DBEEA
(3) C.P. Hall, Krahn-Chemie
(4) 434.6 g mol^{-1}
(5) plasticiser
(6) colourless, clear liquid
(7) -25 °C
(9) 1.01 g cm^{-3}
(10) 1.445
(13) layer btw KBr

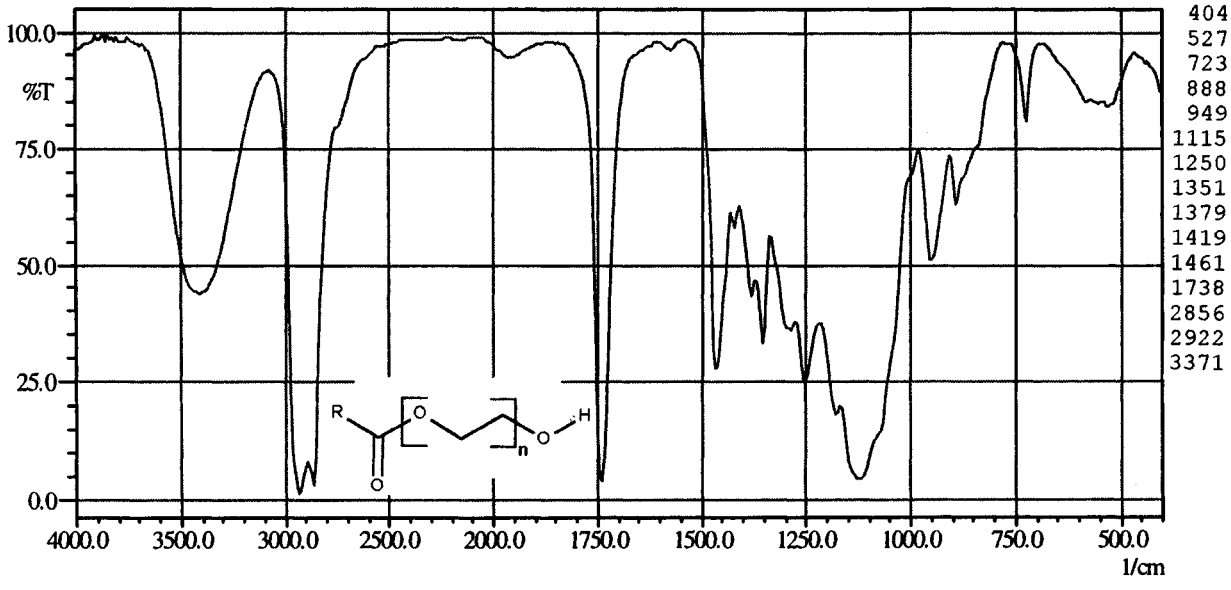
3323

$C_{26}H_{50}O_8$



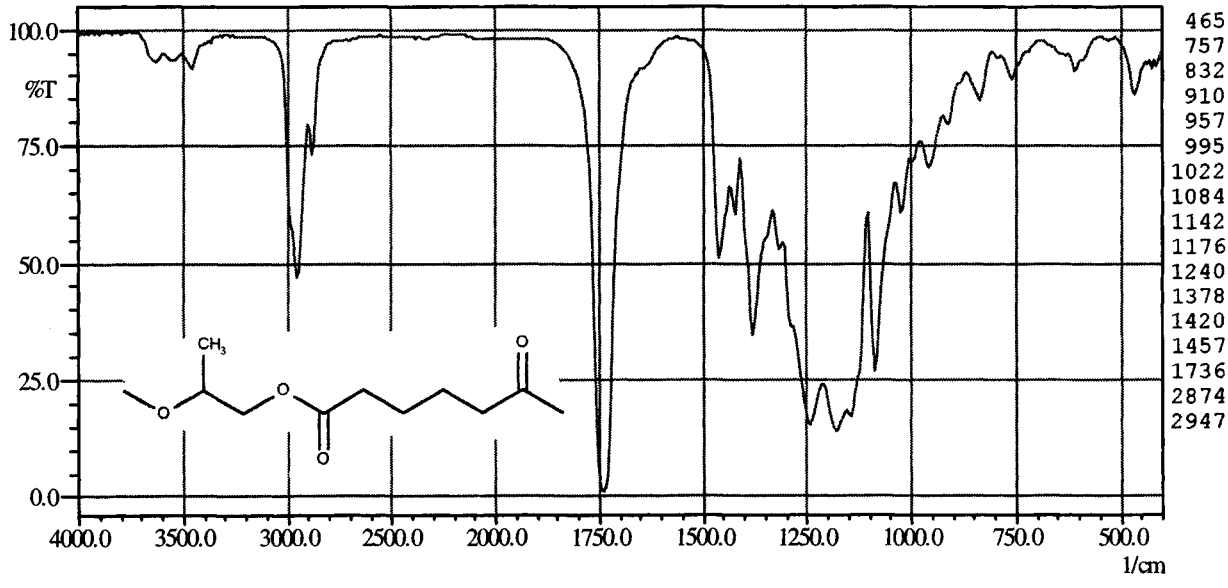
(1) **dibutoxyethoxyethylsebacate**
(2) Plasthall 83 SS
(3) C.P. Hall
(4) 490.7 g mol^{-1}
(5) plasticiser
(6) brown, clear liquid
(7) −10 °C
(9) 0.989 g cm^{-3}
(10) 1.446
(13) layer btw KBr

3323



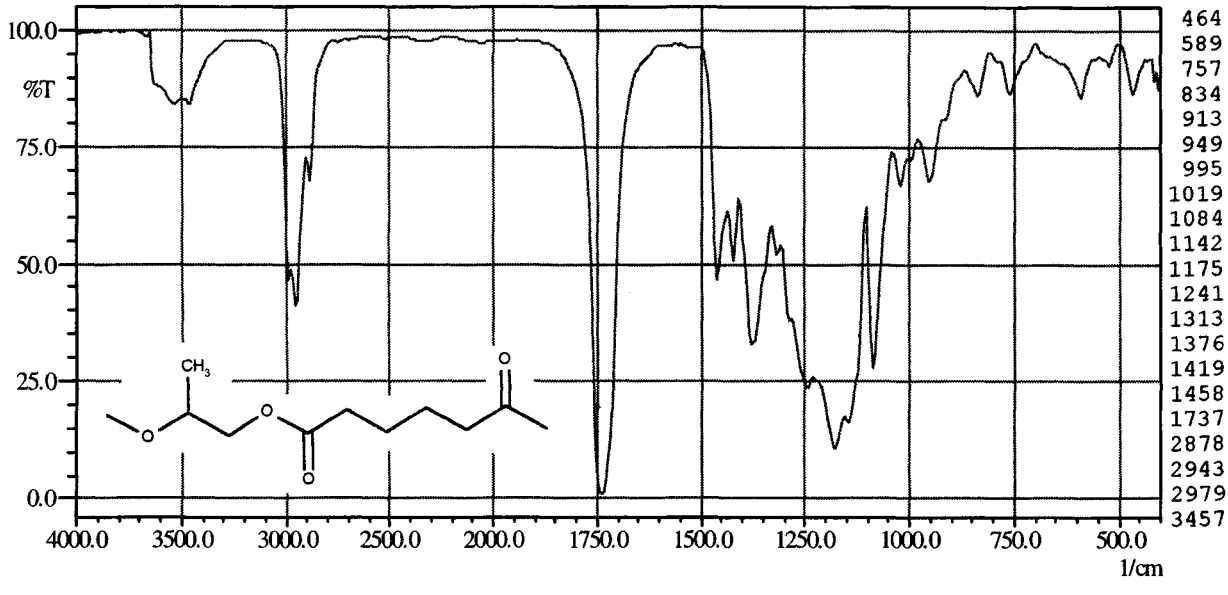
(1) **fatty acid polyglycol ester**
(2) Deplastol 00130344
(3) Henkel
(5) plasticiser
(6) colourless, clear liquid
(9) 0.98 g cm^{-3}
(13) layer btw KBr

3324



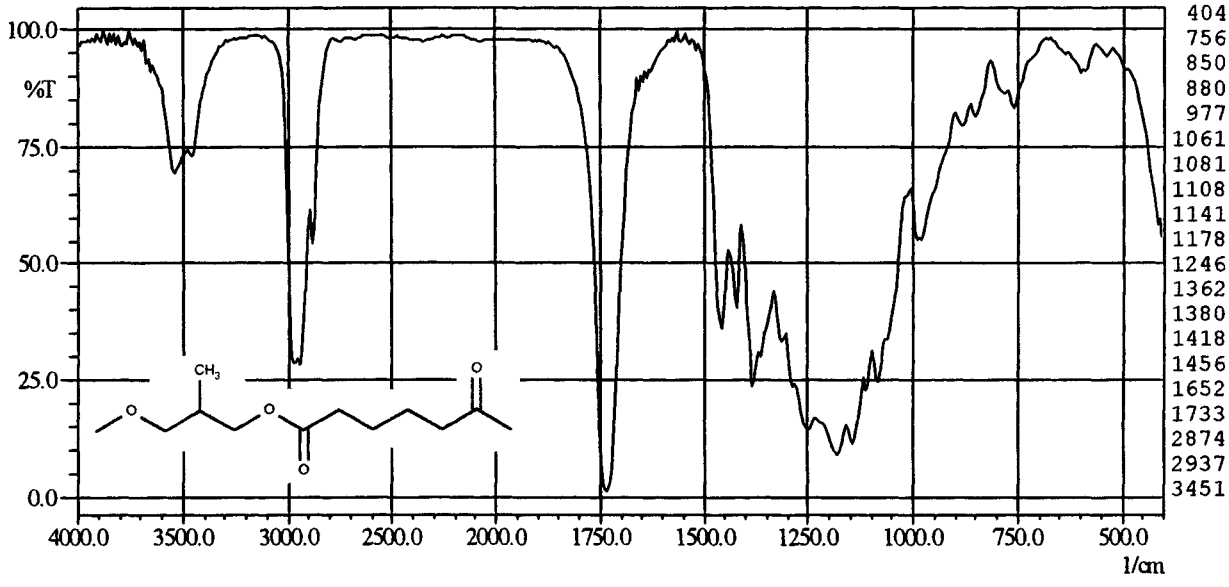
(1) **poly(1,2-propanedioladipate)**
(2) Palamoll 636
(3) BASF
(5) plasticiser
(6) colourless, clear liquid
(9) 1.15 g cm^{-3}
(10) 1.467
(13) layer btw KBr

3324



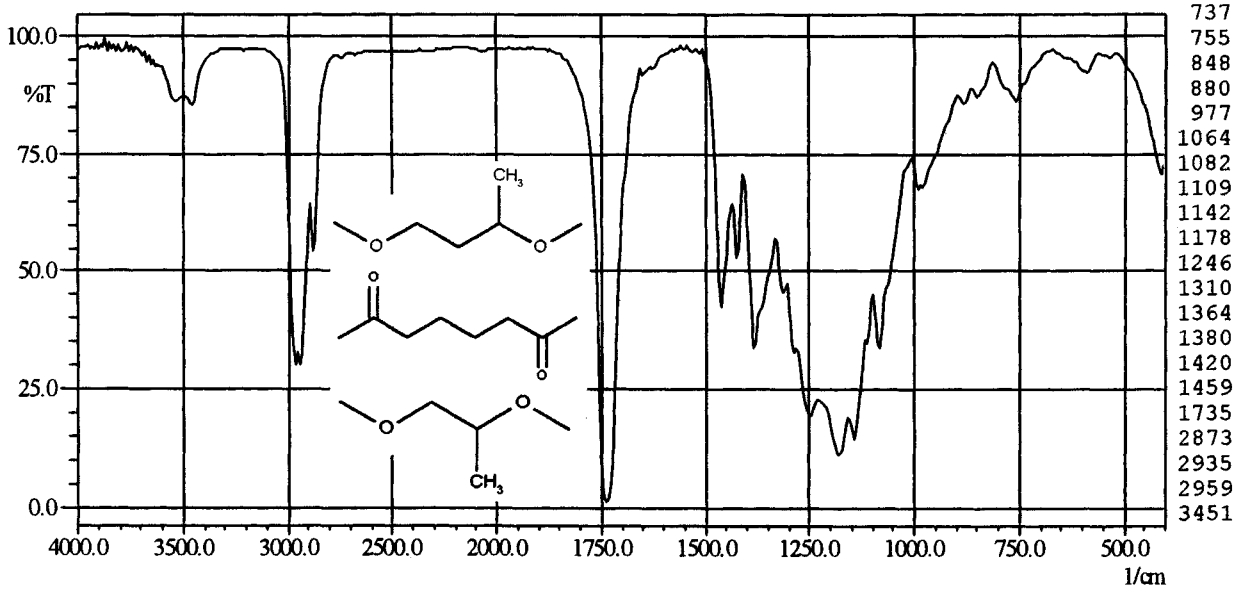
(1) **poly(1,2-propyleneadipate)**
(2) Witamol 615 MEK
(3) Huels
(5) plasticiser
(6) colourless, clear liquid
(13) layer btw KBr
(14) dissolved in butanone

3324



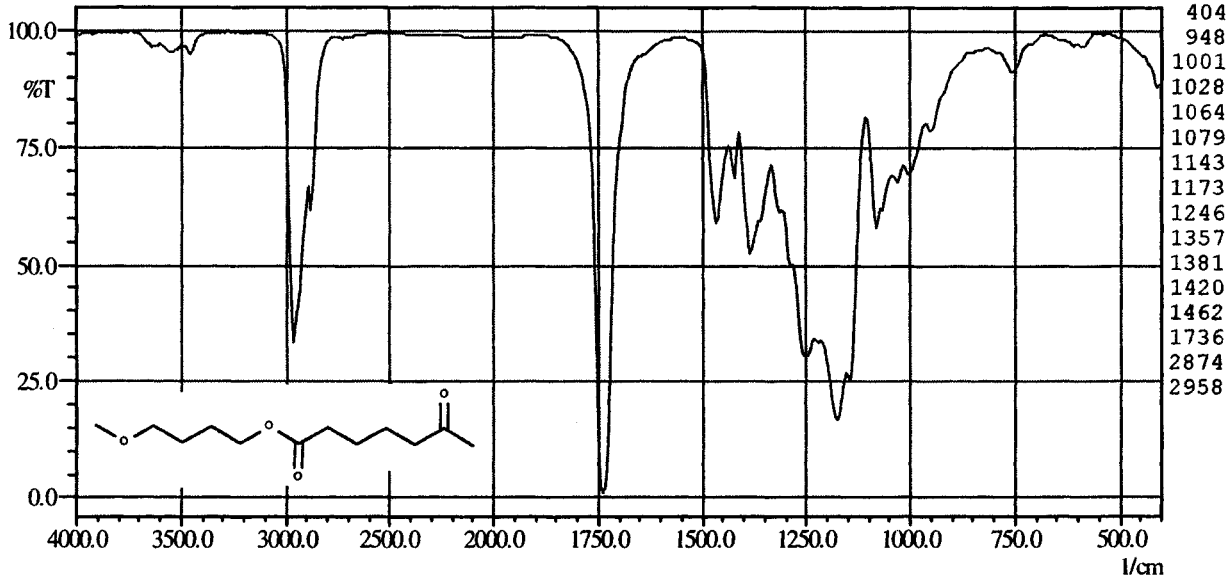
(1) **poly(1,3-butanedioladipate)**
(2) Diolpate 150
(3) Macpherson
(5) plasticiser
(6) colourless, clear liquid
(9) 1.125 g cm^{-3}
(10) 1.471
(13) layer btw KBr

3324



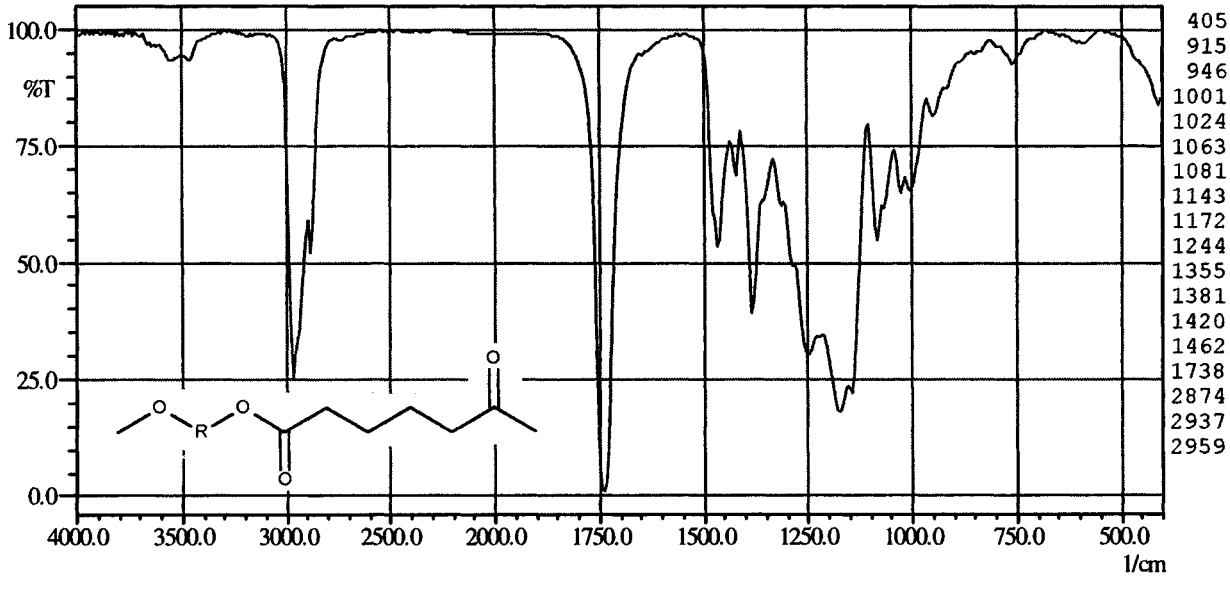
(1) **poly(1,3-butylene-*co*-1,2-propylene adipate)**
(2) Diolpate 214
(3) Macpherson
(4) 1150 g mol^{-1}
(5) plasticiser
(6) colourless, clear liquid
(10) 1.4674
(13) layer btw KBr

3324



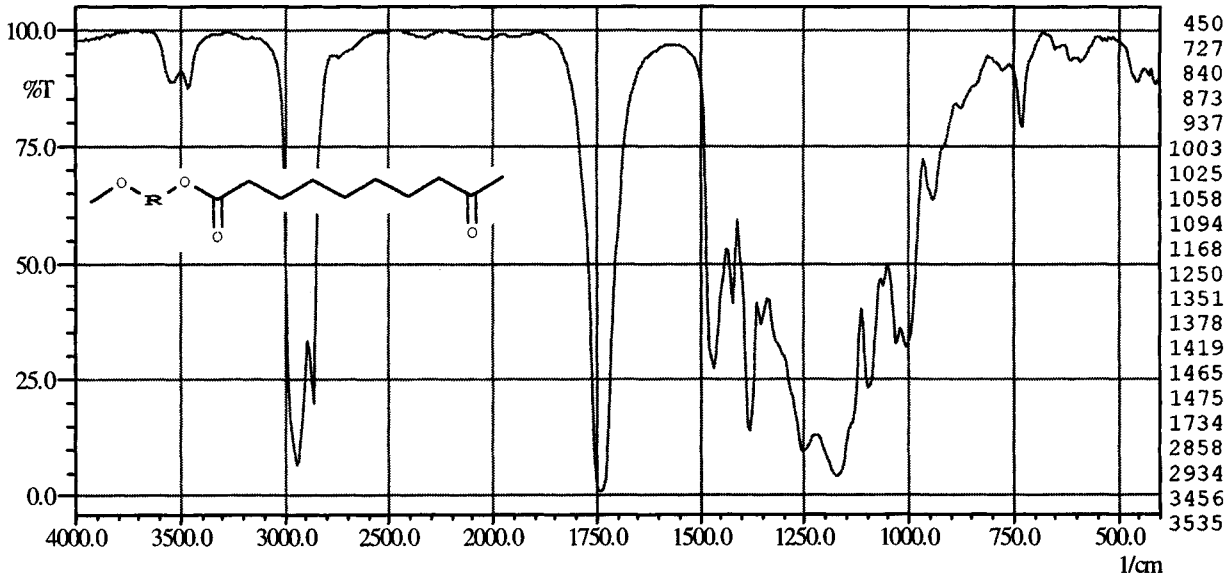
(1) **poly(butanedioladipate)**
(2) Palamoll 646
(3) BASF
(5) plasticiser
(6) colourless, clear liquid
(9) 1.132 g cm^{-3}
(10) 1.47
(13) layer btw KBr

3324



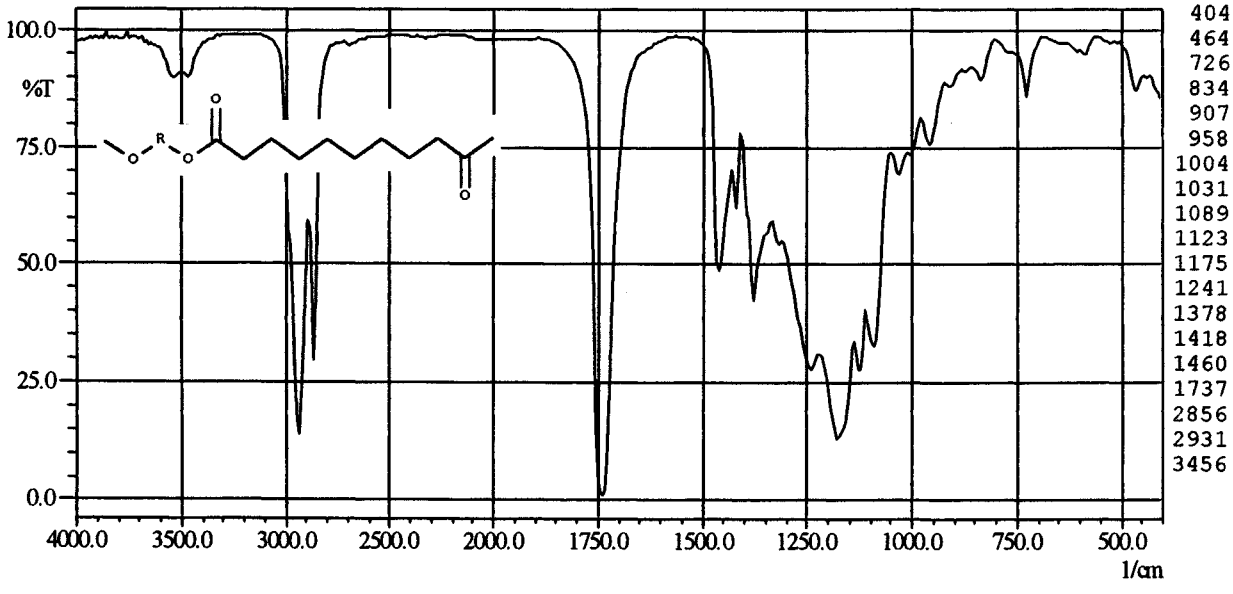
(1) **adipic acid polyester (based on butanediol)**
(2) Palamoll 652
(3) BASF
(5) plasticiser
(6) colourless, clear liquid
(9) 1.055 g cm^{-3}
(10) 1.464
(13) layer btw KBr

3324



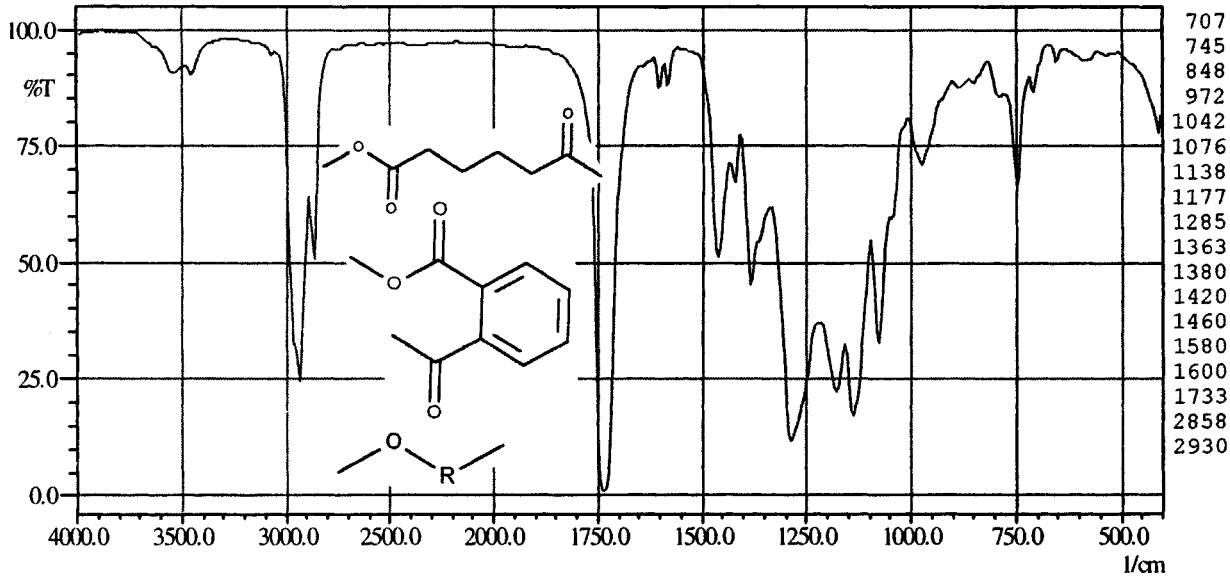
(1) **azelaic polyester**
(2) Priplast 3142
(3) Unichema
(5) plasticiser
(6) colourless, viscous liquid
(13) layer on KBr

3324



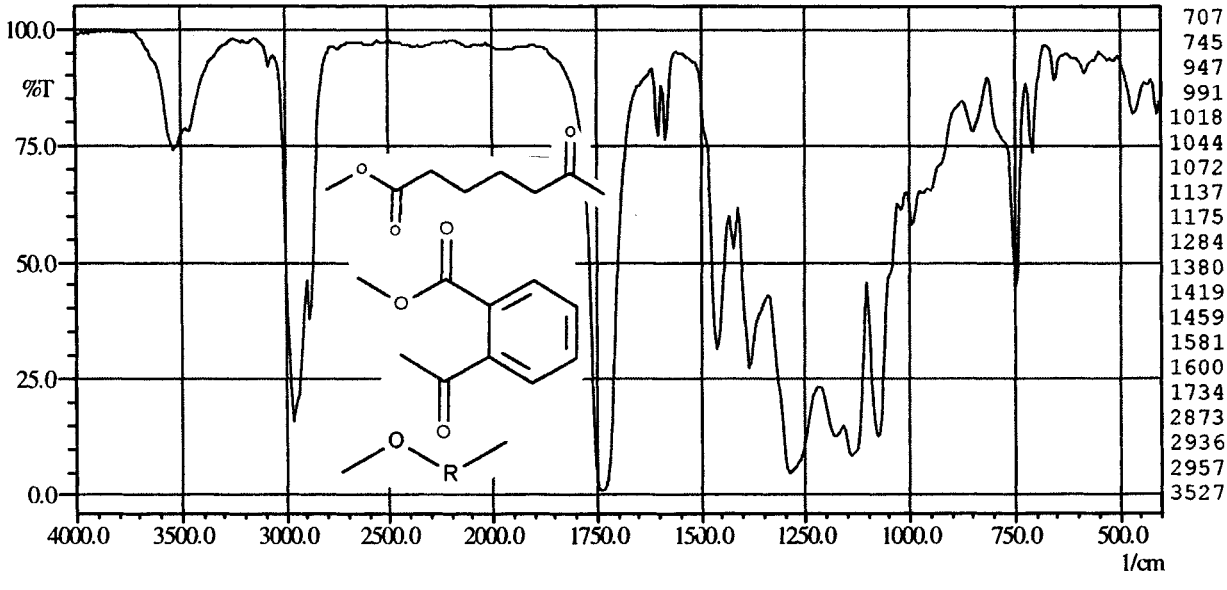
(1) **sebacic acid polyester**
(2) Edenol 1800
(3) Henkel
(5) plasticiser
(6) colourless, clear liquid
(9) 1,06 g cm^{-3}
(10) 1,468
(13) layer btw KBr

3324



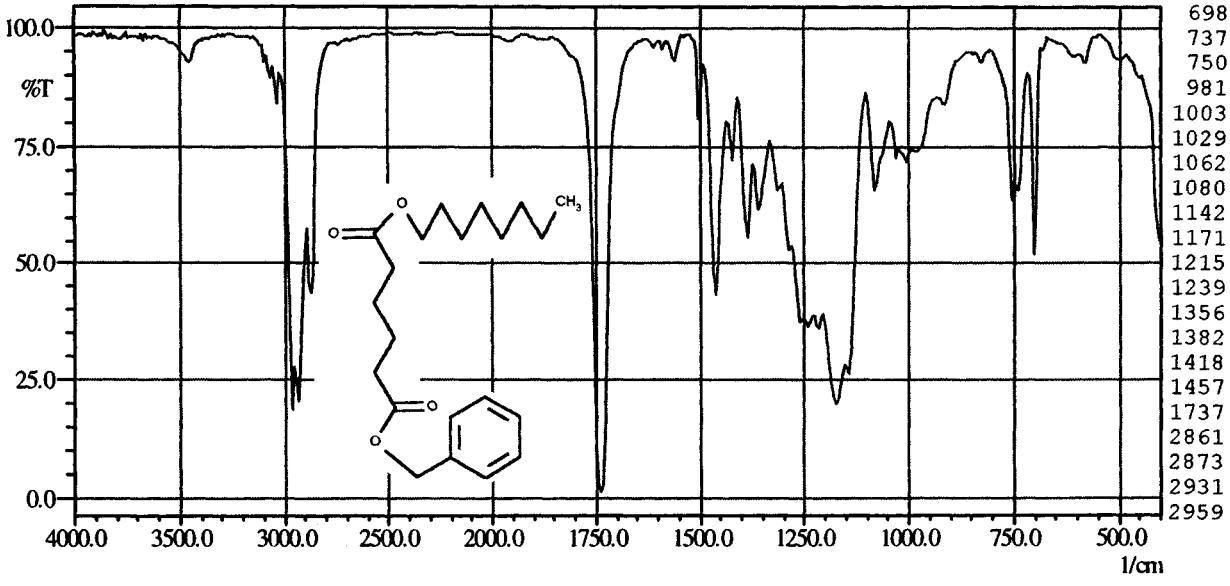
(1) **polyester based on adipic and phthalic acids**
(2) Uraplast RA17
(3) DSM
(5) plasticiser
(6) colourless, clear liquid
(9) 1.06 g cm^{-3}
(10) 1.487
(13) layer btw KBr

3324



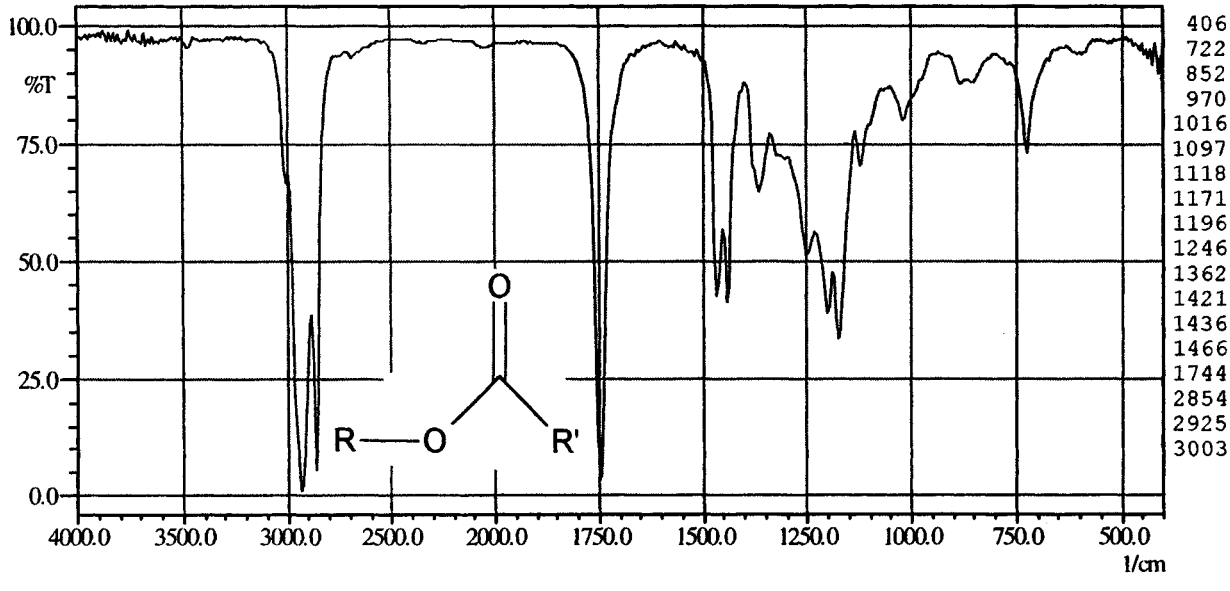
(1) **polyester based on adipic and phthalic acids**
(2) Uraplast RA5
(3) DSM
(5) plasticiser
(6) colourless, clear liquid
(9) 1.12 g cm^{-3}
(10) 1.485
(13) layer btw KBr

3325 $C_{21}H_{32}O_4$



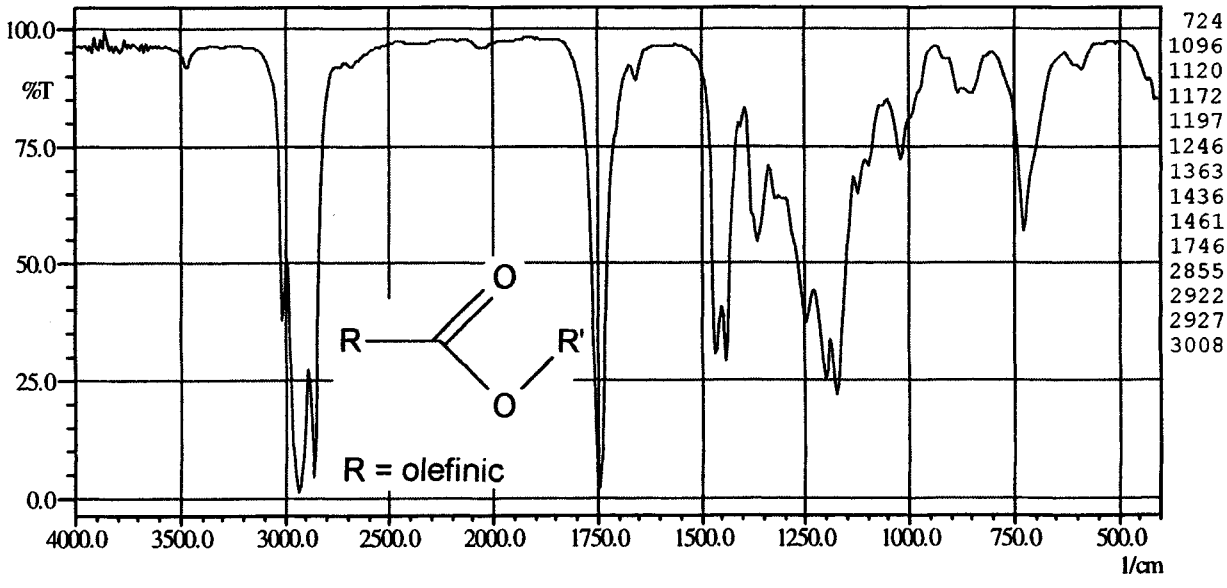
(1) **benzyloctyl adipate**
(2) Adimoll BO
(3) Bayer
(4) 348.5 g mol^{-1}
(5) plasticiser
(6) colourless, clear liquid
(9) 1.005 g cm^{-3}
(13) layer btw KBr

3341



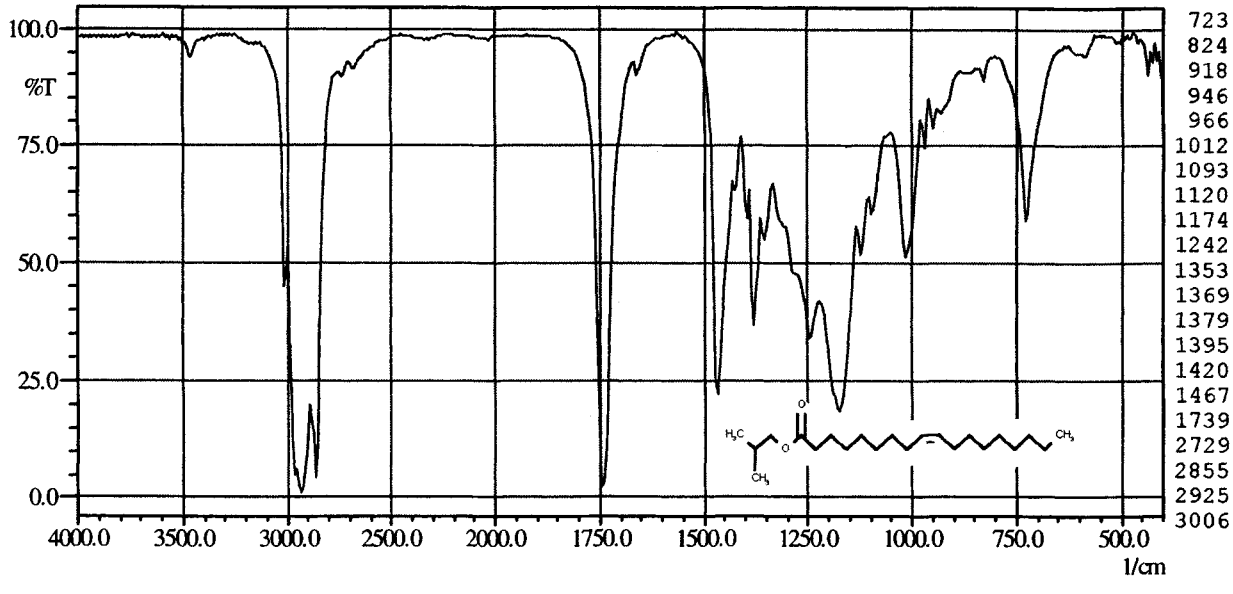
(1) **fatty acid ester**
(2) Edenol W750
(3) Henkel
(5) plasticiser
(6) yellow, clear liquid
(9) 0.88 g cm^{-3}
(13) layer btw KBr

3341



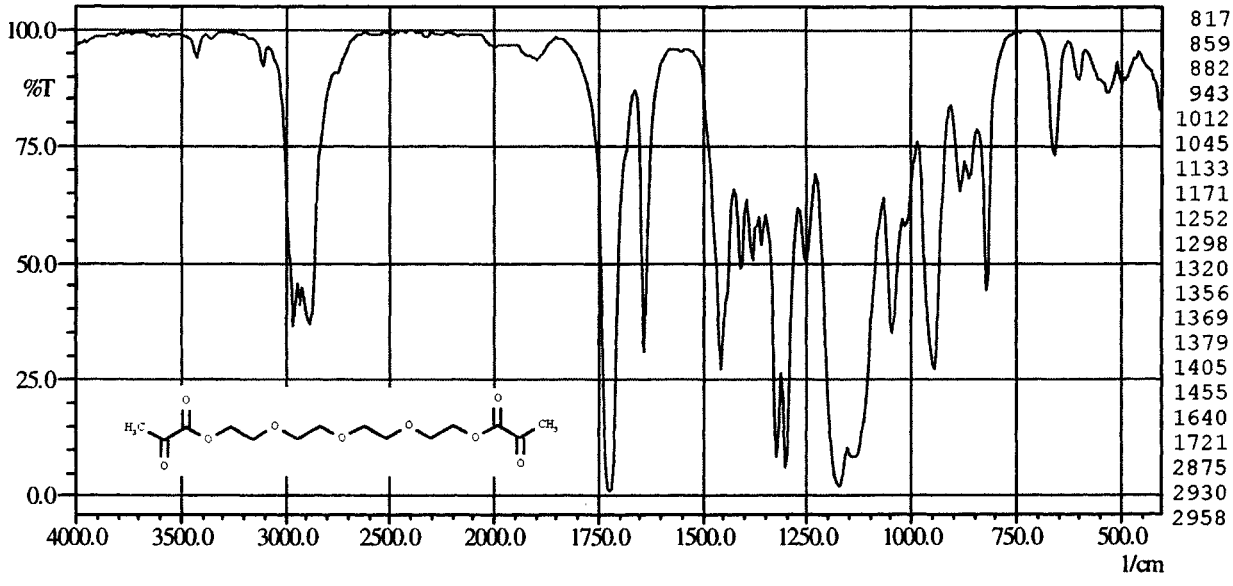
(1) **special unsaturated fatty acid ester**
(2) Edenol W 1385
(3) Henkel
(5) plasticiser
(6) yellowish, clear liquid
(13) layer btw KBr

3342 $C_{22}H_{42}O_2$



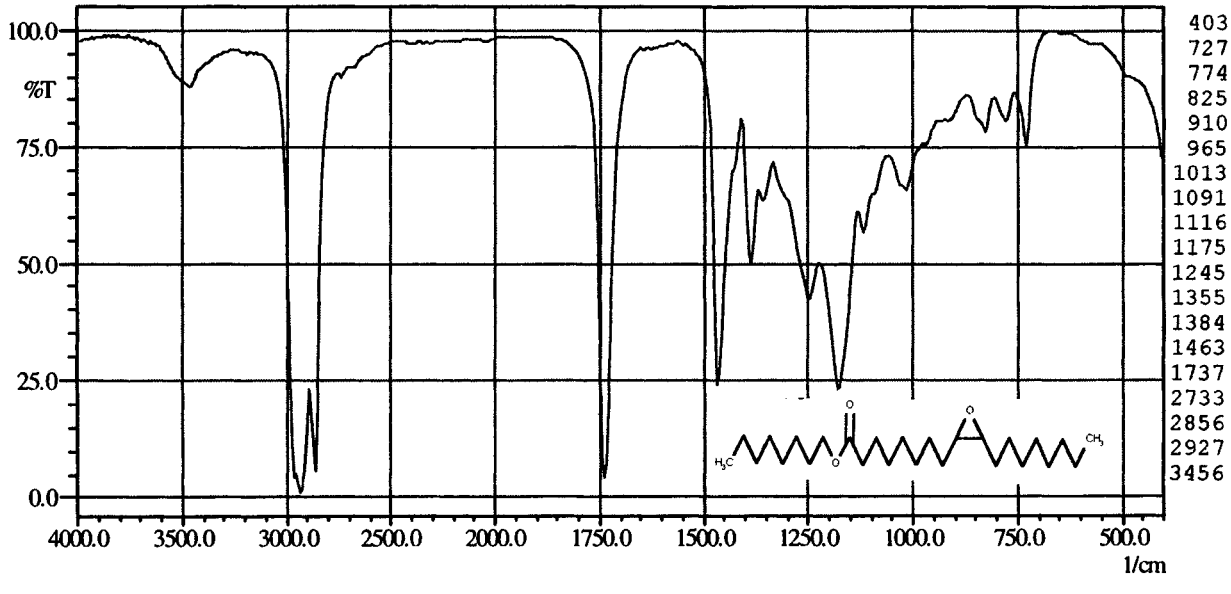
(1) ***i*-butyloleate**
(2) Edenol IBO
(3) Henkel
(4) 338.6 g mol^{-1}
(5) plasticiser
(6) yellow, clear liquid
(9) 0.862 g cm^{-3}
(10) 1.45
(13) layer btw KBr

3344 $C_{16}H_{26}O_7$



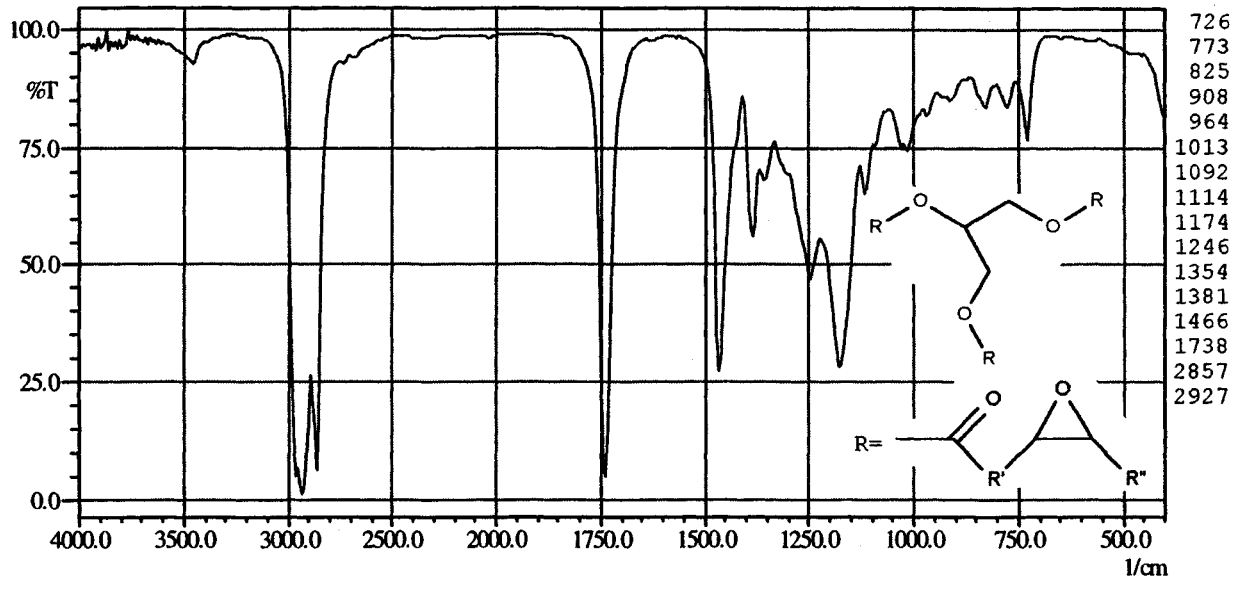
(1) **tetra(oxyethylene)dimethacrylate**
(2) Weichmacher TEDMA
(3) Degussa
(4) 330.4 g mol^{-1}
(5) reactive plasticiser
(6) colourless, clear liquid
(13) layer btw KBr

336 $C_{25}H_{35}O_3$



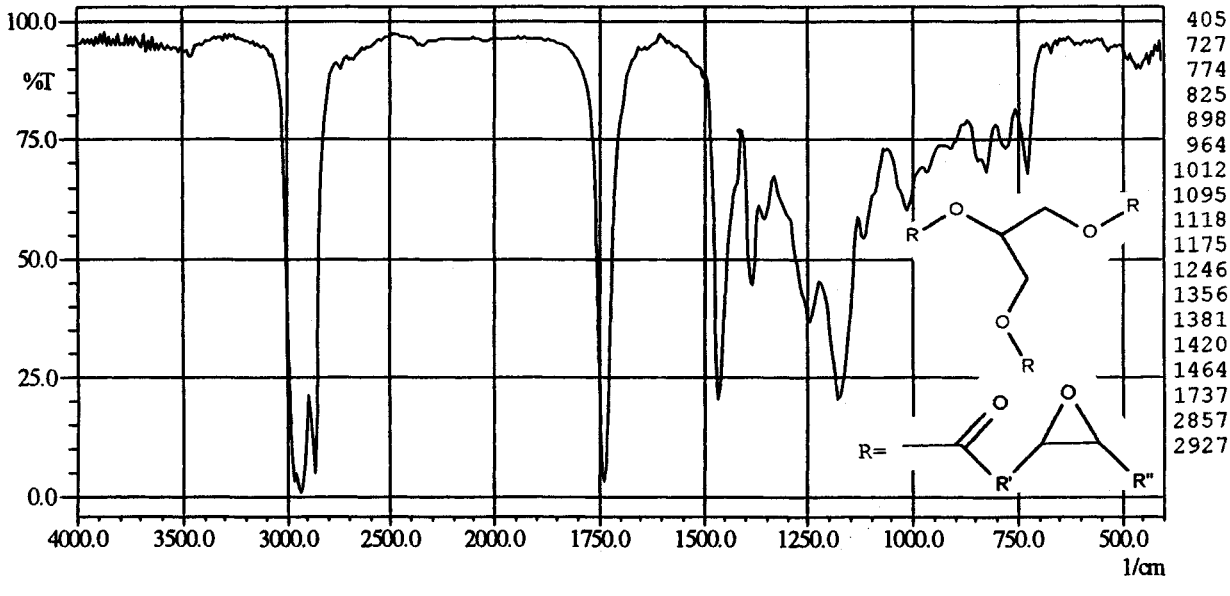
(1) **octylepoxystearate**
(2) Reagens EP/3
(3) Reagens
(4) 383.6 g mol^{-1}
(5) plasticiser
(6) colourless, clear liquid
(9) 0.9 g cm^{-3}
(13) layer btw KBr

336



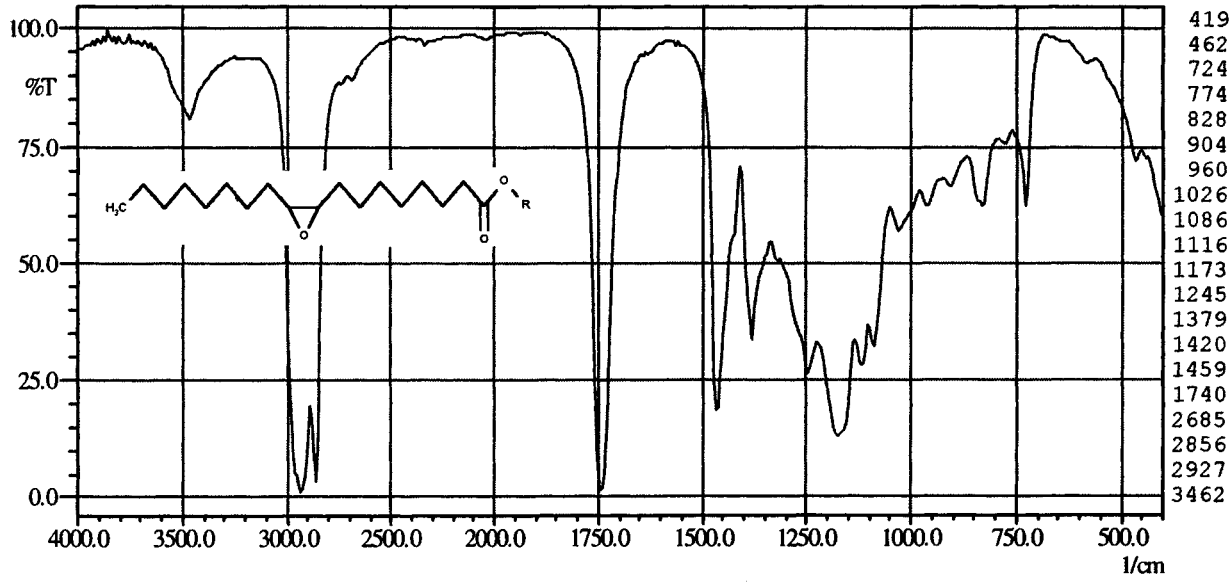
(1) **special epoxidised fatty acid ester**
(2) Edenol B 33
(3) Henkel
(5) plasticiser
(6) colourless, clear liquid
(9) 0.9 g cm^{-3}
(10) 1.455
(13) layer btw KBr

336



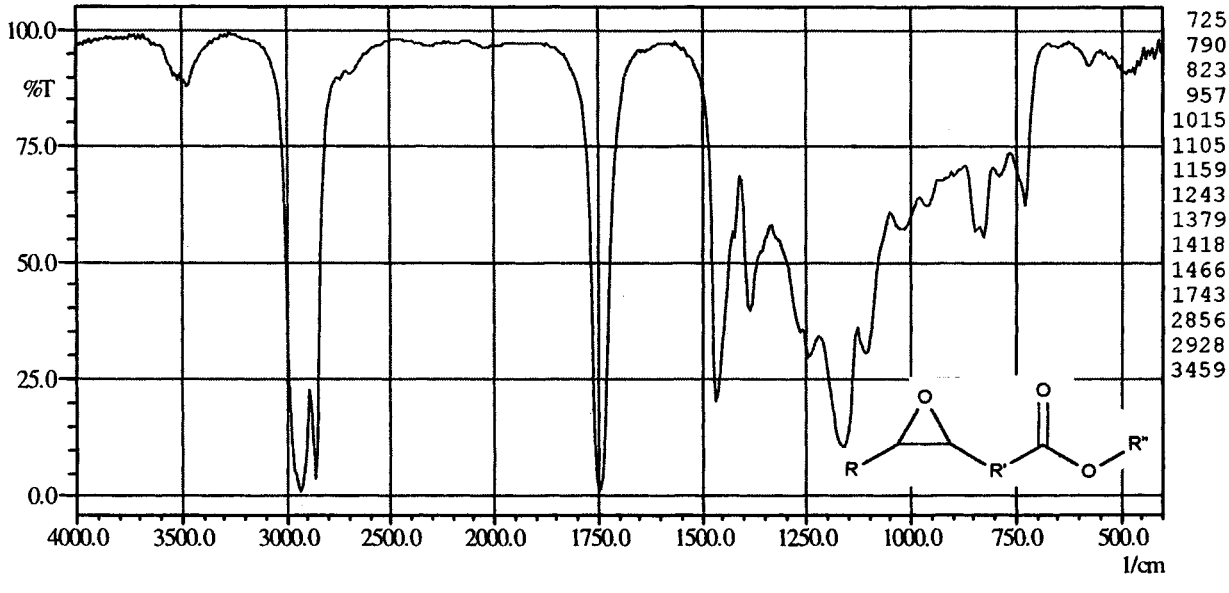
(1) ***i*-alkylepoxystearate**
(2) Edenol B35
(3) Henkel
(4) 380 g mol^{-1}
(5) plasticiser
(6) colourless, clear liquid
(9) 0.91 g cm^{-3}
(10) 1.457
(13) layer btw KBr

336



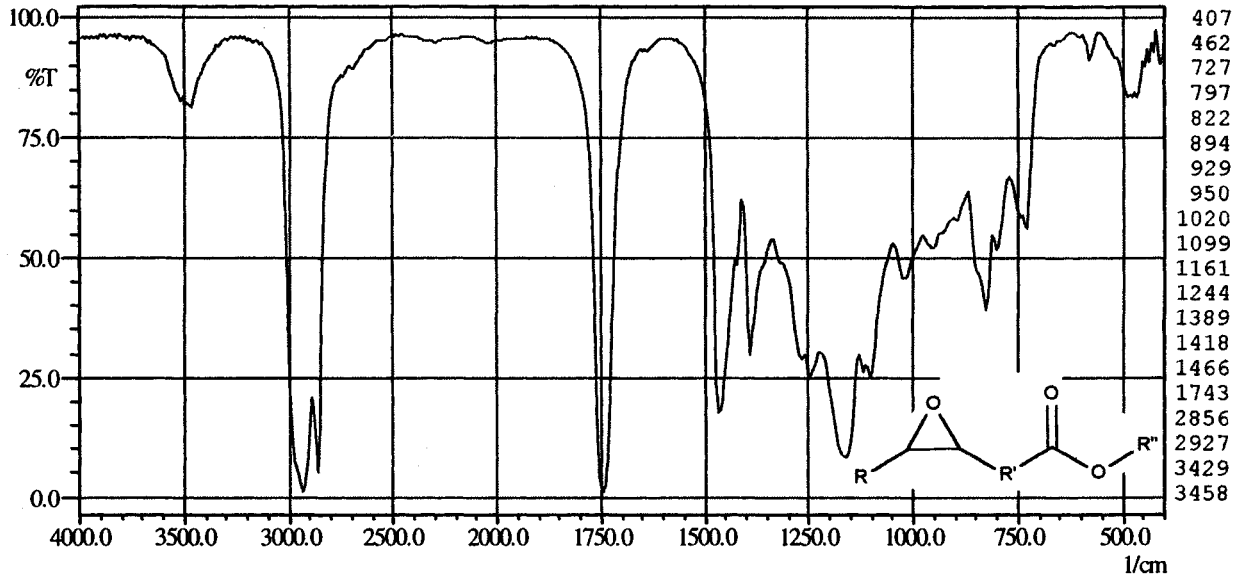
(1) **epoxidised oleic ester**
(2) Priplast 1431
(3) Unichema Chemie
(4) 600 g mol^{-1}
(5) stabilising plasticiser
(6) pale-yellow liquid
(13) layer btw KBr

336



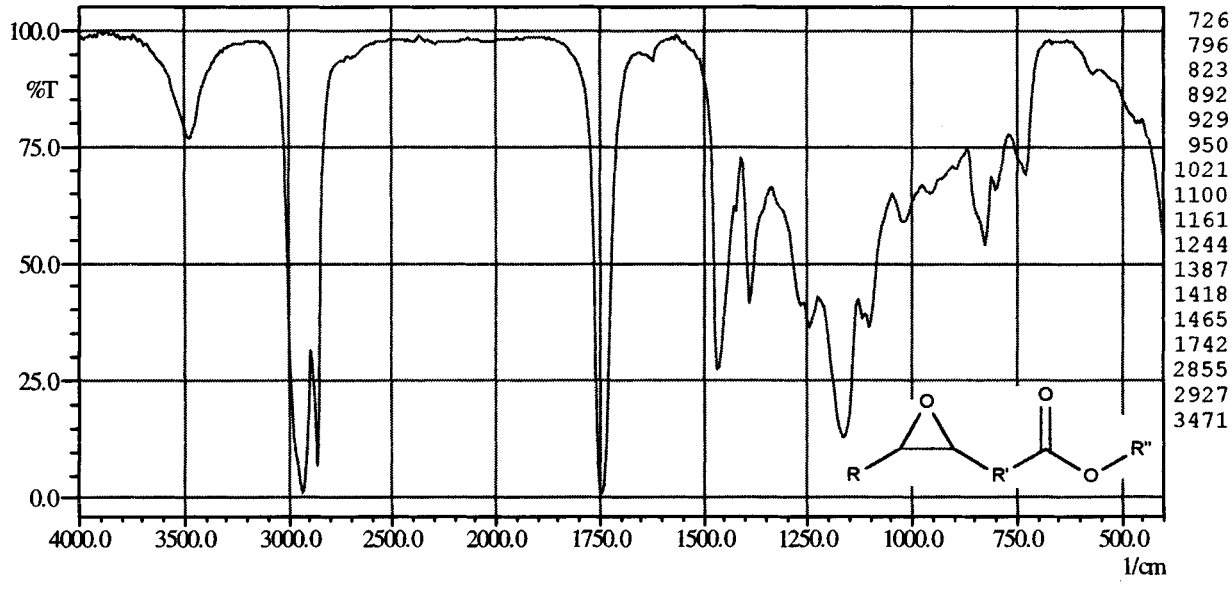
(1) **epoxidised soy bean oil**
(2) Edenol D82
(3) Henkel
(4) 935 g mol^{-1}
(5) plasticiser
(6) yellowish liquid
(9) 0.996 g cm^{-3}
(10) 1.473
(13) layer btw KBr

336



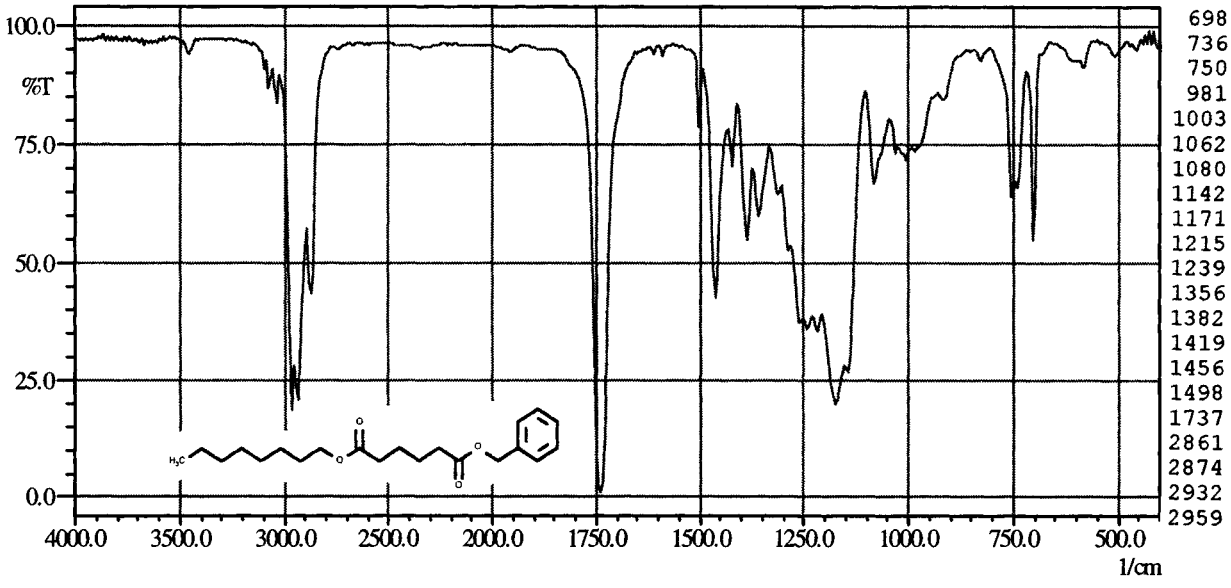
(1) **epoxidised linseed oil**
(2) Edenol B316
(3) Henkel
(4) 960 g mol^{-1}
(5) plasticiser
(6) yellow, clear liquid
(9) 1.03 g cm^{-3}
(10) 1.477
(13) layer btw KBr

336



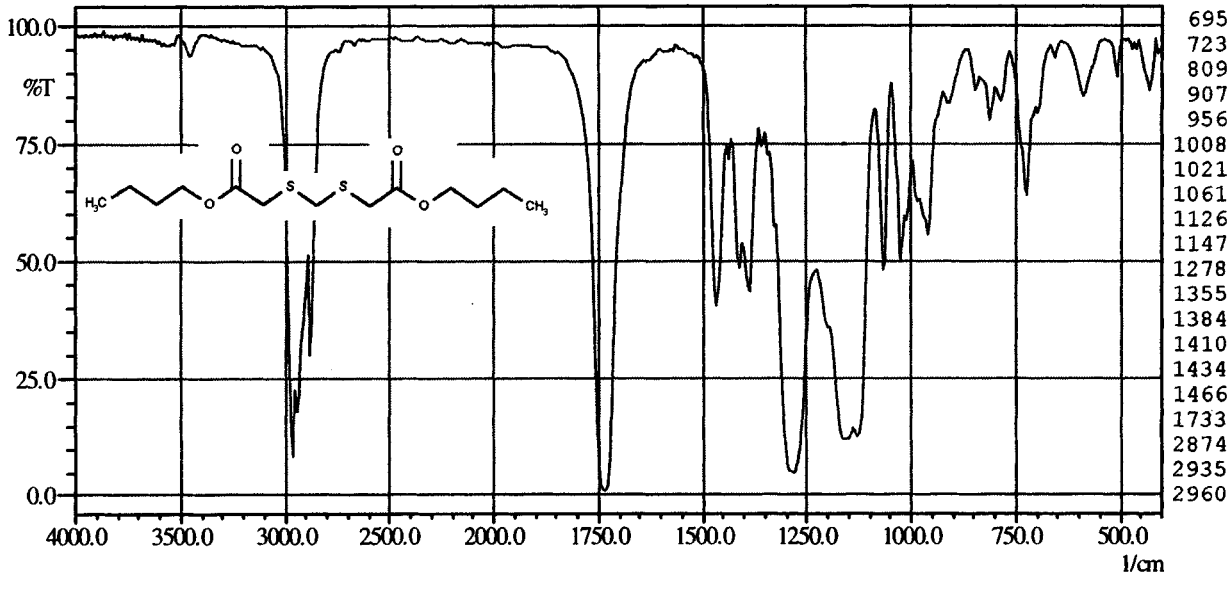
(1) **epoxidised vegetable oil**
(2) Lankroflex L
(3) Harcros
(5) plasticiser
(6) colourless, clear liquid
(13) layer btw KBr

337 $C_{21}H_{32}O_4$



(1) **benzyloctyladipate**
(2) Adimoll BO
(3) Bayer
(4) 348.5 g mol^{-1}
(5) plasticiser
(6) colourless, clear liquid
(8) 245 °C / 1300 Pa
(9) 1 g cm^{-3}
(10) 1.48
(13) layer btw KBr

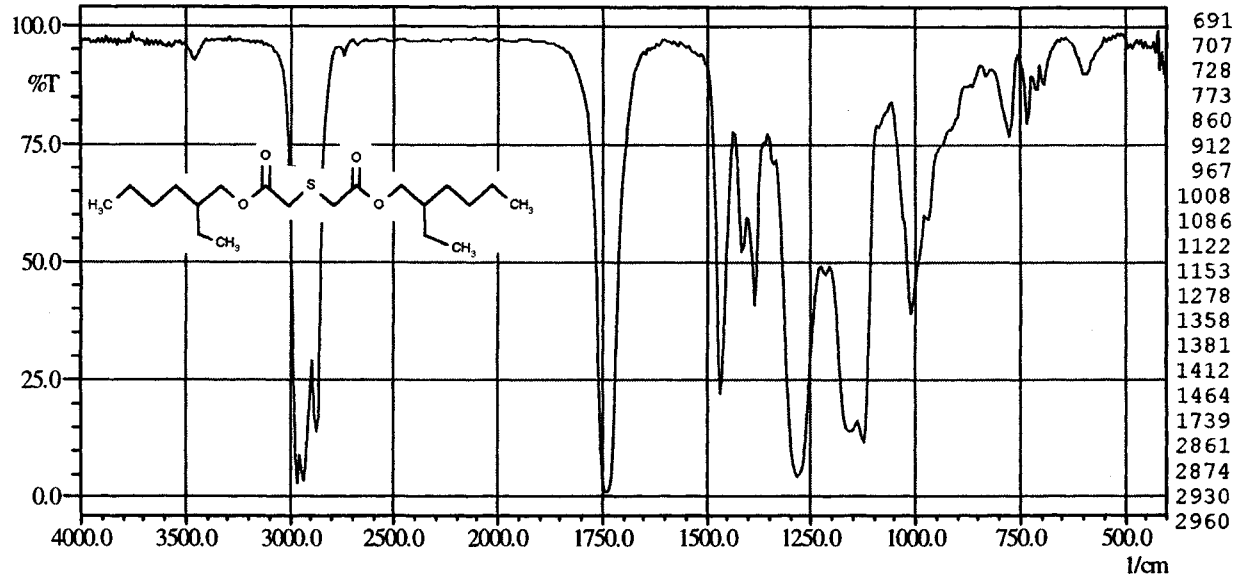
338 $C_{13}H_{24}O_4S_2$



(1) **methylene-*bis*(thioglycolic acid butyl ester)**
(2) Vulkanol 88
(3) Bayer
(4) 308.5 g mol^{-1}
(5) plasticiser
(6) yellowish, clear liquid
(9) 1.1 g cm^{-3}
(10) 1.49
(13) layer btw KBr

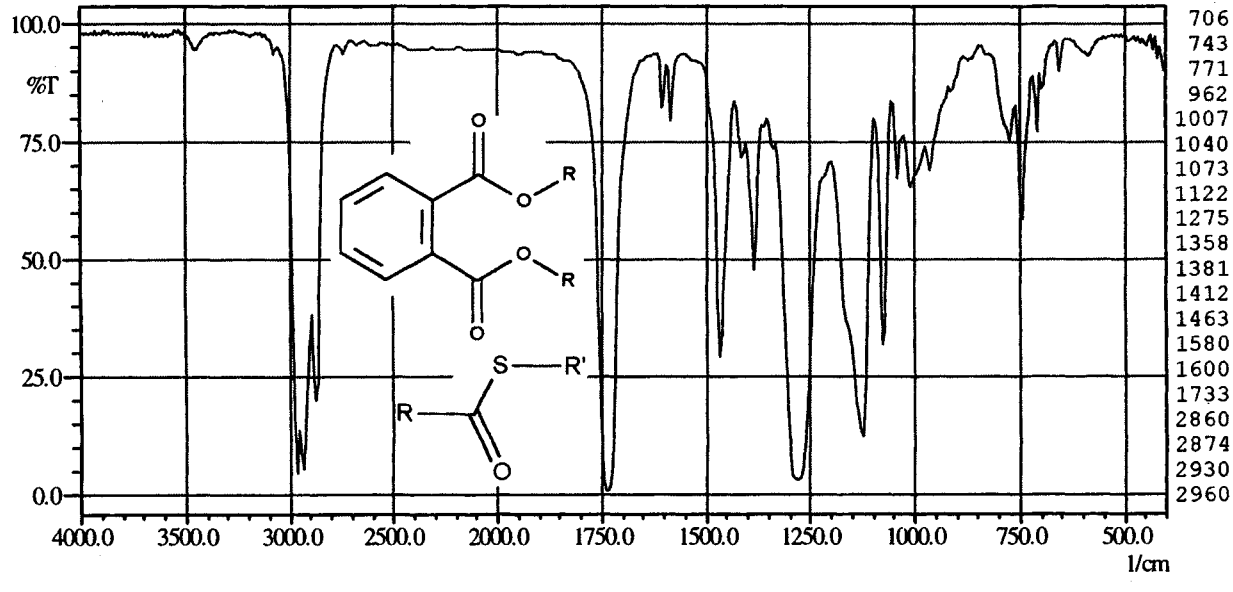
338

$C_{20}H_{38}O_4S$



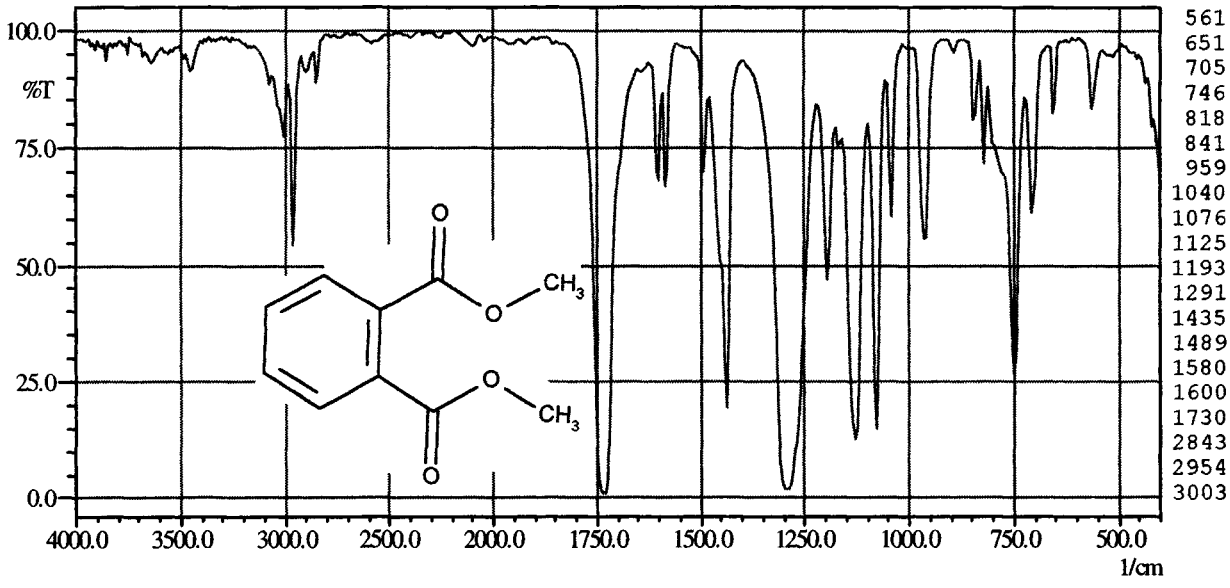
(1) **thiodi(glycolic acid-di-2-ethylhexyl ester)**
(2) Vulkanol 90
(3) Bayer
(4) 374.6 g mol^{-1}
(5) plasticiser
(6) yellow to brownish, clear liquid
(9) 0.98 g cm^{-3}
(10) 1.465
(13) layer btw KBr

338



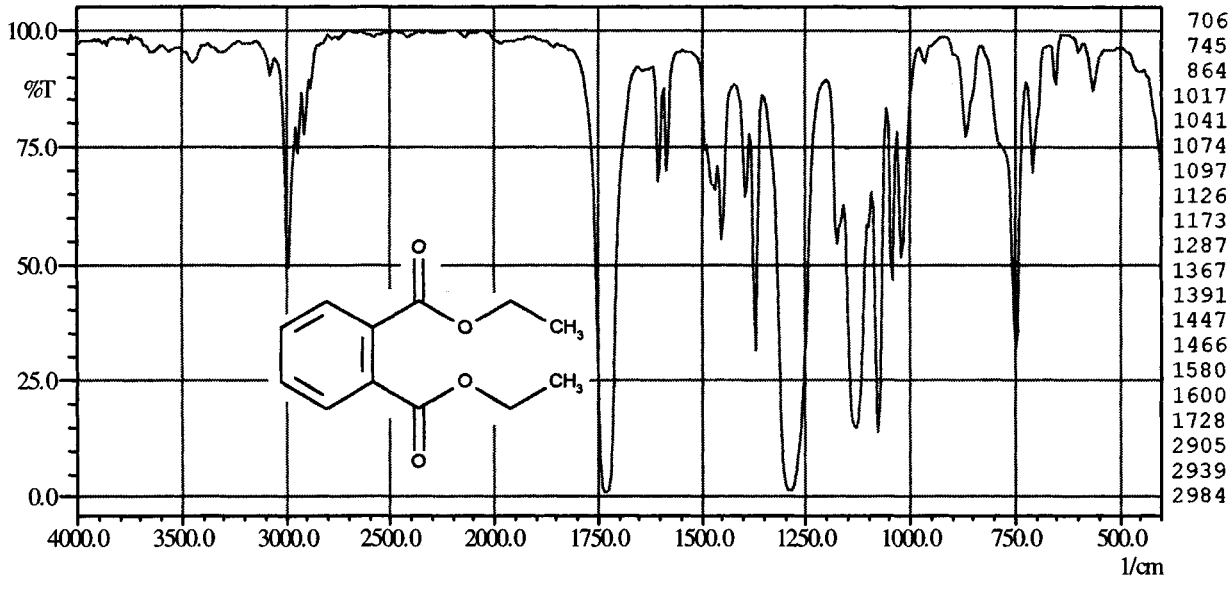
(1) **mixture of thiocarboxylic and carboxylic acid esters**
(2) Vulkanol 81
(3) Bayer
(5) plasticiser
(6) pale yellow, clear liquid
(9) 0.98 g cm^{-3}
(10) 1.475
(13) layer btw KBr

34211 $C_{10}H_{10}O_4$



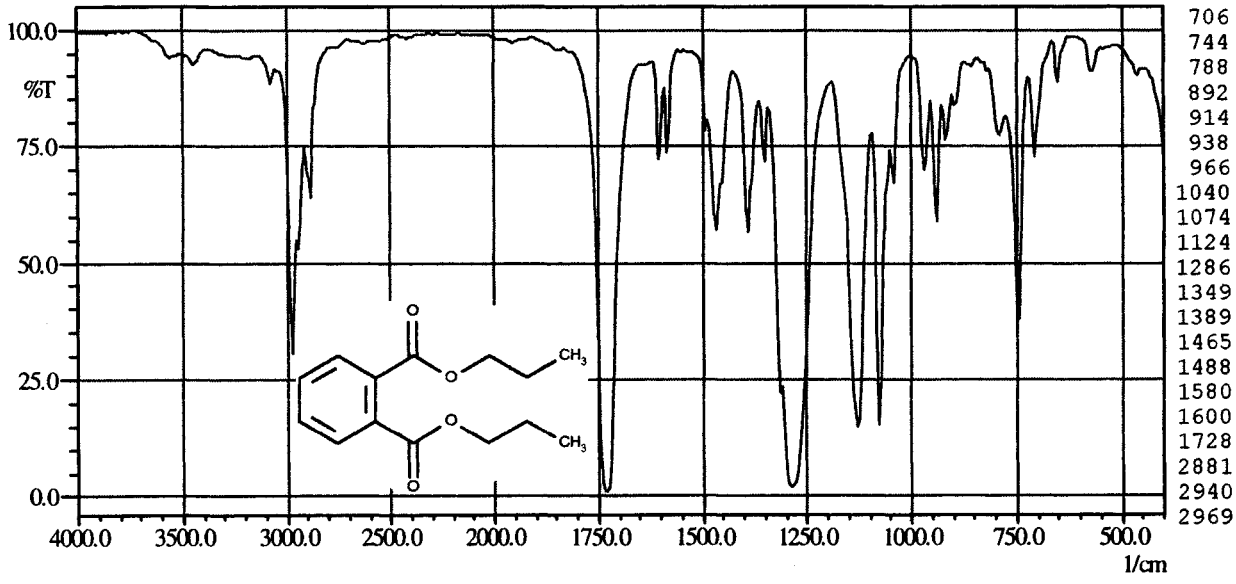
(1) **dimethylphthalate**
(3) Chrompack
(4) 194.2 g mol^{-1}
(5) plasticiser (GC-standard)
(6) colourless, clear liquid
(7) 2 °C
(8) 282 °C
(9) 1.190 g cm^{-3}
(10) 1.515
(13) layer btw KBr

34211 $C_{12}H_{14}O_4$



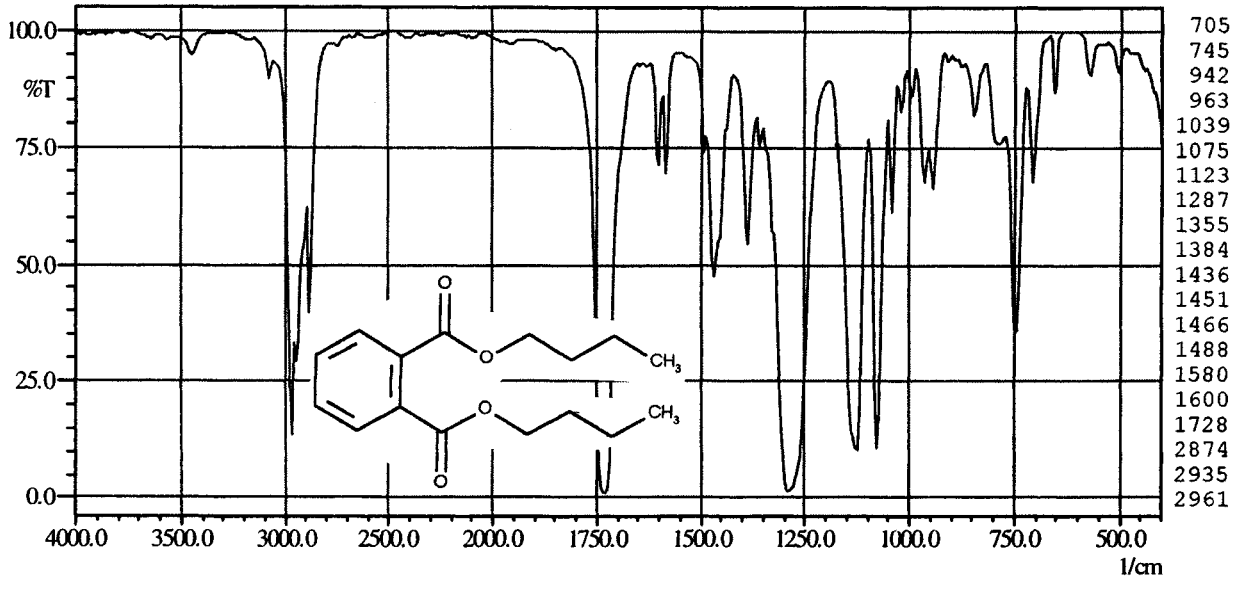
(1) **diethylphthalate**
(3) Chrompack
(4) 222.2 g mol^{-1}
(5) plasticiser (GC-standard)
(6) colourless, clear liquid
(7) 3 °C
(8) 298 °C
(9) 1.118 g cm^{-3}
(10) 1.502
(13) layer btw KBr

34211 $C_{14}H_{18}O_4$



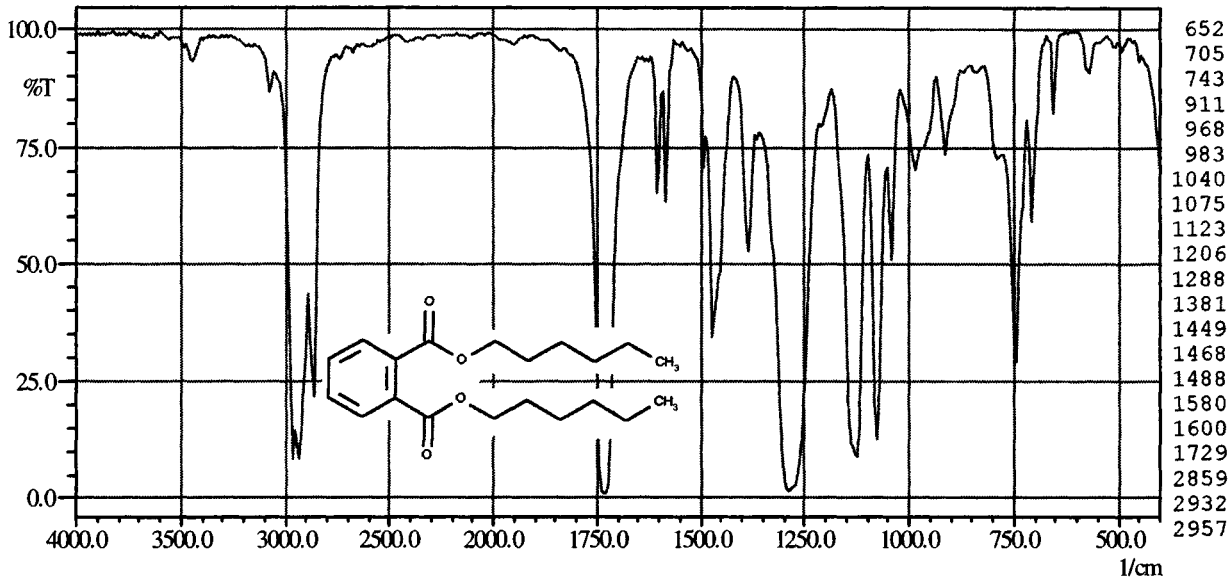
(1) **dipropylphthalate**
(3) Chrompack
(4) 250.3 g mol^{-1}
(5) plasticiser (GC-standard)
(6) colourless, clear liquid
(8) 317 °C
(9) 1.078 g cm^{-3}
(10) 1.497
(13) layer btw KBr

34211 $C_{16}H_{22}O_4$



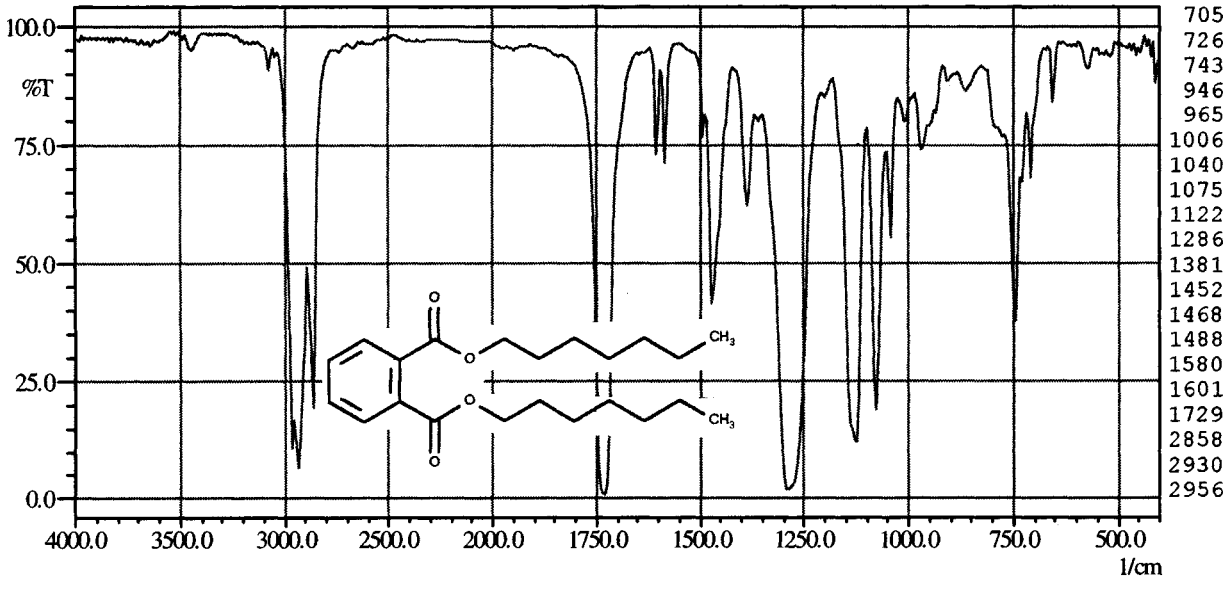
(1) **dibutylphthalate**
(3) Chrompack
(4) 278.3 g mol^{-1}
(5) plasticiser (GC-standard)
(6) colourless, clear liquid
(7) −35 °C
(8) 340 °C
(9) 1.043 g cm^{-3}
(10) 1.492
(13) layer btw KBr

34211 $C_{20}H_{30}O_4$



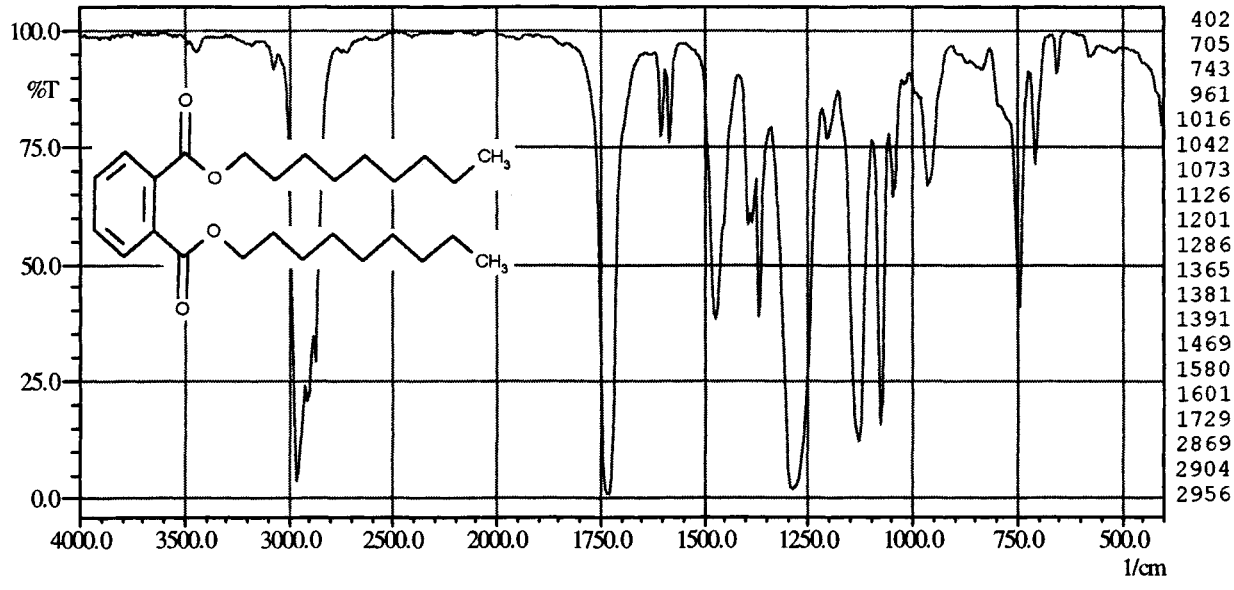
(1) **dihexylphthalate**
(3) Chrompack
(4) 334.5 g mol^{-1}
(5) plasticiser (GC-standard)
(6) colourless, clear liquid
(13) layer btw KBr

34211 $C_{22}H_{34}O_4$



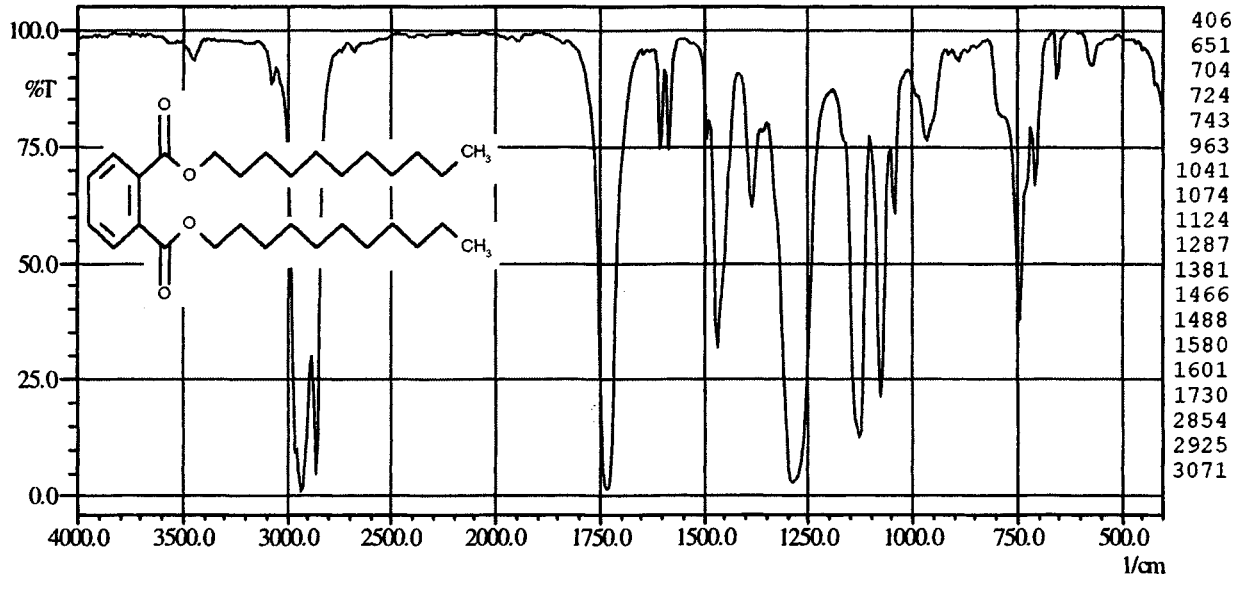
(1) **diheptylphthalate**
(2) Witamol 107
(3) Huels
(4) 362.5 g mol^{-1}
(5) plasticiser
(6) colourless, clear liquid
(9) 0.988 g cm^{-3}
(10) 1.486
(13) layer btw KBr

34211 $C_{26}H_{42}O_4$



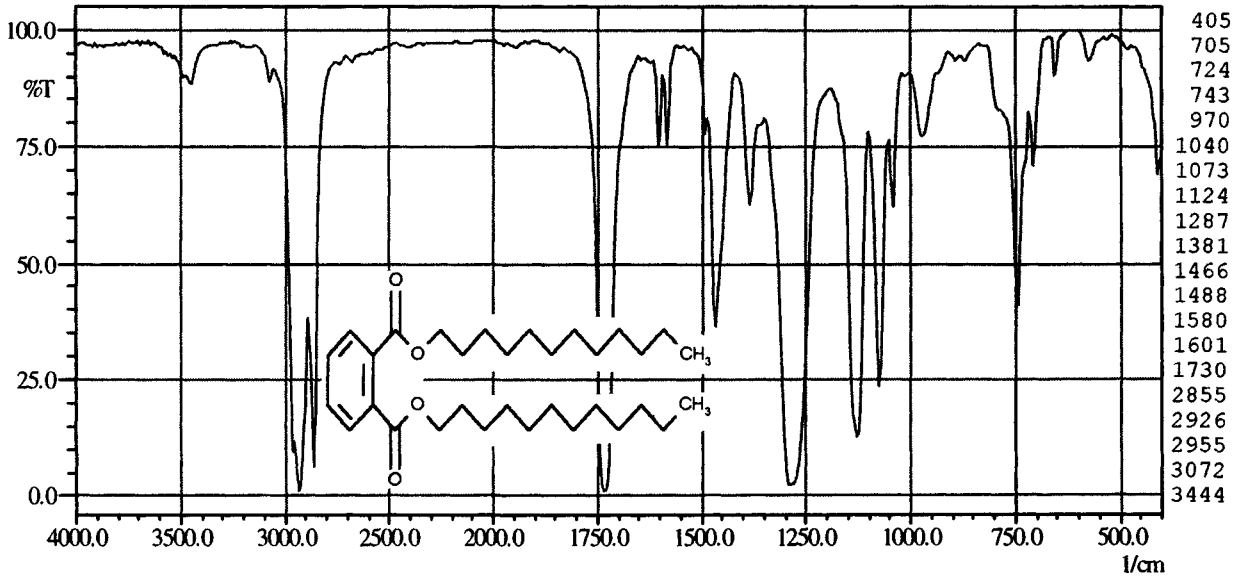
(1) **dinonylphthalate**
(3) Chrompack
(4) 418.6 g mol^{-1}
(5) plasticiser (GC-standard)
(6) colourless, clear liquid
(13) layer btw KBr

34211 $C_{30}H_{50}O_4$



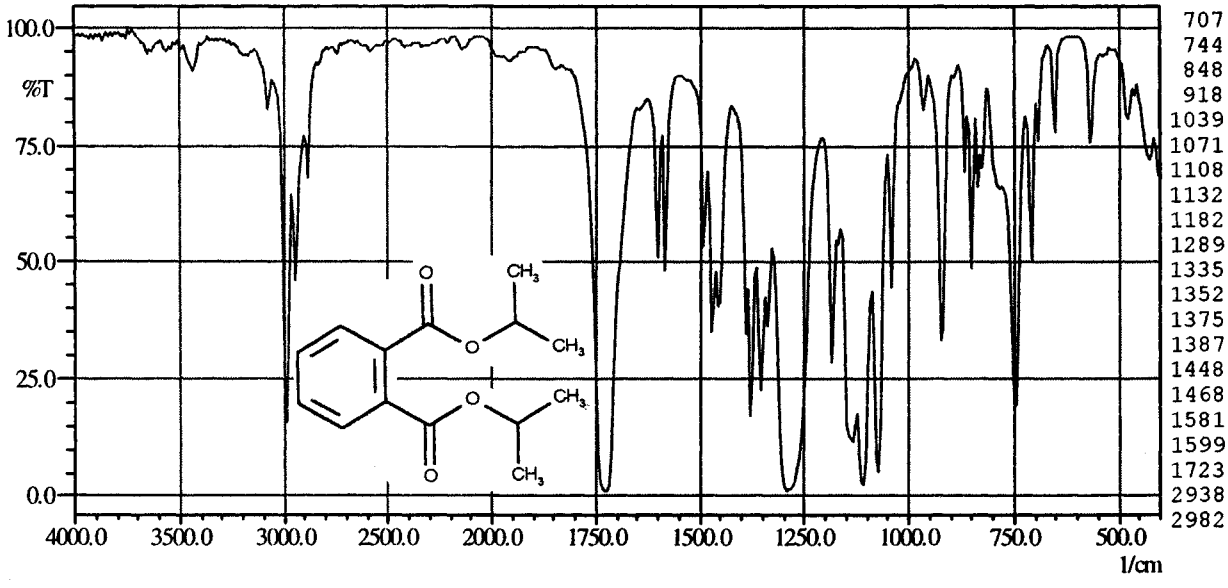
(1) **diundecylphthalate**
(3) Chrompack
(4) 474.7 g mol^{-1}
(5) plasticiser (GC-standard)
(6) colourless, clear liquid
(13) layer btw KBr

34211 $C_{32}H_{54}O_4$



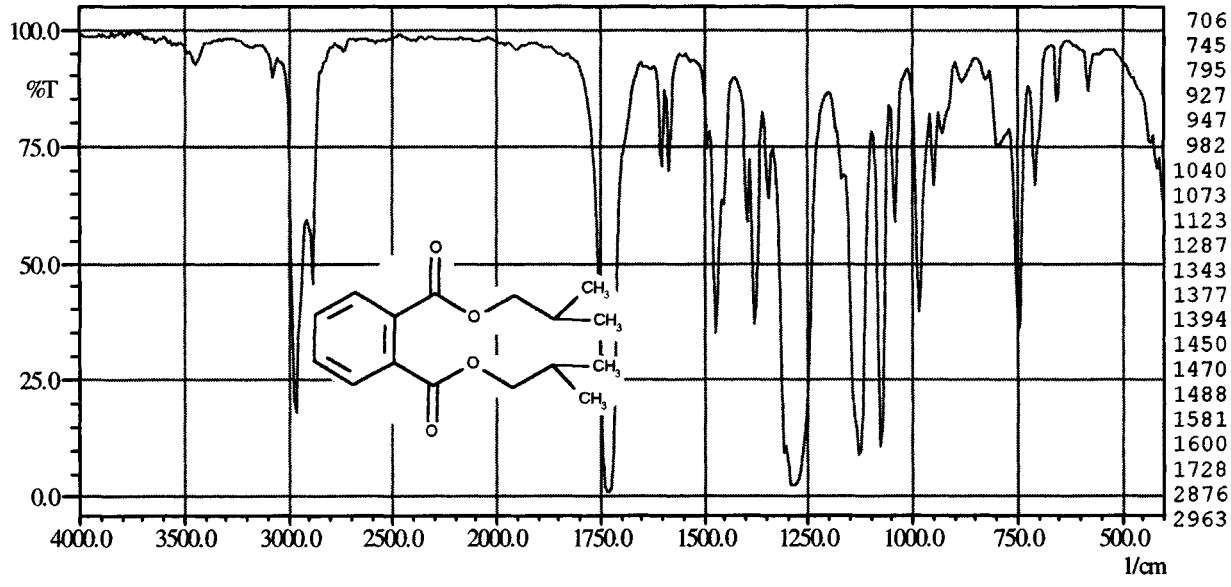
(1) **didodecylphthalate**
(3) Chrompack
(4) 502.8 g mol^{-1}
(5) plasticiser (GC-standard)
(6) colourless, clear liquid
(13) layer btw KBr

34212 $C_{14}H_{18}O_4$



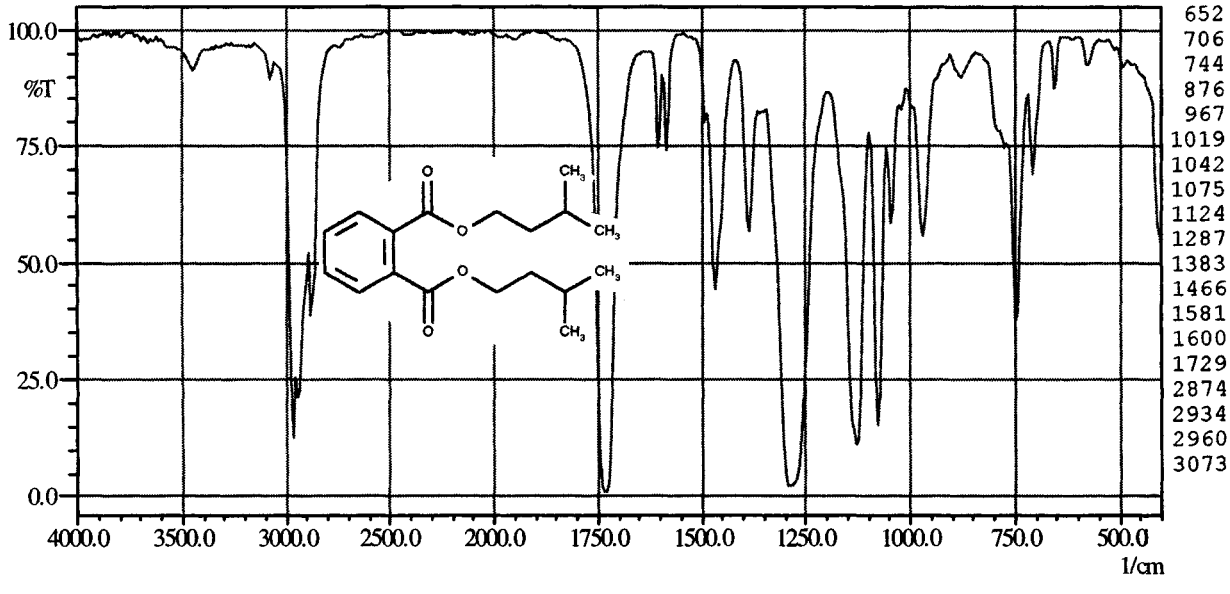
(1) **di-2-propylphthalate**
(3) Chrompack
(4) 250.3 g mol^{-1}
(5) plasticiser (GC-standard)
(6) colourless, clear liquid
(13) layer btw KBr

34212 $C_{16}H_{22}O_4$



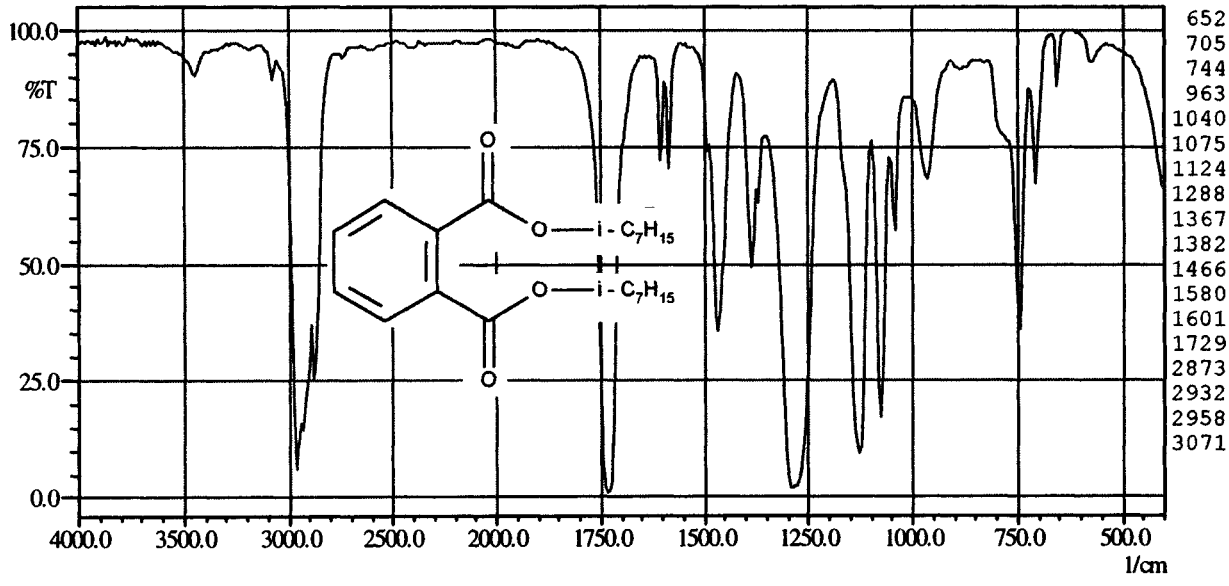
(1) **di-*i*-butylphthalate**
(3) Chrompack
(4) 278.3 g mol^{-1}
(5) plasticiser (GC-standard)
(6) colourless, clear liquid
(13) layer btw KBr

34212 $C_{18}H_{26}O_4$



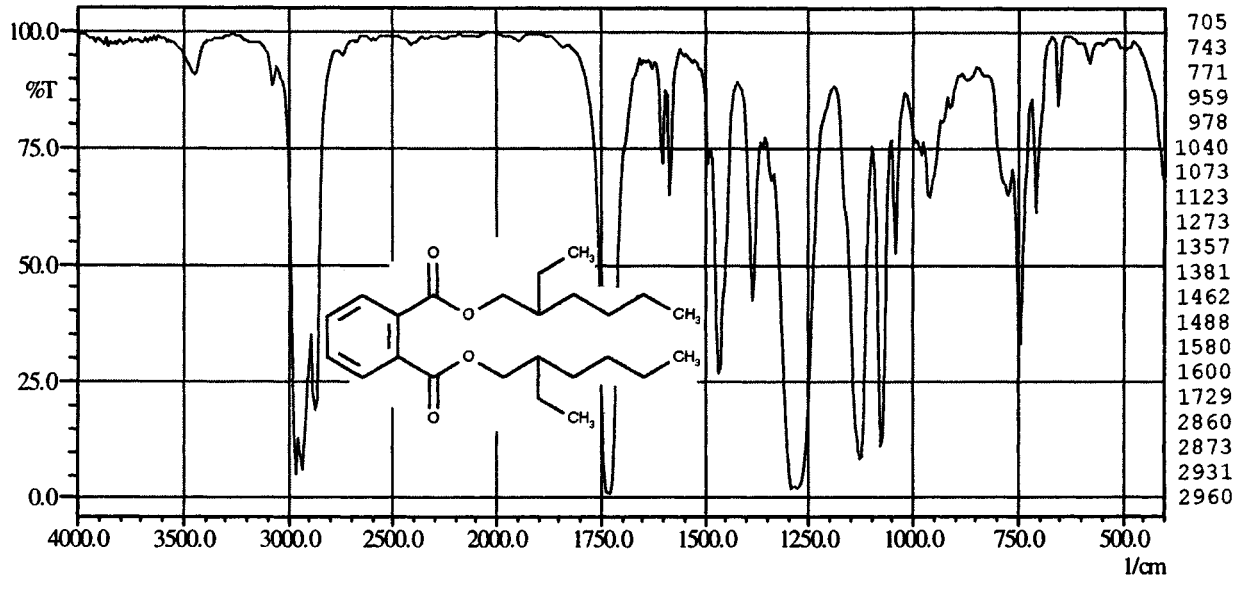
(1) **di-*i*-pentylphthalate**
(2) Palatinol CE 5539 (DIPP)
(3) BASF
(4) 306.4 g mol^{-1}
(5) plasticiser
(6) colourless, clear liquid
(8) 213 °C / 700 Pa
(9) 1.023 g cm^{-3}
(10) 1.49
(13) layer btw KBr

34212 $C_{22}H_{34}O_4$



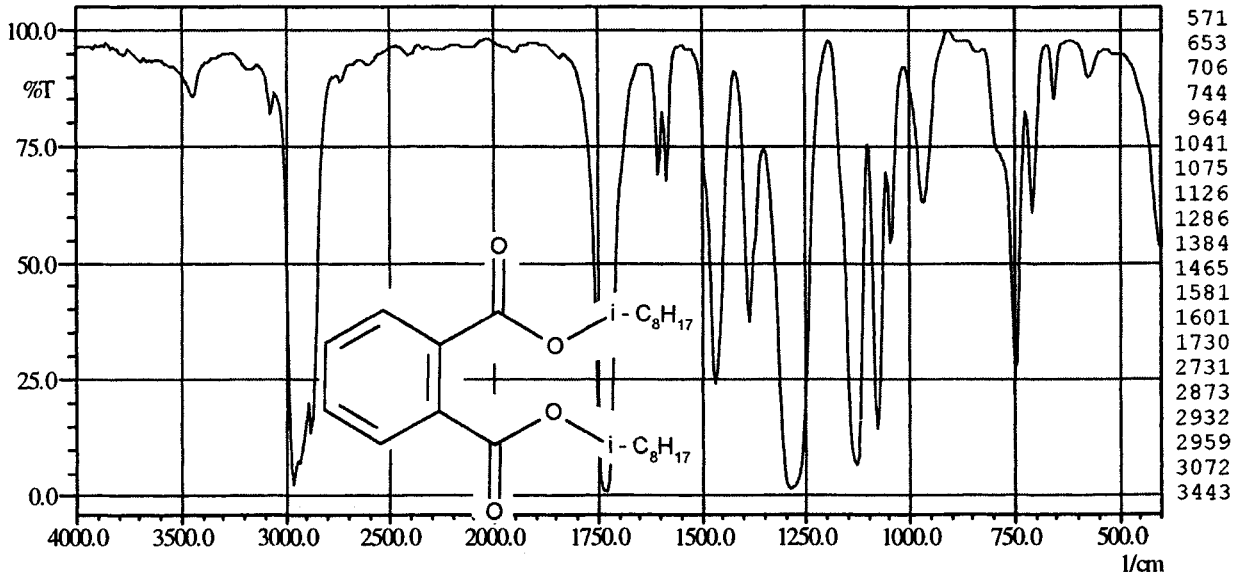
(1) **di-*i*-heptylphthalate**
(2) DIHP J 77
(3) Exxon Chemical
(4) 362.5 g mol^{-1}
(5) plasticiser
(6) colourless, clear liquid
(7) –40 °C
(9) 0.991 g cm^{-3}
(10) 1.487
(13) layer btw KBr

34212 $C_{24}H_{38}O_4$



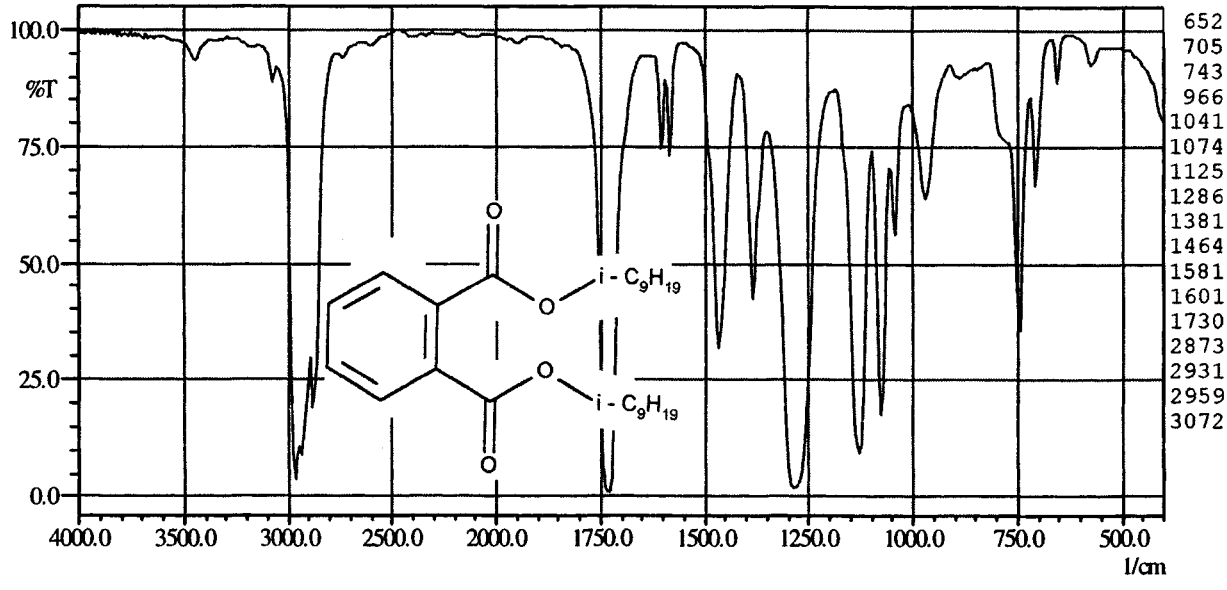
(1) **di(2-ethylhexyl)phthalate**
(2) Witamol 100
(3) Dynamit Nobel
(4) 390.6 g mol^{-1}
(5) plasticiser
(6) colourless, clear liquid
(13) layer btw KBr

34212 $C_{24}H_{38}O_4$



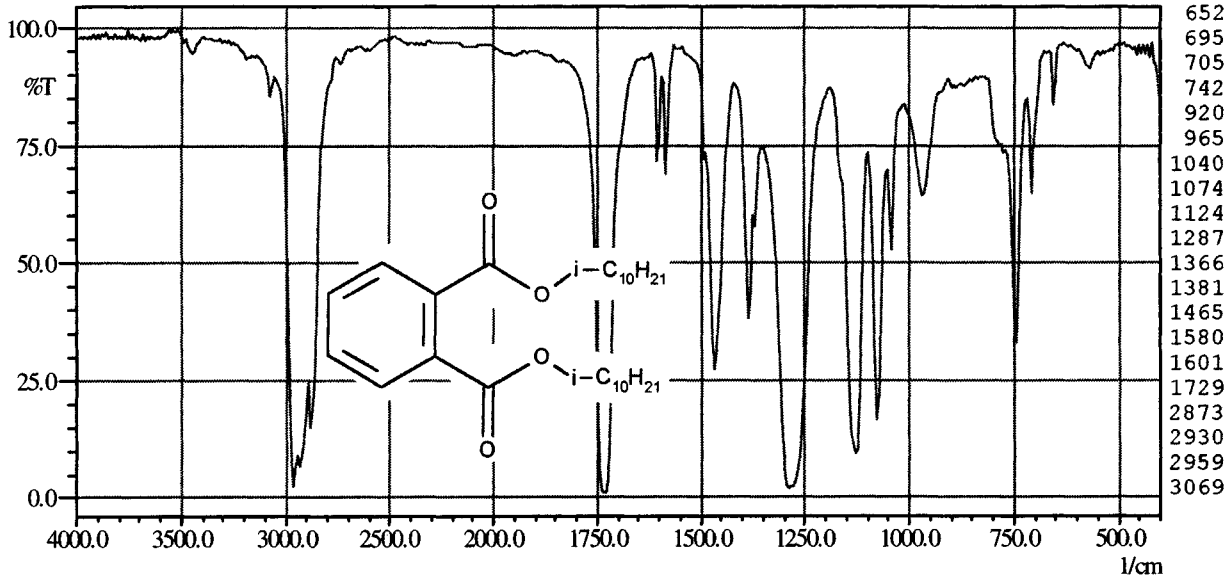
(1) **di-*i*-octylphthalate**
(2) Jayflex DIOP
(3) Exxon Chemical
(4) 390.6 g mol^{-1}
(5) plasticiser (PVC)
(6) colourless, clear liquid
(9) 0.983 g cm^{-3}
(10) 1.486
(13) layer btw KBr

34212 $C_{26}H_{42}O_4$



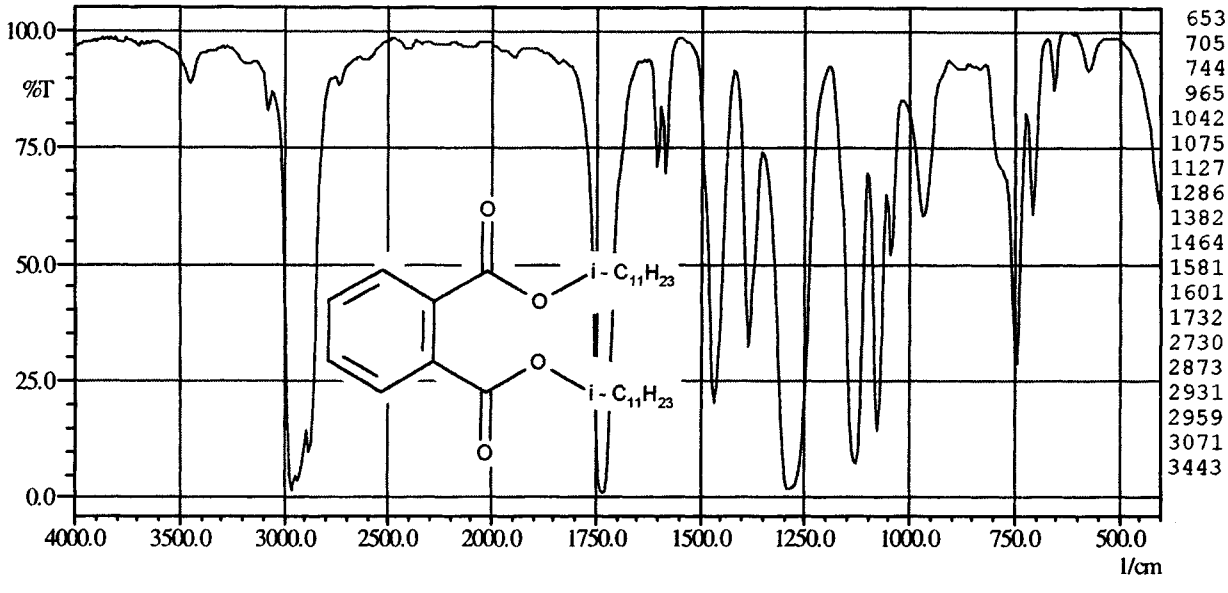
(1) **di-*i*-nonylphthalate**
(2) Palatinol DINP
(3) BASF
(4) 418.6 g mol^{-1}
(5) plasticiser
(6) colourless, clear liquid
(8) 257 °C / 700 Pa
(9) 0.978 g cm^{-3}
(10) 1.486
(13) layer btw KBr
(14) structure of *i*-nonyl is undefined

34212 $C_{28}H_{46}O_4$



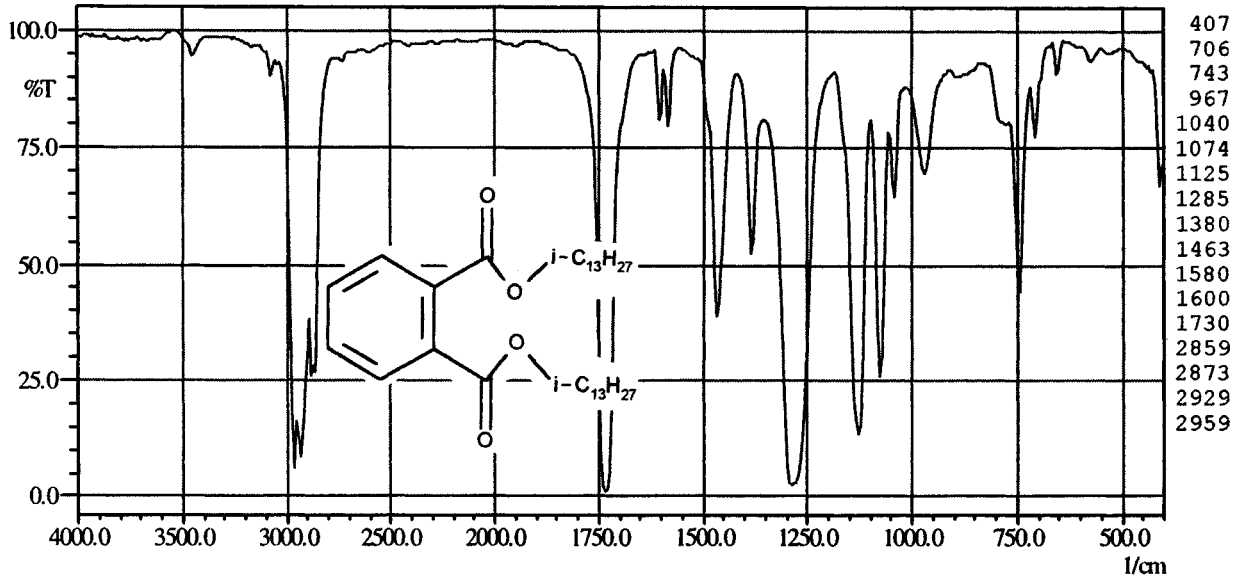
(1) **di-*i*-decylphthalate**
(2) Genomoll 180
(3) Hoechst
(4) 446.7 g mol^{-1}
(5) plasticiser
(6) colourless, clear liquid
(13) layer btw KBr
(14) structure of *i*-decyl is undefined

34212 $C_{30}H_{50}O_4$



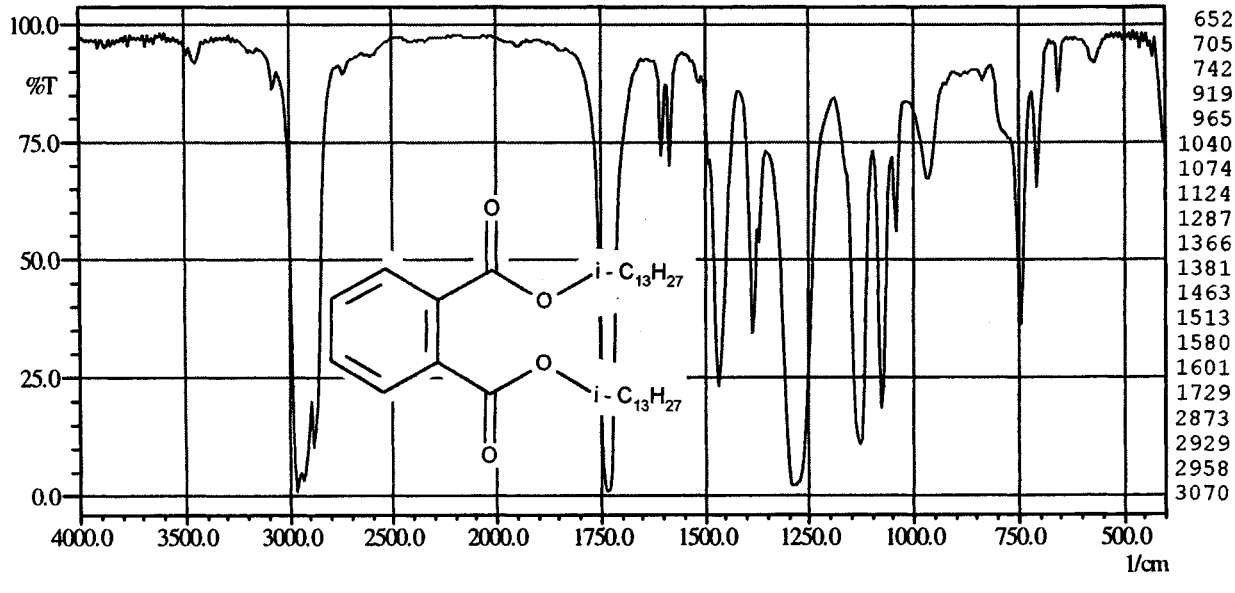
(1) **di-*i*-undecylphthalate**
(2) Jayflex DIUP
(3) Exxon Chemical
(4) 474.7 g mol^{-1}
(5) plasticiser (PVC)
(6) colourless, clear liquid
(9) 0.962 g cm^{-3}
(10) 1.485
(13) layer btw KBr
(14) structure of *i*-undecyl is undefined

34212 $C_{34}H_{58}O_4$



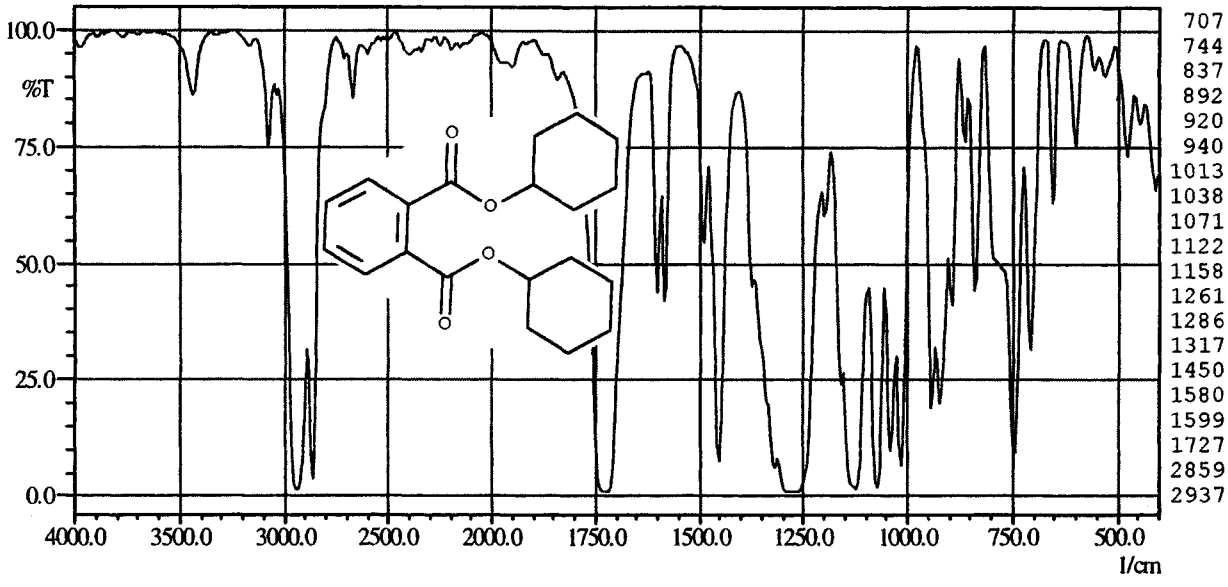
(1) **di-*i*-tridecylphthalate**
(2) Vestinol TD stab.
(3) Huels
(4) 530.8 g mol^{-1}
(5) plasticiser
(6) colourless, clear liquid
(9) 0.952 g cm^{-3}
(10) 1.485
(13) layer btw KBr
(14) with stabiliser, structure of *i*-tridecyl is undefined

34212 $C_{34}H_{58}O_4$



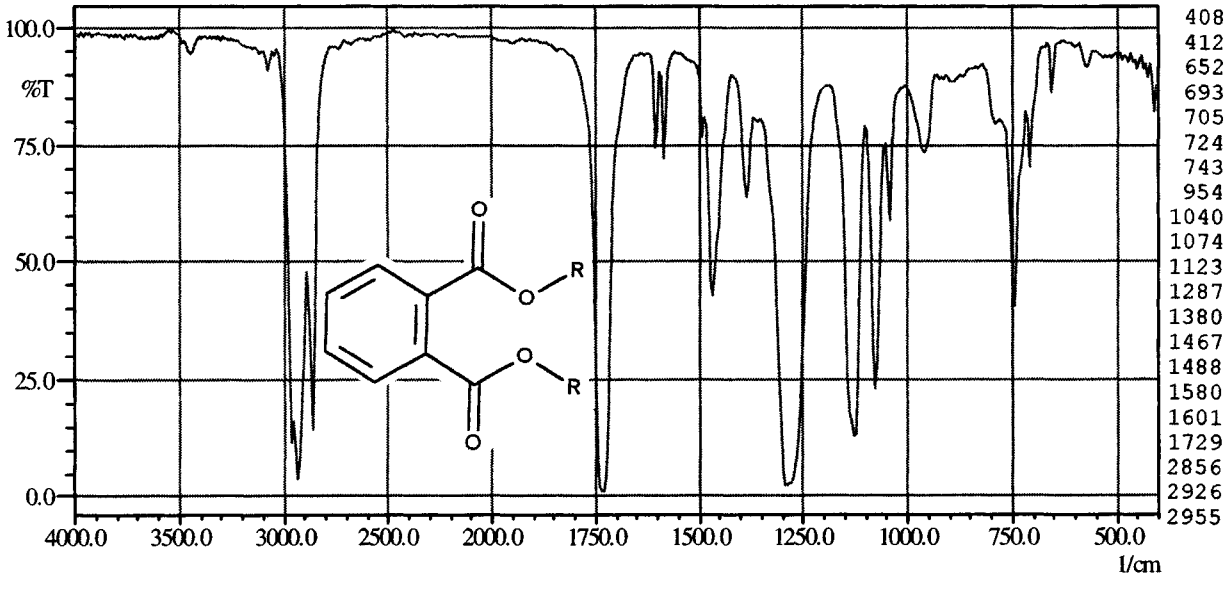
(1) **di-*i*-tridecylphthalate**
(2) Edenol W300S
(3) Henkel
(4) 530.8 g mol^{-1}
(5) plasticiser
(6) yellow liquid
(9) 0.95 g cm^{-3}
(10) 1.484
(13) layer btw KBr
(14) structure of *i*-tridecyl is undefined

34213 $C_{20}H_{26}O_4$



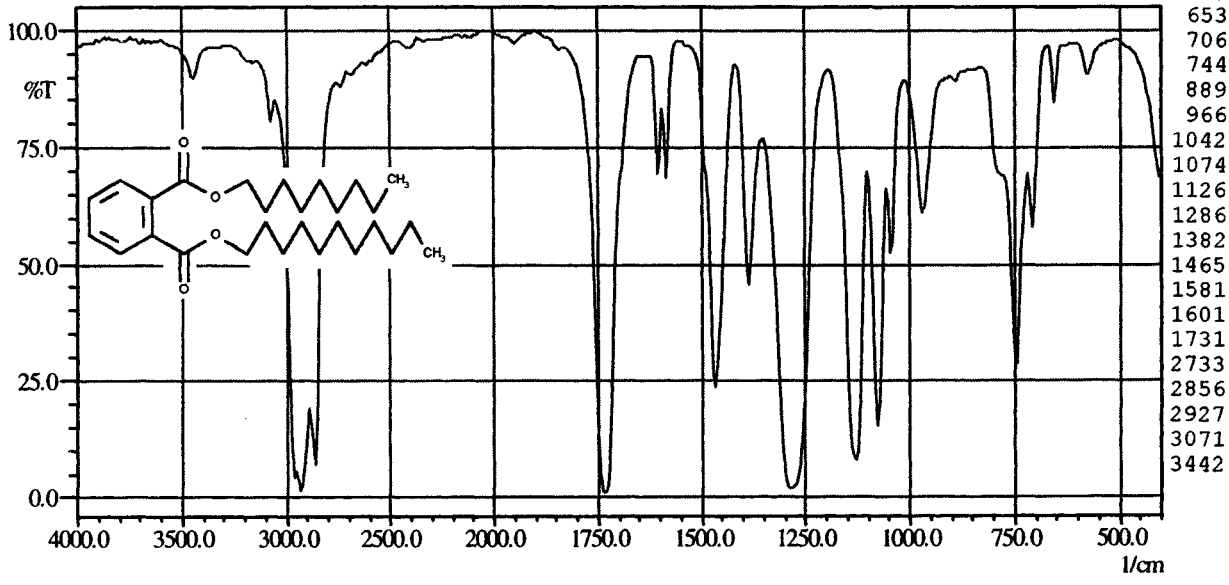
(1) **dicyclohexylphthalate**
(2) Unimoll 66
(3) Bayer
(4) 330.4 g mol^{-1}
(5) plasticiser
(6) colourless solid
(7) 64 °C
(8) 248 °C
(9) 1.15 g cm^{-3}
(13) molten, layer btw KBr

34214



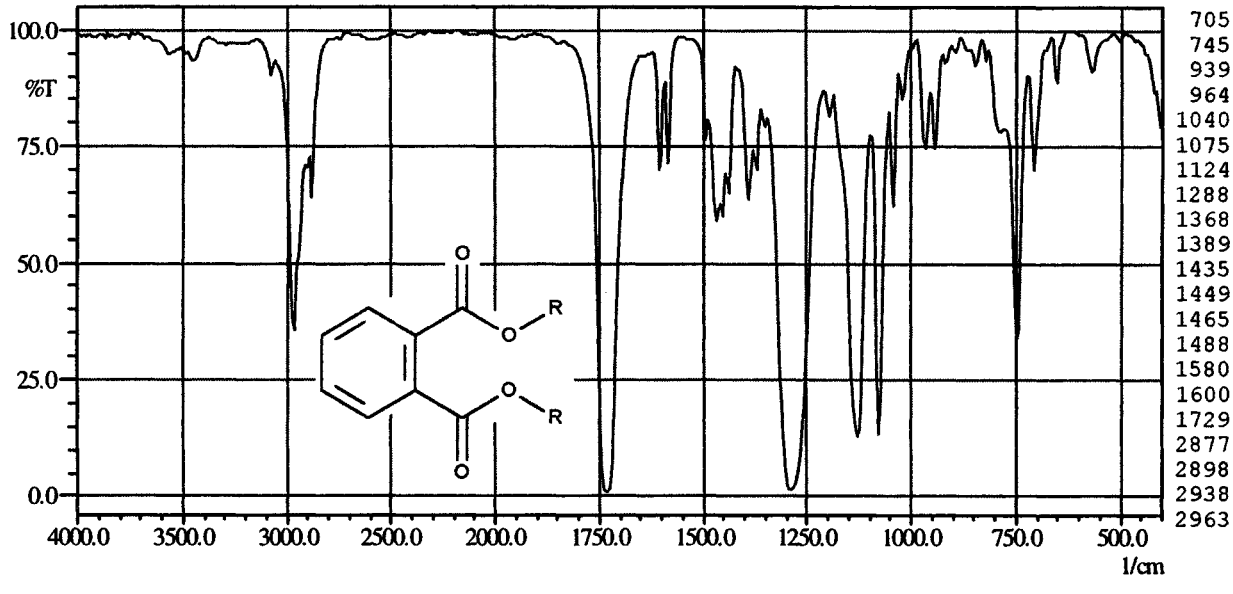
(1) **di(C_6...C_{10}-alkyl)phthalate**
(2) Witamol 110
(3) Huels
(4) 395 g mol^{-1}
(5) plasticiser
(6) colourless, clear liquid
(9) 0.982 g cm^{-3}
(10) 1.483
(13) layer btw KBr

34214 $C_{28}H_{46}O_4$



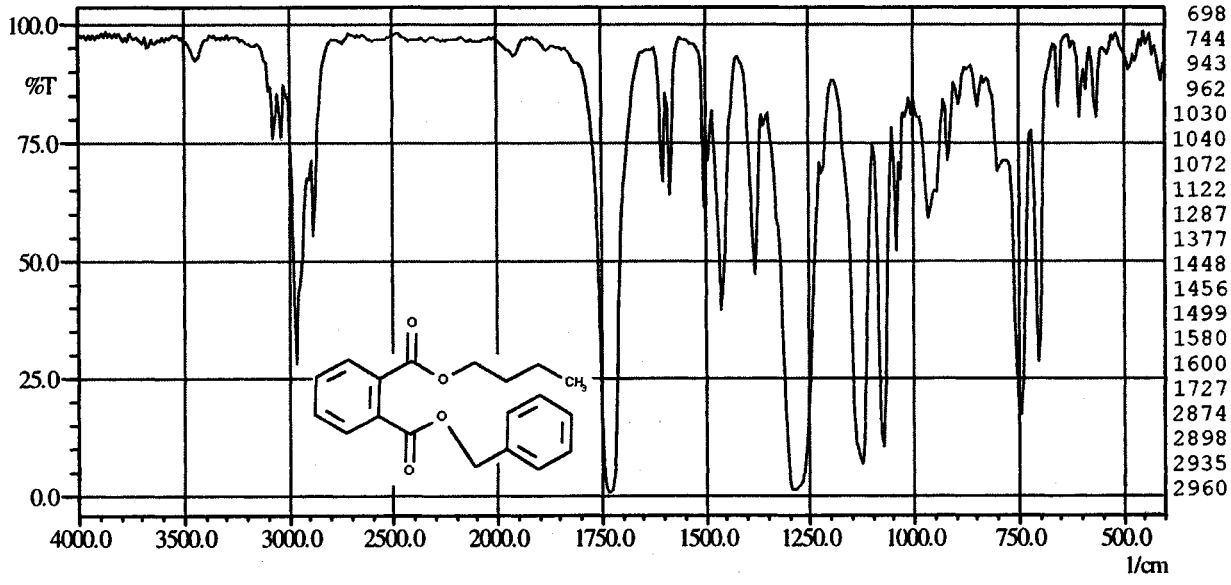
(1) **nonylundecylphthalate**
(2) Jayflex 911P
(3) Exxon Chemical
(4) 446.7 g mol^{-1}
(5) plasticiser (PVC)
(6) colourless, clear liquid
(7) −50 °C
(9) 0.962 g cm^{-3}
(10) 1.483
(13) layer btw KBr

34214



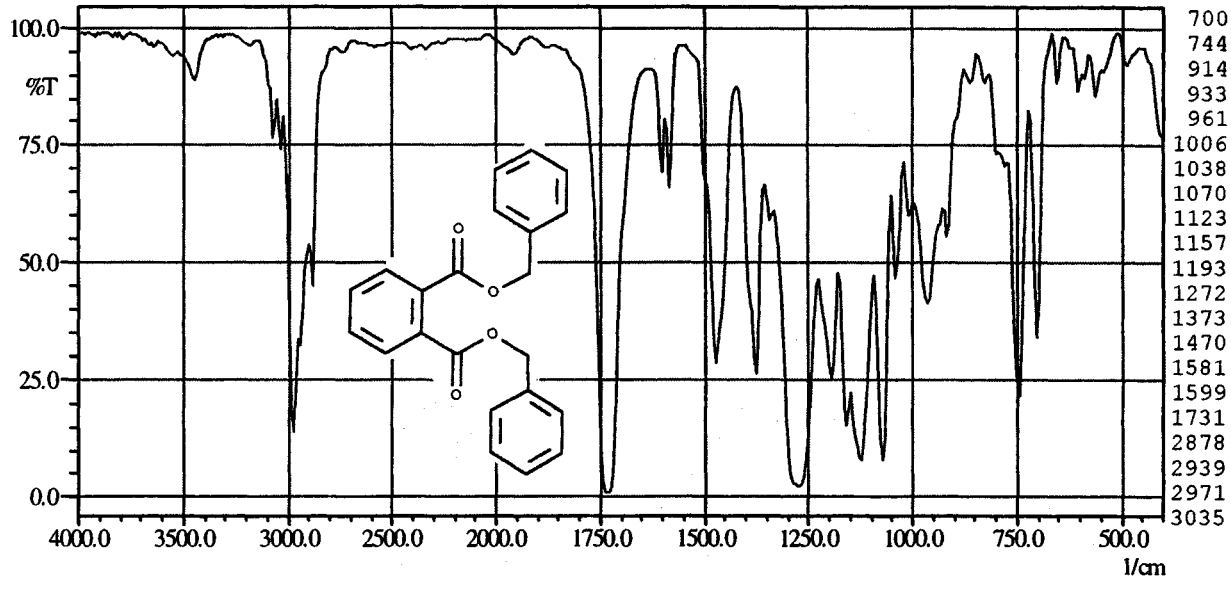
(1) **mixture of phthalic acid esters**
(2) Calibration Mixture 84C
(3) Chrompack
(5) plasticiser (GC-calibration mixture)
(6) colourless, clear liquid
(13) layer btw KBr

34215 $C_{19}H_{20}O_4$



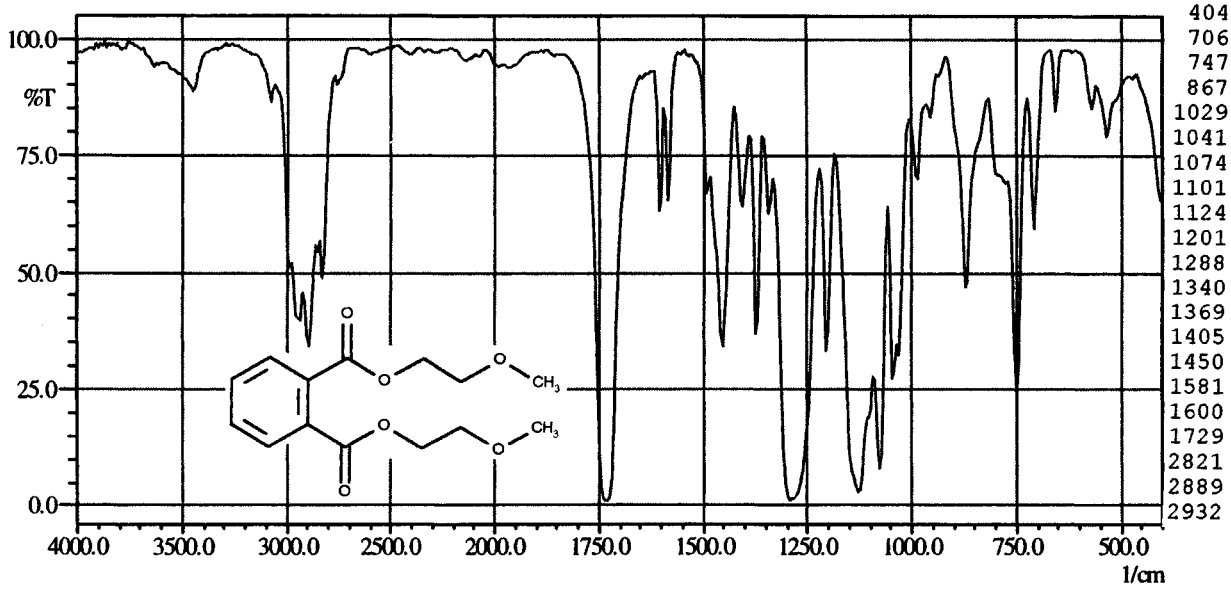
(1) **benzylbutylphthalate**
(2) Unimoll BB
(3) Bayer
(4) 312.4 g mol^{-1}
(5) plasticiser
(6) colourless, clear, low-viscous liquid
(8) 245 °C / 1300 Pa
(9) 1.13 g cm^{-3}
(10) 1.54
(13) layer btw KBr

34215 $C_{22}H_{18}O_4$



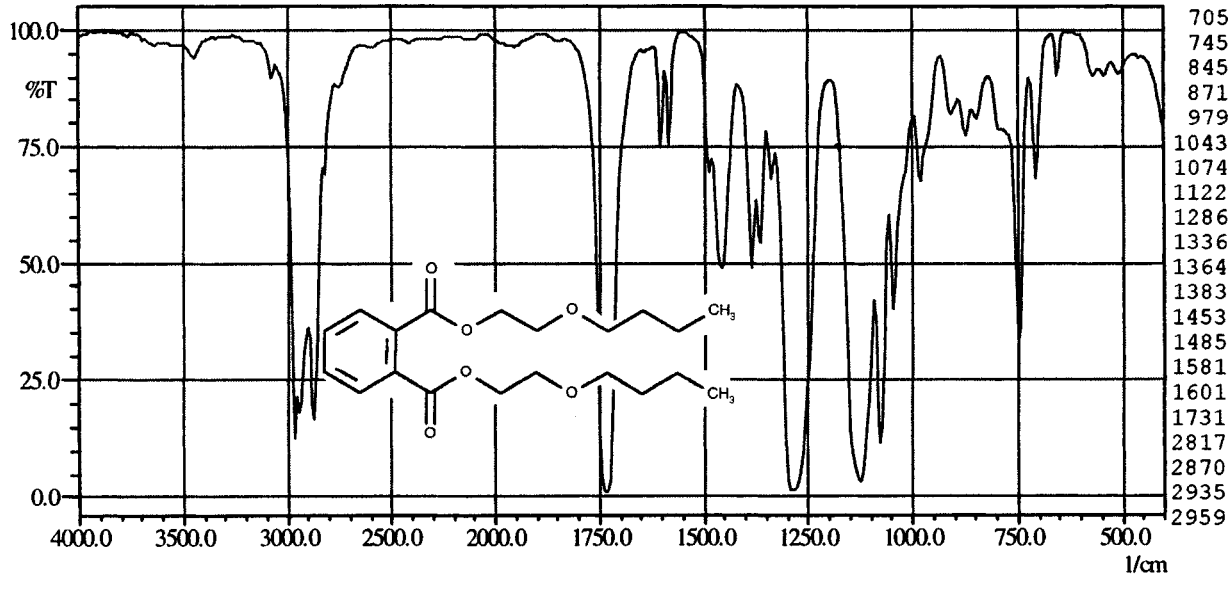
(1) **dibenzylphthalate**
(2) Santicizer 278
(3) Monsanto
(4) 346.4 g mol^{-1}
(5) plasticiser
(6) colourless, clear, oily liquid
(9) 1.097 g cm^{-3}
(10) 1.518
(13) layer btw KBr

34217 $C_{14}H_{18}O_6$



(1) **dimethoxyethylphthalate**
(2) Palatinol O
(3) BASF
(4) 282.3 g mol^{-1}
(5) plasticiser
(6) colourless, clear liquid
(13) layer btw KBr

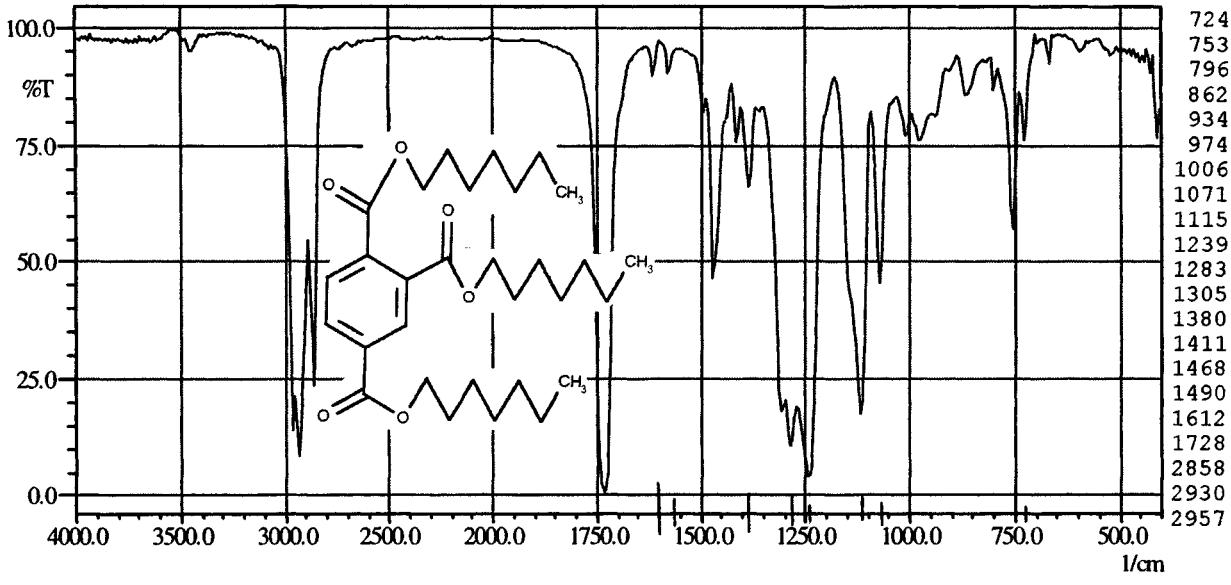
34217 $C_{20}H_{30}O_6$



(1) **dibutoxyethylphthalate**
(2) Palatinol K (CE 5531)
(3) BASF
(4) 366.5 g mol^{-1}
(5) plasticiser
(6) colourless, clear liquid
(8) 248 °C
(9) 1.6 g cm^{-3}
(10) 1.486
(13) layer btw KBr

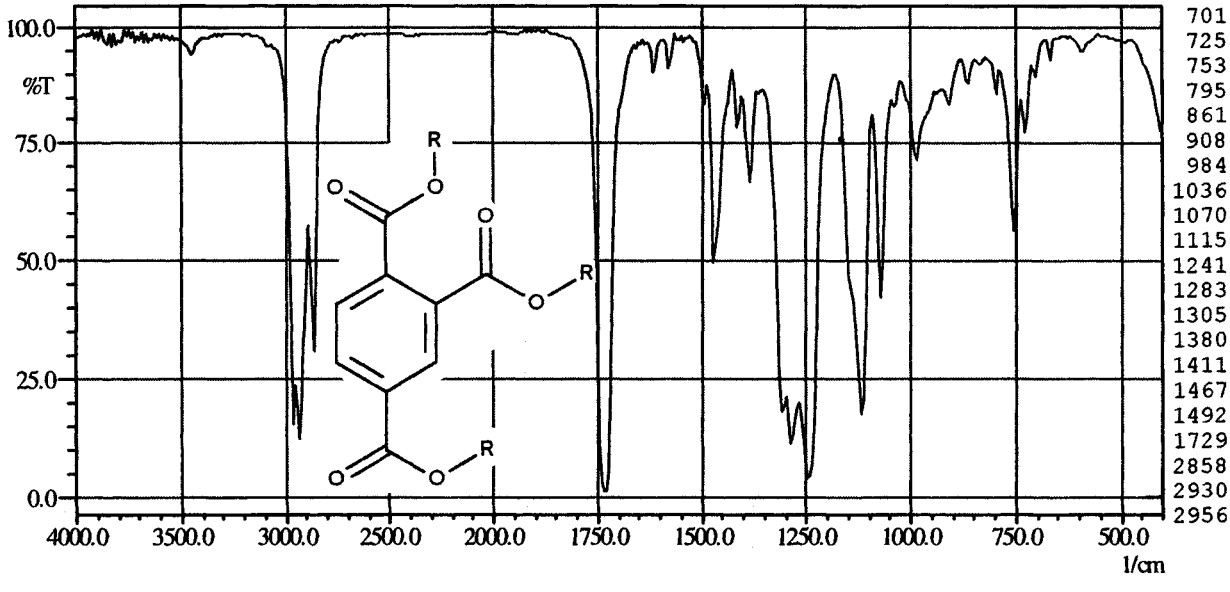
3424

$C_{30}H_{48}O_6$



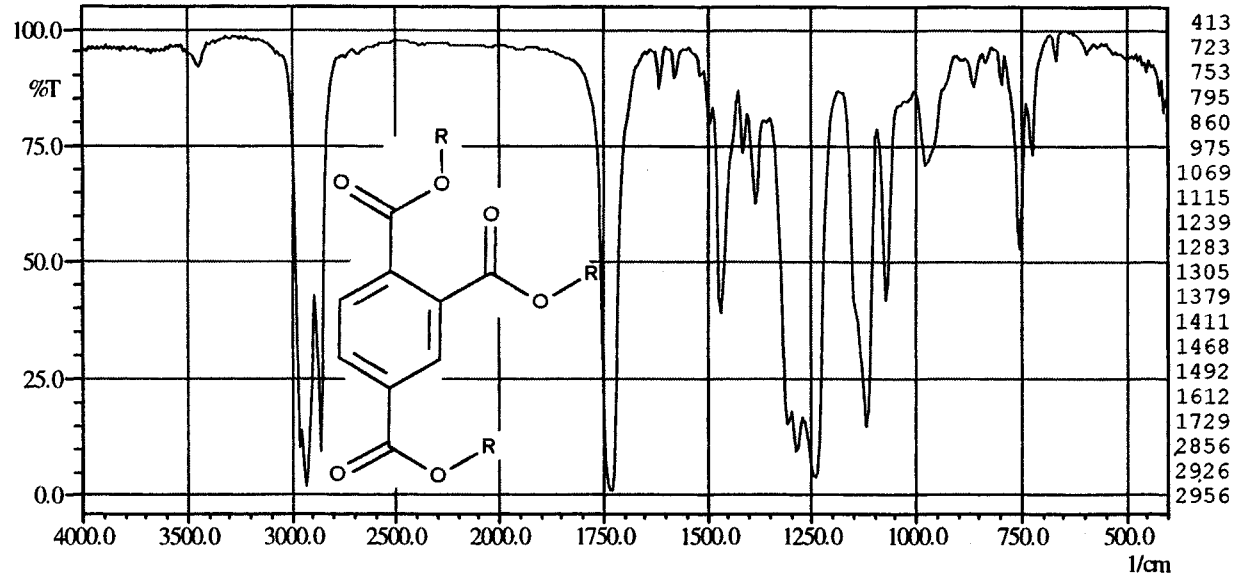
(1) **triheptyltrimellitate**
(2) Witamol 207 stab
(3) Huels
(4) 504.7 g mol^{-1}
(5) plasticiser
(6) colourless, clear liquid
(9) 0.995 g cm^{-3}
(10) 1.485
(13) layer btw KBr

3424



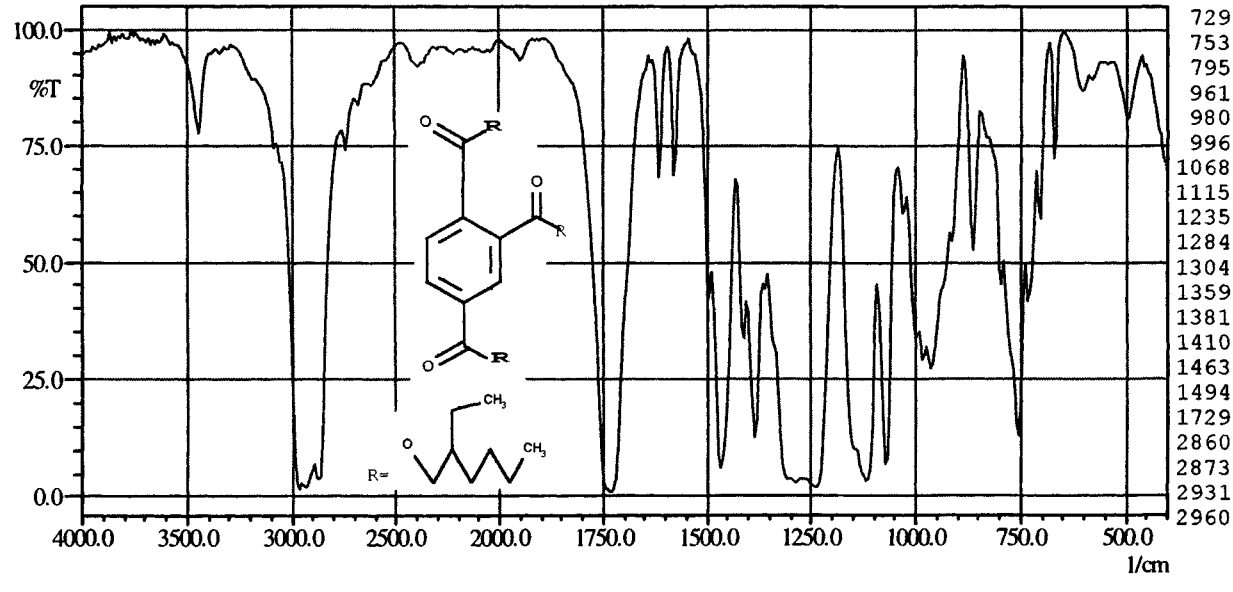
(1) **tri(C_6...C_8-alkyl)trimellitate**
(2) Linplast 68 TM
(3) Condea
(5) plasticiser
(6) colourless, clear liquid
(7) −52 °C
(9) 1.01 g cm^{-3}
(13) layer btw KBr

3424



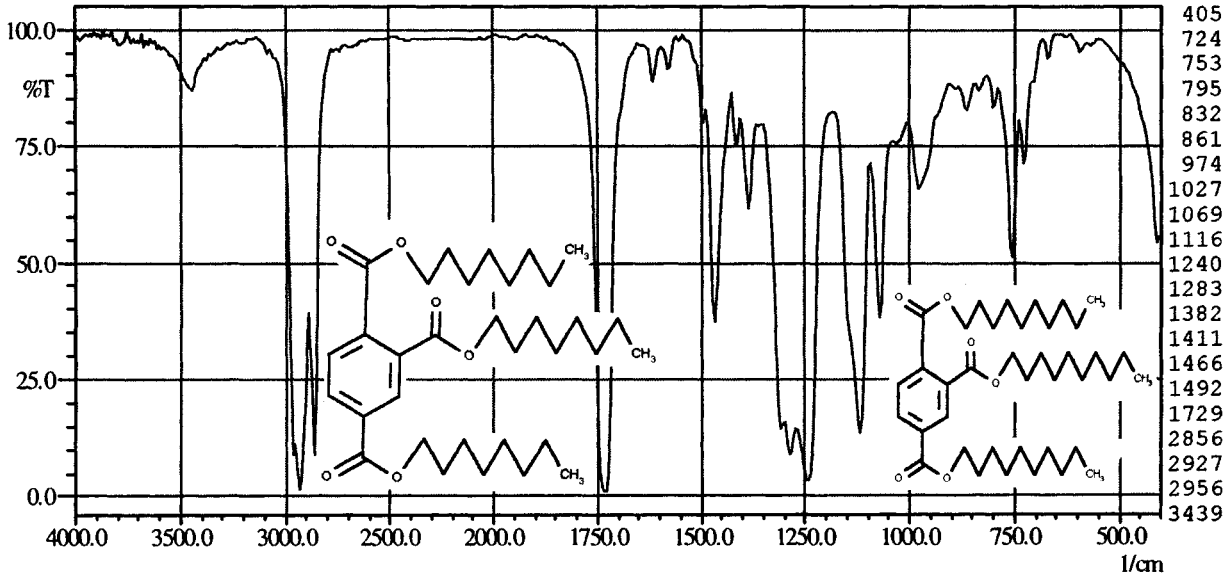
(1) **tri(C_8...C_{10}-alkyl)trimellitate**
(2) Witamol 218 stab.
(3) Huels
(4) 590 g mol^{-1}
(5) plasticiser
(6) colourless, clear liquid
(9) 0.975 g cm^{-3}
(10) 1.483
(13) layer btw KBr
(14) with stabiliser

3424 **$C_{33}H_{54}O_6$**



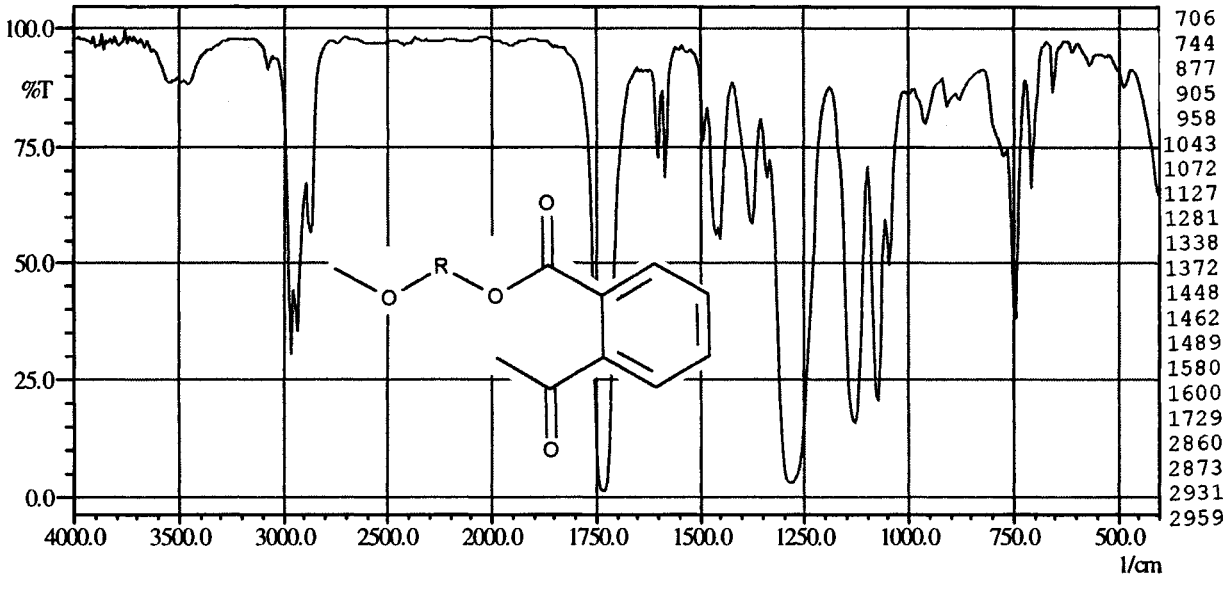
(1) **tri(2-ethylhexyl)trimellitate**
(2) Hexaplas OTM
(3) ICI
(4) 546.8 g mol^{-1}
(5) plasticiser
(6) colourless, clear liquid
(9) 0.991 g cm^{-3}
(10) 1.486
(13) layer btw KBr

3424



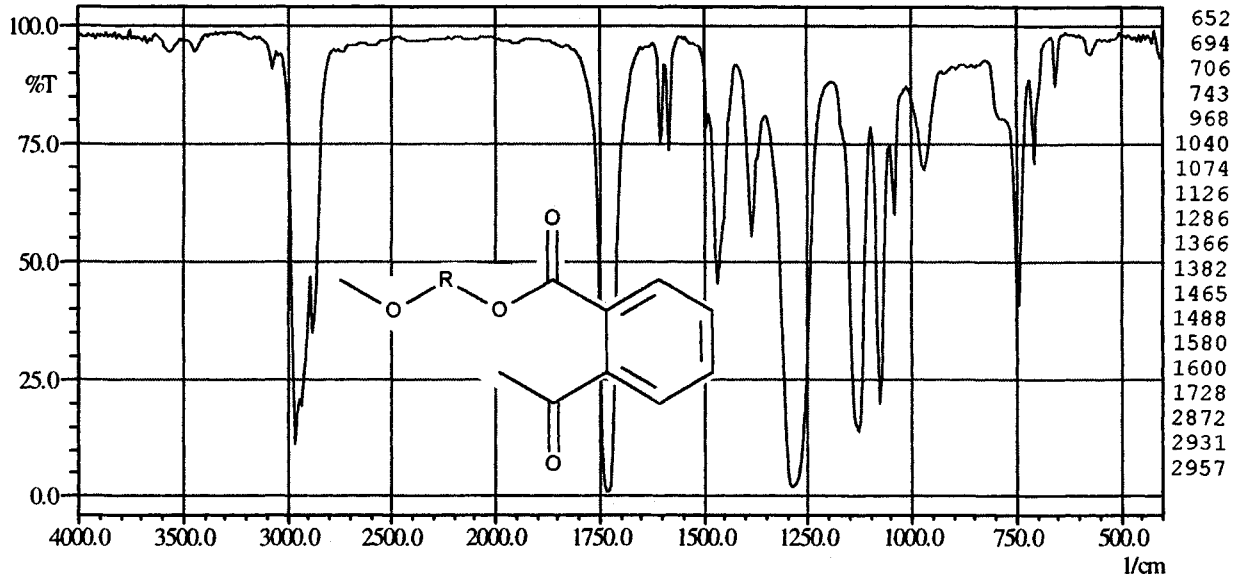
(1) **mixture of trioctyl and tridecyl trimellitate**
(2) Hexaplas L810TM
(3) ICI
(4) 592 g mol^{-1}
(5) plasticiser
(6) colourless, clear liquid
(9) 0.973 g cm^{-3}
(10) 1.481
(13) layer btw KBr

3426



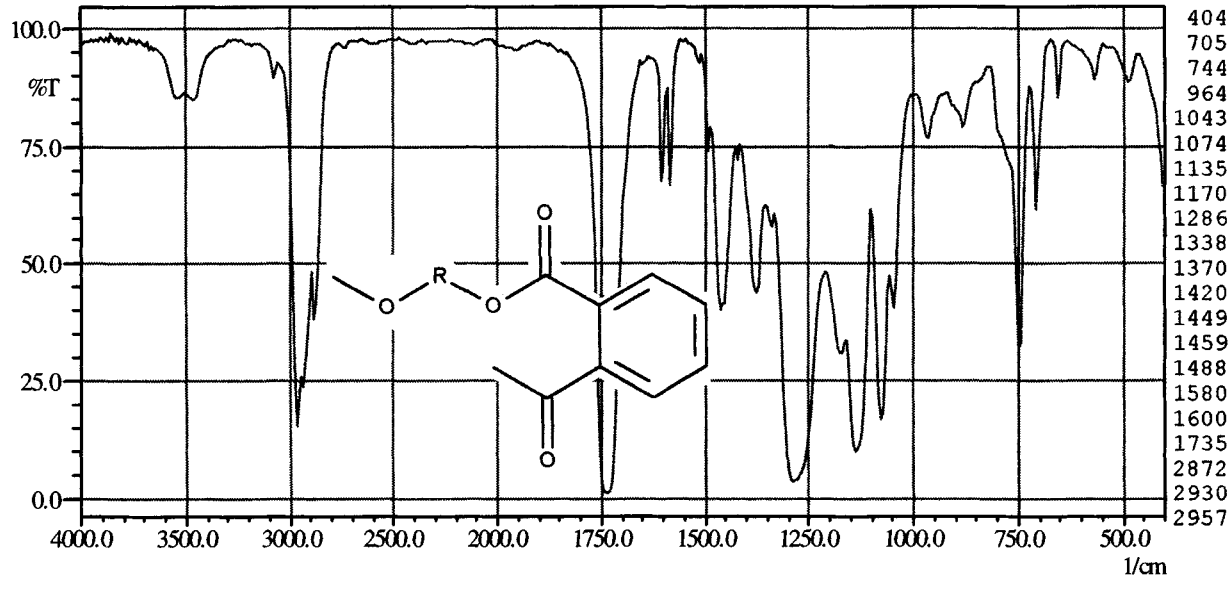
(1) **polymer, linear, saturated phthalate**
(2) Uraplast W4
(3) DSM
(5) plasticiser
(6) colourless, clear liquid
(9) 1.13 g cm^{-3}
(10) 1.514
(13) layer btw KBr

3426



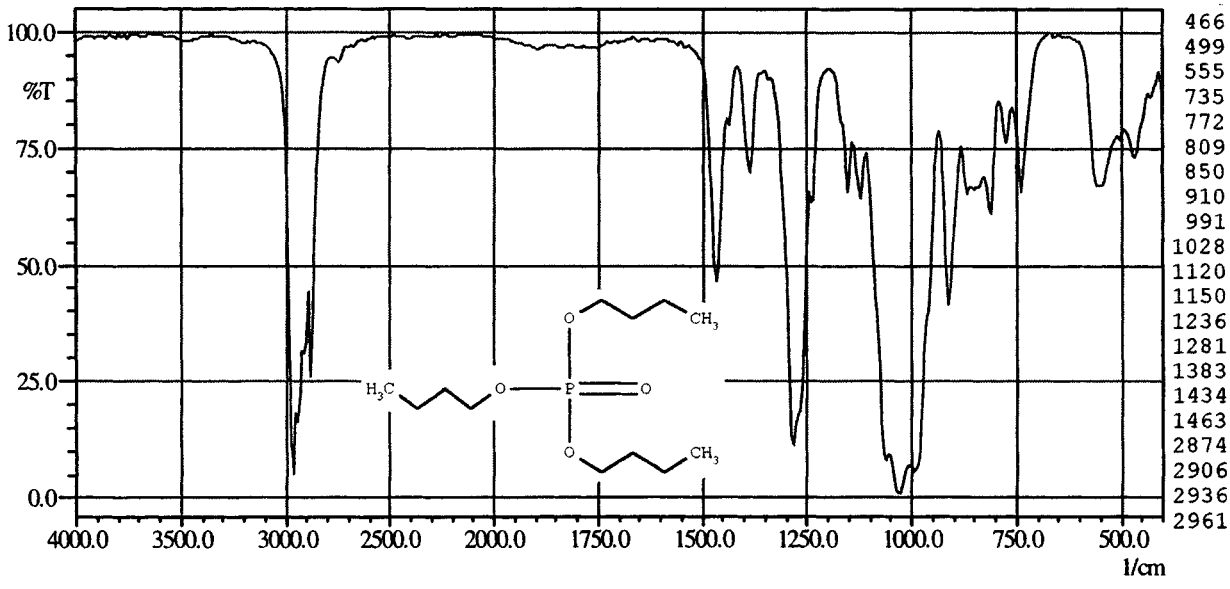
(1) **phthalic acid polyester**
(2) Ultramoll PP
(3) Bayer
(5) plasticiser
(6) colourless, clear, low-viscous liquid
(9) 1.04 g cm^{-3}
(10) 1.503
(13) layer btw KBr

3426



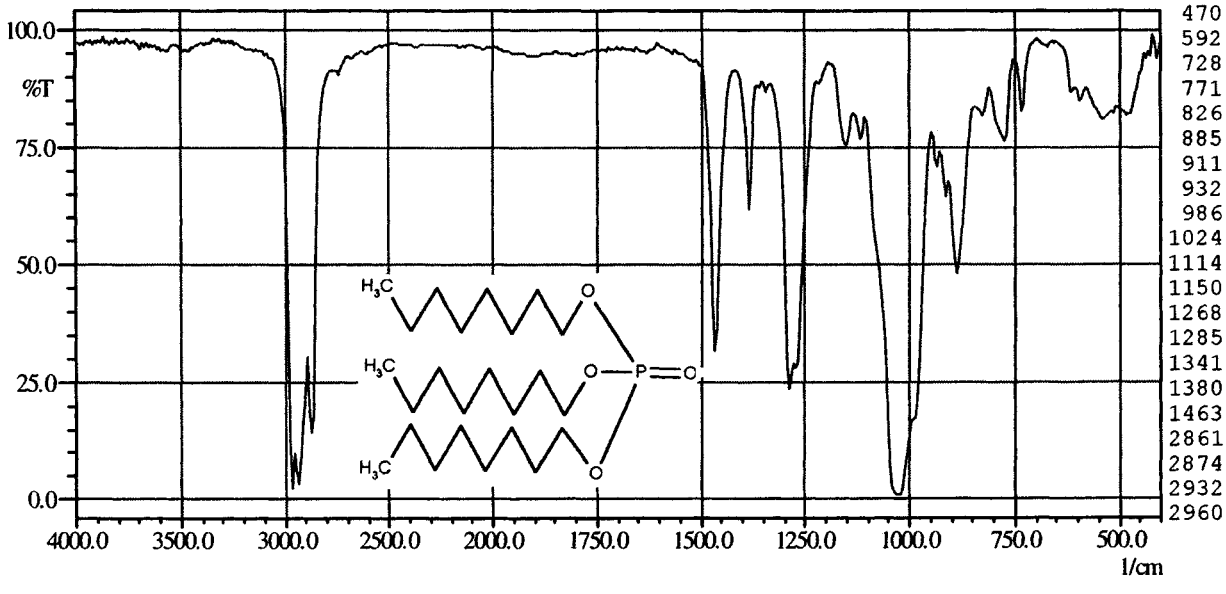
(1) **phthalic polyester**
(2) Paraplex G31
(3) C. P. Hall , Krahn-Chemie
(5) plasticiser
(6) colourless, clear liquid
(9) 1.1 g cm^{-3}
(10) 1.503
(13) layer btw KBr

361 $PC_{12}H_{27}O_4$



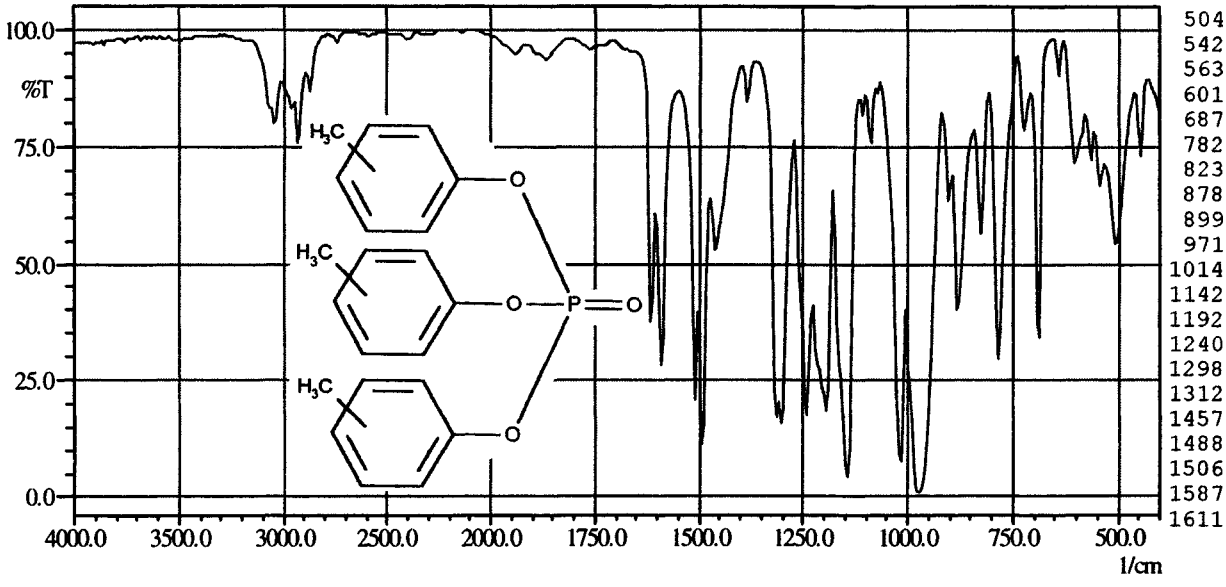
(1) **tributylphosphate**
(3) Freudenberg (Brunne collection)
(4) 266.3 g mol^{-1}
(5) plasticiser
(6) colourless, clear liquid
(13) layer on KBr

361 $C_{24}H_{51}O_4P$



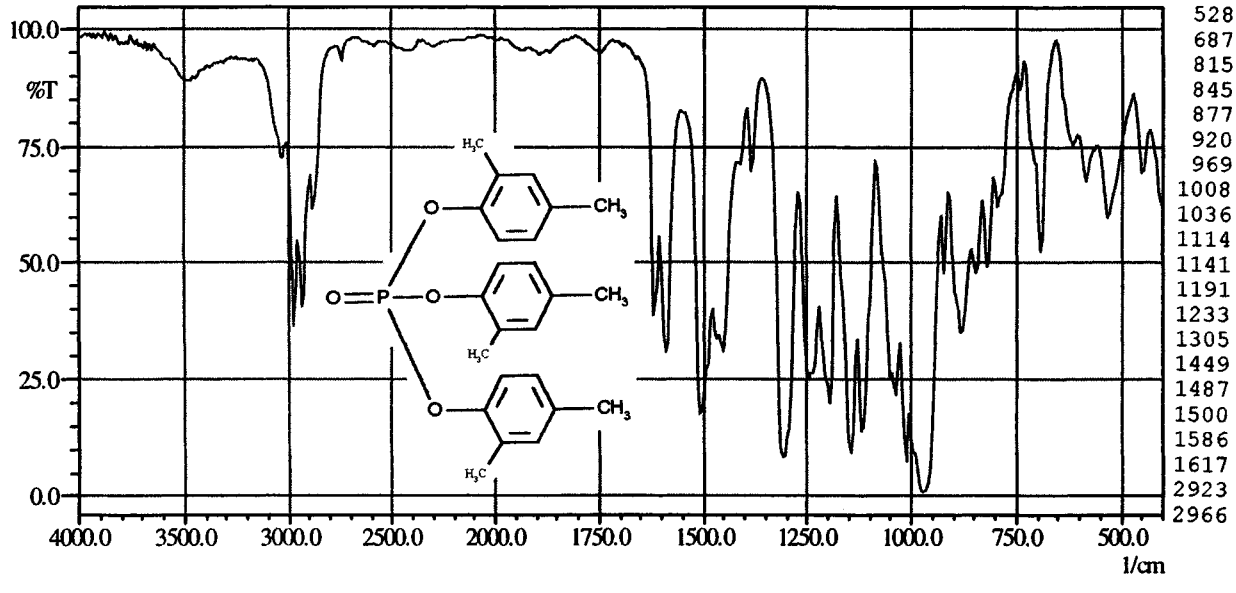
(1) **trioctylphosphate**
(2) Disflamoll TOF
(3) Bayer
(4) 434.7 g mol^{-1}
(5) plasticiser
(6) colourless, clear liquid
(8) 210 °C / 500 Pa
(9) 0.92 g cm^{-3}
(10) 1.443
(13) layer btw KBr

362 $C_{21}H_{21}O_7P$



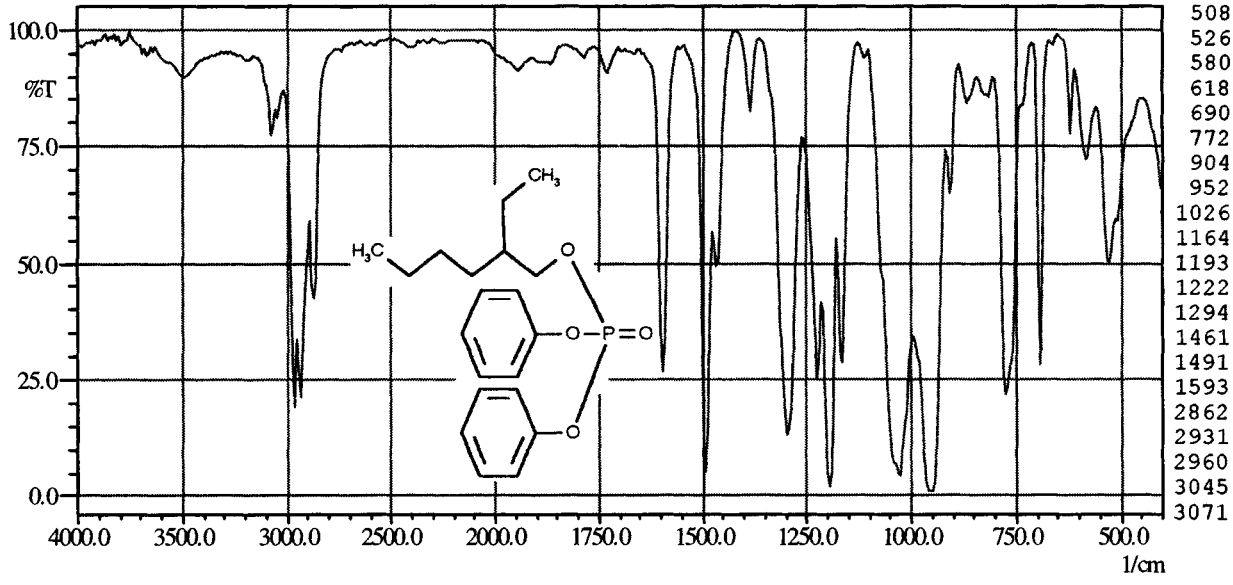
(1) **tricresylphosphate**
(2) Disflamoll TKP
(3) Bayer
(4) 416.4 g mol^{-1}
(5) plasticiser
(6) colourless, pale-yellow, clear liquid
(8) 245 °C / 500 Pa
(9) 1.18 g cm^{-3}
(10) 1.559
(13) layer btw KBr
(14) mixture of isomers

362 $C_{24}H_{27}O_4P$



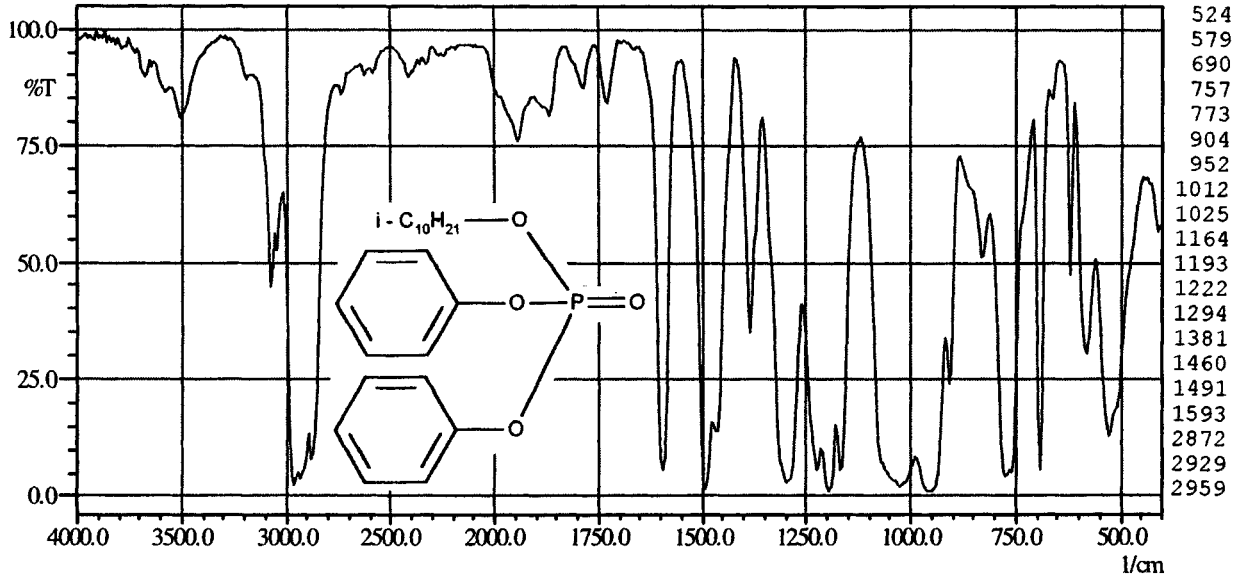
(1) **trixylenylphosphate**
(2) Reomol TXP
(3) Ciba-Geigy
(4) 410.5 g mol^{-1}
(5) plasticiser
(6) colourless, clear liquid
(13) layer btw KBr

362 $C_{20}H_{27}O_4P$



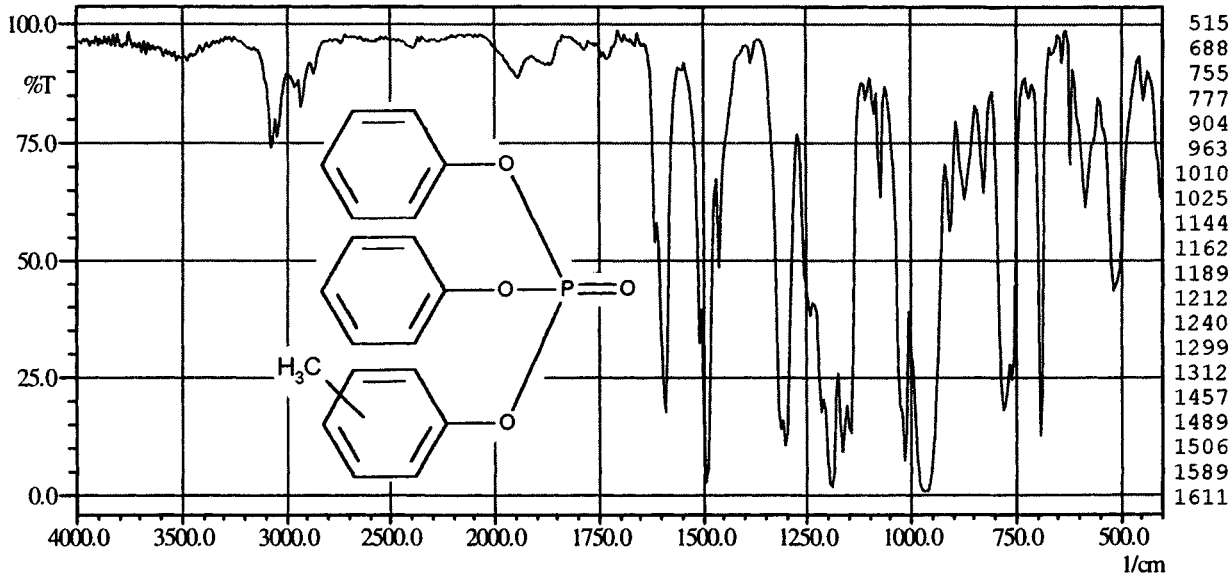
(1) **2-ethylhexyldiphenylphosphate**
(2) Santicizer 141
(3) Monsanto, Brenntag
(4) 362.4 g mol^{-1}
(5) plasticiser
(6) colourless, clear, oily liquid
(9) 1.88 g cm^{-3}
(10) 1.511
(13) layer btw KBr

362 $C_{22}H_{31}O_4P$



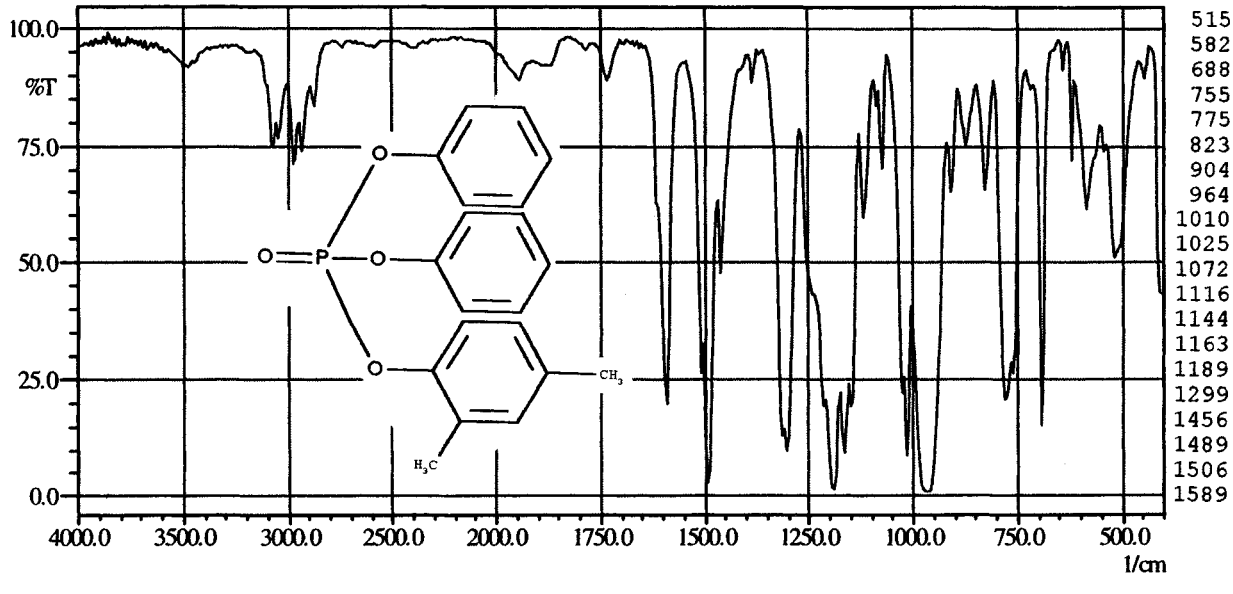
(1) ***i*-decyldiphenylphosphate**
(2) Santicizer 148
(3) Monsanto
(4) 390.5 g mol^{-1}
(5) plasticiser
(6) colourless, clear, oily liquid
(8) 245 °C
(9) 1.066 g cm^{-3}
(10) 1.504
(13) layer btw KBr
(14) structure of *i*-decyl is undefined

362 $C_{19}H_{17}O_4P$



(1) **cresyldiphenylphosphate**
(2) Disflamoll DPK
(3) Bayer
(4) 340.3 g mol^{-1}
(5) plasticiser
(6) colourless, clear liquid
(8) 23 °C / 500 Pa
(9) 1.2 g cm^{-3}
(10) 1.563
(13) layer btw KBr

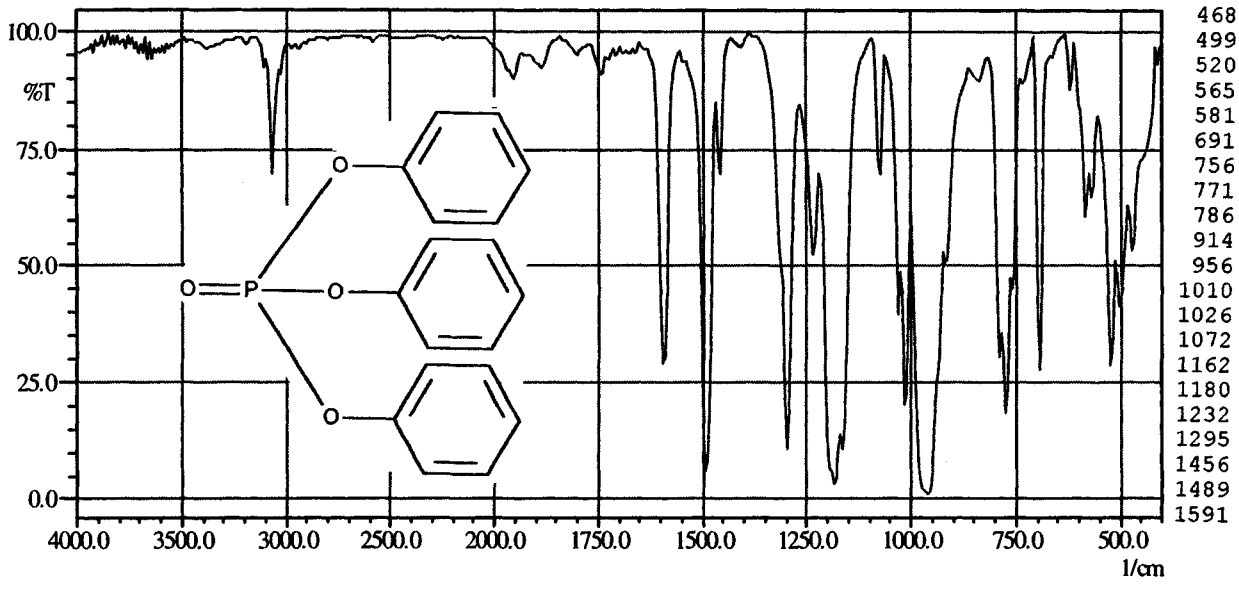
362 $C_{20}H_{190}O_4P$



(1) **2,4-xylyldiphenylphosphate**
(2) Reomol CDP
(3) Ciba-Geigy
(4) 354.4 g mol^{-1}
(5) plasticiser
(6) colourless, clear liquid
(13) layer btw KBr

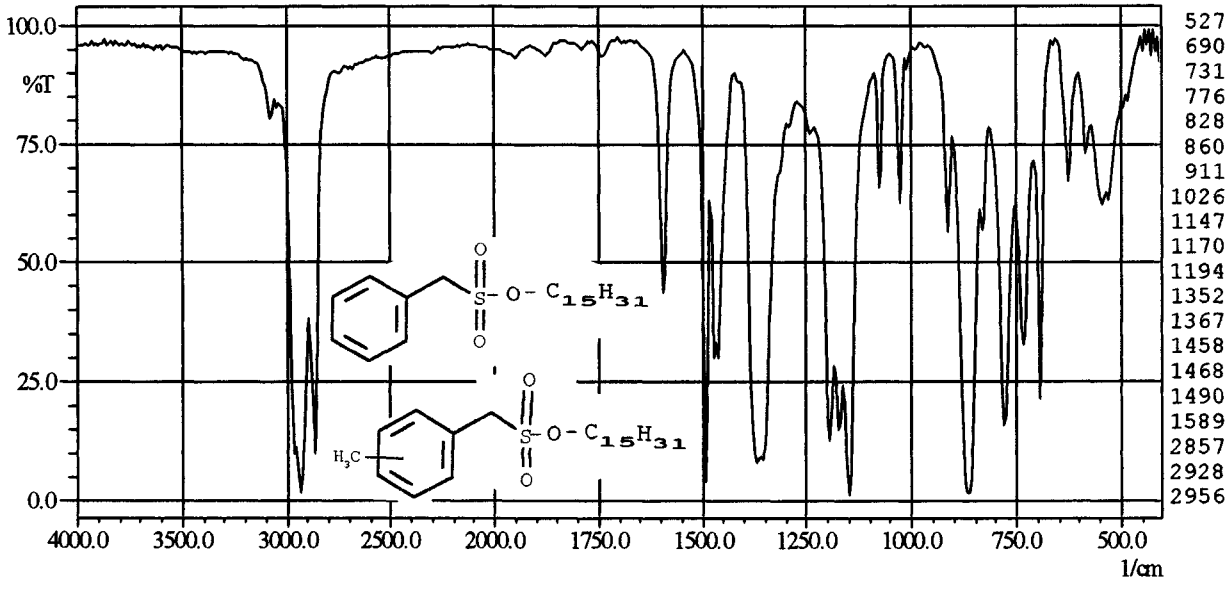
Previous Page

363 $C_{18}H_{15}O_4P$



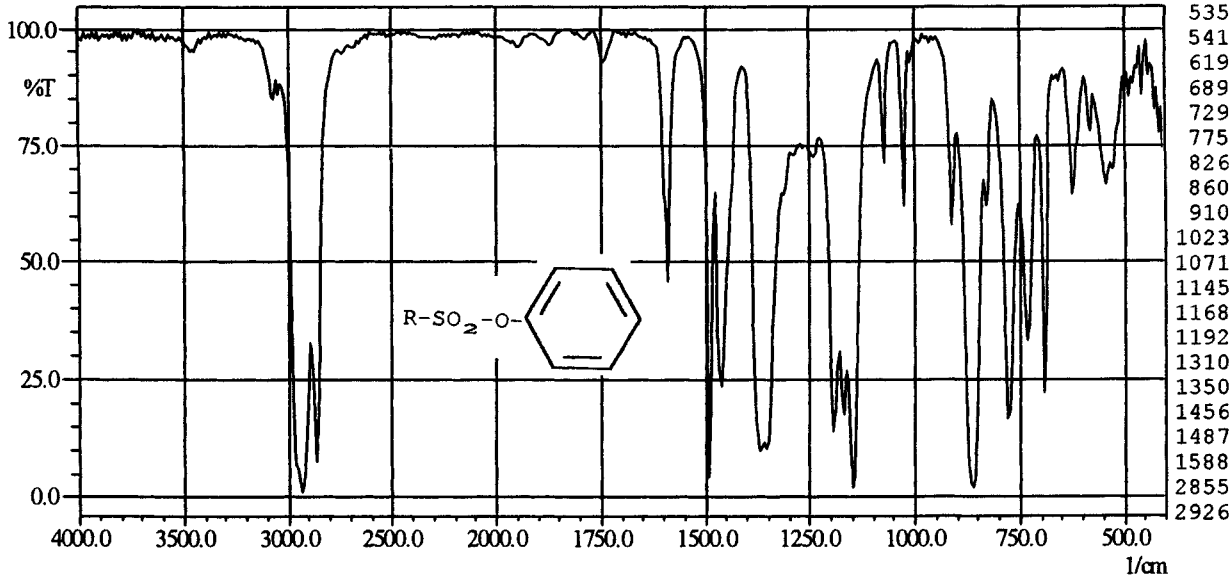
(1) **triphenylphosphate**
(2) Disflamoll TP
(3) Bayer
(4) 326.3 g mol^{-1}
(5) plasticiser
(6) colourless solid
(7) 48 °C
(8) 245 °C / 1500 Pa
(9) 1.25 g cm^{-3}
(10) 1.555
(13) KBr pellet

371 $C_{21}H_{36}O_3S, C_{22}H_{38}O_3S$



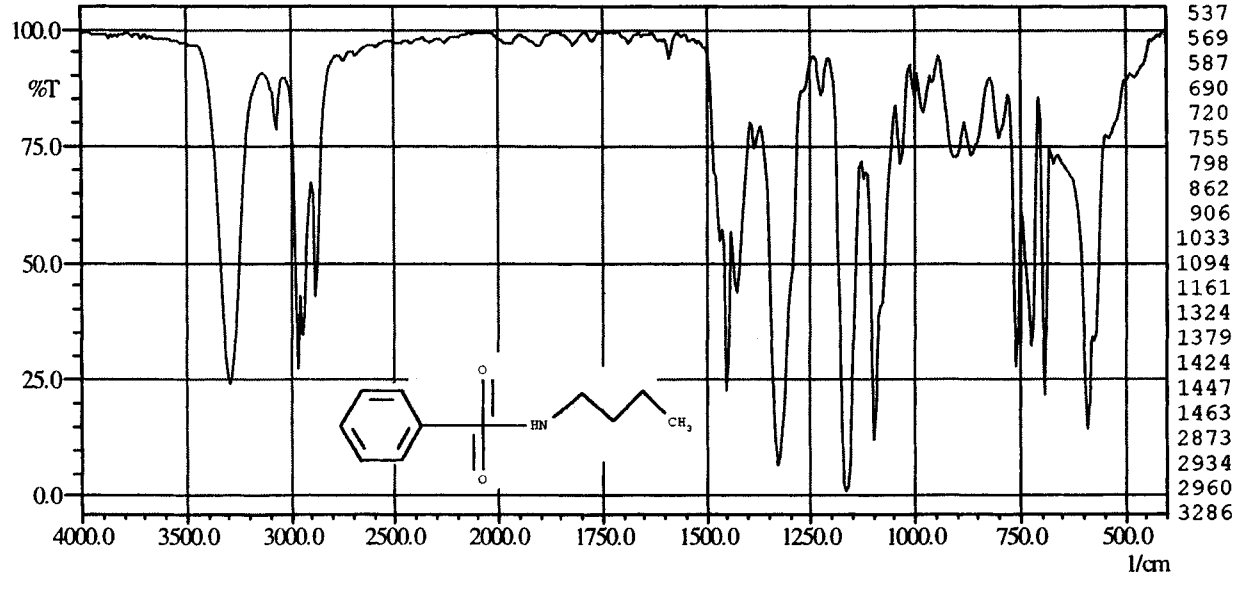
(1) **pentadecanesulfonic acid phenol and cresol esters**
(2) Mesamoll
(3) Bayer
(4) 368.4, 382.4 g mol^{-1}
(5) plasticiser
(6) colourless, clear liquid
(13) layer btw KBr

371



(1) **phenolic ester of aliphatic sulfonic acid**
(2) Weichmacher KL 3-3030
(3) Mercura
(5) plasticiser
(6) colourless, clear liquid
(13) layer btw KBr

372 $C_{10}H_{15}NO_2S$



(1) **N-butylbenzenesulfonamide**
(2) Cetamoll BMB
(3) Bayer
(4) 213.3 g mol^{-1}
(5) plasticiser
(6) colourless, clear liquid
(13) layer btw KBr

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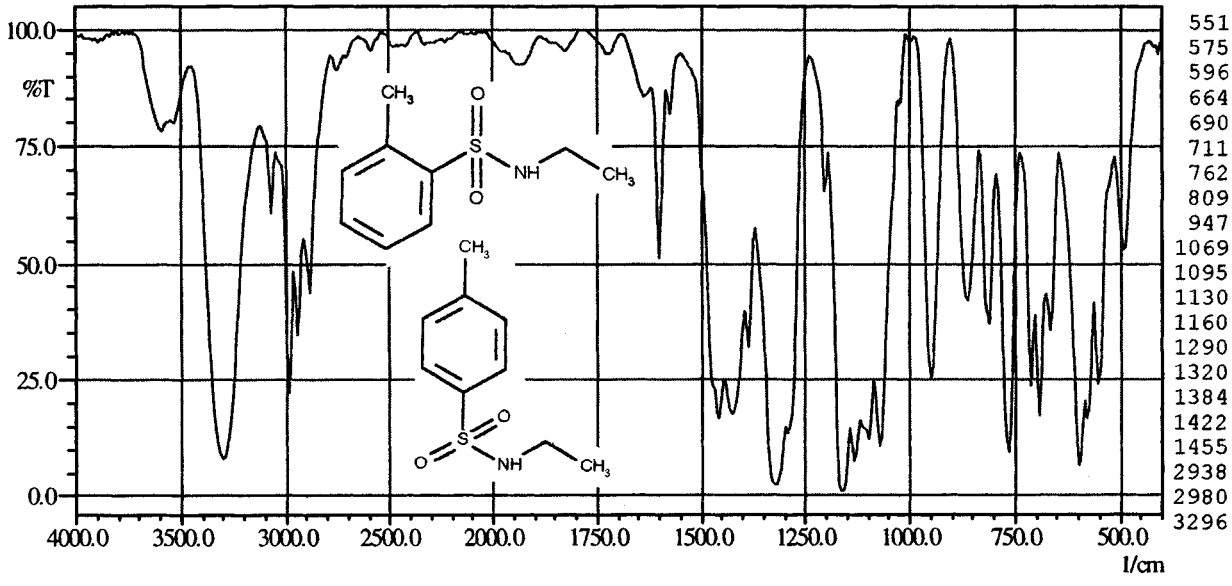
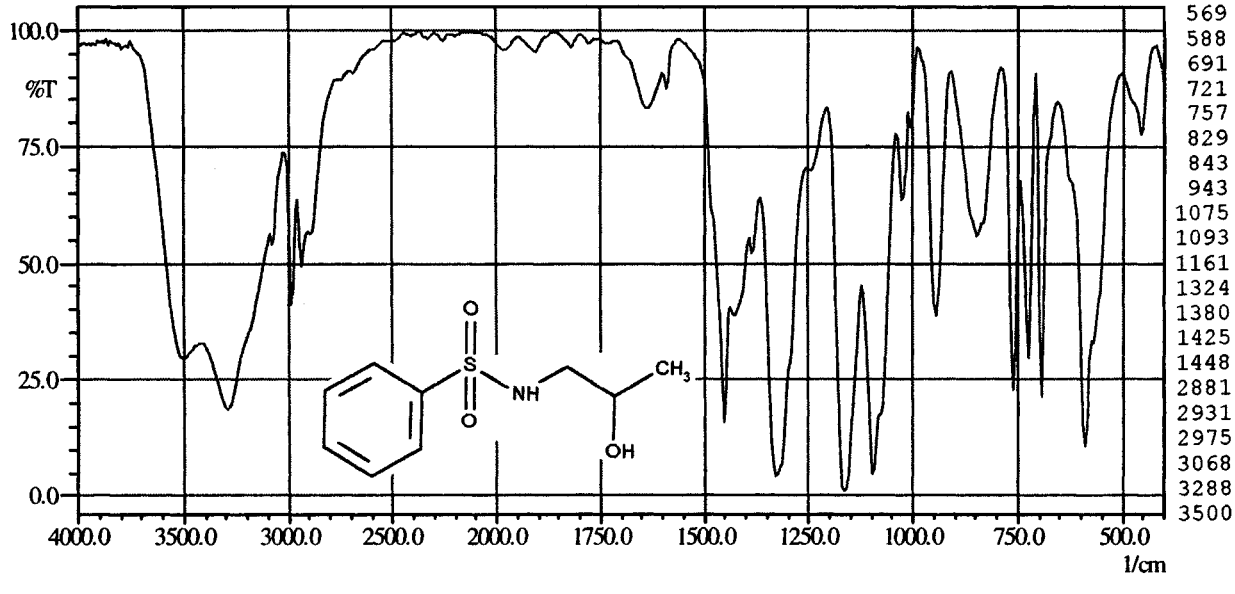
372



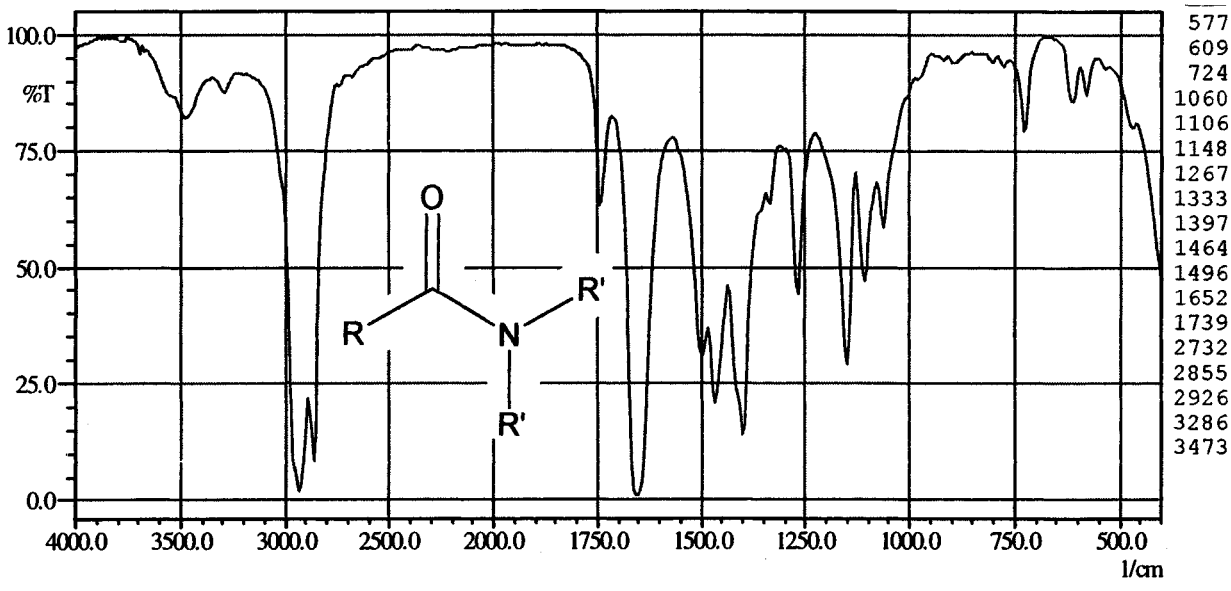
(1) **mixture of *o*- and *p*-N-ethyltoluenesulfonamide**
(2) Isaplast 5975
(3) Th. Boehme
(5) plasticiser for melt adhesives
(6) viscous liquid
(9) 1.18 g cm^{-3}
(13) layer btw KBr

372 $C_9H_{13}NO_3S$



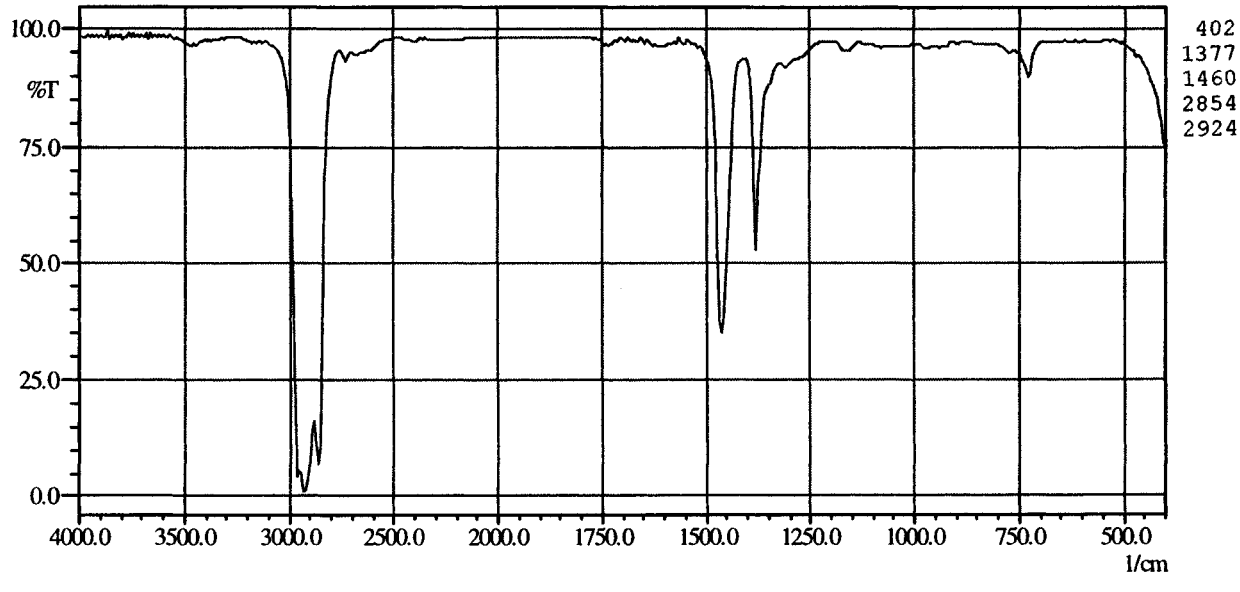
(1) **N-(2-hydroxypropyl)benzenesulfonamide**
(2) Isaplast
(3) Th. Boehme
(5) plasticiser for PU, PE, PA
(6) viscous, clear liquid
(13) layer btw KBr

382



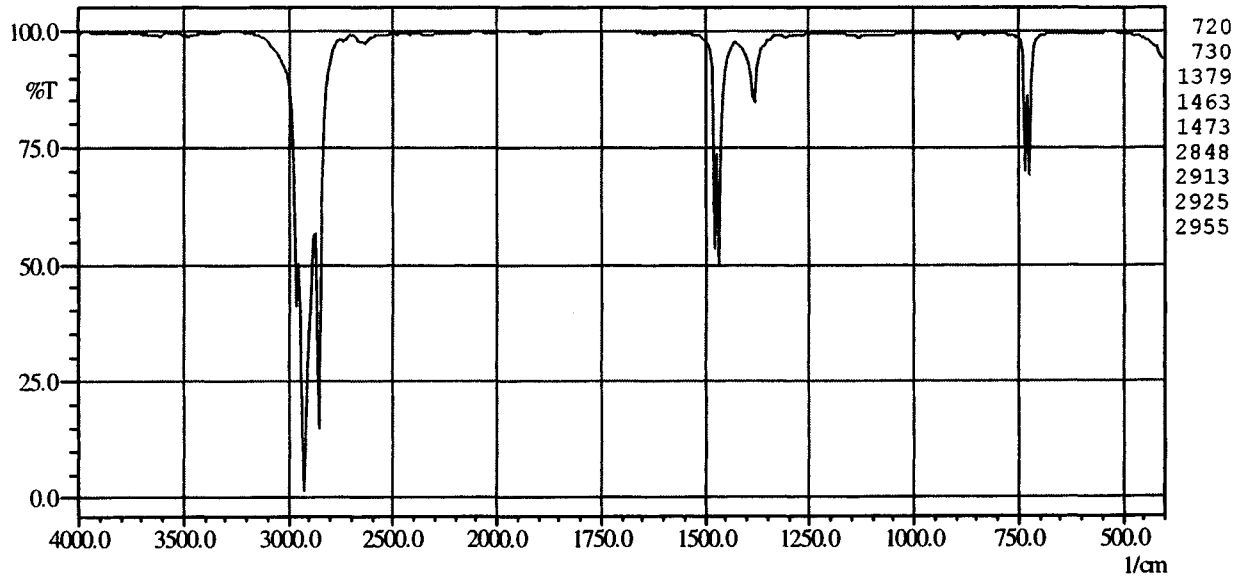
(1) **N,N-disubstituted fatty acid amide**
(2) Hallcomid M-8-10
(3) C.P. Hall
(5) plasticiser
(6) yellow, clear liquid
(13) layer btw KBr

4111



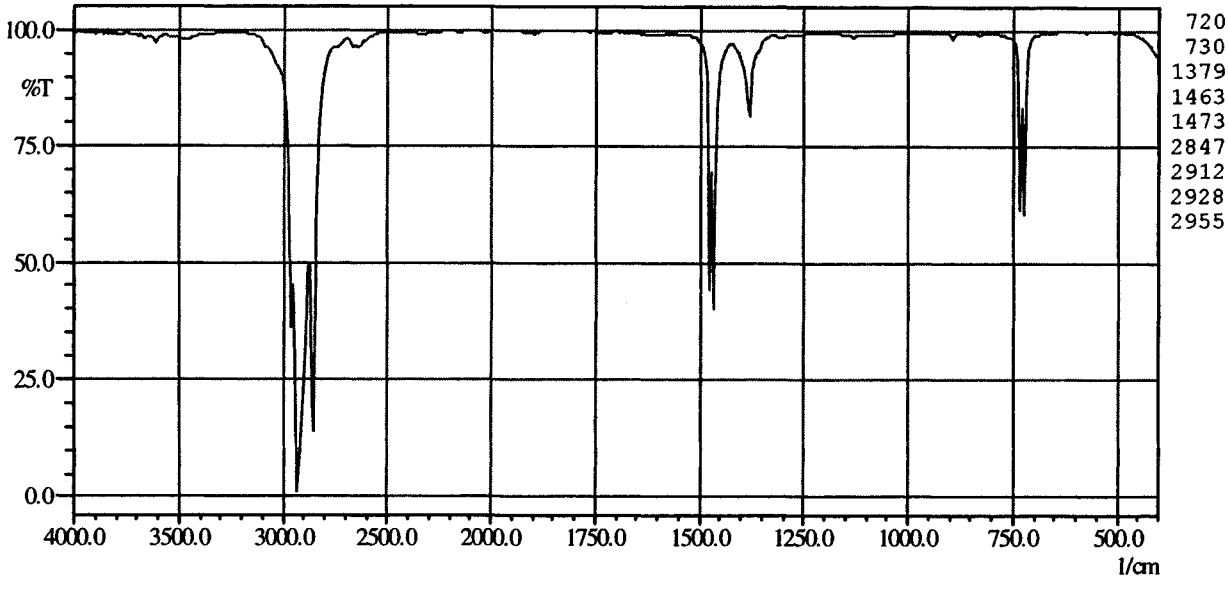
(1) **higher paraffinic hydrocarbons**
(2) Irgawax 366
(3) Ciba-Geigy
(5) lubricant
(6) colourless, clear liquid
(9) 0.87 g cm^{-3}
(10) 1.478
(13) layer btw KBr

4111



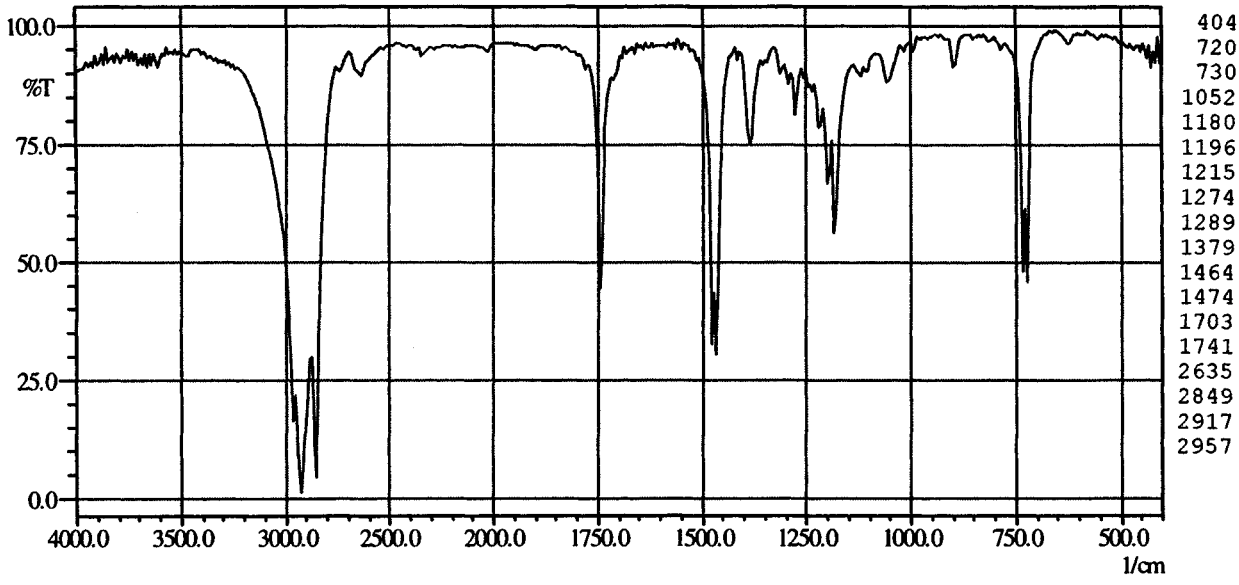
(1) **paraffin wax with low melting point**
(2) Naftolube SP 17
(3) Chemson
(5) lubricant
(6) colourless solid
(13) recrystallised film from melt

4111



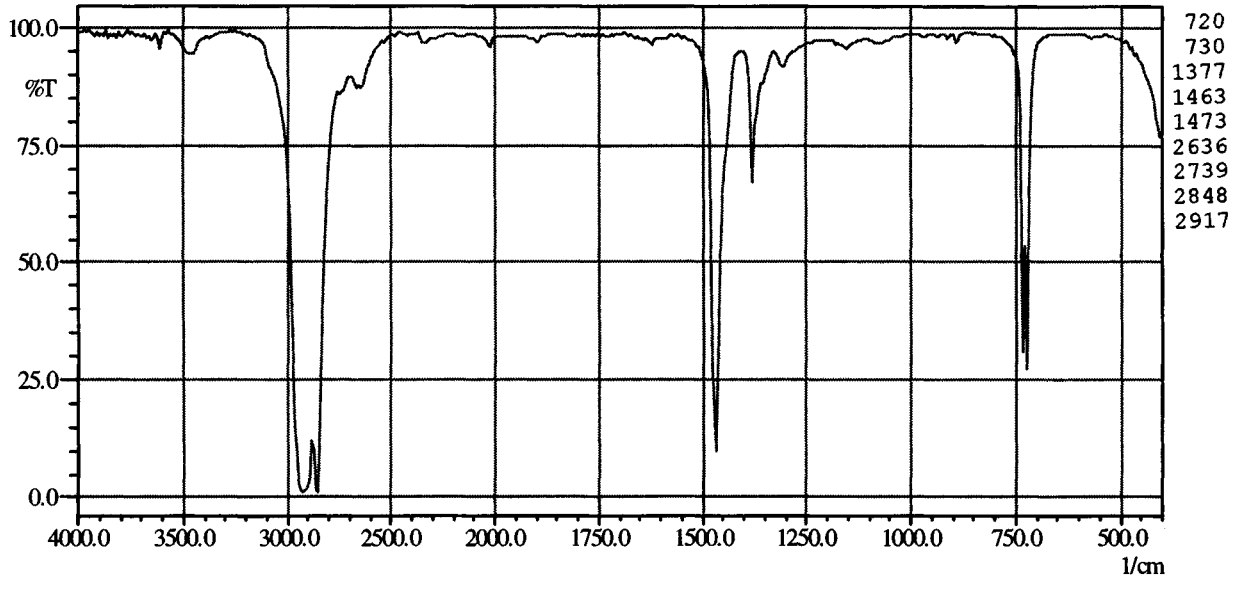
(1) **paraffin wax with high melting point**
(2) Naftolube SP 18
(3) Chemson
(5) lubricant
(6) colourless solid
(13) recrystallised film from melt

4111



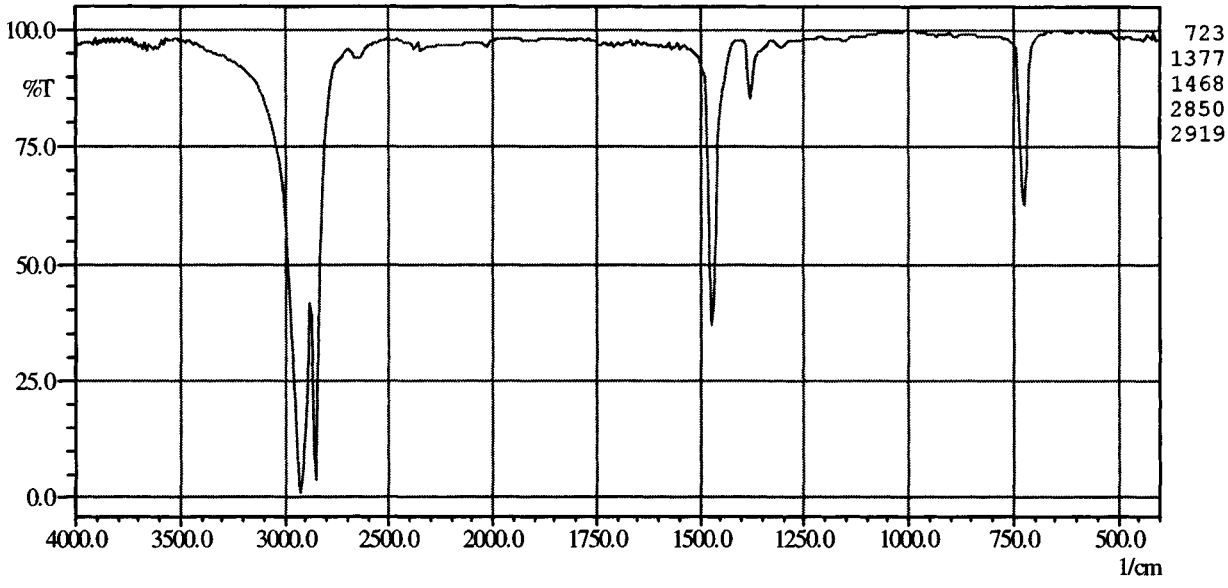
(1) **hydrocarbon wax with aliphatic ester groups**
(2) Baerolub L-KM
(3) Baerlocher
(5) lubricant
(6) colourless solid
(7) 55 °C
(9) 0.9 g cm^{-3}
(13) KBr pellet

4112



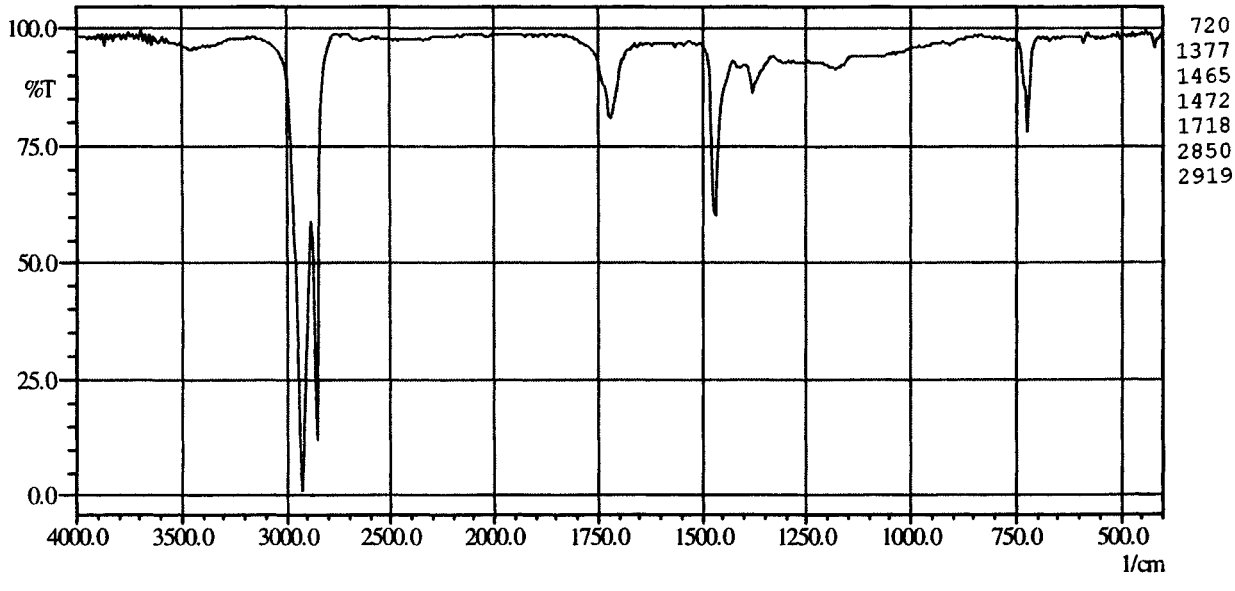
(1) **polyethylene wax**
(2) Naftolube PEF
(3) Chemson
(5) lubricant
(6) colourless solid
(13) recrystallised film from melt btw KBr

4112



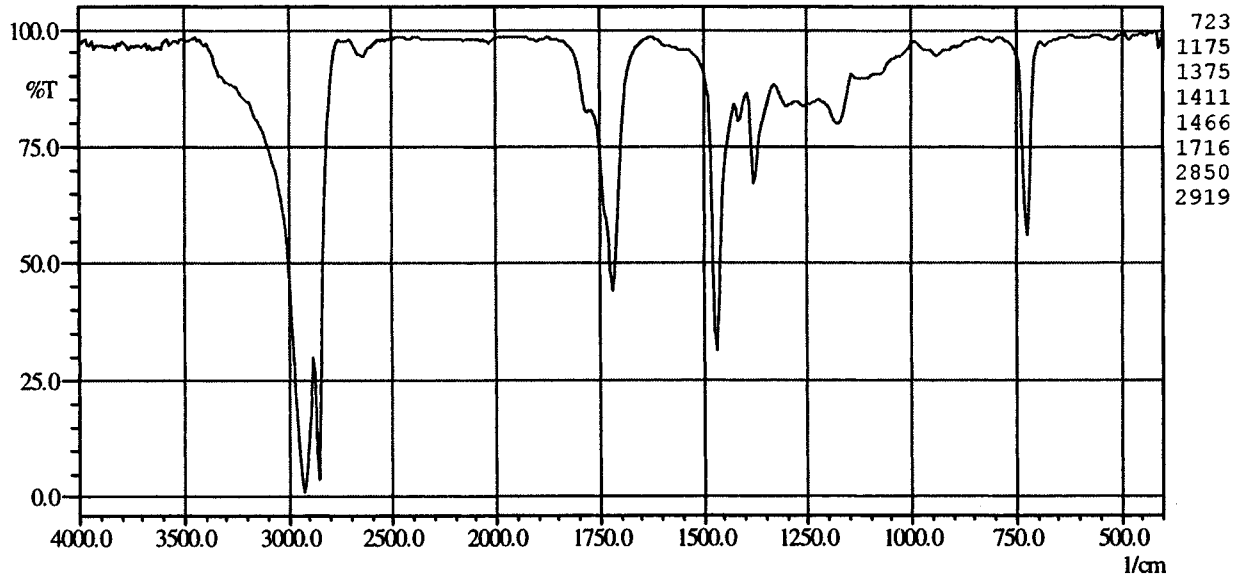
(1) **polyethylene wax, non-polar**
(2) Hoechst-Wachs PE 520
(3) Hoechst
(5) lubricant
(6) colourless granules
(9) 0.93 g cm^{-3}
(13) KBr pellet

41131



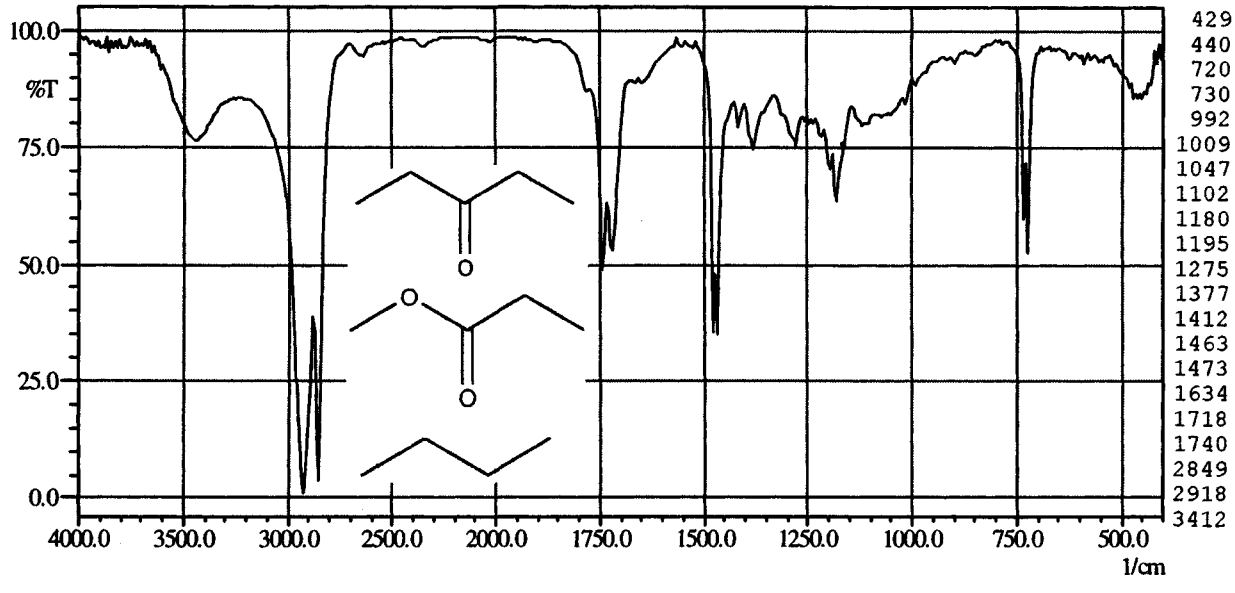
(1) **oxidized polyethylene wax**
(2) Naftolube OPE
(3) Chemson
(5) lubricant
(6) colourless solid
(13) KBr pellet

41131



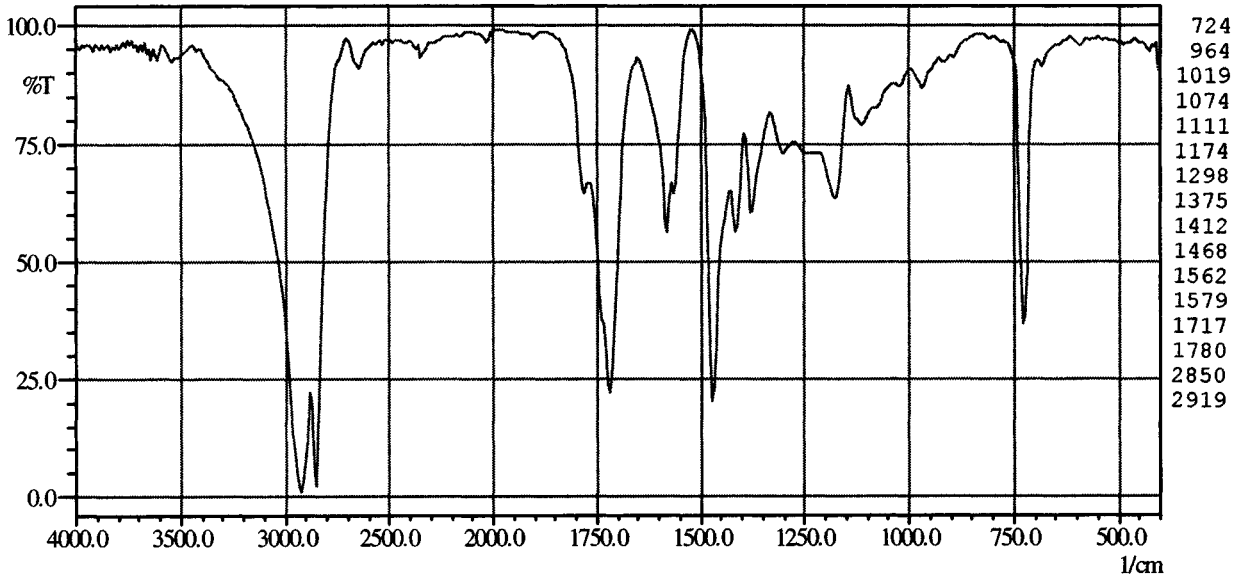
(1) **polyethylene wax, polar**
(2) Hostalub H 12
(3) Hoechst
(5) lubricant
(6) colourless solid
(9) 0.95 g cm^{-3}
(13) KBr pellet

41131



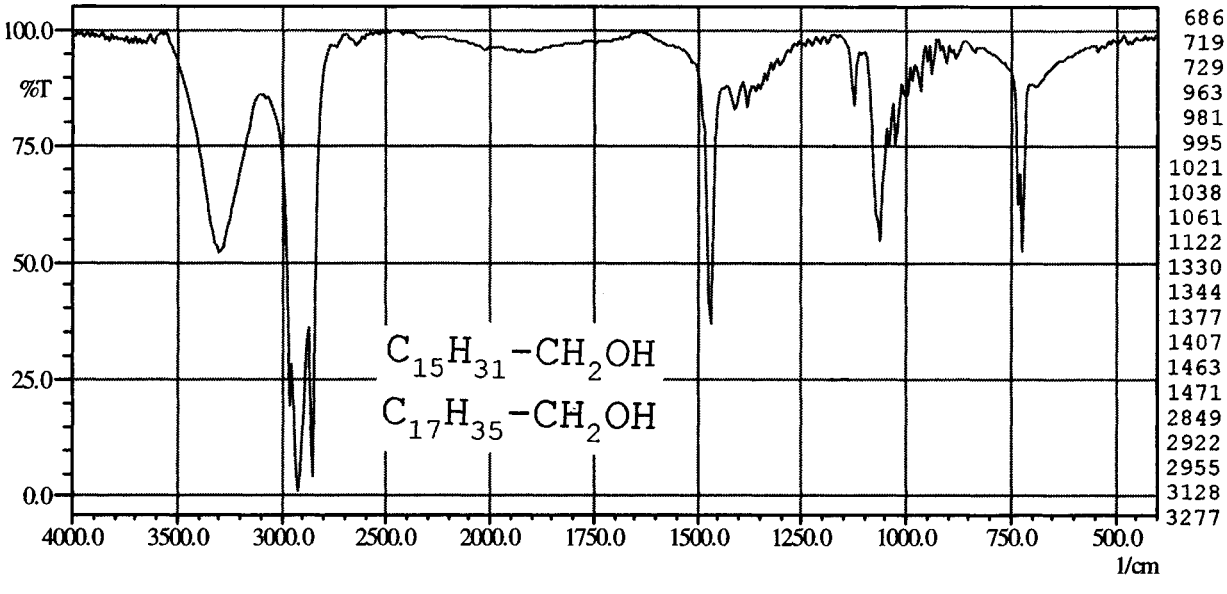
(1) **oxidized hydrocarbon wax**
(2) Baerolub L-AX
(3) Baerlocher
(5) lubricant
(6) colourless solid
(7) 97.5 °C
(9) 0.9 g cm^{-3}
(13) KBr pellet

41131



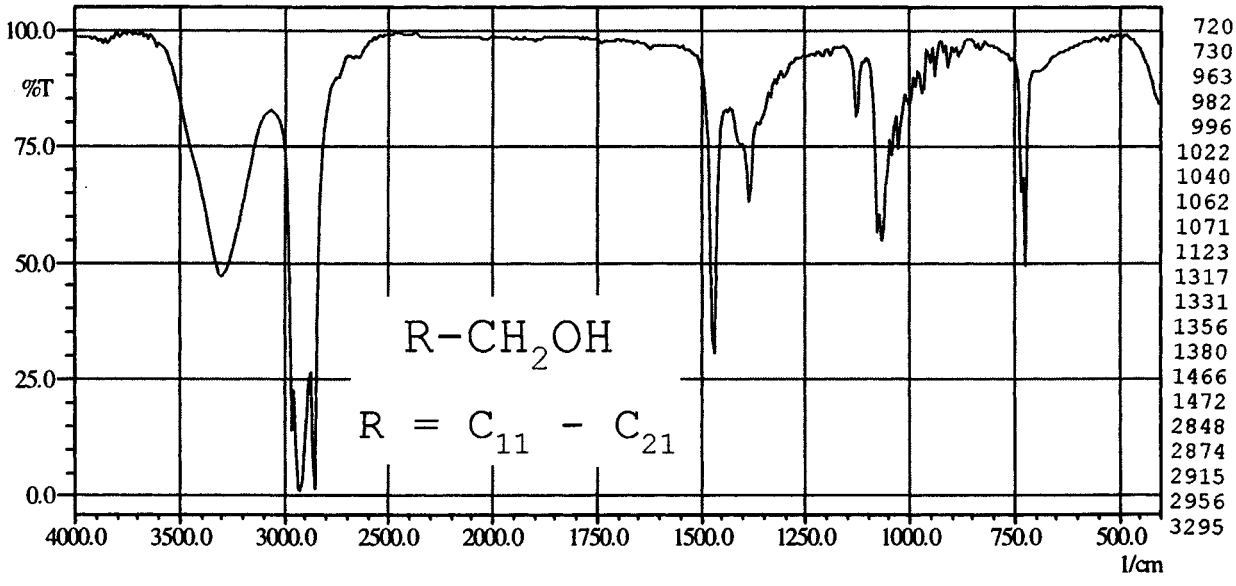
(1) **partially oxidized, partially saponified polyethylene wax**
(2) Irgawax 372
(3) Ciba-Geigy
(5) lubricant
(6) yellowish solid
(13) KBr pellet

412 $C_{16}H_{34}O+C_{18}H_{38}O$



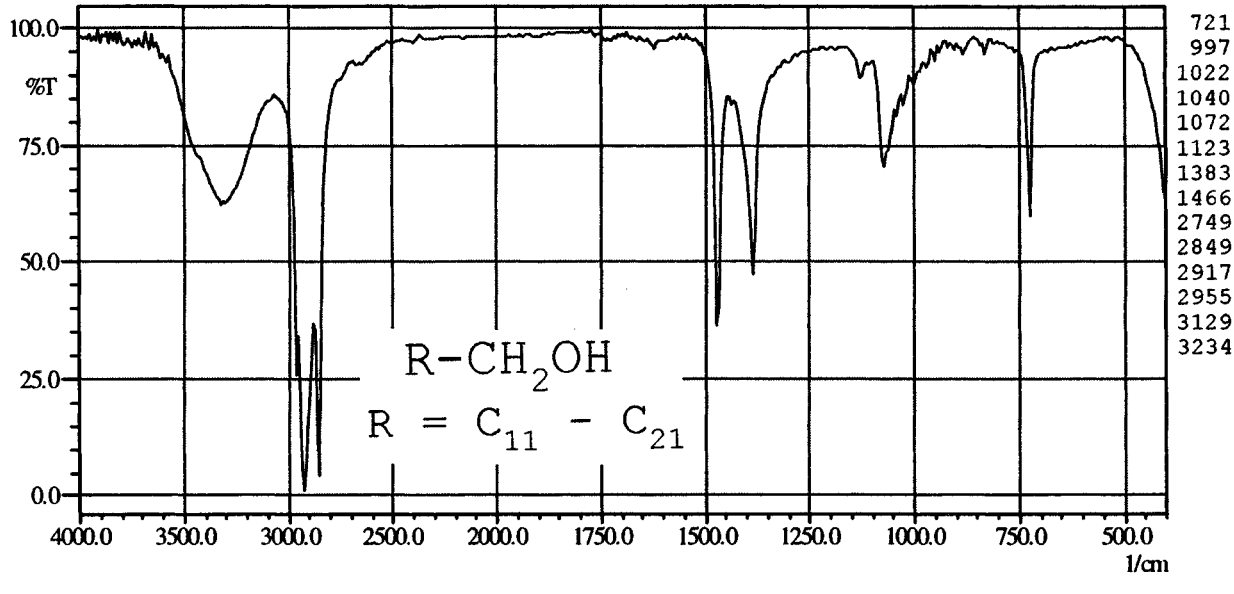
(1) **cetyl-stearyl alcohol**
(2) Realube C/18
(3) Reagens
(4) 513 g mol^{-1}
(5) lubricant
(6) colourless solid
(7) 46 °C
(13) KBr pellet

412



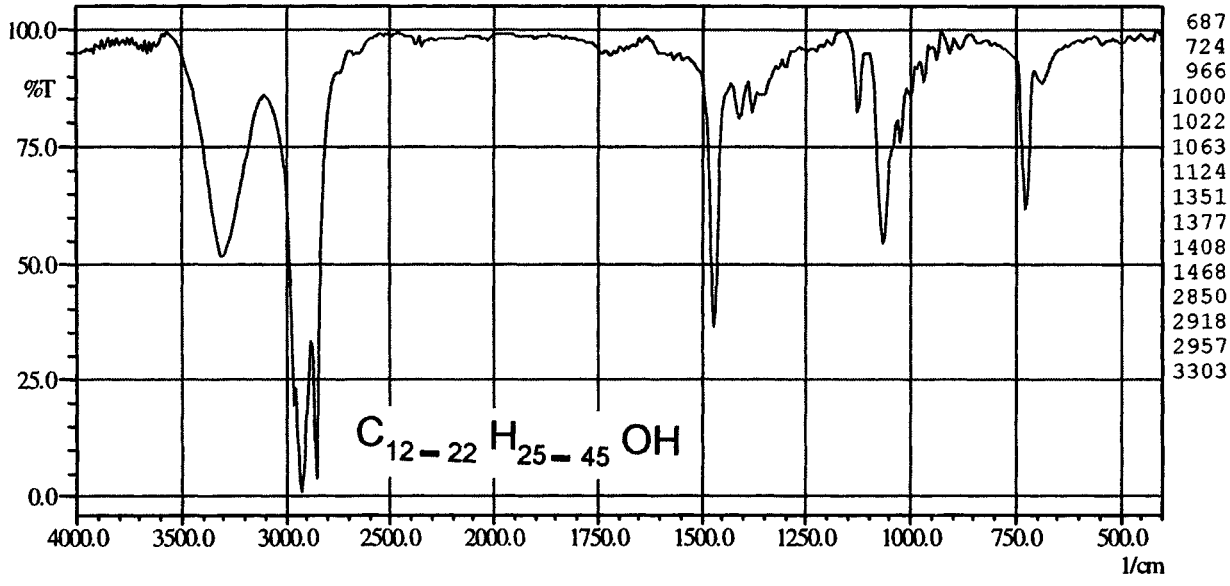
(1) **saturated fatty alcohol**
(2) Naftolube SRL
(3) Chemson
(5) lubricant
(6) colourless solid
(13) recrystallised film from melt

412



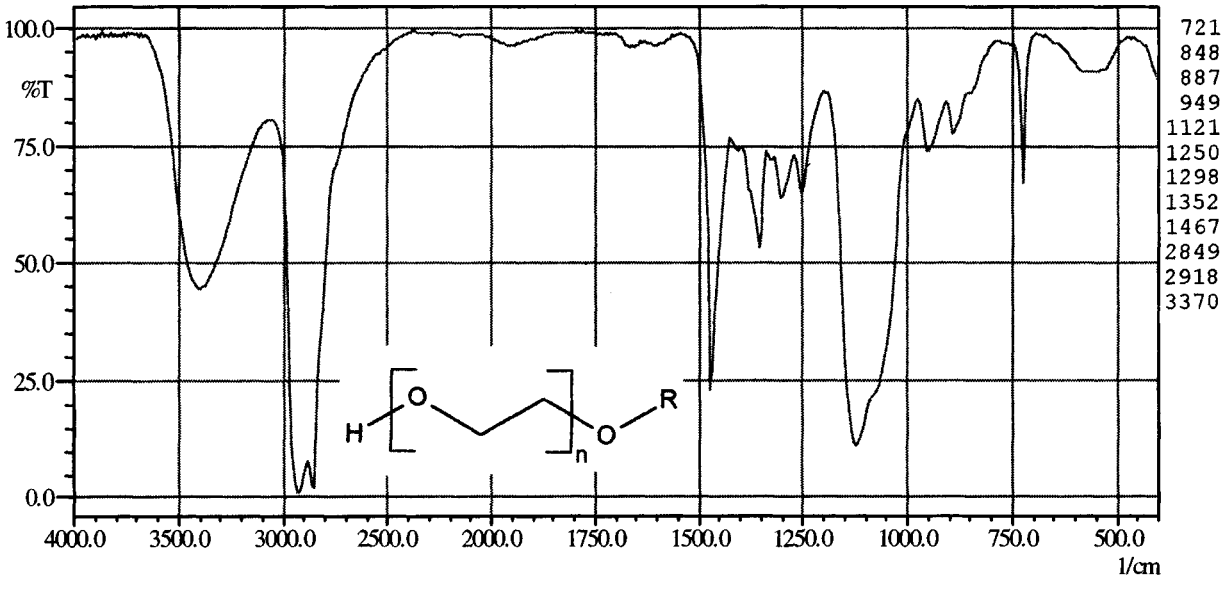
(1) **saturated fatty alcohol**
(2) Loxiol EP 52
(3) Henkel
(5) lubricant
(6) colourless solid
(7) 51 °C
(9) 0.82 g cm^{-3}
(10) 1.436
(13) recrystallised film from melt

412



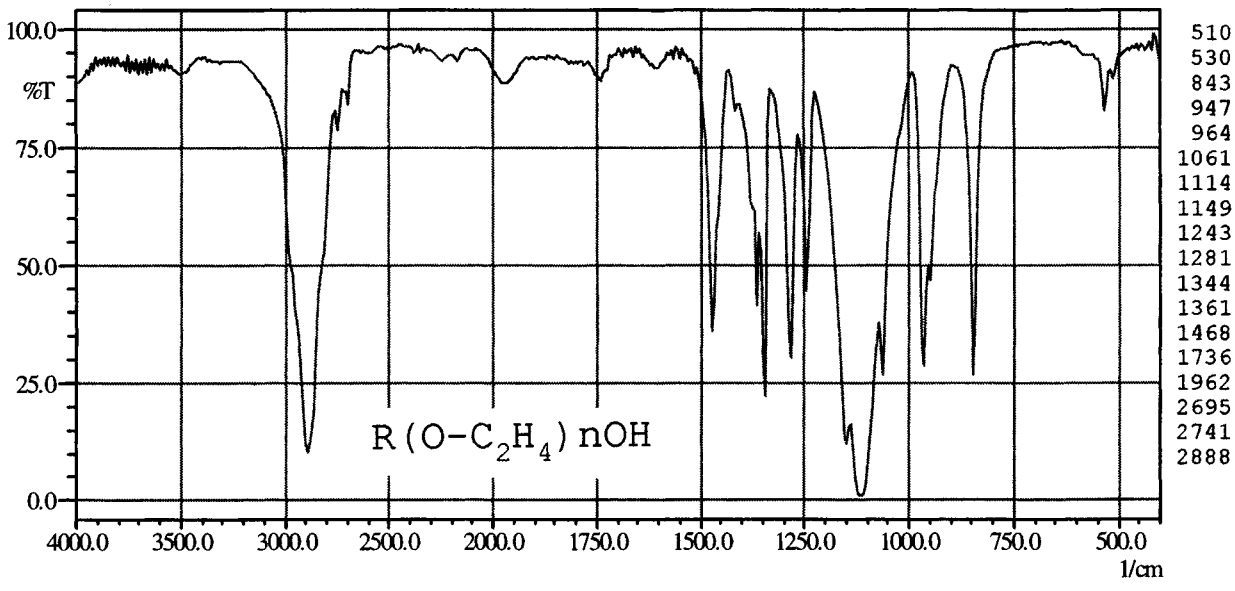
(1) **saturated fatty alcohol**
(2) Irgawax 365
(3) Ciba-Geigy
(5) lubricant
(6) colourless solid
(7) 49.5 °C
(13) KBr pellet

412



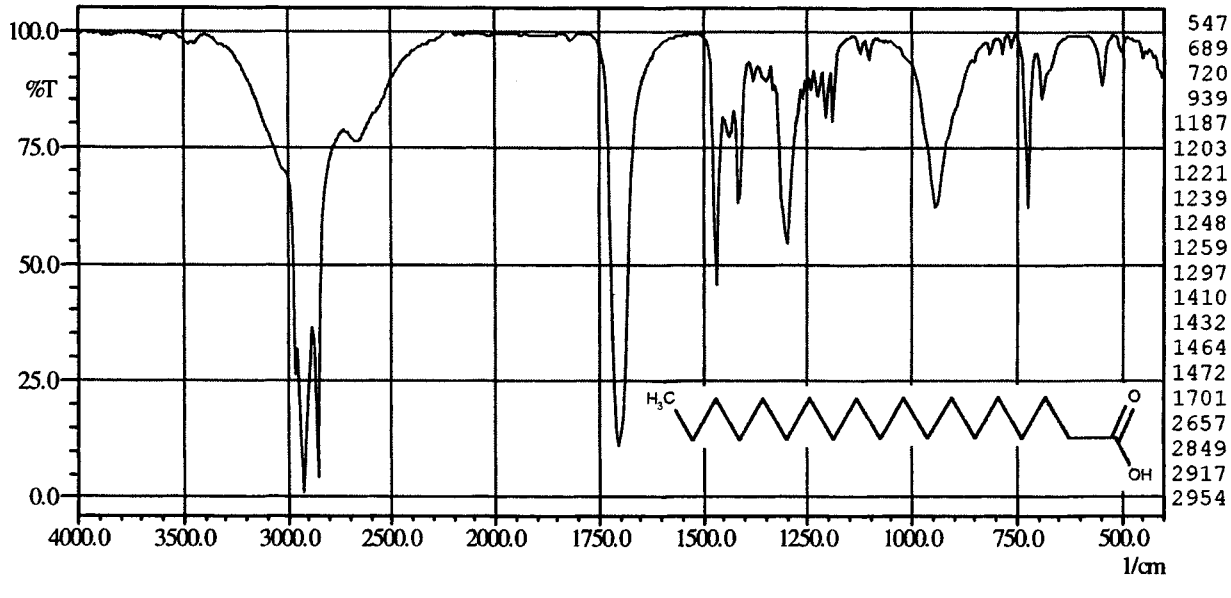
(1) **fatty alcohol-ethyleneoxide adduct**
(2) Tebestat PE 1
(3) Dr. Th. Boehme
(5) antistatic
(6) yellowish wax
(13) dried i.v., layer btw KBr

412



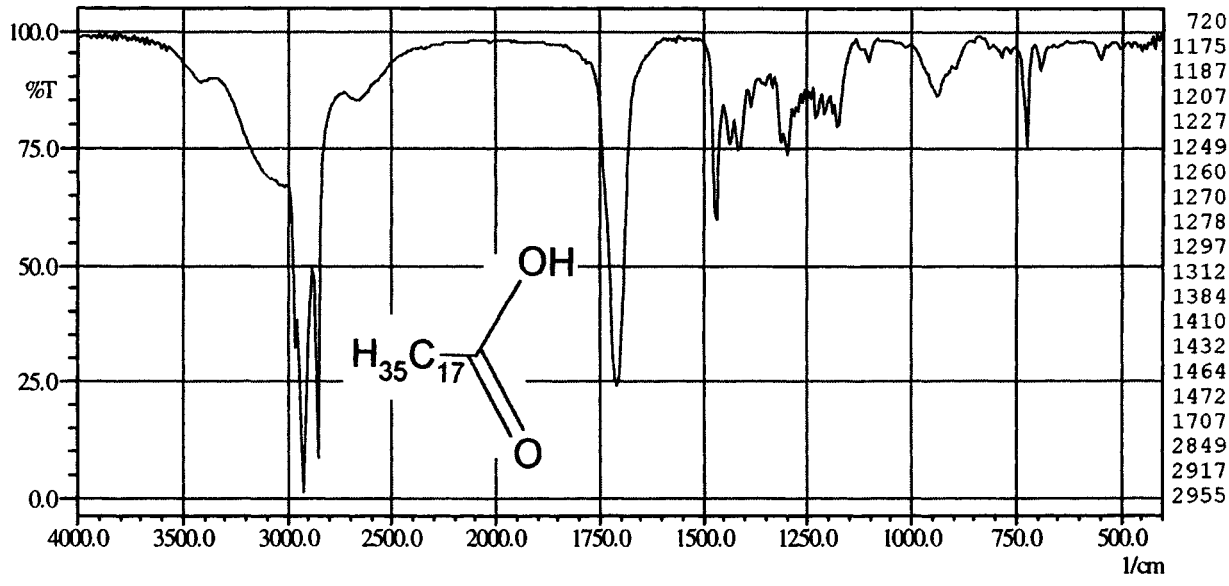
(1) **etherified poly(oxyethylene)**
(2) Loxiol EP 304
(3) Henkel
(5) lubricant
(6) almost colourless flakes
(13) KBr pellet

4131 $C_{18}H_{36}O_2$



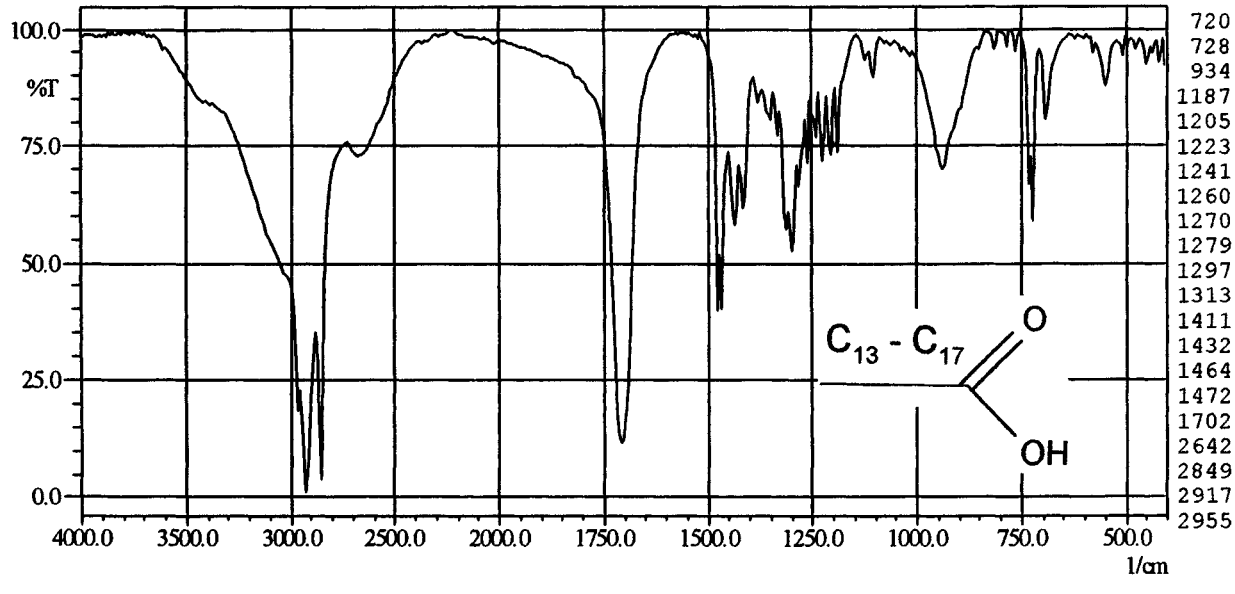
(1) **stearic acid**
(2) Naftozin N
(3) Chemetall
(4) 284.5 g mol^{-1}
(5) lubricant
(6) waxy solid
(13) recrystallised film on KBr

4131 $C_{18}H_{36}O_2$



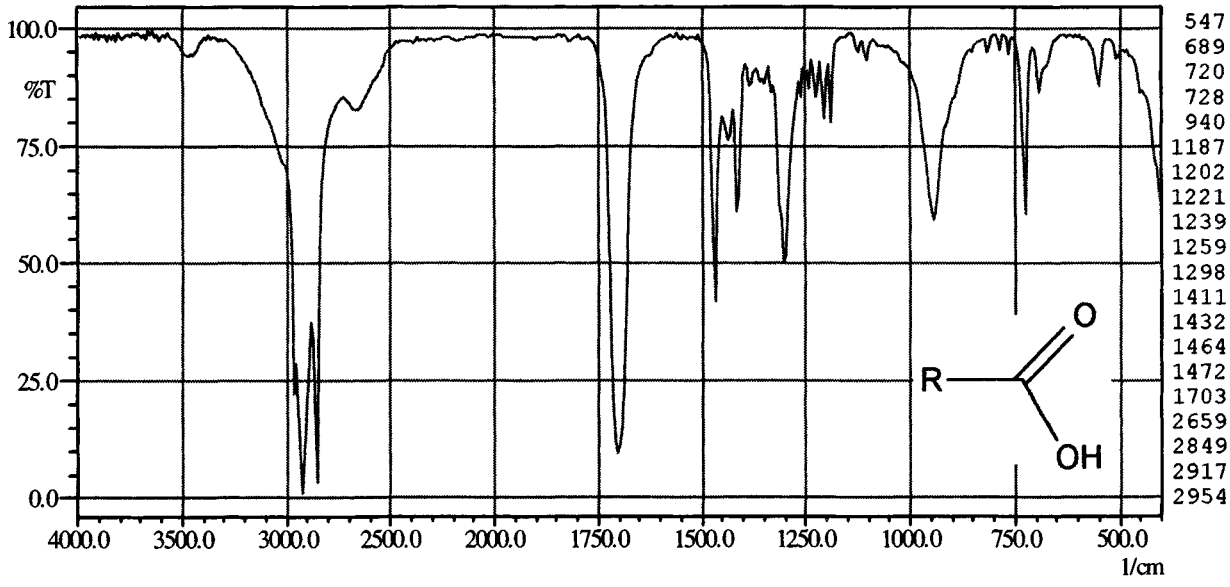
(1) **special stearic acid**
(2) Ligalub Se
(3) Peter Greven Fettchemie
(4) 284.5 g mol^{-1}
(5) lubricant
(6) colourless solid
(13) KBr pellet

4131



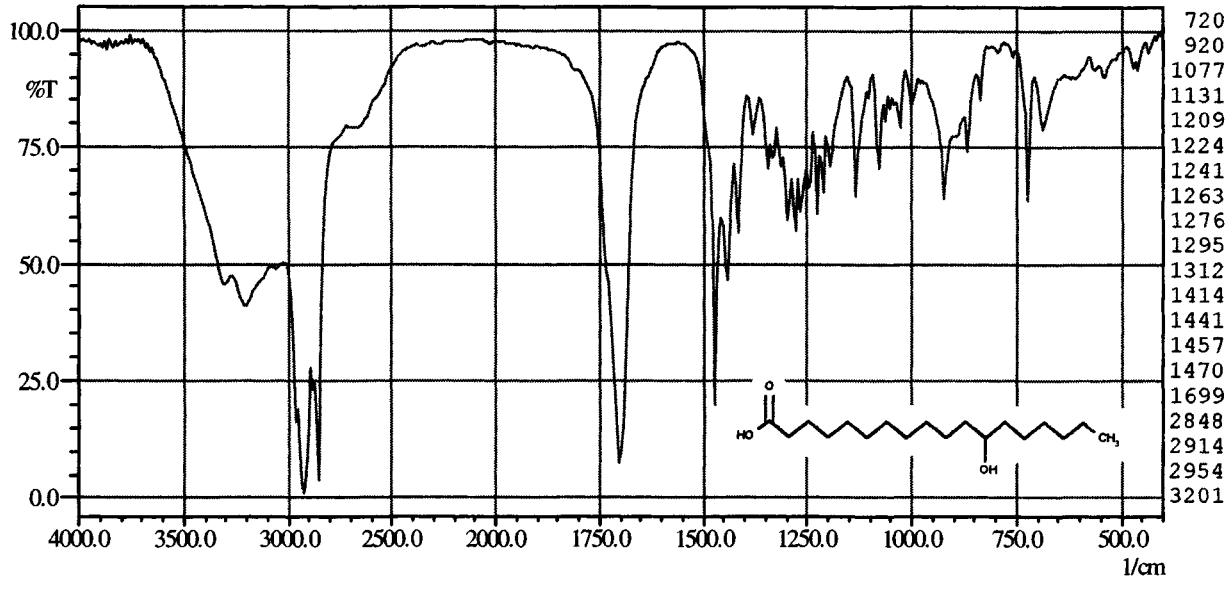
(1) **mixture of fatty acids**
(2) Baerolub FTA
(3) Baerlocher
(5) lubricant
(6) colourless solid
(7) 59 °C
(9) 0.96 g cm^{-3}
(13) KBr pellet

4131



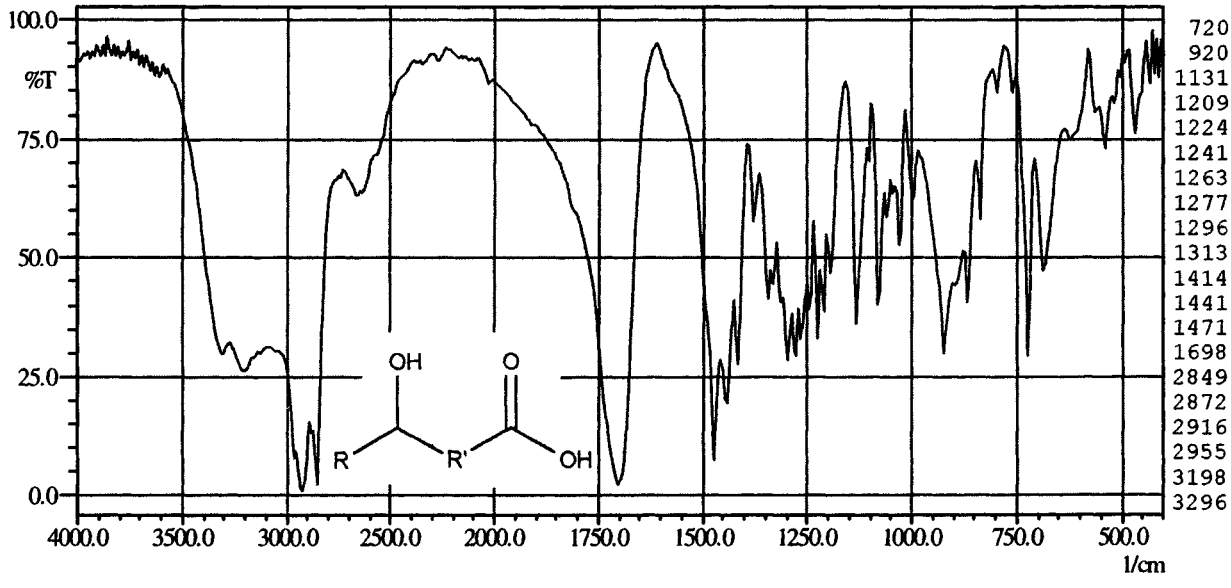
(1) **fatty acid**
(2) Realube PS
(3) Reagens
(5) lubricant
(6) colourless solid
(7) 55 °C
(9) 0.85 g cm^{-3}
(13) recrystallised film from melt btw KBr

4132 $C_{18}H_{36}O_3$



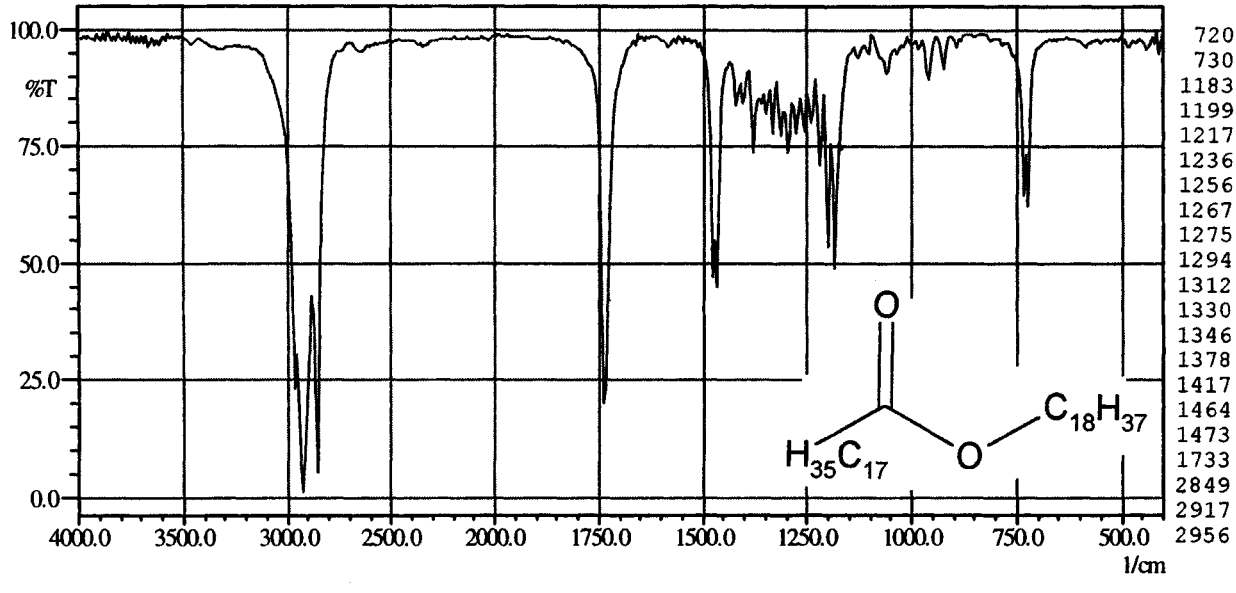
(1) **12-hydroxystearic acid**
(2) Loxiol G 21
(3) Henkel
(4) 300.5 g mol^{-1}
(5) lubricant
(6) colourless solid (beaded)
(7) 75.5 °C
(9) 0.89 g cm^{-3}
(10) 1.442
(13) KBr pellet

4132



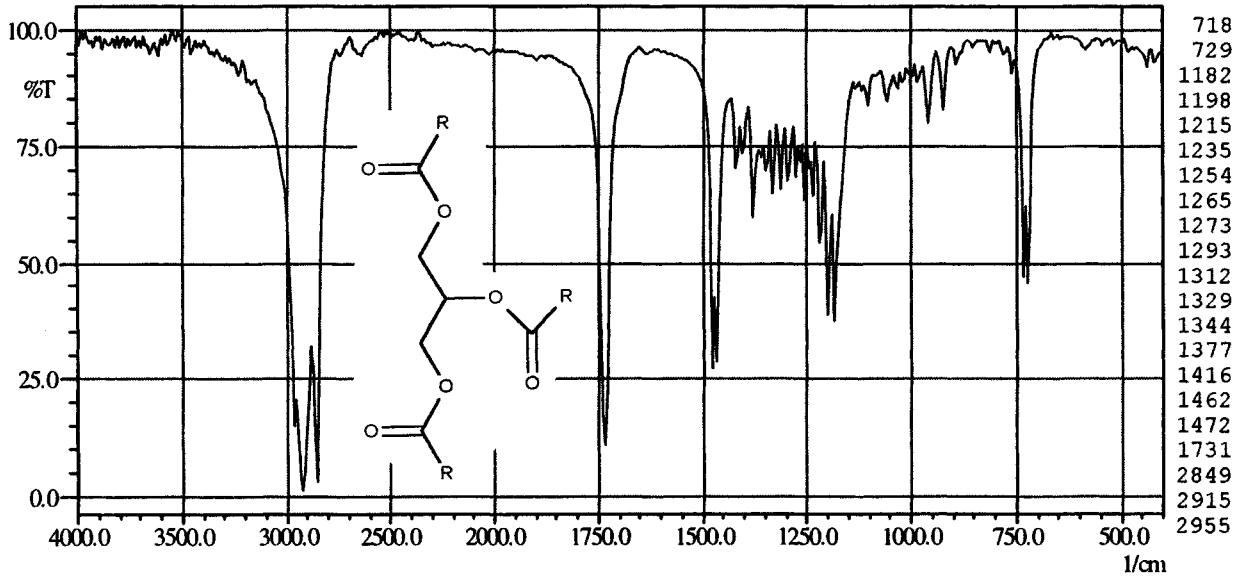
(1) **mixture of hydroxyfatty acids**
(2) Baerolub FTO
(3) Baerlocher
(5) lubricant
(6) colourless solid
(7) 72.5 °C
(9) 1.01 g cm^{-3}
(13) KBr pellet

4133 $C_{36}H_{72}O_2$



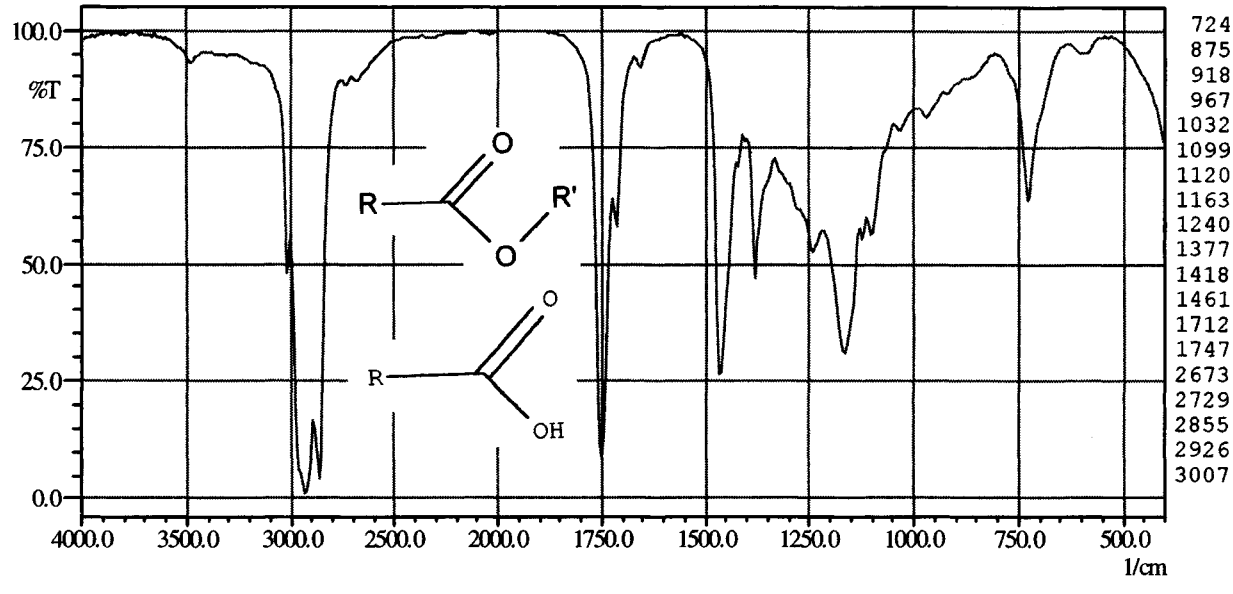
(1) **stearylstearate**
(2) Ligalub 36 Fe
(3) Peter Greven Fettchemie
(4) 537.0 g mol^{-1}
(5) lubricant
(6) colourless solid
(7) 55.5 °C
(8) >220 °C
(13) KBr pellet

4133



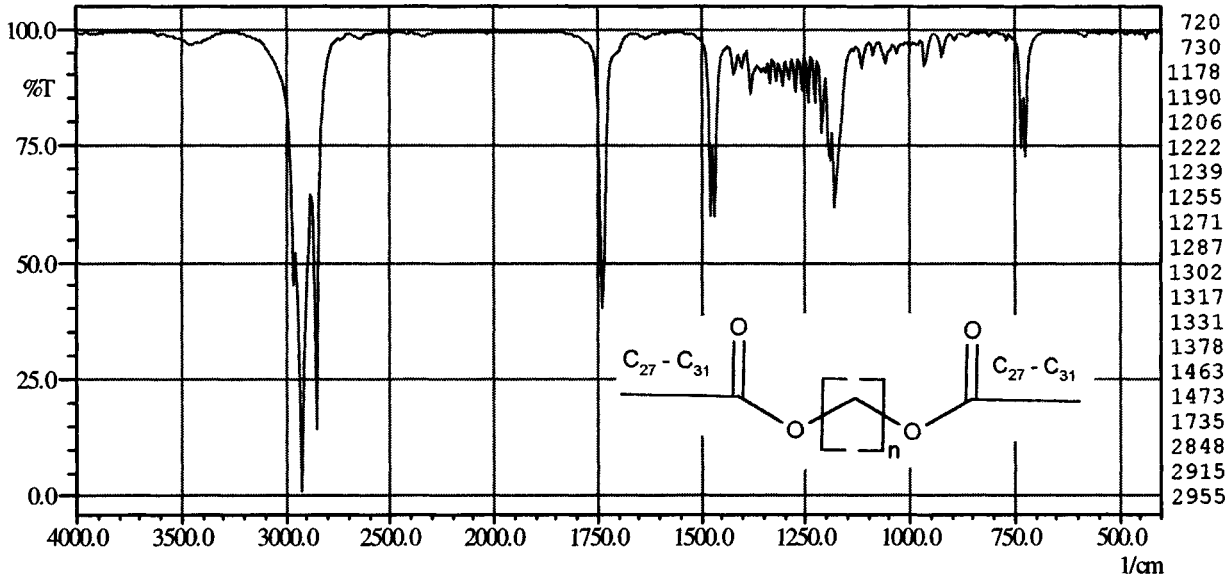
(1) **C_{16}, C_{18} ester wax**
(2) Realube SS/16–18
(3) Reagens
(5) lubricant
(6) colourless solid
(7) 50 °C
(13) KBr pellet

4133+4131



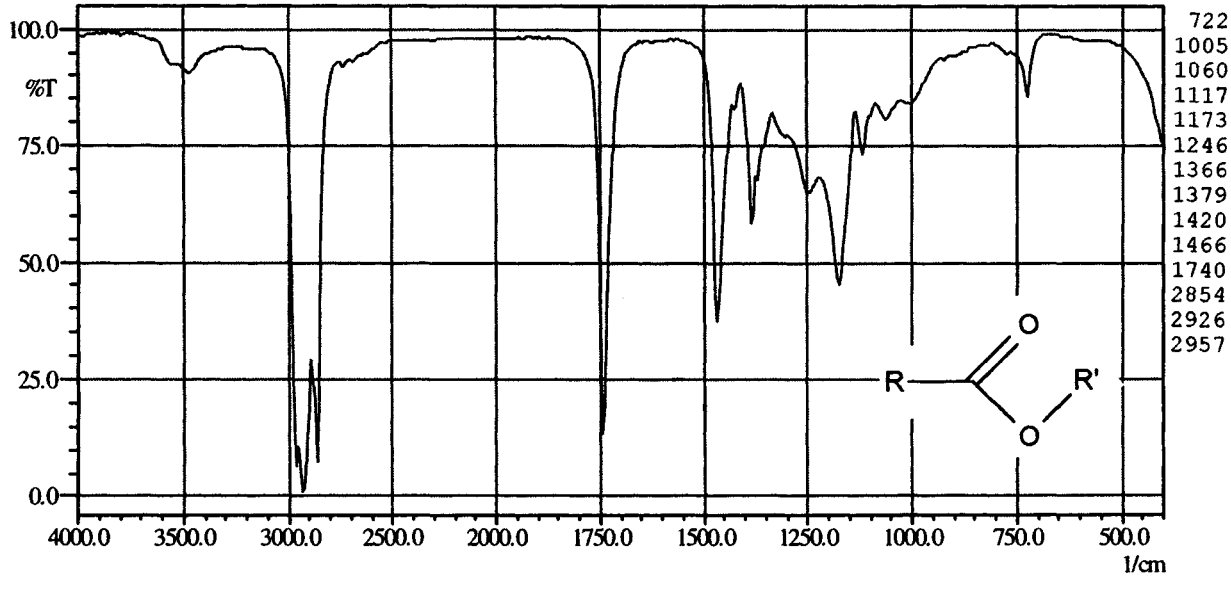
(1) **fatty acid ester + acid**
(2) Baerolub L-PO-1
(3) Baerlocher
(5) lubricant
(6) colourless, clear liquid
(9) 0.9 g cm^{-3}
(13) layer btw KBr

4133



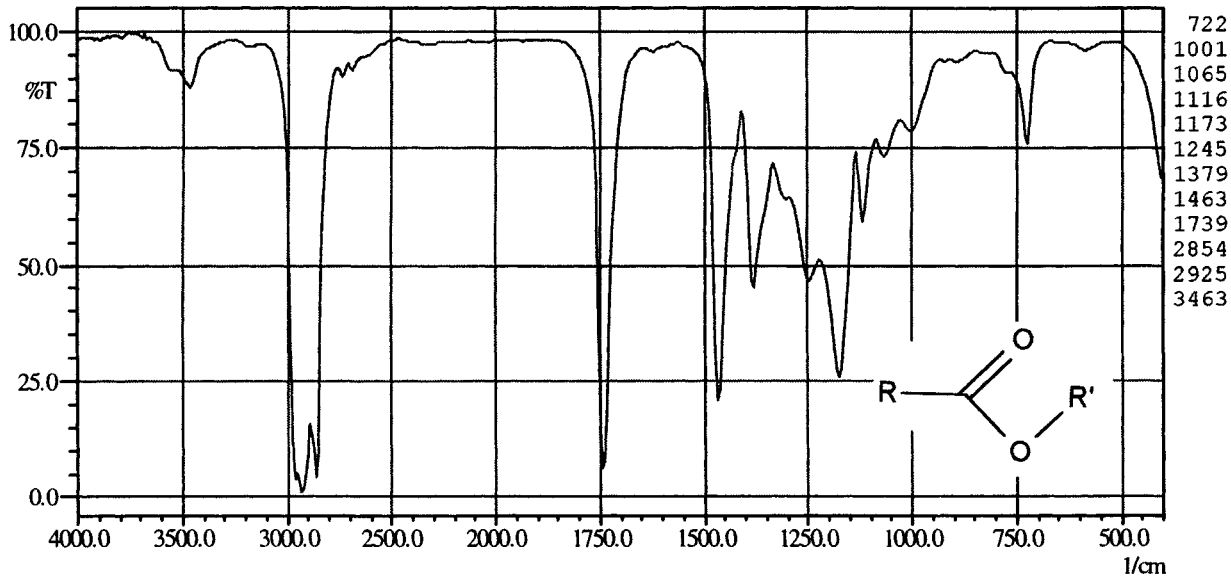
(1) **aliphatic ester wax**
(2) Loxiol G 47
(3) Henkel
(5) lubricant
(6) colourless solid
(7) 62 °C
(9) 0.819 g cm^{-3}
(10) 1.435
(13) KBr pellet

4133



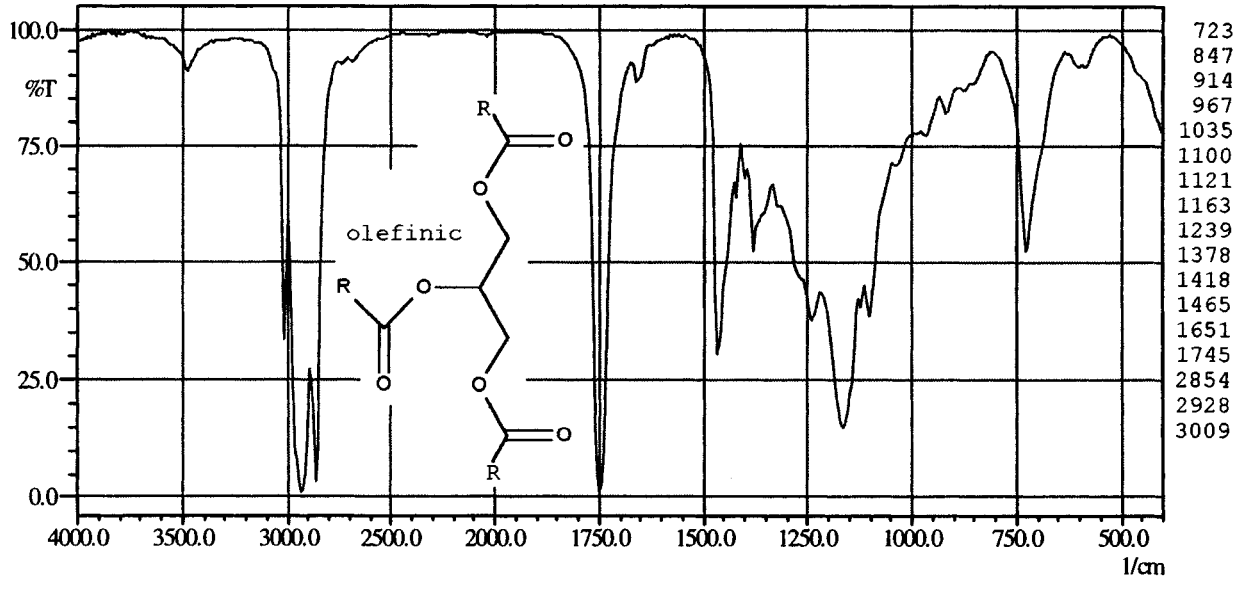
(1) **fatty acid ester**
(2) Baerolub L-PK
(3) Baerlocher
(5) lubricant
(6) colourless, clear liquid
(9) 0.86 g cm^{-3}
(13) layer btw KBr

4133



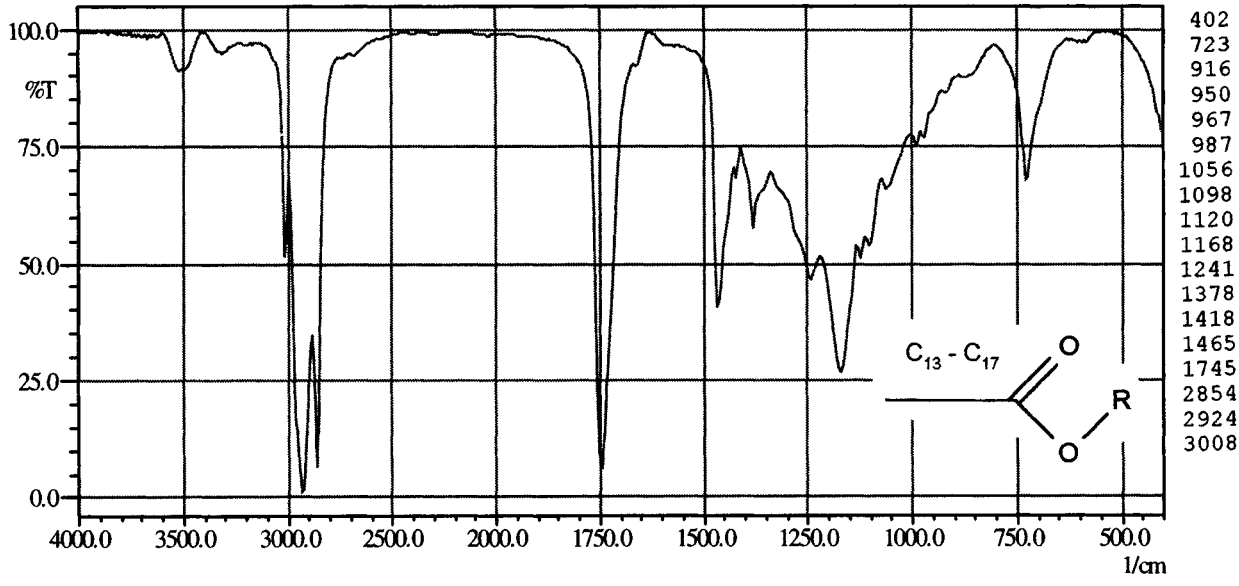
(1) **long-chain aliphatic ester**
(2) Realube TR
(3) Reagens
(5) lubricant for PVC
(6) colourless, clear liquid
(7) 3 °C
(9) 0.86 g cm^{-3}
(13) layer btw KBr

4133



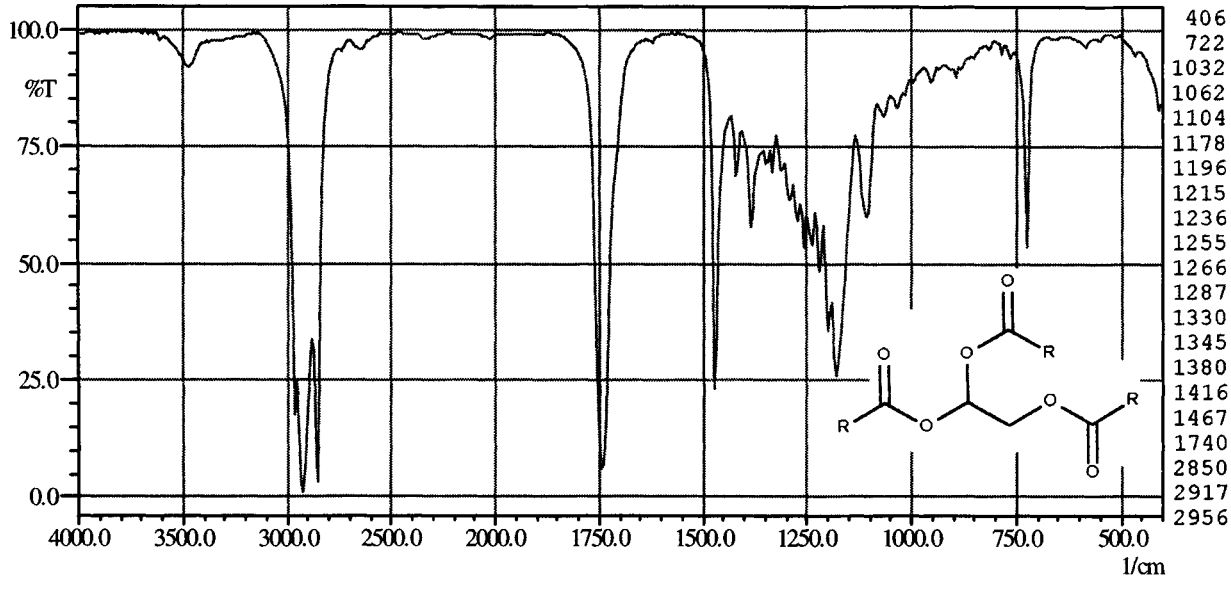
(1) **glycerol ester of unsaturated fatty acids**
(2) Swedlub FG-4
(3) Swedstab
(5) lubricant
(6) colourless, clear, oily liquid
(9) 0.92 g cm^{-3}
(10) 1.47
(13) layer btw KBr

4133



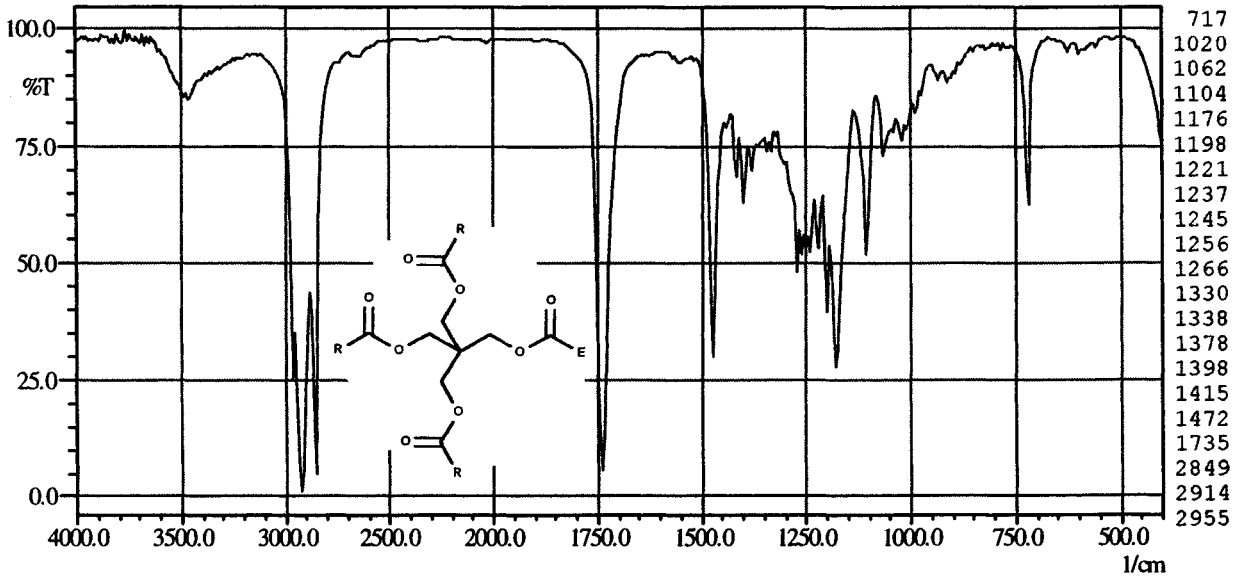
(1) **unsaturated fatty acid ester**
(2) Ligalub 40/1
(3) Peter Greven Fettchemie
(5) lubricant
(6) yellow, clear liquid
(7) –2 °C
(8) >250 °C
(13) layer btw KBr

4133



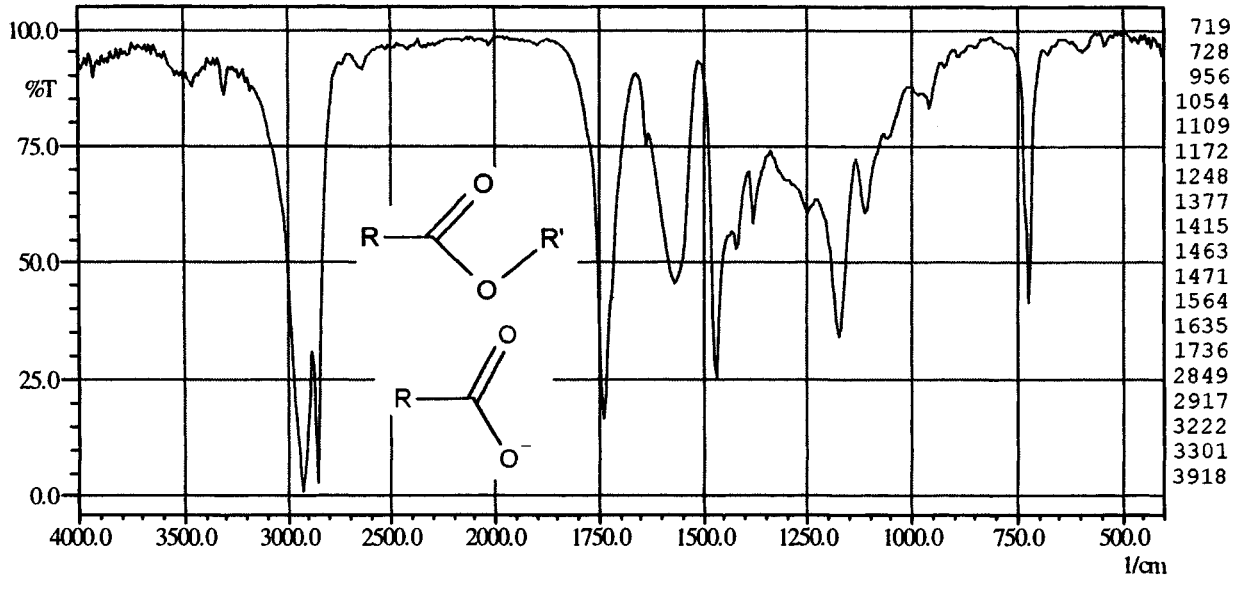
(1) **fatty acid triglycerol ester**
(2) Realube SI
(3) Reagens
(5) lubricant
(6) colourless solid
(7) 60 °C
(13) recrystallised film from melt btw KBr

4133



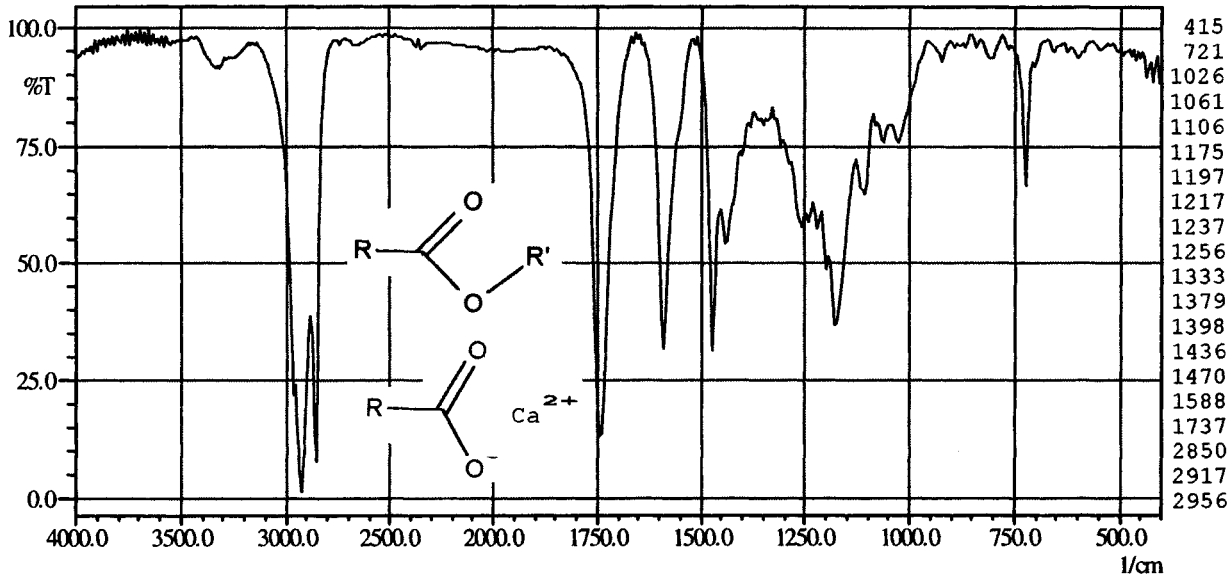
(1) **pentaerythrol fatty ester**
(2) Loxiol EP 861
(3) Henkel
(5) lubricant
(6) colourless solid (beaded)
(7) 61.5 °C
(9) 0.879 g cm^{-3}
(10) 1.443
(13) recrystallised film from melt

4133



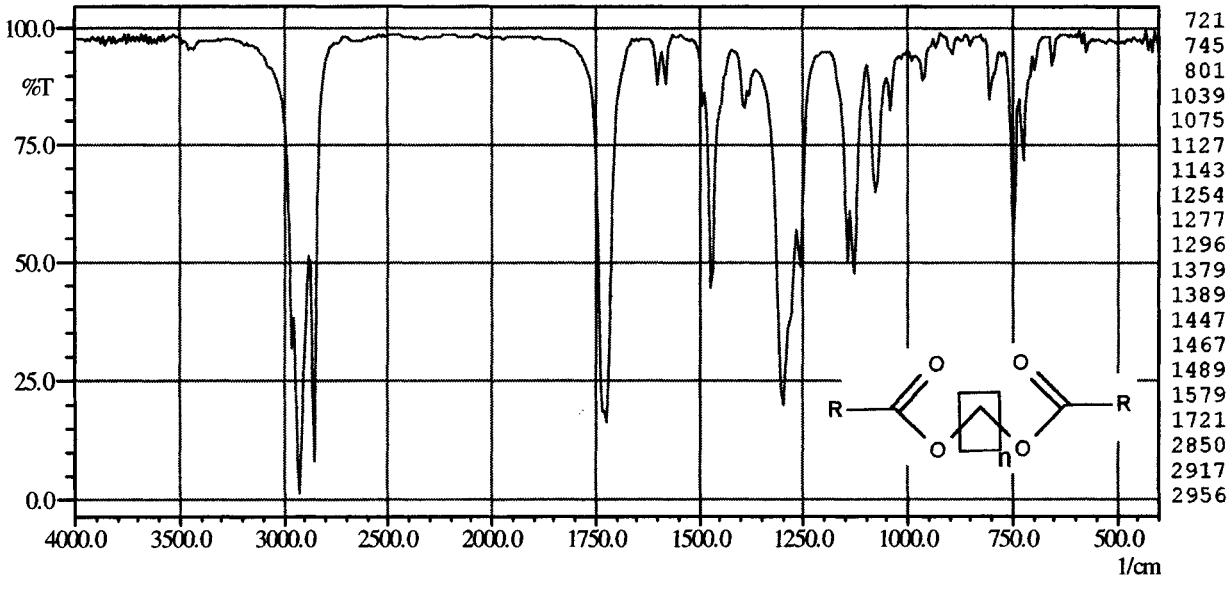
(1) **montanic ester carboxylate**
(2) Hostalub We 4
(3) Hoechst
(5) lubricant
(6) yellowish solid
(9) 1.01 g cm^{-3}
(13) KBr pellet

4133+4139



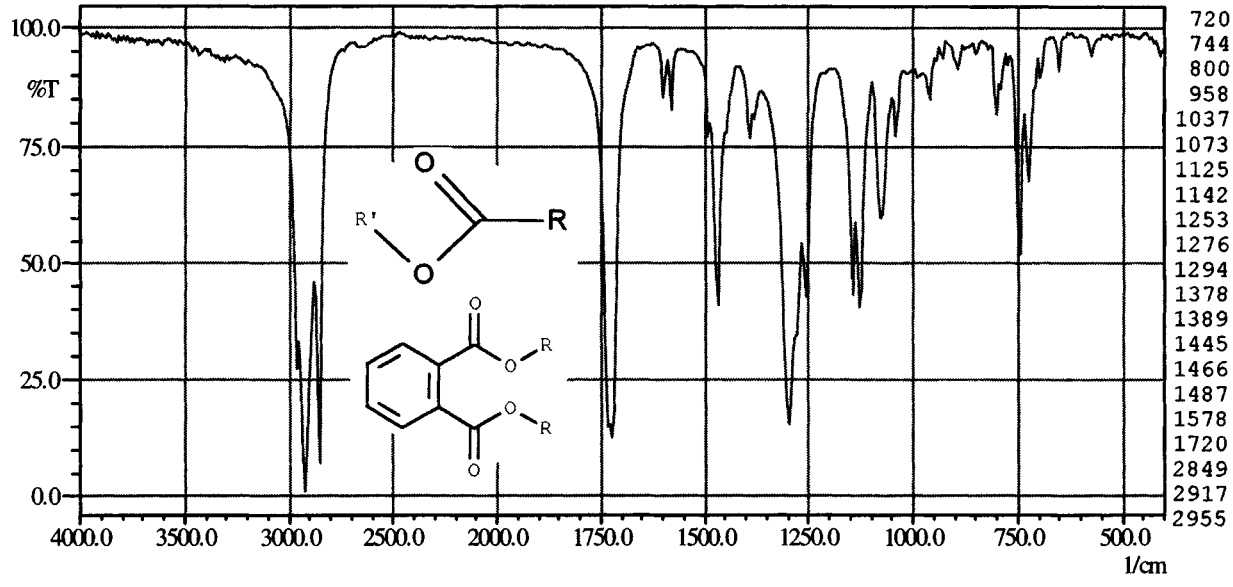
(1) **complex ester of saturated fatty acids**
(2) Baerolub A 275
(3) Baerlocher
(5) lubricant
(6) yellowish solid
(7) 120 °C
(13) KBr pellet
(14) contains Ca soap

4133



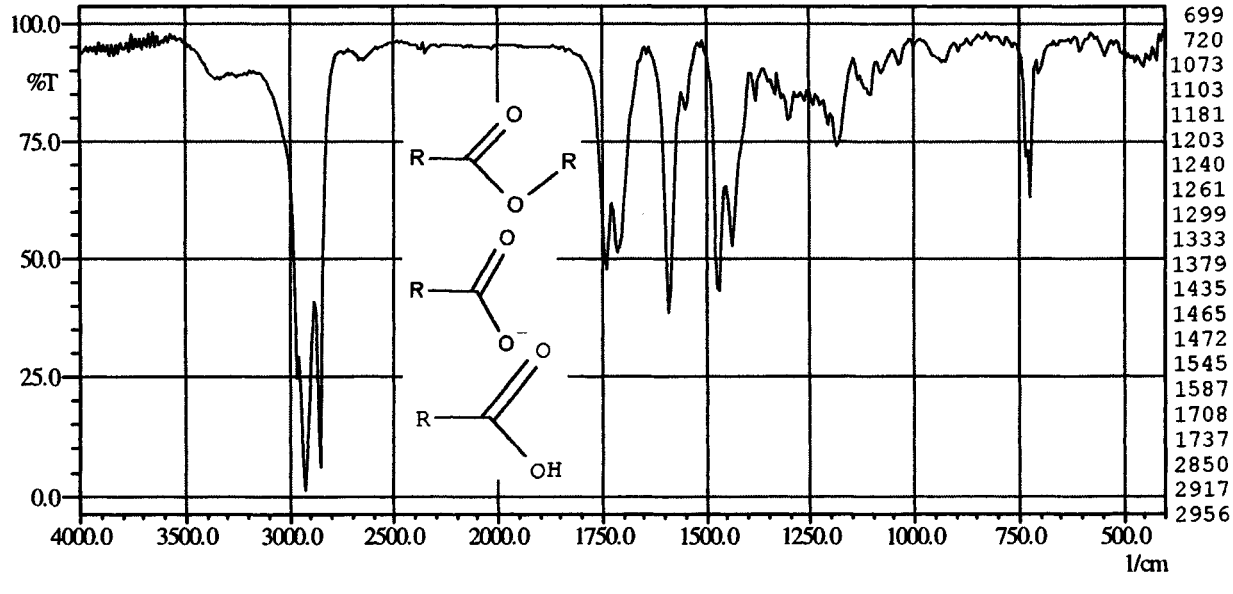
(1) **aliphatic ester wax with some phthalate ester**
(2) Naftolube ELP
(3) Chemson
(5) lubricant
(6) colourless solid
(13) KBr pellet

4133+3421



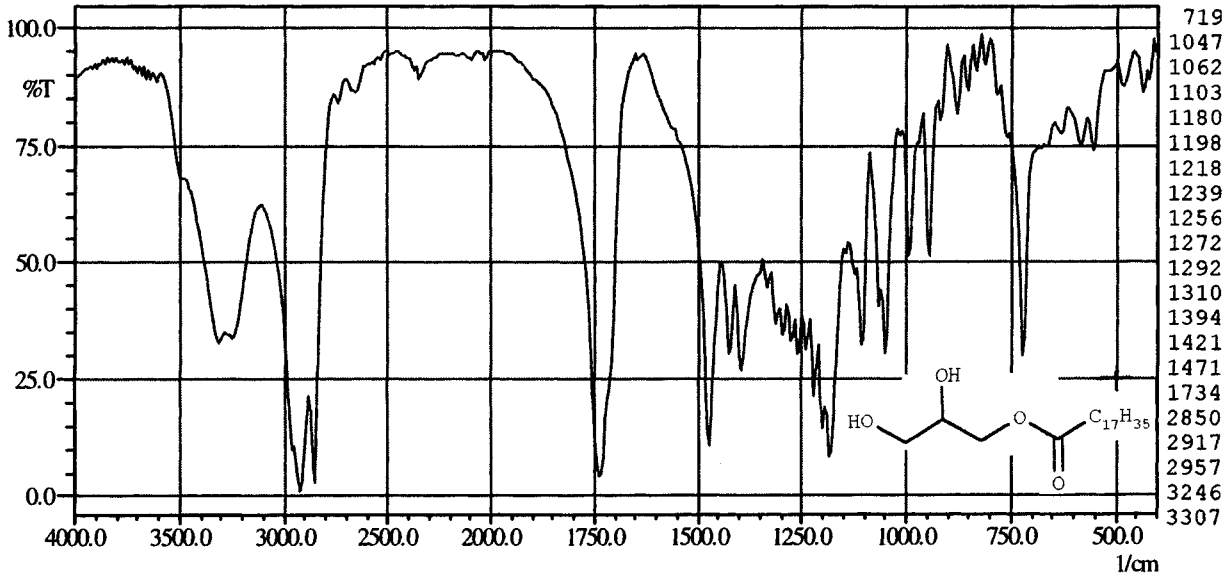
(1) **aliphatic ester wax + phthalate ester**
(2) Realube SD
(3) Reagens
(5) lubricant
(6) colourless solid
(7) 43 °C
(13) KBr pellet

4133+4131+4139



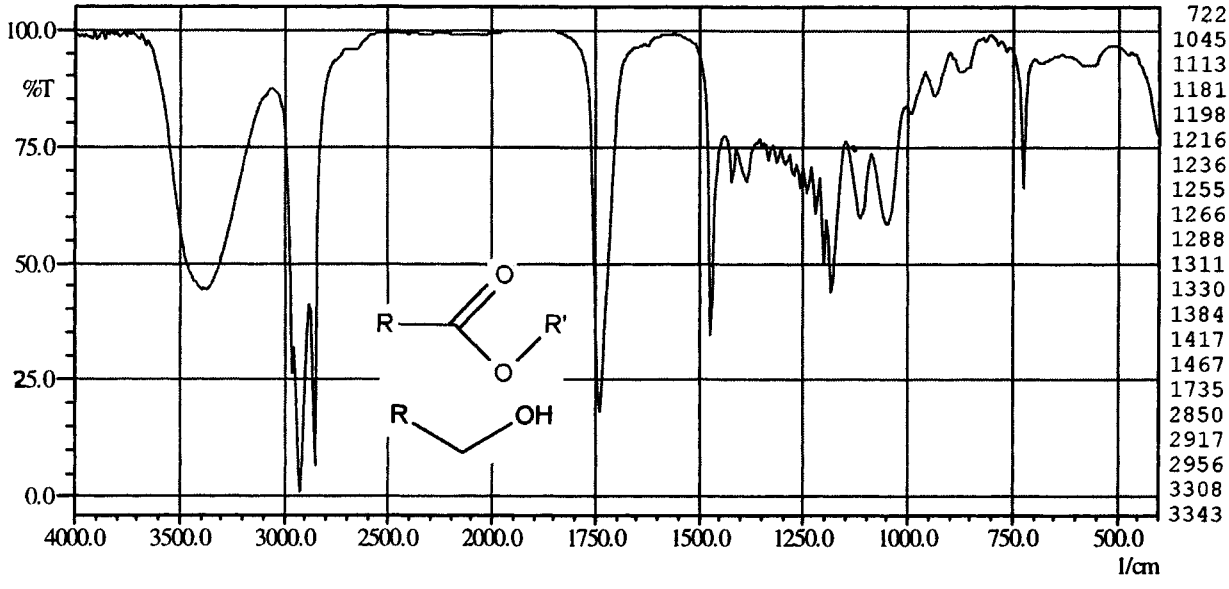
(1) **ester acid carboxylate**
(2) Baerolub GL 5 DO
(3) Baerlocher
(6) yellowish solid
(7) 80 °C
(5) combination lubricant
(13) KBr pellet

4134 $C_{21}H_{42}O_4$



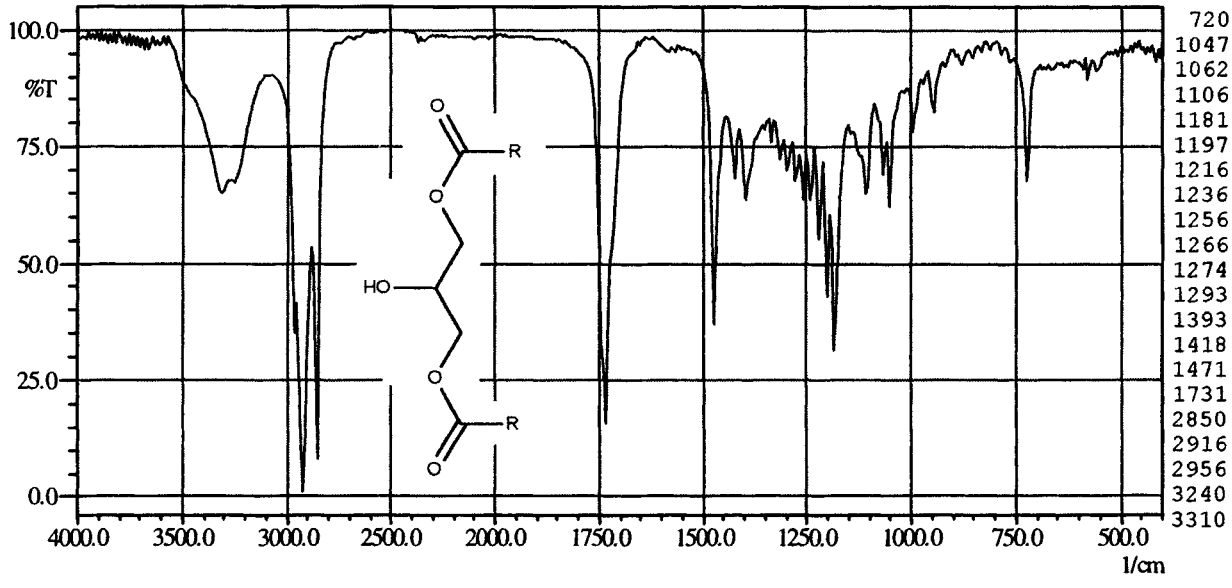
(1) **glycerolmonostearate**
(2) Swedlub HG 55
(3) Swedstab
(4) 358.6 g mol^{-1}
(5) lubricant
(6) slightly yellowish flakes
(7) 56.5 °C
(9) 0.908 g cm^{-3}
(10) 1.441
(13) KBr pellet

4134



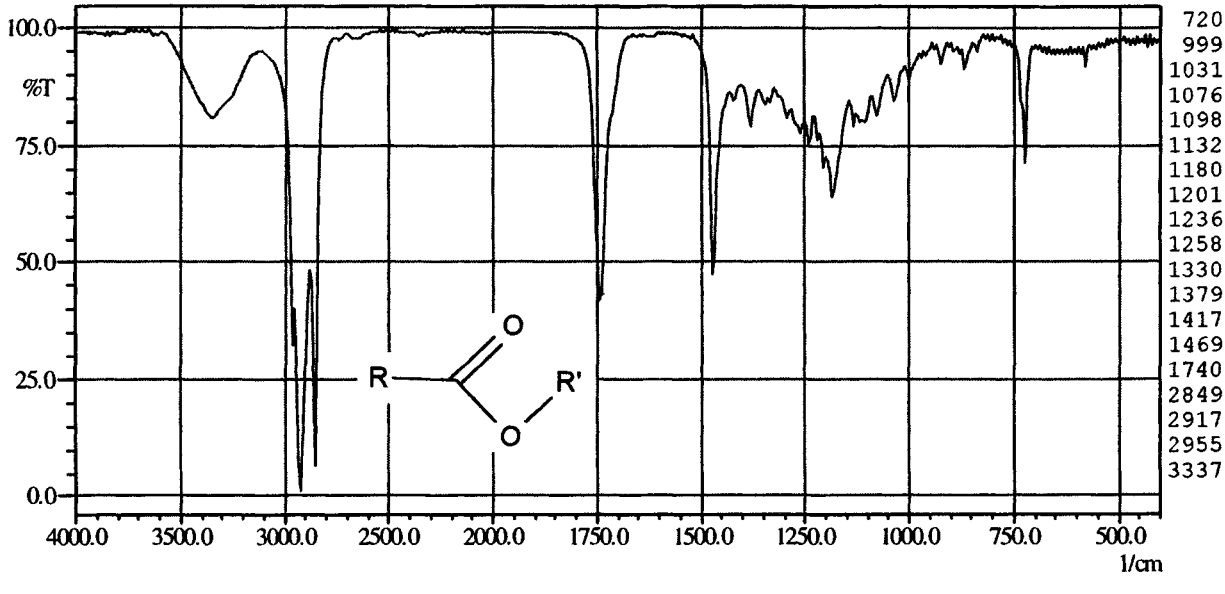
(1) **wax esteralcohol, partial ester of glycerol**
(2) Realube GMS
(3) Reagens
(5) lubricant
(6) colourless solid
(7) 56 °C
(13) KBr pellet

4134



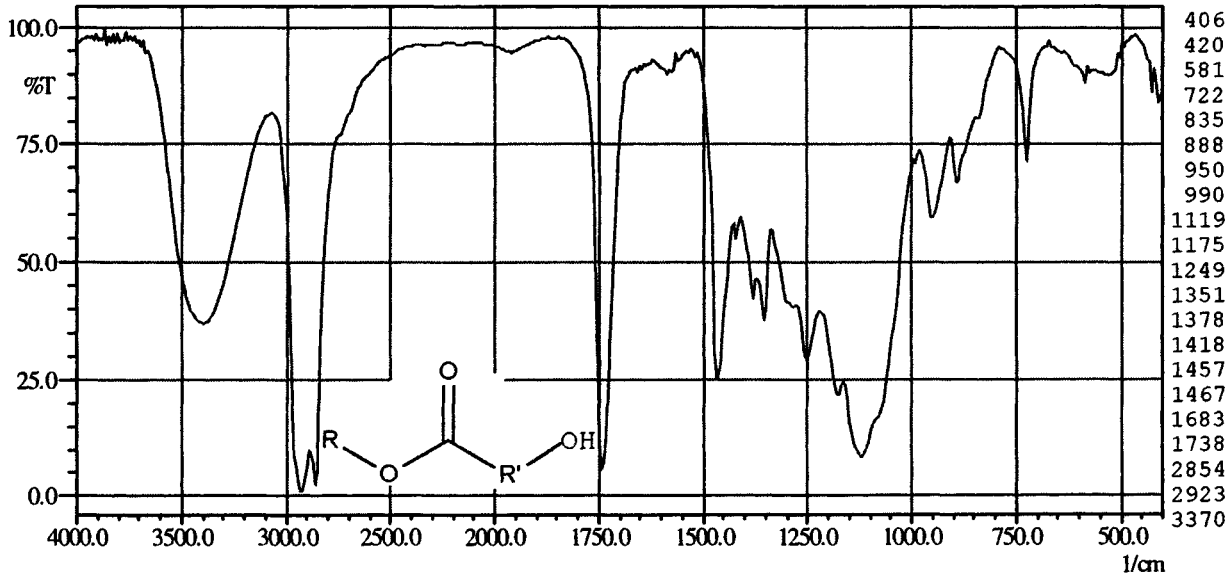
(1) **glycerol partial ester of saturated fatty acids**
(2) Baerolub L-MS
(3) Baerlocher
(5) lubricant
(6) colourless solid
(7) 58.5 °C
(9) 0.95 g cm^{-3}
(13) KBr pellet

4134



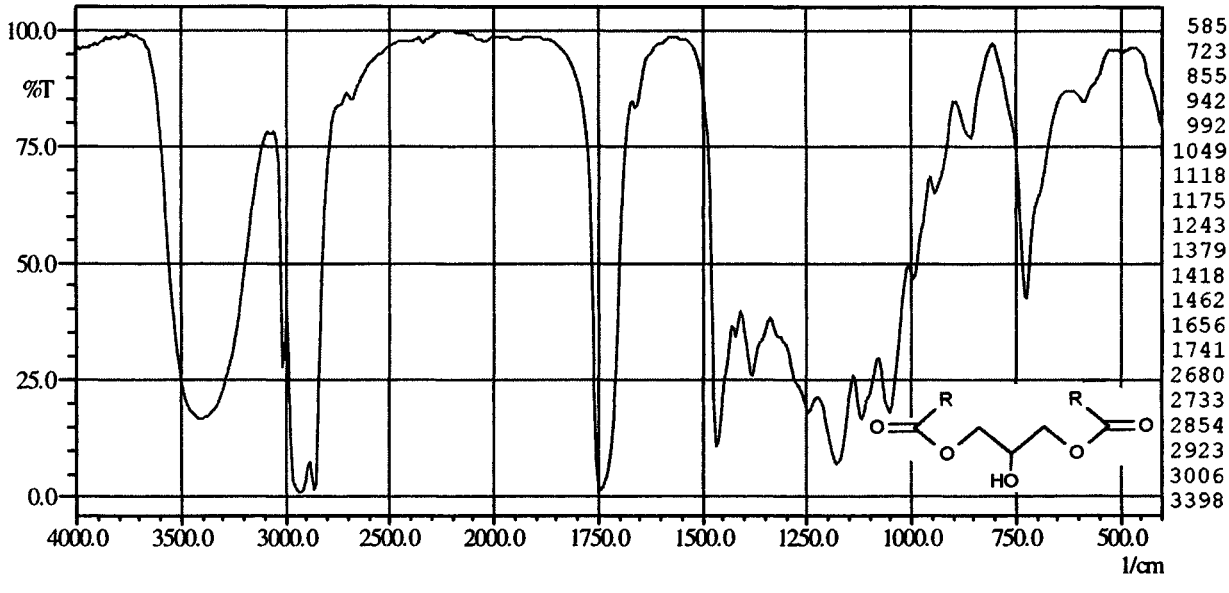
(1) **fatty acid ester with OH groups**
(2) Baerolub LM 4
(3) Baerlocher
(5) combination lubricant
(6) colourless solid
(7) 75 °C
(9) 0.96 g cm^{-3}
(13) KBr pellet

4134



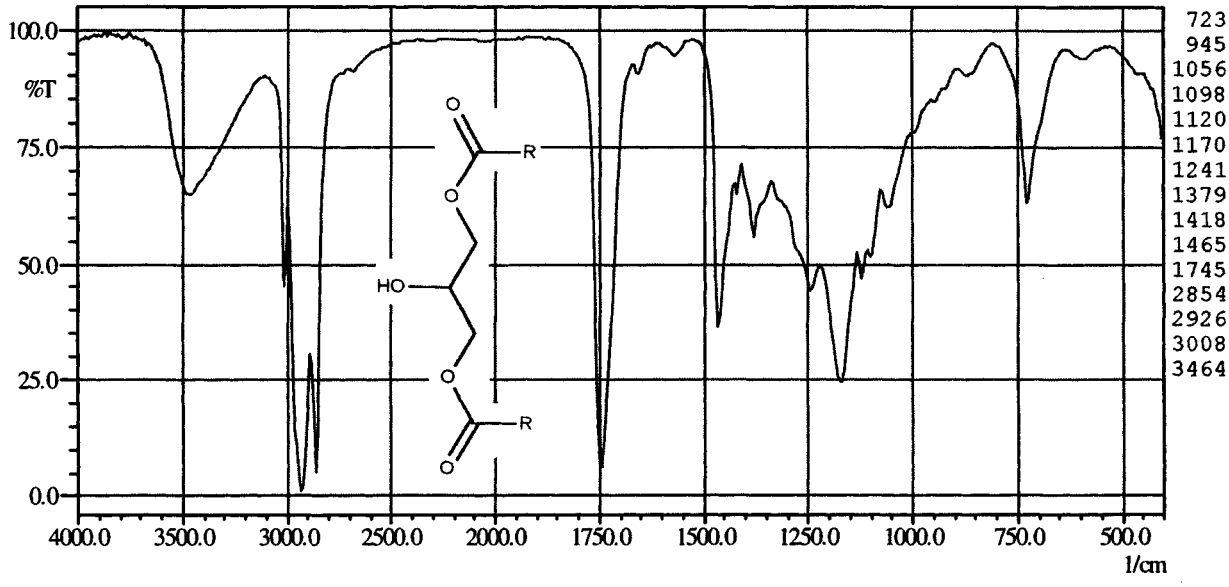
(1) **mixture of aliphatic esteralcohols**
(2) Tebestat HSE 81
(3) Dr. Th. Boehme
(5) antistatic
(6) yellowish, clear liquid
(8) 200 °C
(13) layer btw KBr

4134



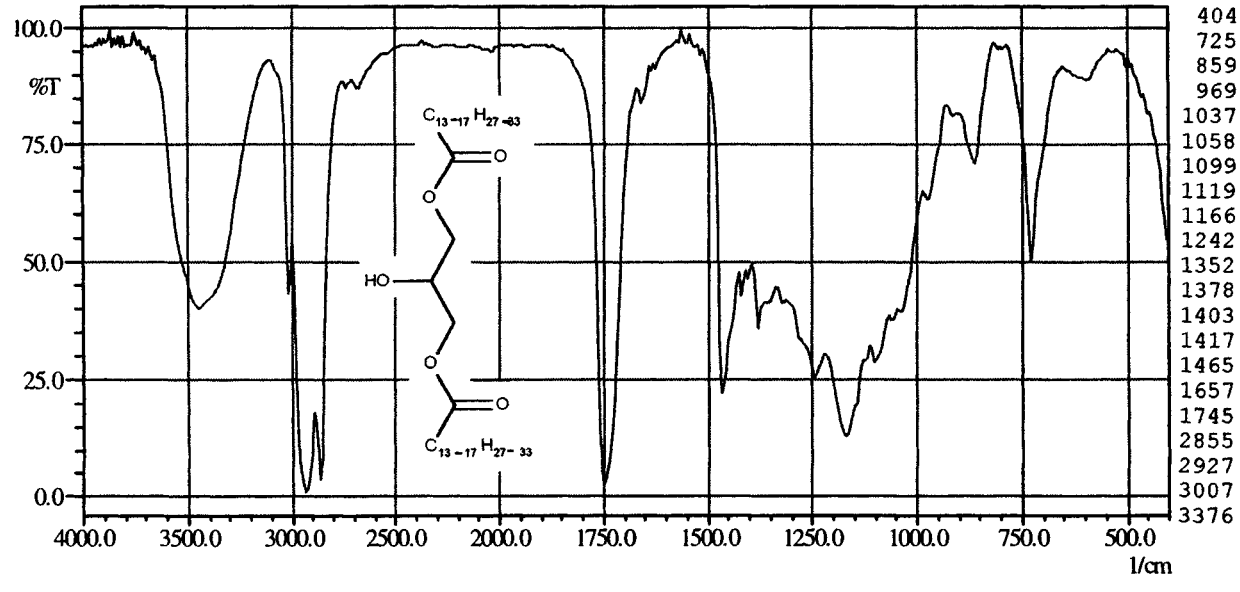
(1) **glycerol partial ester of oleic acid**
(2) Realube GMO
(3) Reagens
(5) lubricant for PVC
(6) light yellowish, clear liquid
(7) 25 °C
(13) layer btw KBr

4134



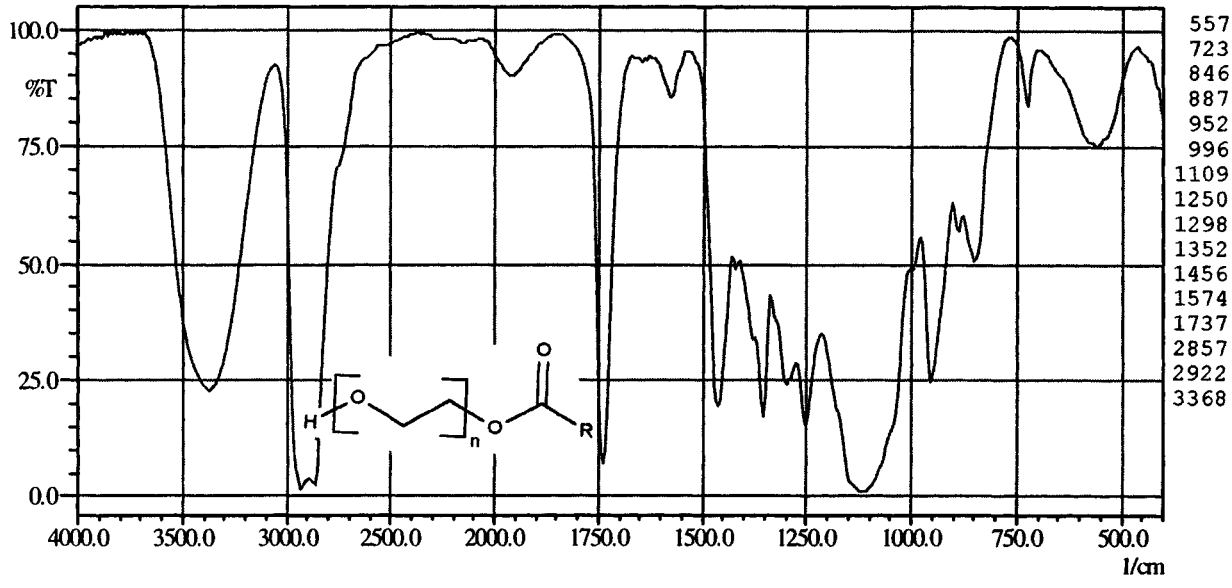
(1) **glycerol partial ester of unsaturated fatty acid**
(2) Baerolub L-PL
(3) Baerlocher
(5) lubricant
(6) yellowish, clear liquid
(9) 0.93 g cm^{-3}
(13) layer btw KBr

4134



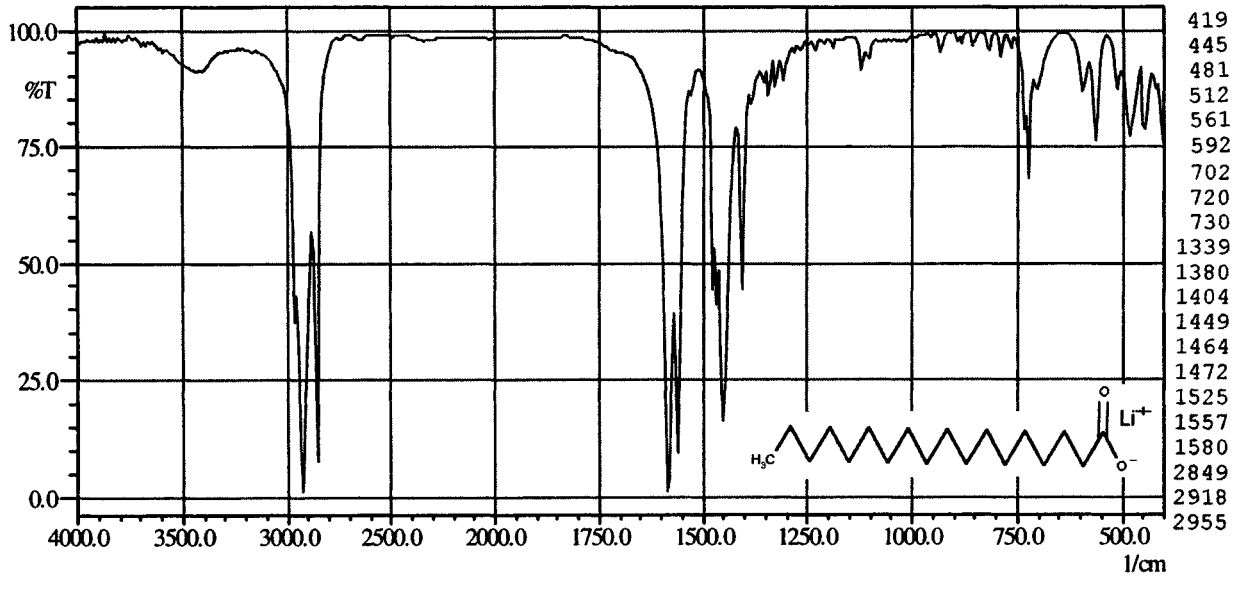
(1) **glycerol partial ester of unsaturated fatty acids**
(2) Irgawax 361
(3) Ciba-Geigy
(5) lubricant
(6) light yellowish, clear, oily liquid
(9) 0.96 g cm^{-3}
(10) 1.475
(13) layer btw KBr

4135



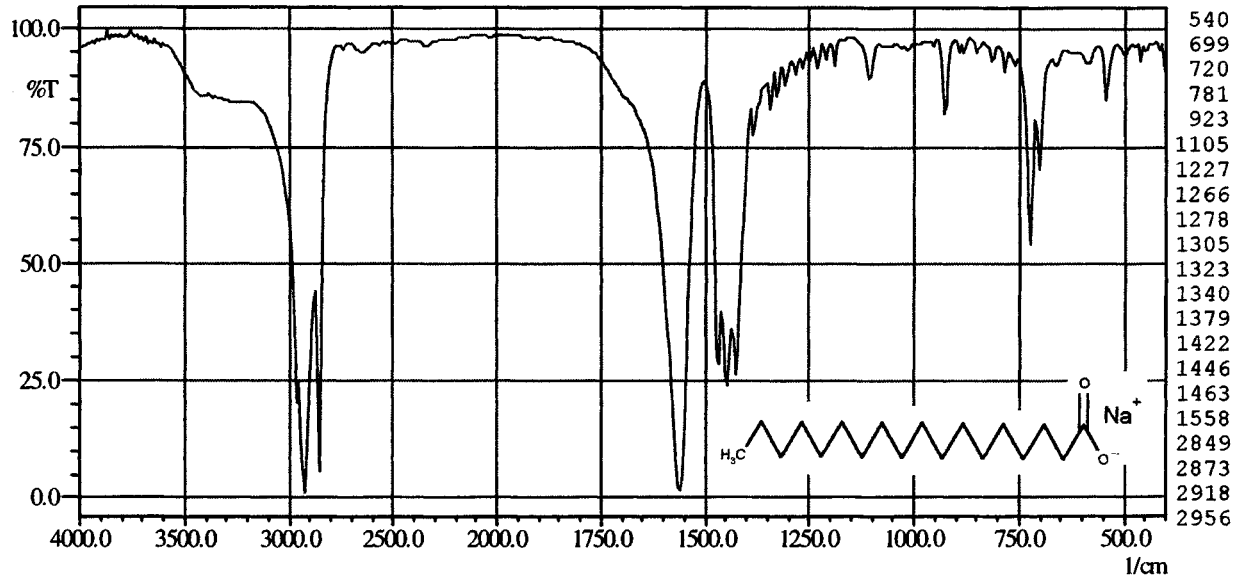
(1) **partially esterified poly(oxyethylene)**
(2) Baerostat 318 S
(3) Baerlocher
(5) antistatic
(6) colourless, clear liquid
(9) 1.035 g cm^{-3}
(13) layer btw KBr
(14) contains H2O

4139 $C_{18}H_{35}O_2Li$



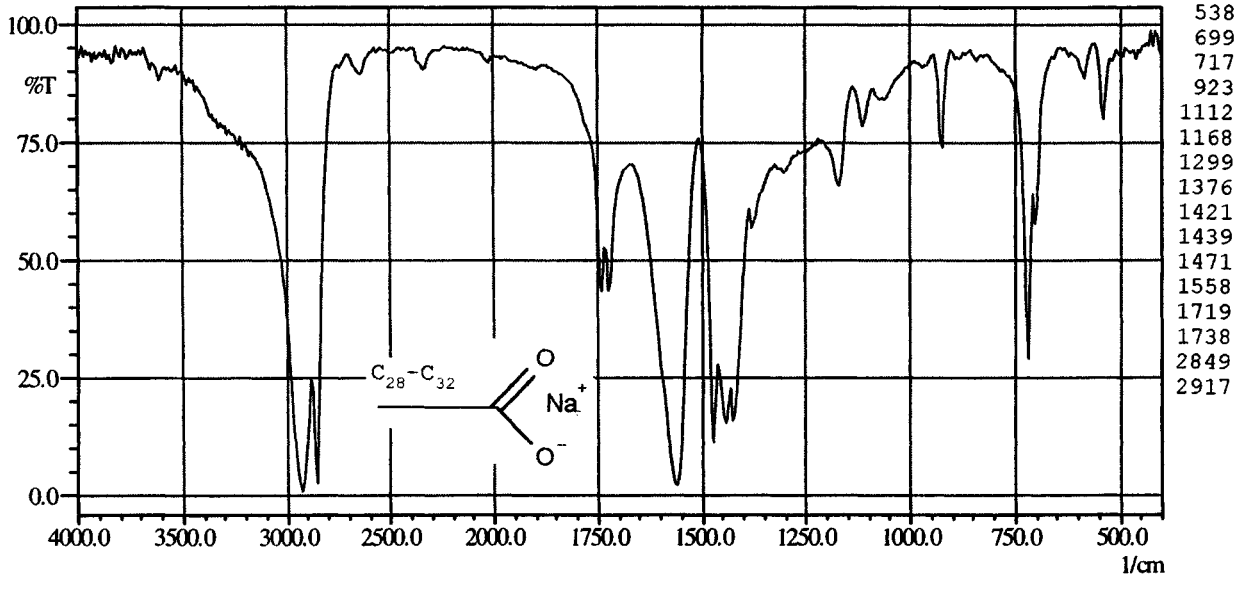
(1) **Li stearate**
(2) Liga Lithiumsterat
(3) Peter Greven Fettchemie
(4) 290.4 g mol^{-1}
(5) lubricant
(6) colourless solid
(13) KBr pellet

4139 $C_{18}H_{35}O_2Na$



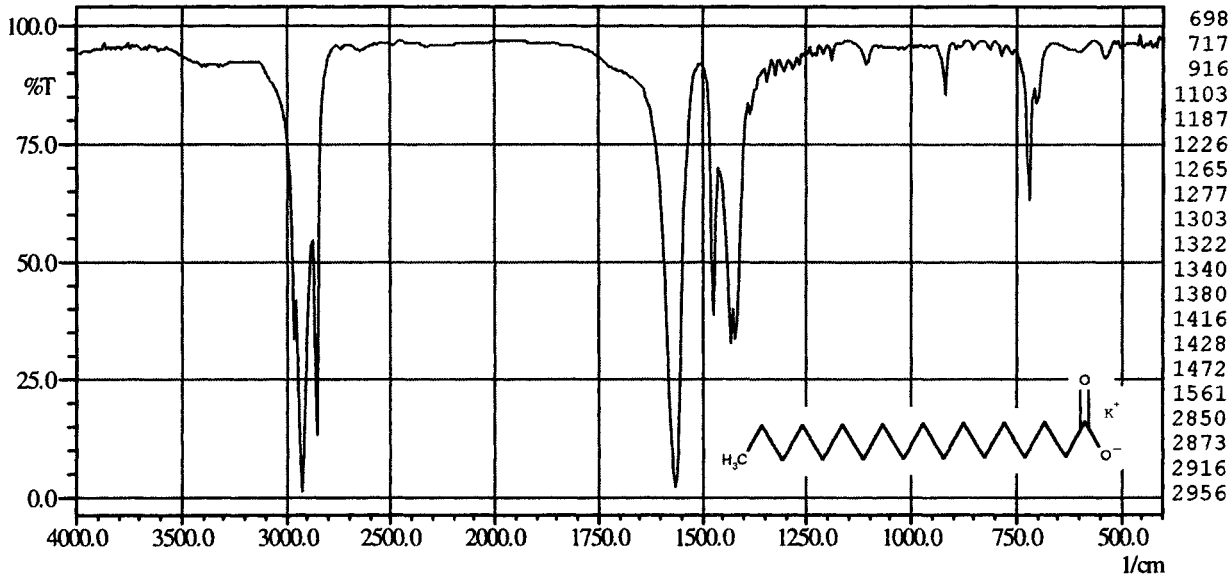
(1) **Na stearate**
(2) Liga Natriumsterat R/D
(3) Peter Greven Fettchemie
(4) 306.5 g mol^{-1}
(5) emulsifying agent
(6) colourless to yellowish solid
(13) KBr pellet

4139



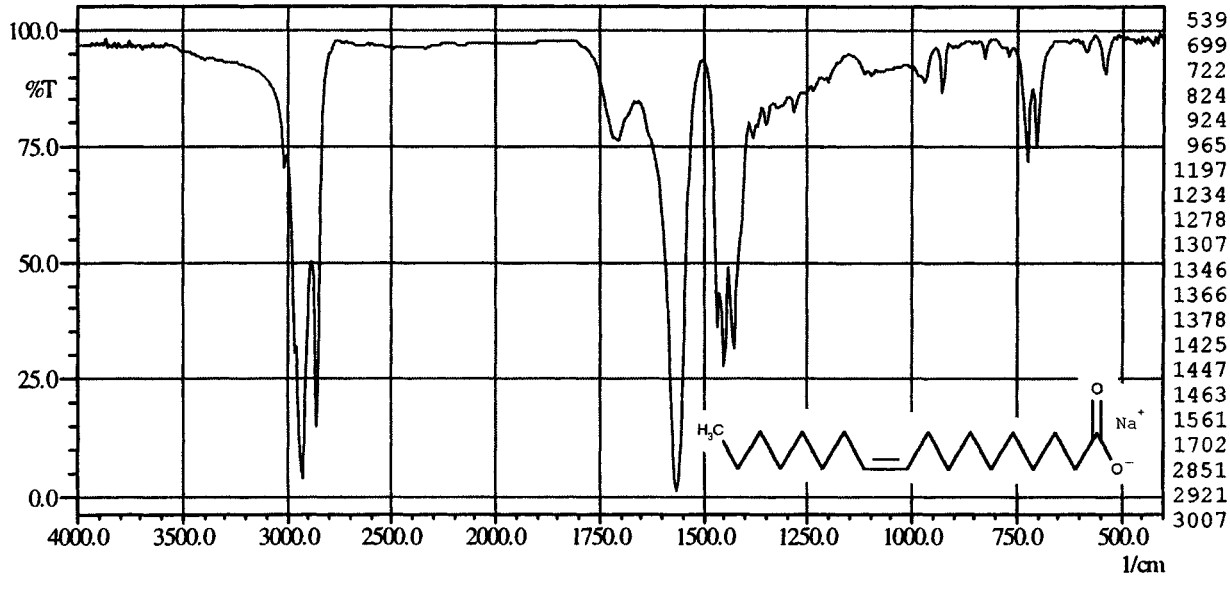
(1) **linear (C_{28}-C_{32}) carboxylic acid, Na-salt**
(2) Hostamont NaV 101
(3) Hoechst
(5) lubricant
(6) pale-yellowish solid
(7) 170 °C
(13) KBr pellet
(14) contains ester groups

4139 $C_{18}H_{35}O_2K$



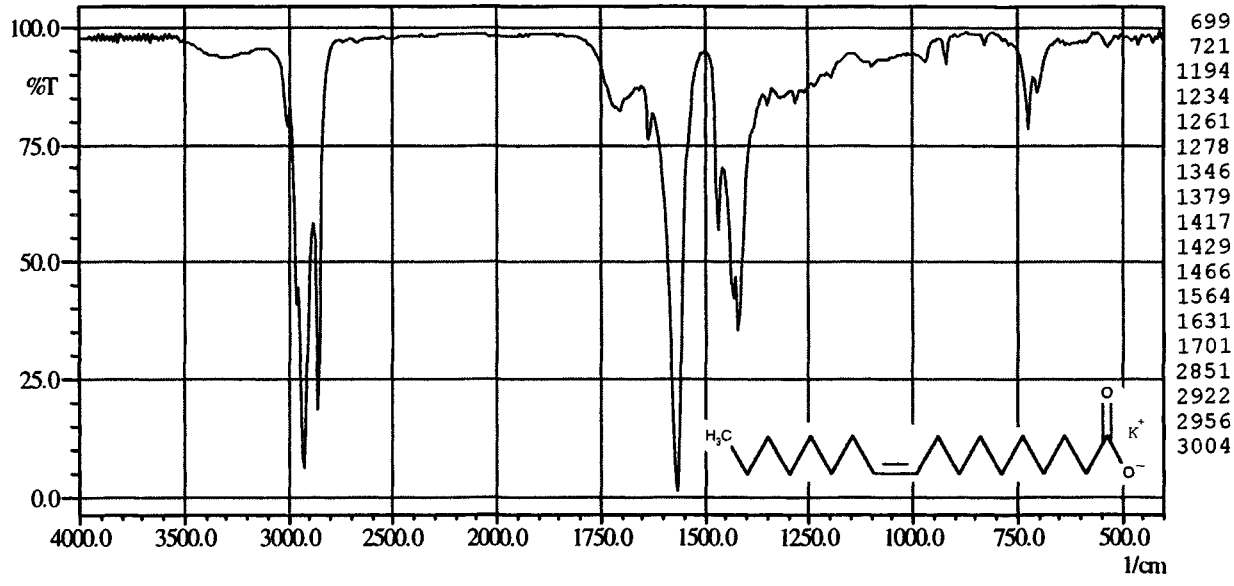
(1) **K stearate**
(2) Liga Kaliumsterat R/D
(3) Peter Greven Fettchemie
(4) 322.6 g mol^{-1}
(5) foaming agent
(6) colourless to yellowish solid
(13) KBr pellet

4139 $C_{18}H_{33}O_2Na$



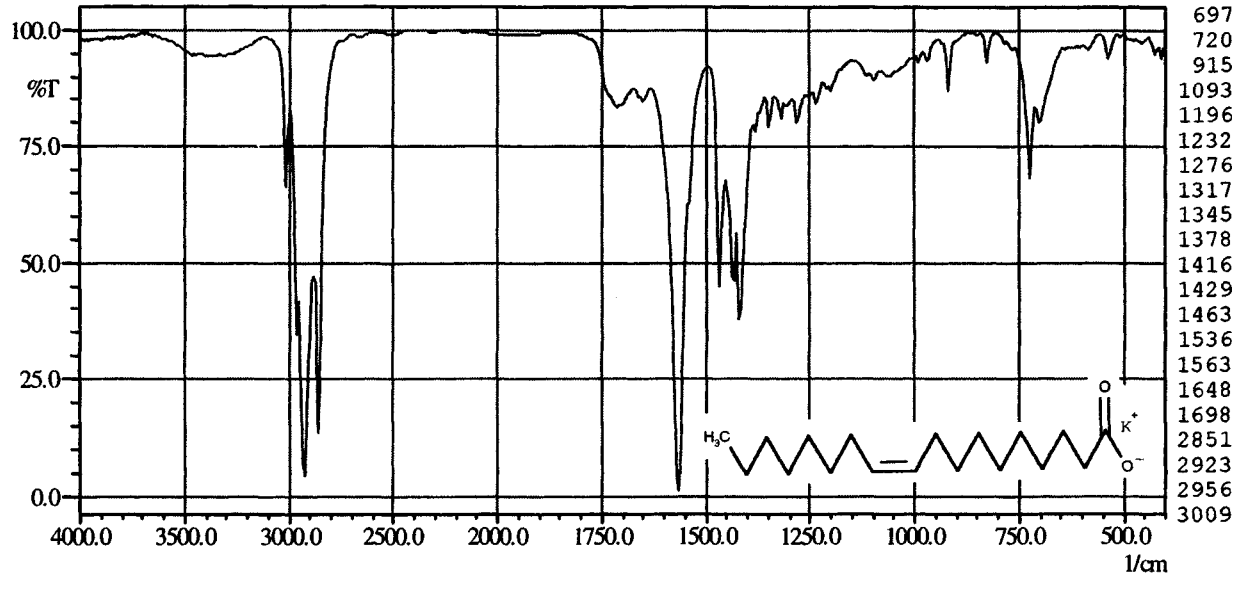
(1) **Na oleate**
(2) Liga Natriumoleat
(3) Peter Greven Fettchemie
(4) 304.5 g mol^{-1}
(5) emulsifying agent
(6) yellowish solid
(13) KBr pellet

4139 $C_{18}H_{33}O_2K$



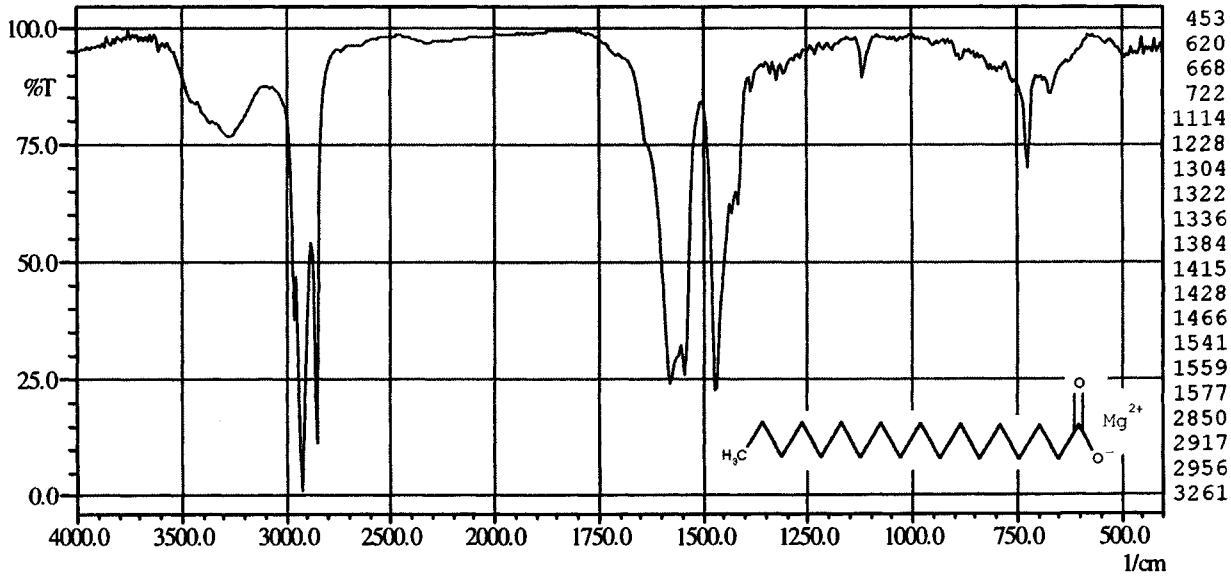
(1) **K oleate**
(2) Liga Kaliumoleat 90 %
(3) Peter Greven Fettchemie
(4) 320.6 g mol^{-1}
(5) lubricant
(6) yellowish solid
(13) KBr pellet

4139 $C_{18}H_{33}O_2K$



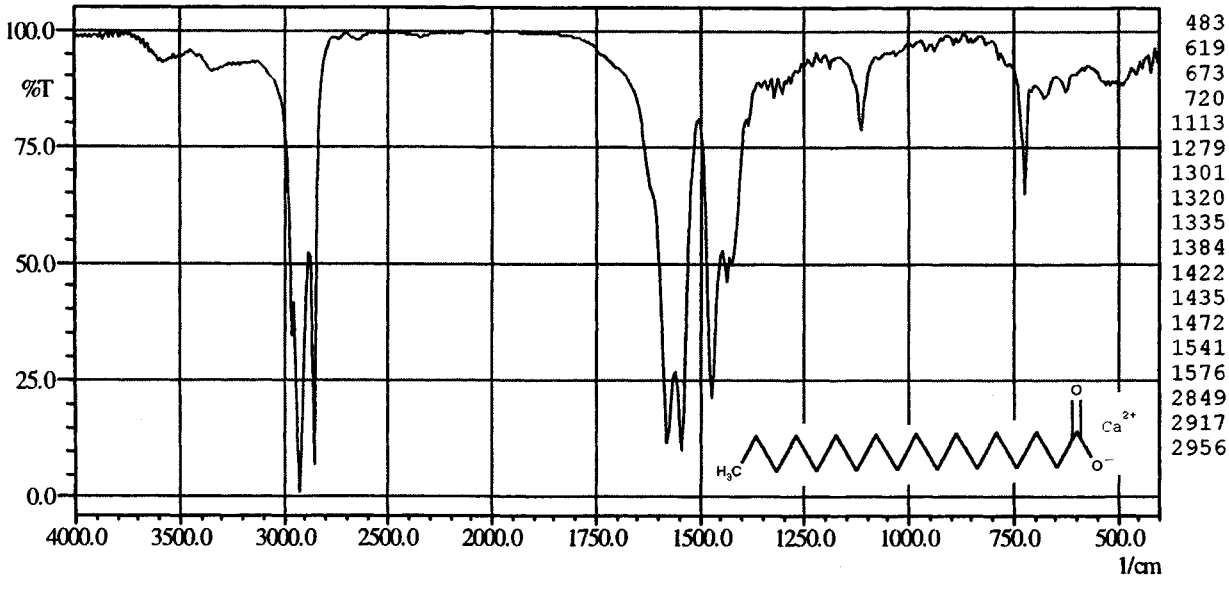
(1) **K salts of unsaturated fatty acids (predominantly K oleate)**
(2) Rhenodiv LE
(3) Rhein-Chemie
(4) 320.6 g mol^{-1}
(5) lubricant
(6) yellowish, soft paste
(13) dried layer on KBr

4139 $C_{36}H_{70}O_4Mg$



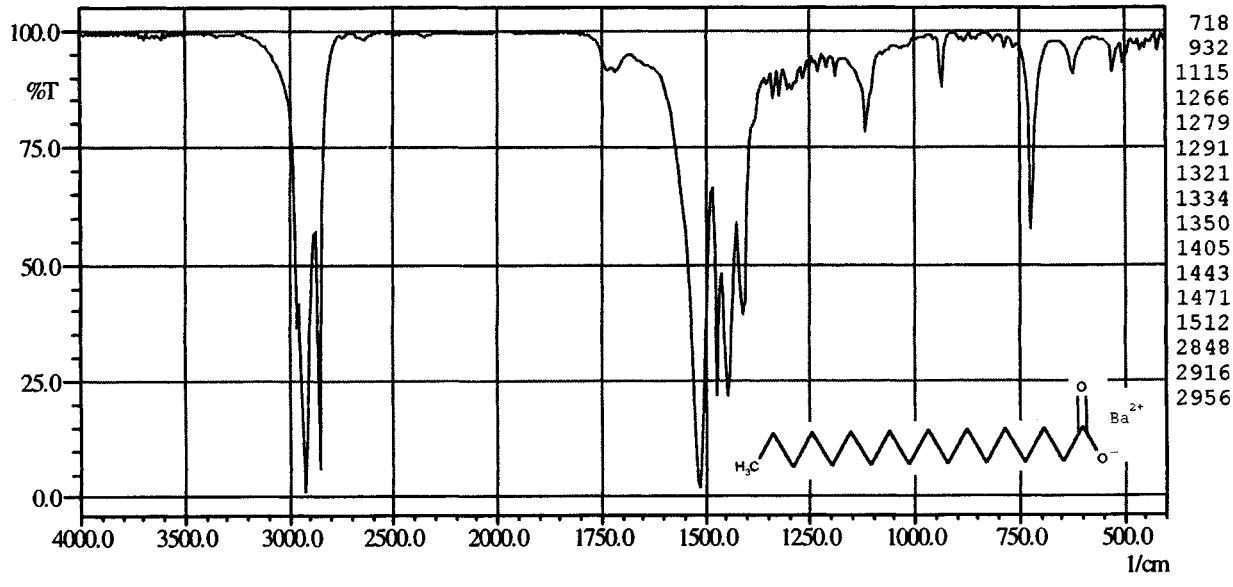
(1) **Mg stearate**
(2) Liga Magnesiumsterat MG tech.
(3) Peter Greven Fettchemie
(4) 591.3 g mol^{-1}
(5) lubricant
(6) colourless solid
(7) 140 °C
(13) KBr pellet

4139 $C_{36}H_{70}O_4Ca$



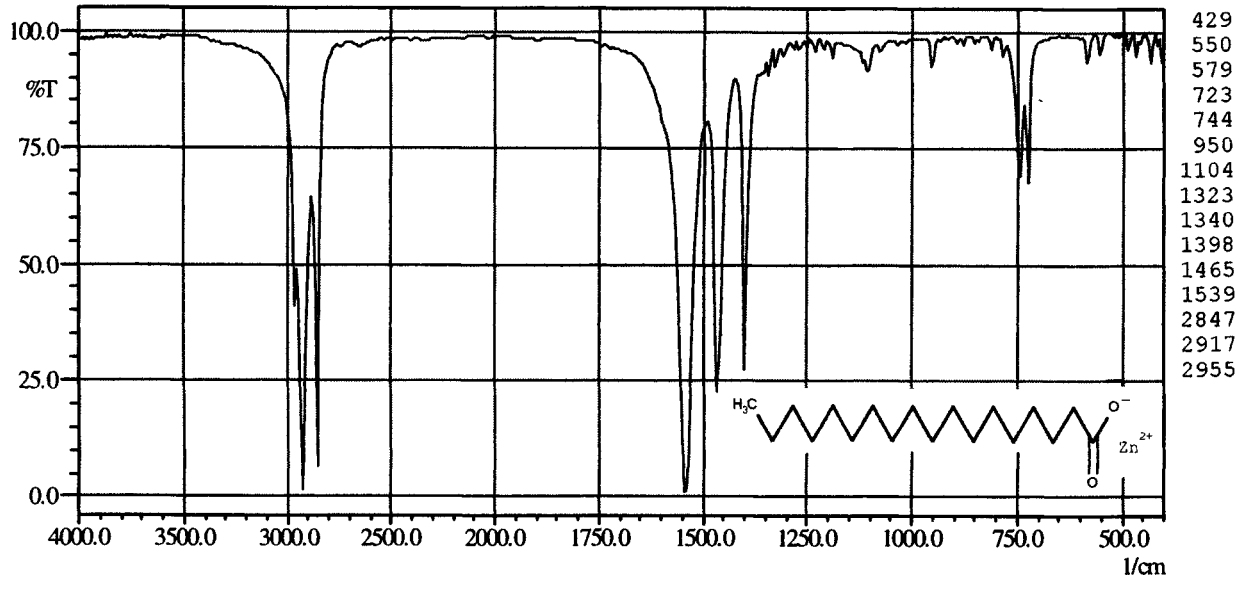
(1) **Ca stearate**
(2) Liga Calciumsterat CA 800
(3) Peter Greven Fettchemie
(4) 607.0 g mol^{-1}
(5) lubricant, stabiliser
(6) colourless solid
(13) KBr pellet

4139 $C_{36}H_{70}O_4Ba$



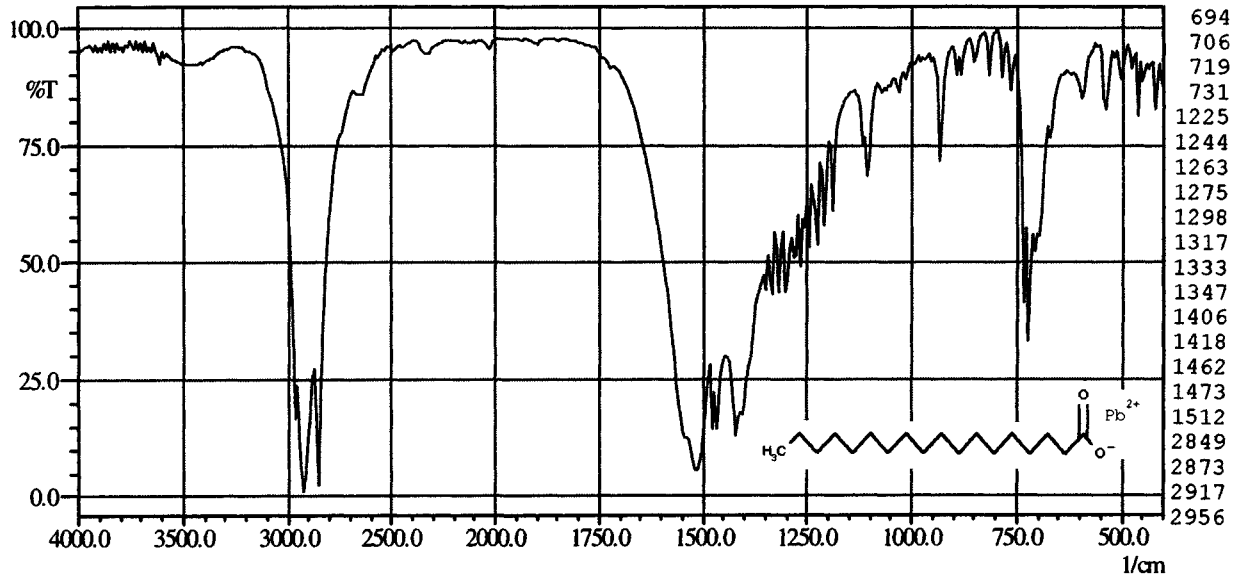
(1) **Ba stearate**
(2) Liga Bariumsterat
(3) Peter Greven Fettchemie
(4) 704.3 g mol^{-1}
(5) lubricant, stabiliser component
(6) colourless solid
(7) 200 °C
(13) KBr pellet

4139 $C_{36}H_{70}O_4Zn$



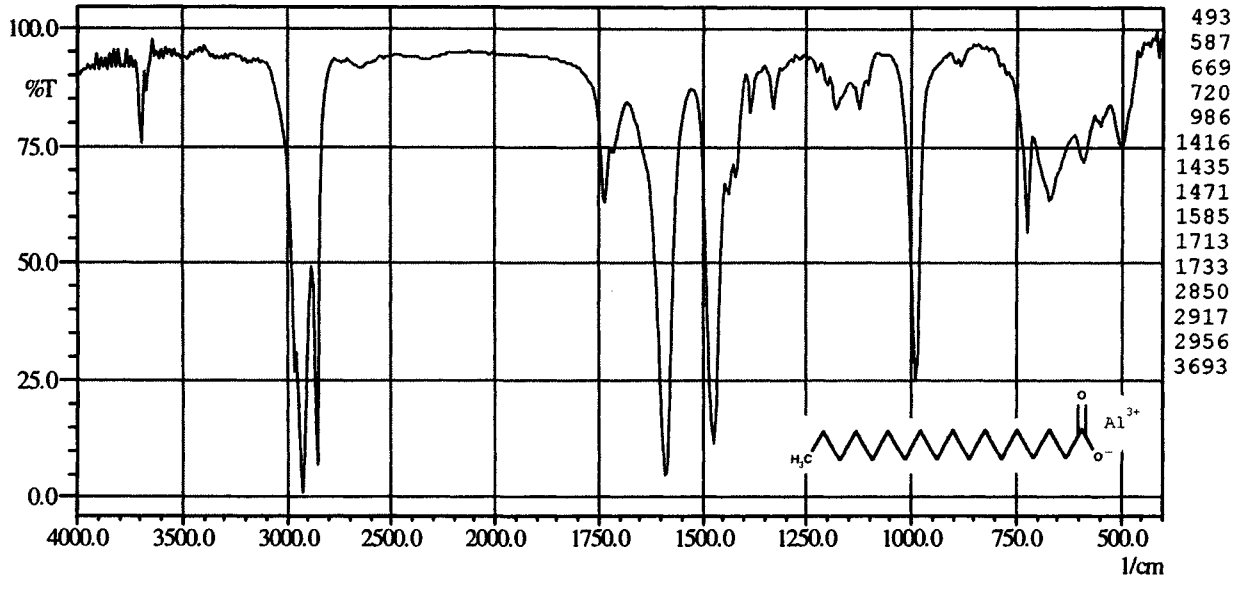
(1) **Zn stearate**
(2) Stabiol ZN 592
(3) Henkel
(4) 632.3 g mol^{-1}
(5) co-stabiliser
(6) colourles solid
(7) 120 °C
(9) 1.13 g cm^{-3}
(13) KBr pellet

4139 $C_{36}H_{70}O_4Pb$



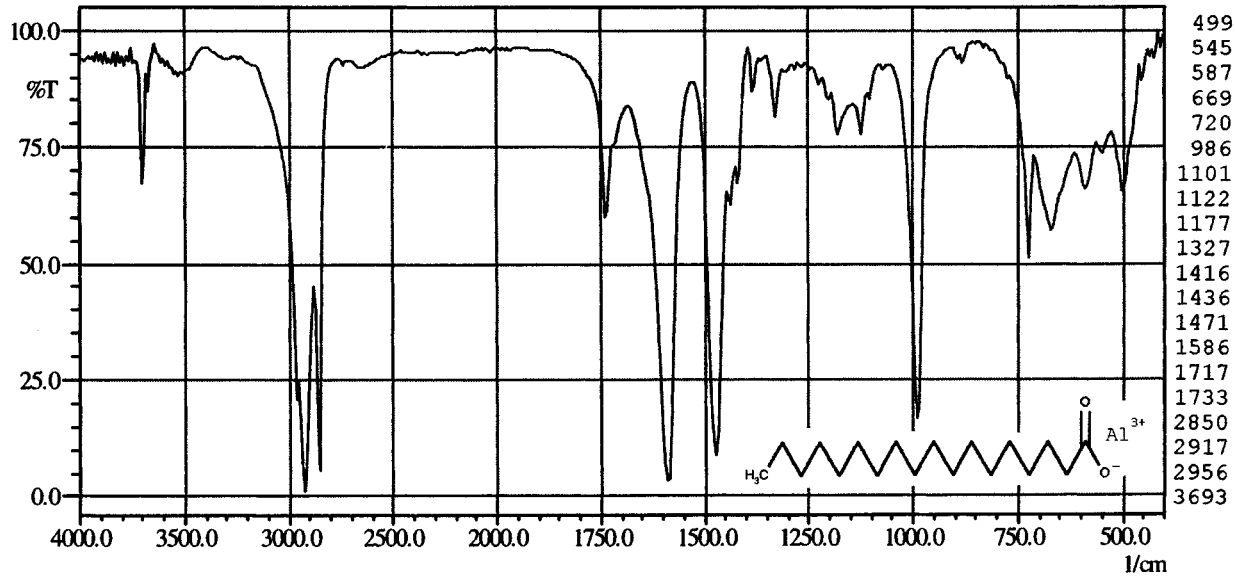
(1) **Pb stearate**
(2) Liga Bleistearat B 28
(3) Peter Greven Fettchemie
(4) 774.2 g mol^{-1}
(5) lubricant
(6) colourless solid
(7) 105 °C
(13) KBr pellet

4139 $C_{54}H_{105}O_6Al$



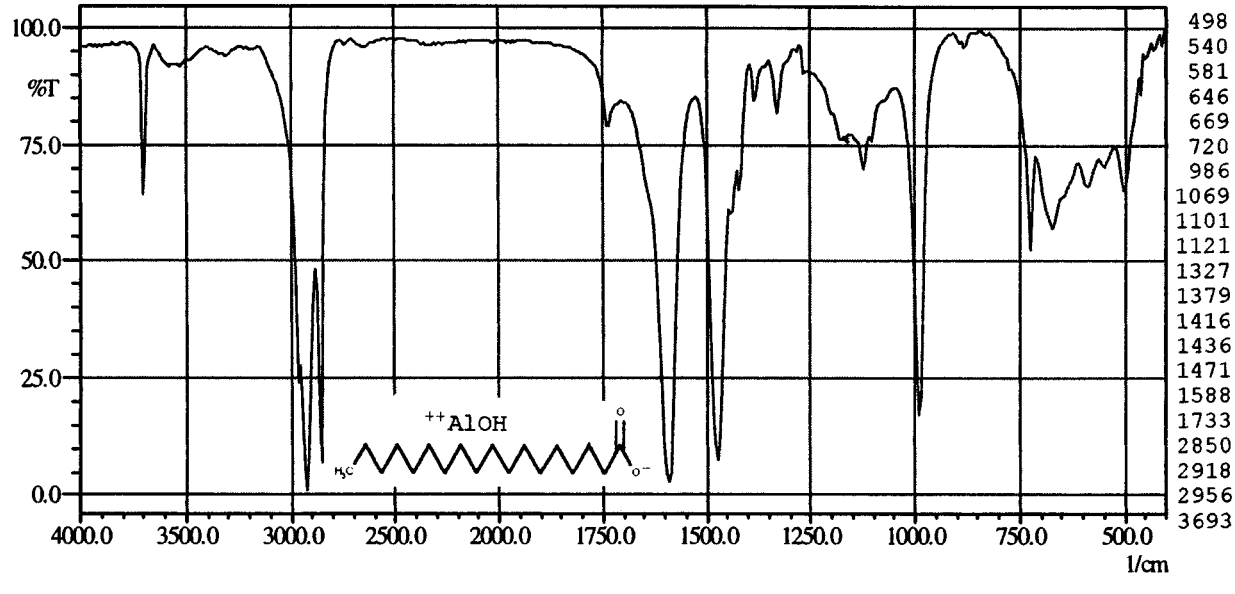
(1) **Al tristearate**
(2) Liga Aluminiumsterat TR
(3) Peter Greven Fettchemie
(4) 877.4 g mol^{-1}
(5) lubricant, stabiliser
(6) colourless solid
(13) KBr pellet

4139 $C_{54}H_{105}O_6Al$



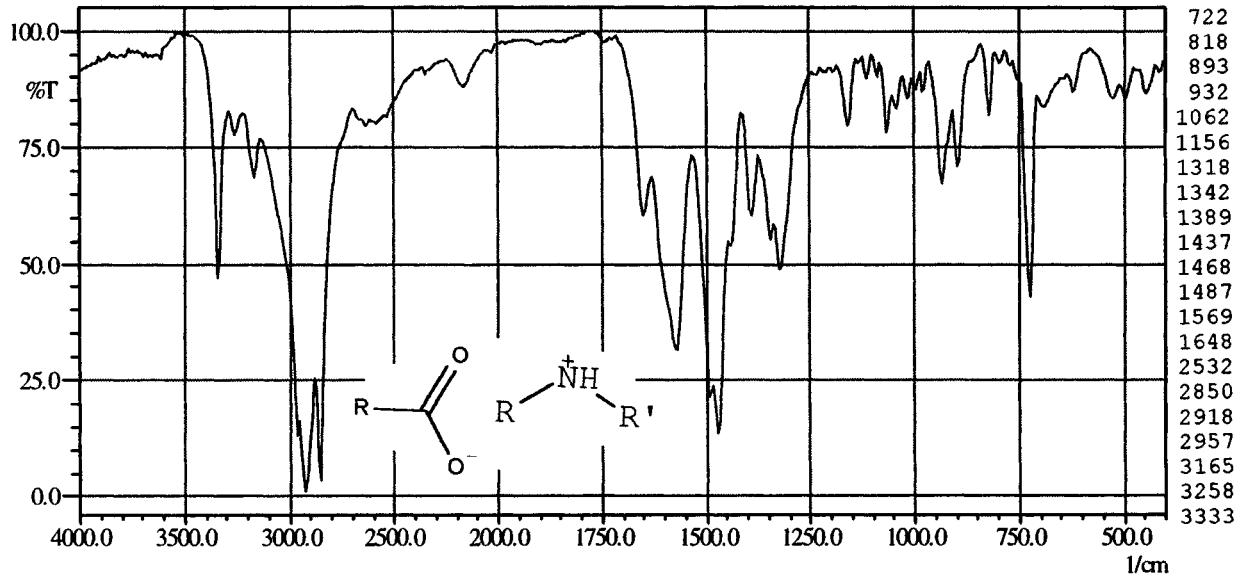
(1) **Al di-tri-stearate**
(2) Liga Aluminiumsterat DT
(3) Peter Greven Fettchemie
(4) 877.4 g mol^{-1}
(5) lubricant, stabiliser
(6) colourless solid
(7) 135 °C
(13) KBr pellet

4139 $C_{36}H_{75}O_5Al$



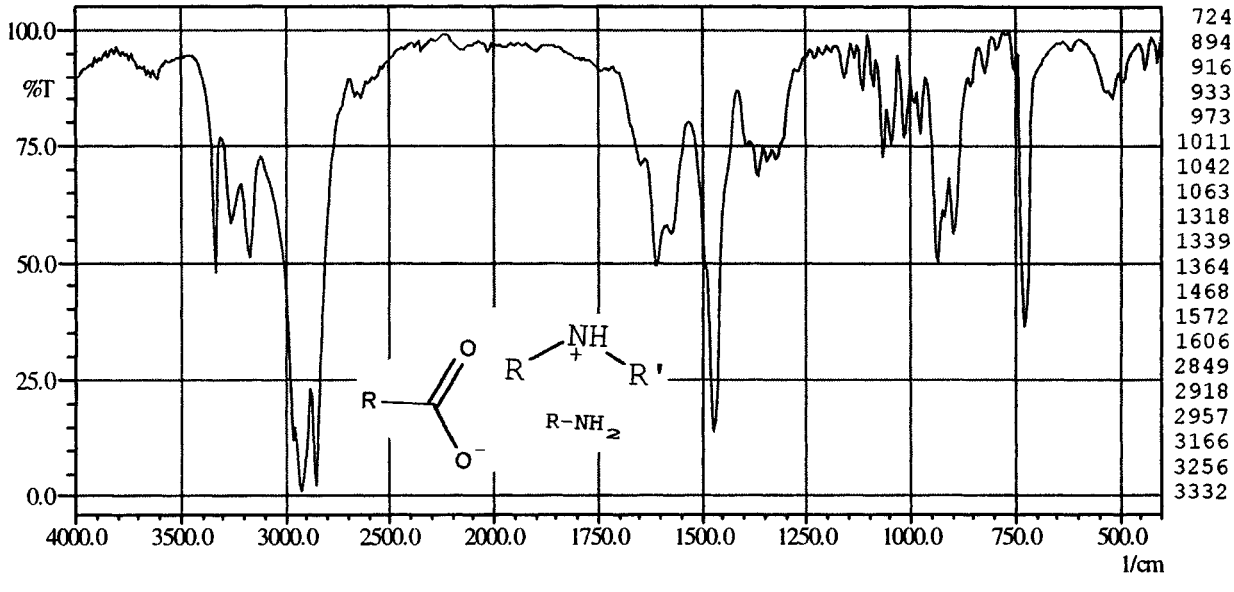
(1) **Al distearate**
(2) Liga Aluminiumstearat D2
(3) Peter Greven Fettchemie
(4) 615 g mol^{-1}
(5) lubricant, stabiliser
(6) colourless solid
(13) KBr pellet

414



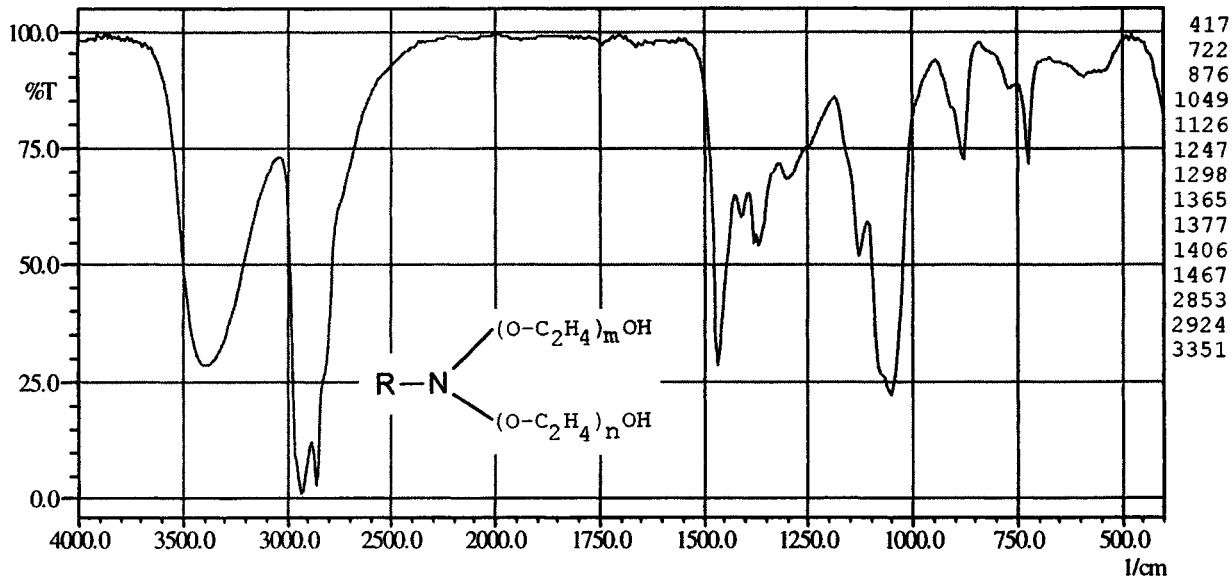
(1) **fatty amine**
(2) Armeen HTD
(3) Akzo Chemie
(5) lubricant
(6) colourless flakes
(13) KBr pellet

414



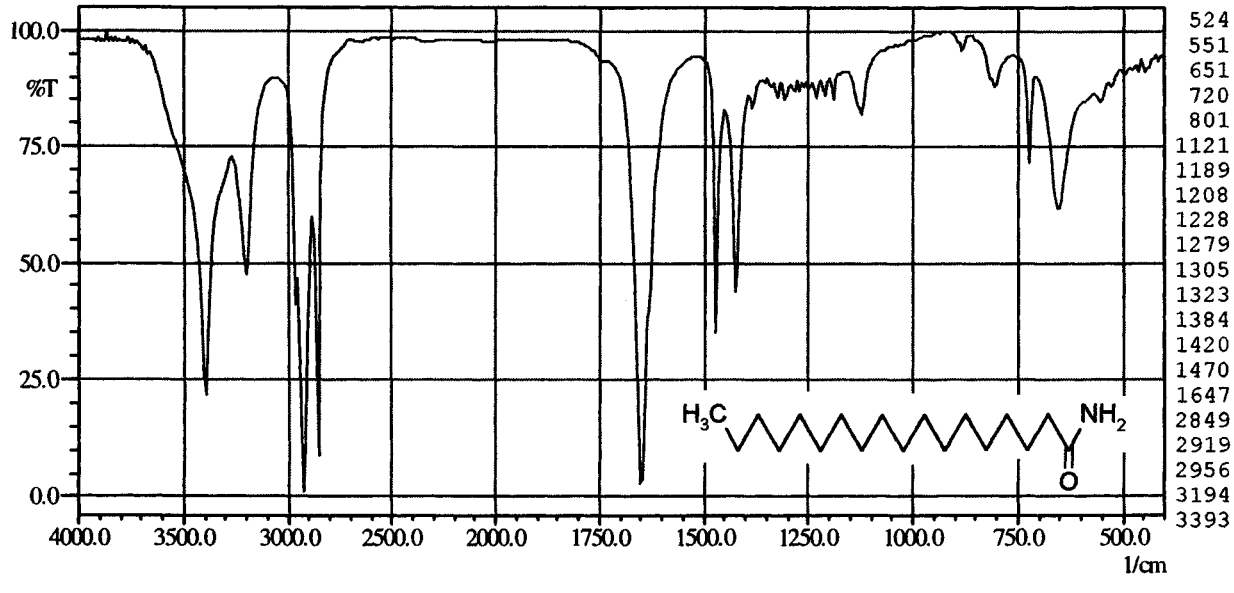
(1) **fatty amine**
(2) Armeen IOD
(3) Akzo Chemie
(5) lubricant
(6) colourless flakes
(13) KBr pellet

414



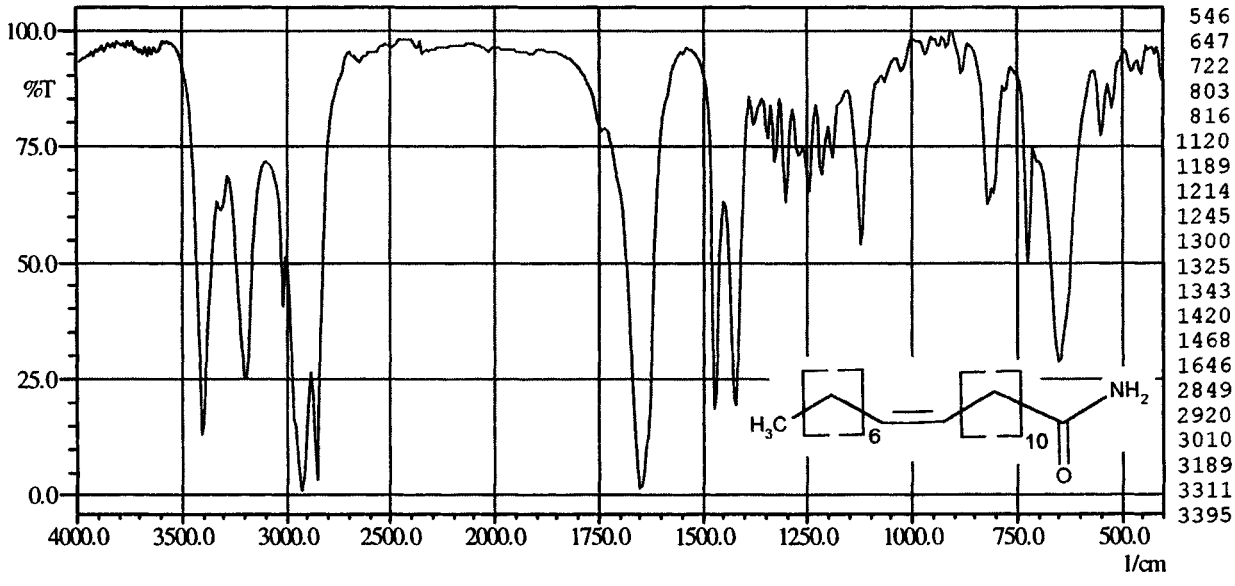
(1) **ethoxylated fatty amine**
(2) Hostastat FA 14
(3) Hoechst
(5) antistatic
(6) yellowish, clear, low viscosity liquid
(7) 5 °C
(9) 0.9 g cm^{-3}
(13) layer btw KBr

415 $C_{18}H_{37}NO$



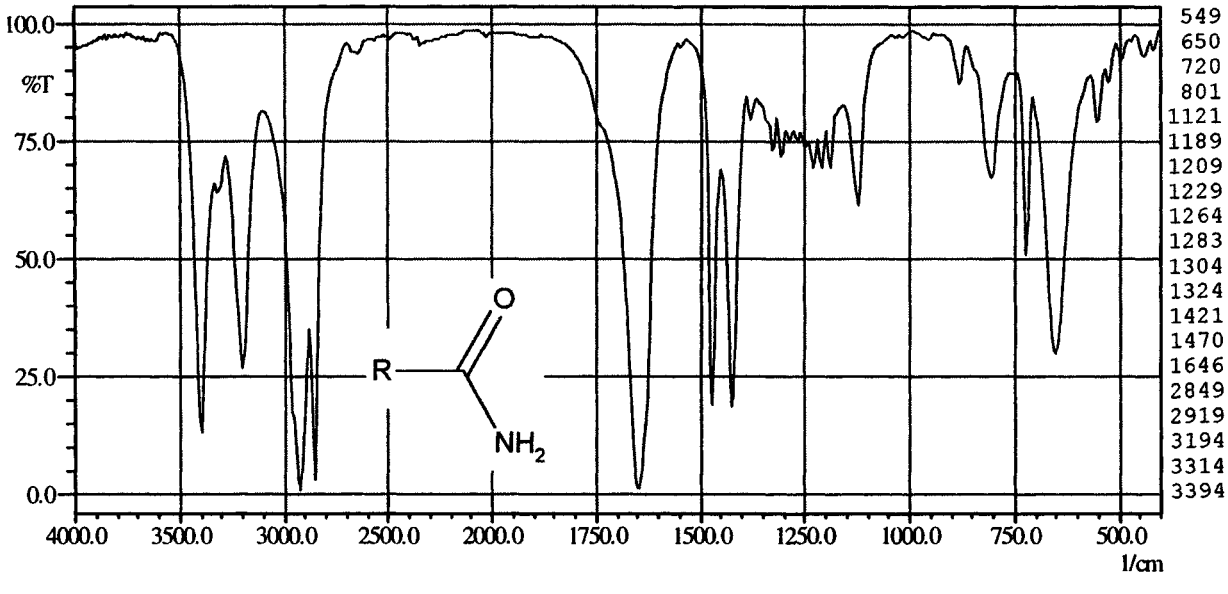
(1) **stearylamide**
(2) Loxamid S
(3) Henkel
(4) 283.5 g mol^{-1}
(5) separating agent
(6) colourless beads
(7) 97.5 °C
(13) KBr pellet

415 $C_{22}H_{43}NO$



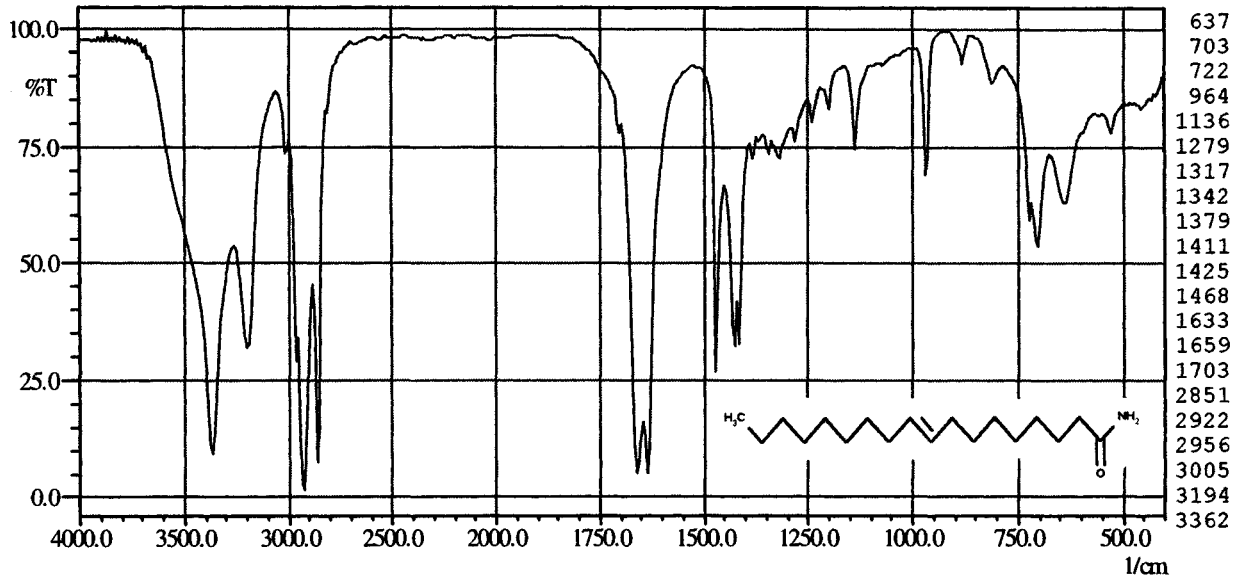
(1) **erucamide**
(2) Armid E
(3) Akzo Chemie
(4) 337.6 g mol^{-1}
(5) lubricant, antiblocking agent
(6) slightly yellowish flakes
(13) KBr pellet

415



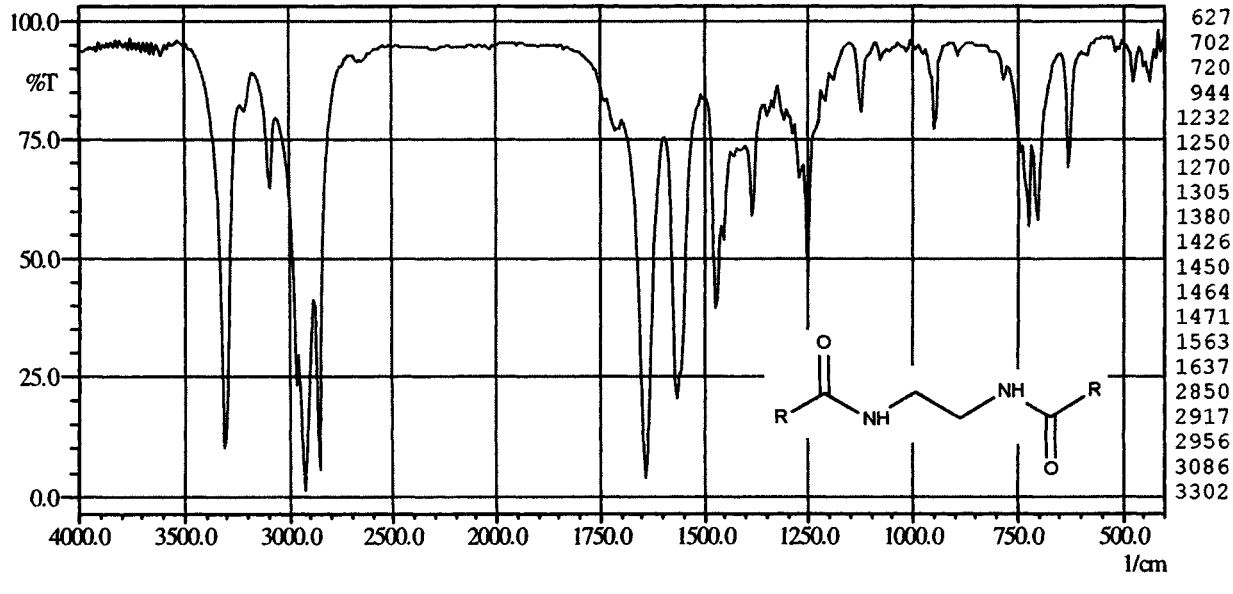
(1) **hydrogenated tallowamide**
(2) Armid HT
(3) Akzo Chemie
(5) lubricant, antiblocking agent
(6) colourless flakes
(13) KBr pellet

415 $C_{18}H_{35}NO$



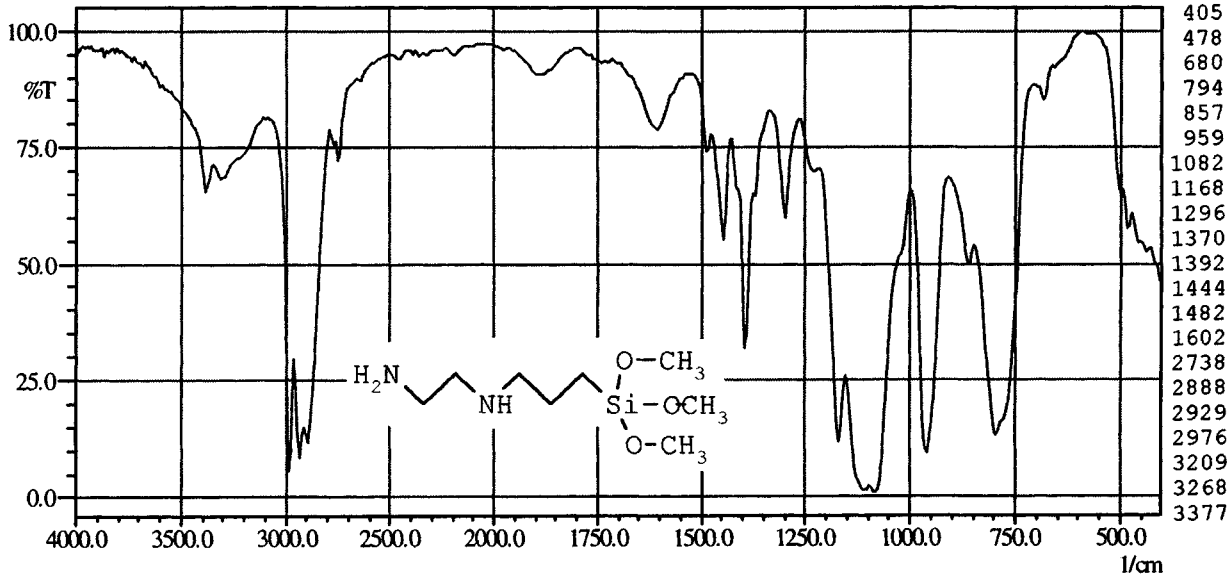
(1) **oleylamide, partially isomerised to elaidic amide**
(2) Loxamid OA
(3) Henkel
(4) 281.5 g mol^{-1}
(5) lubricant, slip agent
(6) colourless solid
(7) 73.5 °C
(13) KBr pellet

415



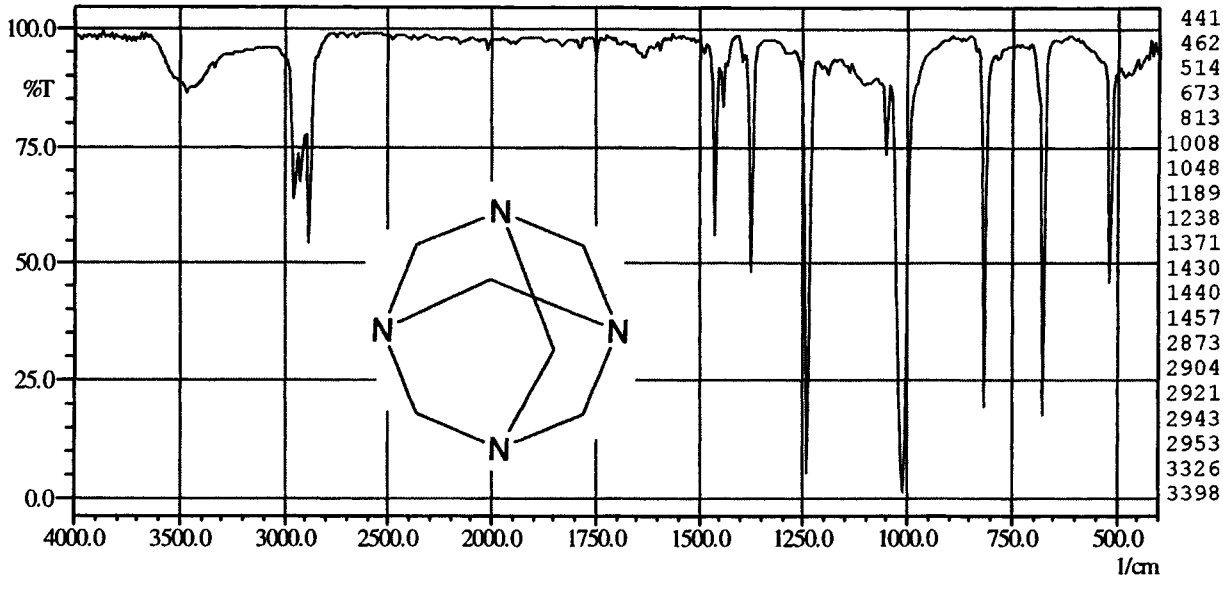
(1) **secondary amide wax**
(2) Baerolub L-AK
(3) Baerlocher
(5) lubricant
(6) colourless solid
(7) 139 °C
(9) 1.02 g cm^{-3}
(13) KBr pellet

4211 $SiH_8H_{22}N_2O_3$



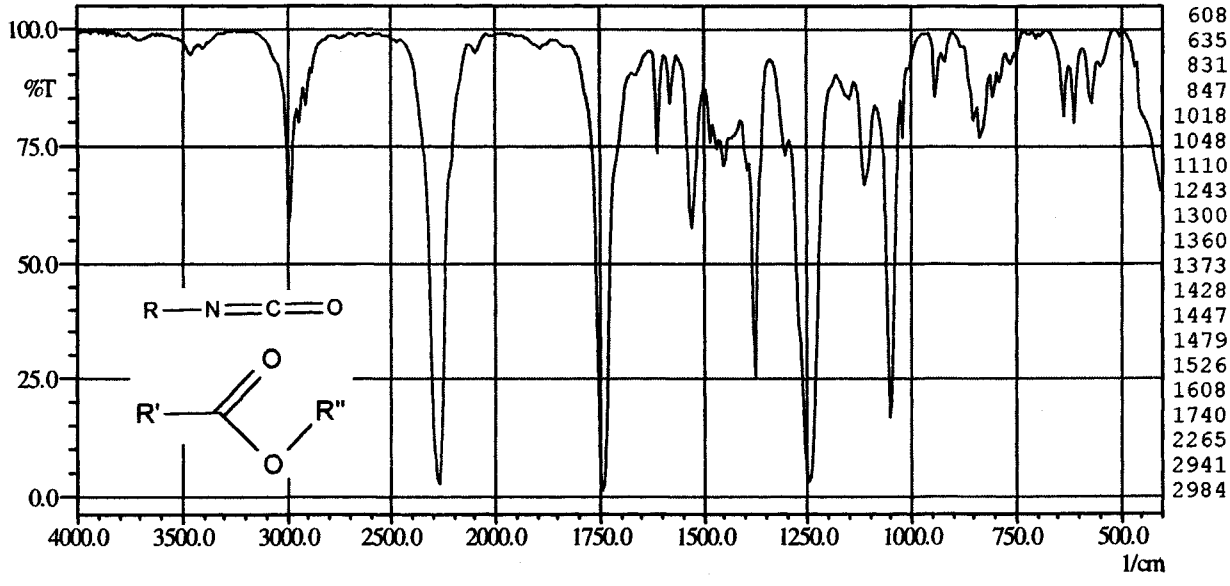
(1) **3-(2-aminoethylamino)propyltrimethoxysilane**
(2) Silane A 1100
(3) Freudenberg (Brunne collection)
(4) 222.4 g mol^{-1}
(5) adhesion promoter between inorganic substances
(6) colourless, clear liquid
(13) layer btw KBr

425 $C_6H_{12}N_4$



(1) **hexamethylenetetramine, 1,3,5,7-tetraazaadamantane**
(2) Cohedur H 30
(3) Bayer
(4) 140.2 g mol^{-1}
(5) adhesion agent
(6) colourless solid
(7) 280 °C
(9) 1.3 g cm^{-3}
(13) KBr pellet

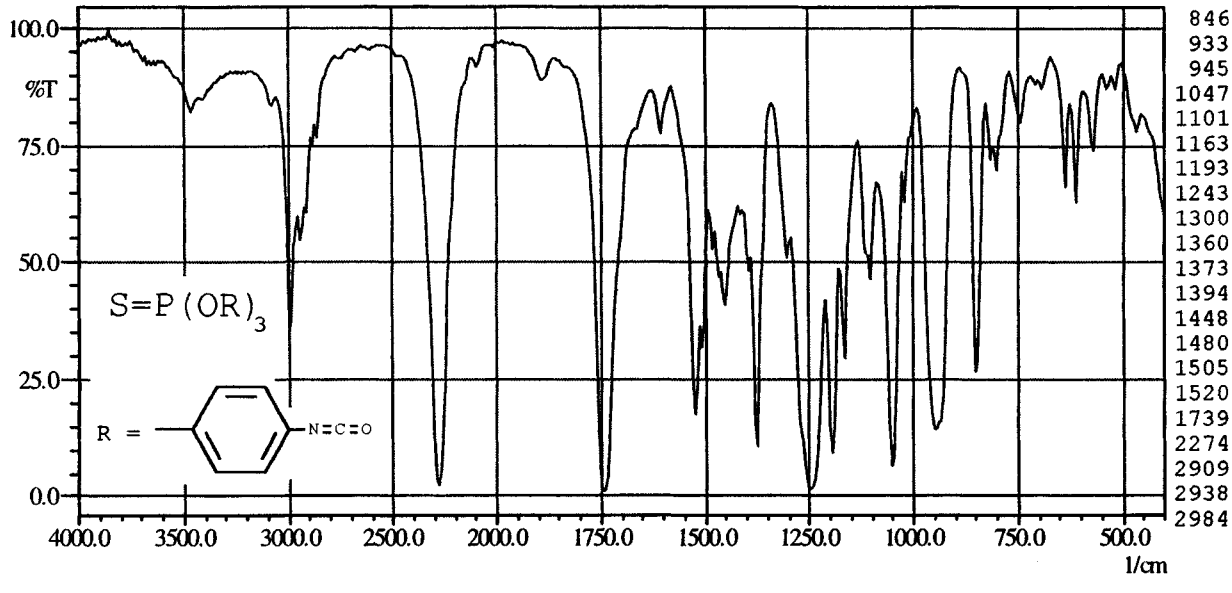
425



(1) **isocyanate with ester groups**
(2) Desmodur RE
(3) Bayer
(5) adhesion agent
(6) yellowish, clear liquid
(13) layer btw KBr

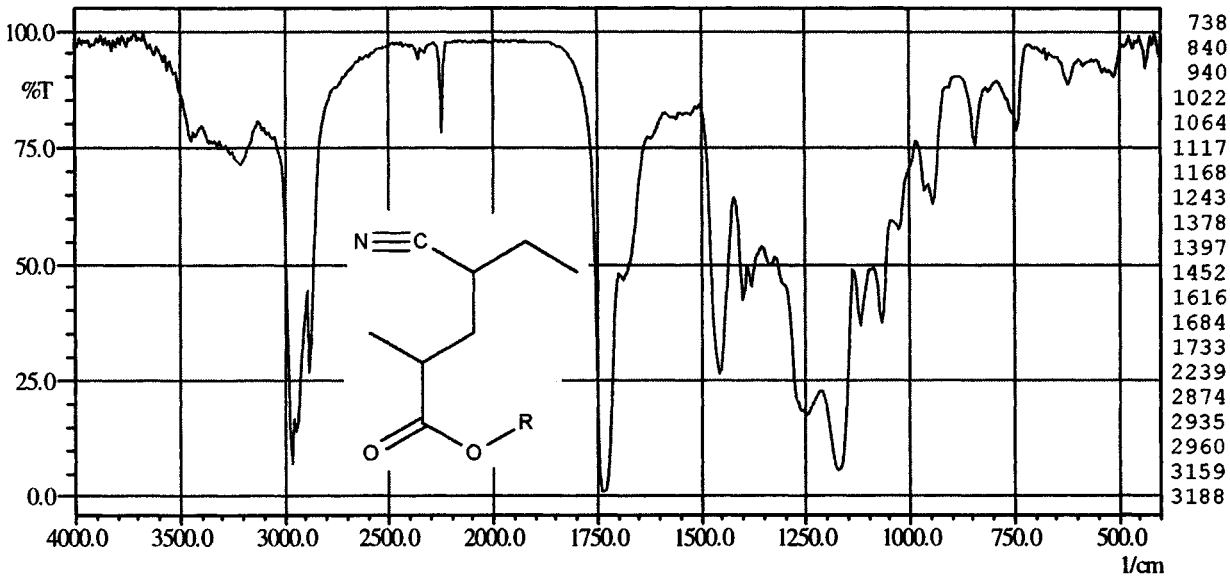
425

$C_{21}H_{12}N_3O_6$



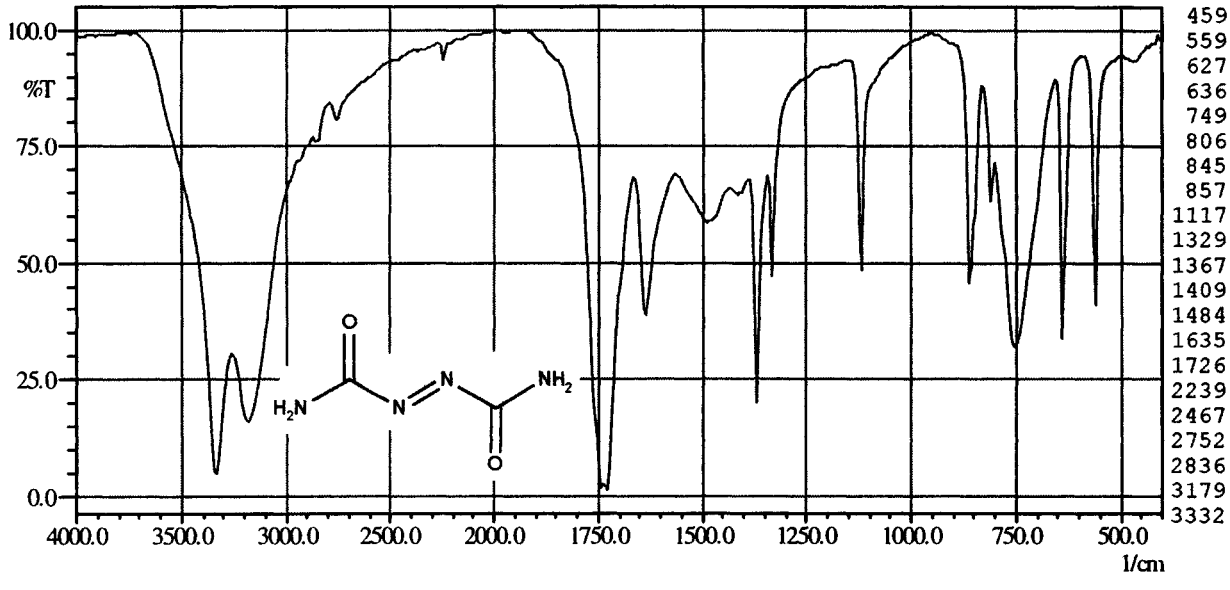
(1) **20% solution of thionophosphoric acid *tris*-(*p*-isocyanatophenyl)ester in CH_2Cl_2**
(2) Desmodur RF/E
(3) Bayer
(4) 465.4 g mol^{-1}
(5) adhesion agent
(6) pale brownish-yellow, clear liquid
(9) 1.32 g cm^{-3}
(13) dried layer on KBr
(14) structure is simplified, aliphatic substituents

425



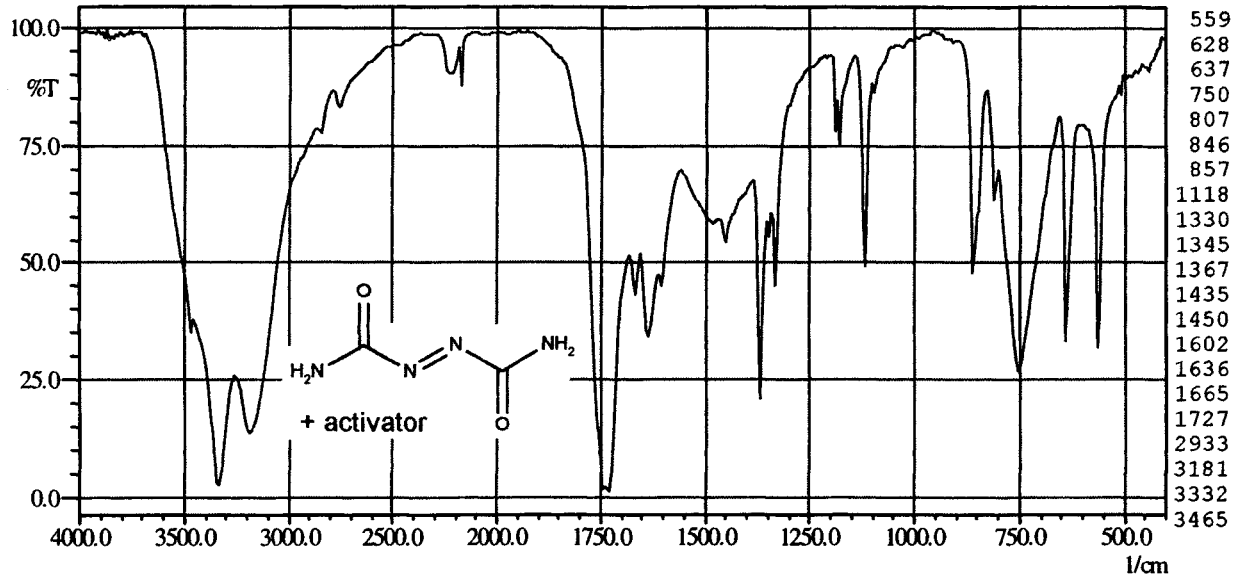
(1) **poly(acrylic ester-*co*-acrylonitrile)**
(2) Acralen AFR
(3) Bayer
(5) adhesion agent, adhesion improver
(6) yellowish, clear liquid
(9) 1.03 g cm^{-3}
(13) layer on KRS-5

4411 $C_2H_4N_4O_2$



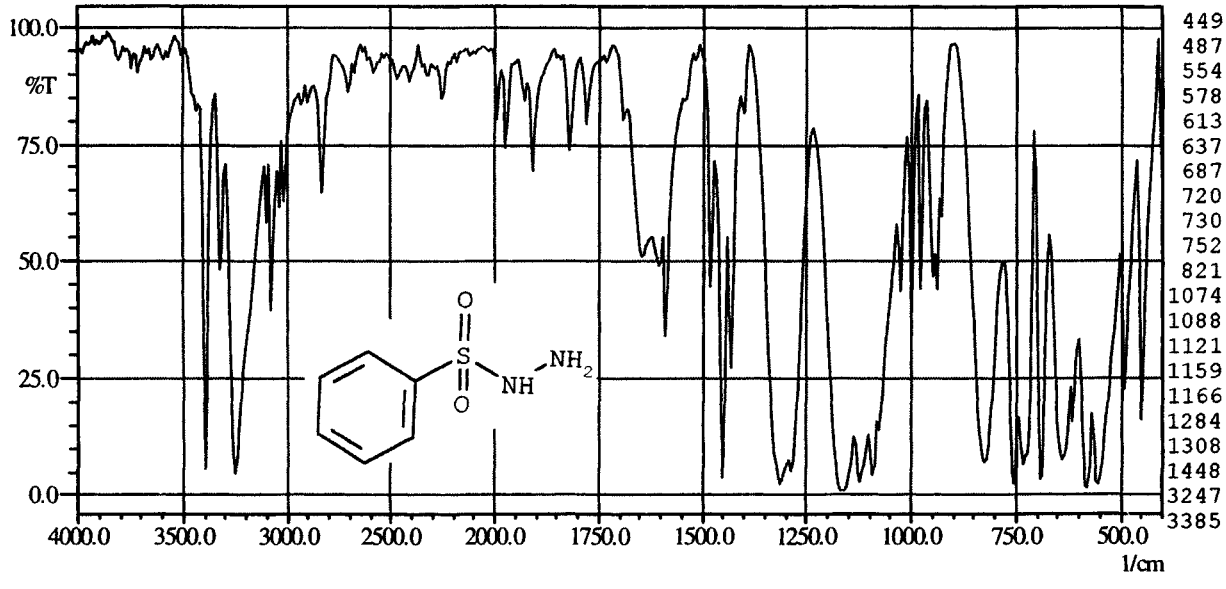
(1) **azodicarboxamide**
(2) Porofor ADC/M Pulver
(3) Bayer
(4) 116.1 g mol^{-1}
(5) blowing agent
(6) colourless solid
(13) KBr pellet

4411



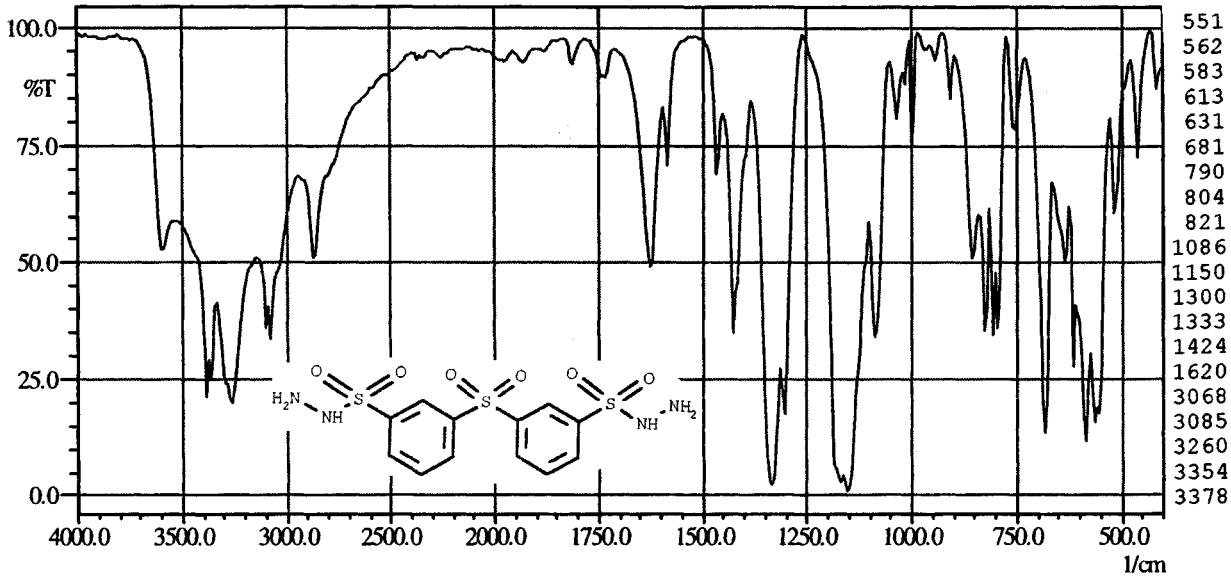
(1) **azodicarbamide and activator (9:1)**
(2) Porofor ADC/K
(3) Bayer
(5) blowing agent
(6) ochre-coloured solid
(13) KBr pellet

4412 $C_6H_8N_2O_2S$



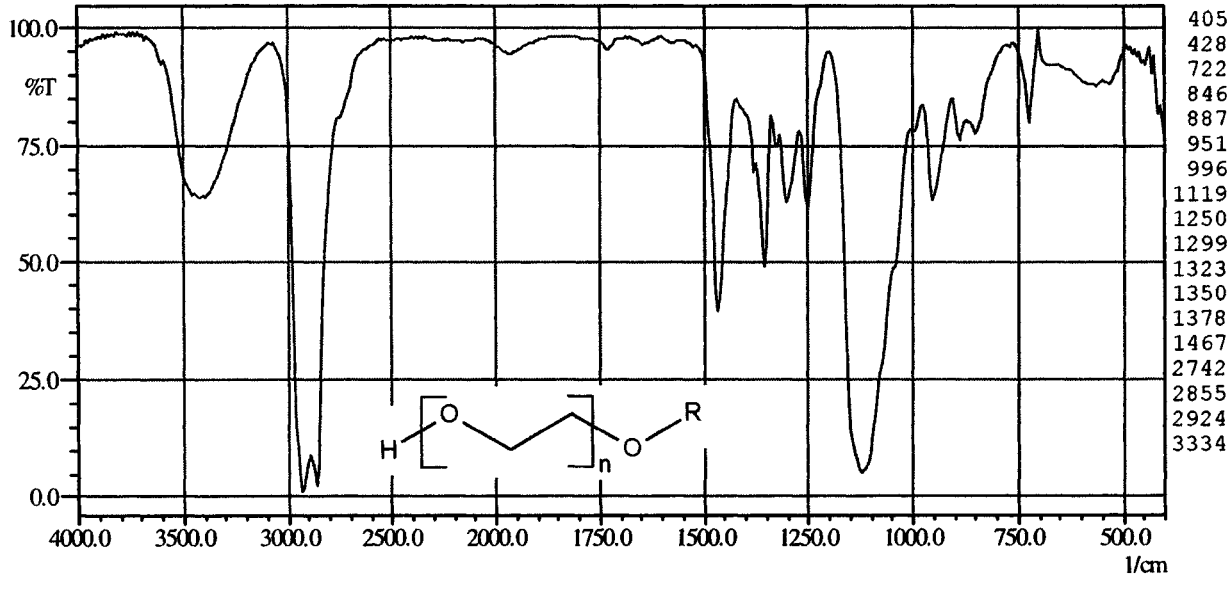
(1) **benzenesulfonohydrazide**
(2) Porofor BSH
(3) Bayer
(4) 172.2 g mol^{-1}
(5) blowing agent
(6) colourless solid
(13) KBr pellet

4412 $C_{12}H_{14}N_4O_6S_3$



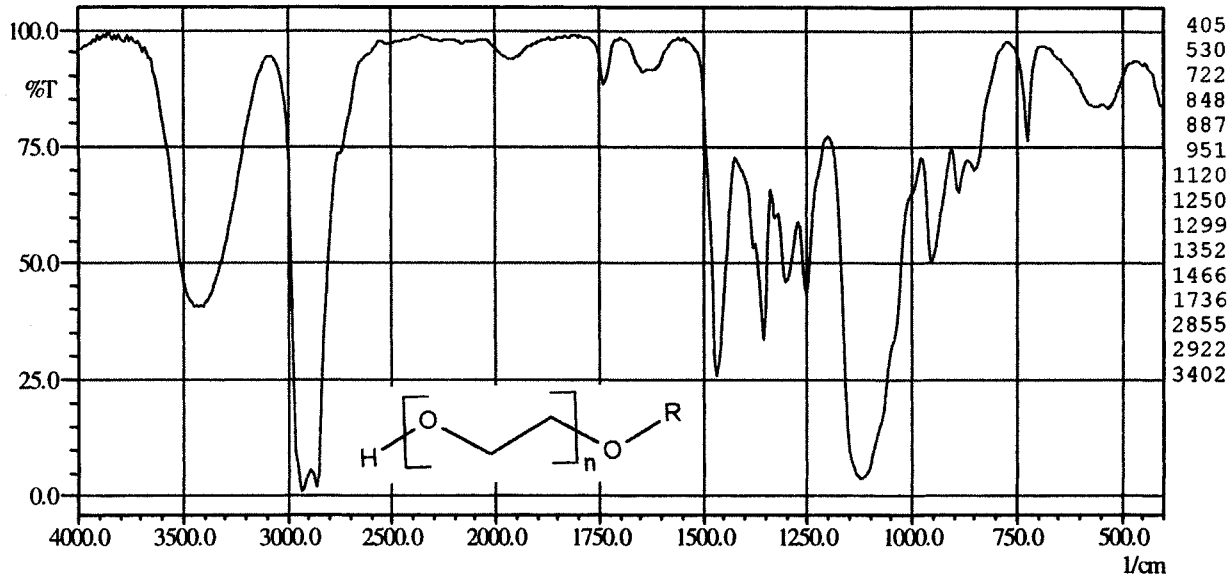
(1) **3,3'-diphenylsulfonedisulfonohydrazide**
(2) Porofor D 33
(3) Bayer
(4) 406.4 g mol^{-1}
(5) blowing agent
(6) colourless solid
(13) KBr pellet

451



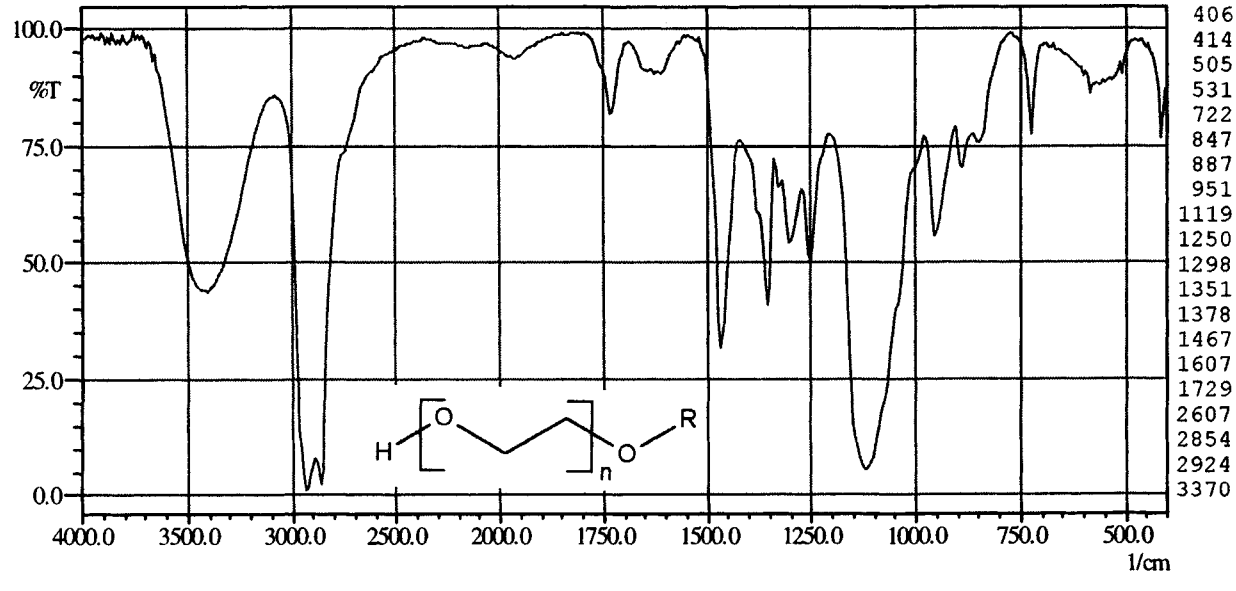
(1) **ethoxylated fatty alcohol**
(2) Meister H 9268
(3) Meister
(5) antistatic
(6) colourless liquid
(7) 13 °C
(9) 0.96 g cm^{-3}
(13) layer btw KBr

451



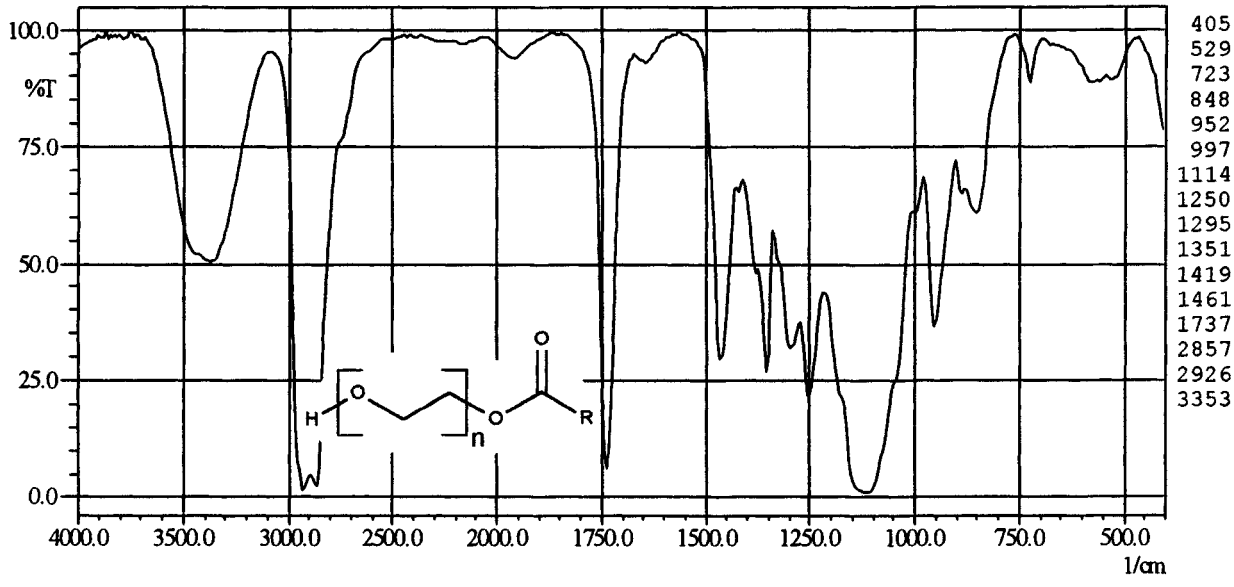
(1) **fatty alcohol-ethylene oxide adduct, poly(oxyethylene) etheralcohol**
(2) Dehydat 3204
(3) Henkel
(5) antistatic
(6) colourless, clear liquid
(9) 0.95 g cm^{-3}
(13) layer btw KBr

451



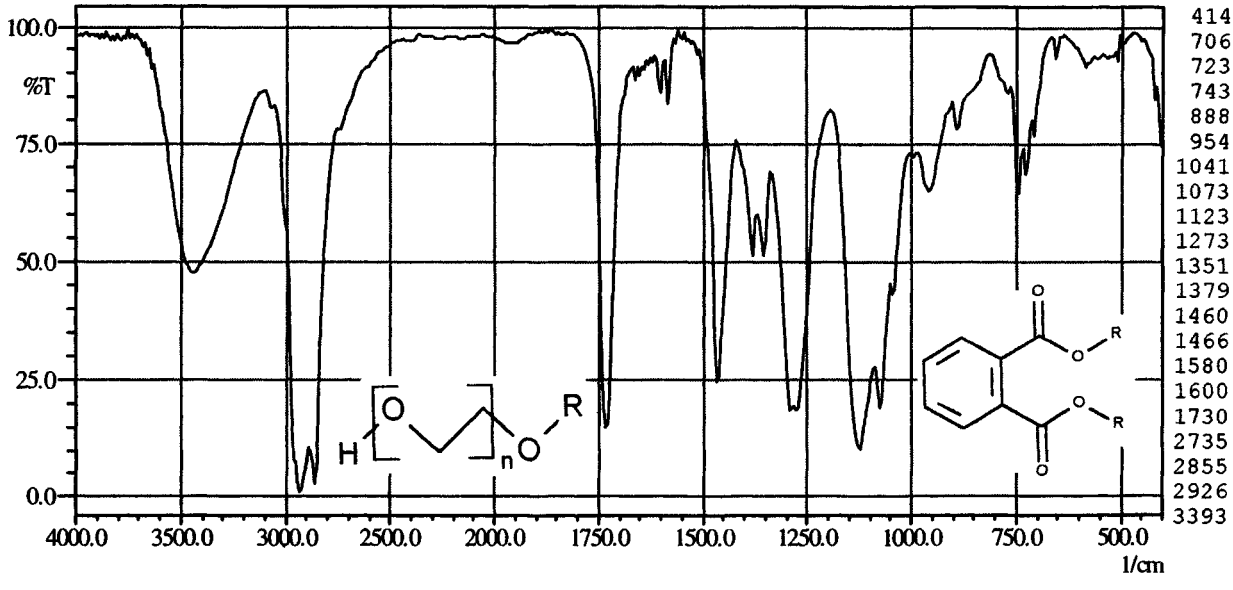
(1) **substituted fatty alcohol-ethyleneoxide adduct**
(2) Atepas K
(3) Dr. Th. Boehme
(5) viscosity modifier, plasticiser
(6) colourless, clear, viscous liquid
(7) 5 °C
(13) layer btw KBr

451



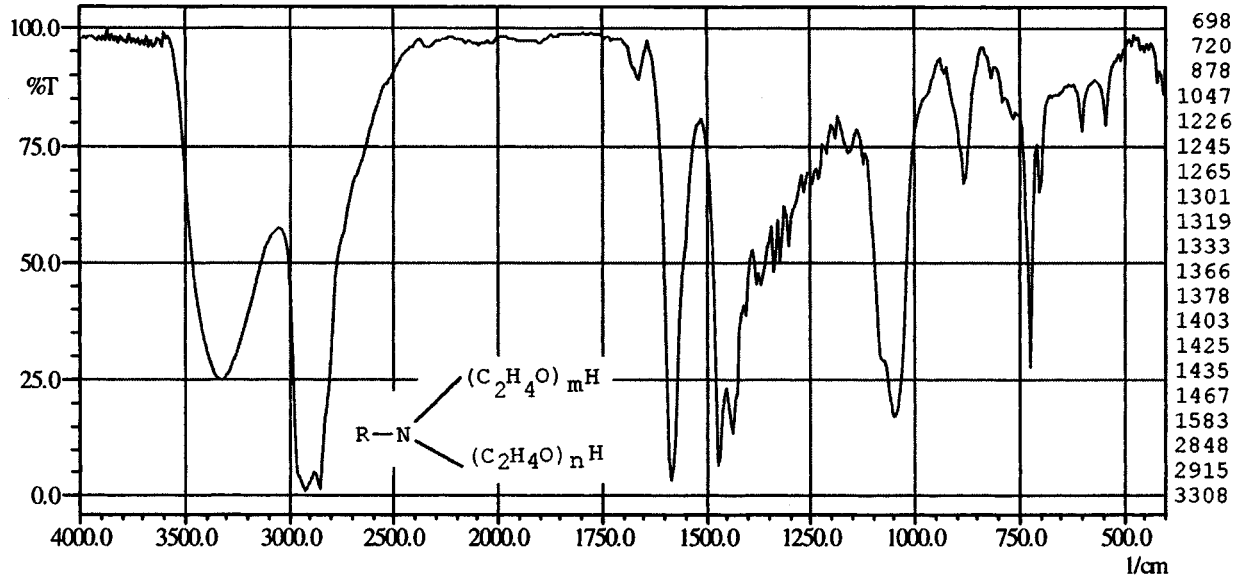
(1) **fatty acid-ethyleneoxide adduct, poly(oxyethylene)ester**
(2) Dehydat 22
(3) Henkel
(5) antistatic
(6) colourless, clear, oily liquid
(9) 1.033 g cm^{-3}
(13) layer btw KBr

451



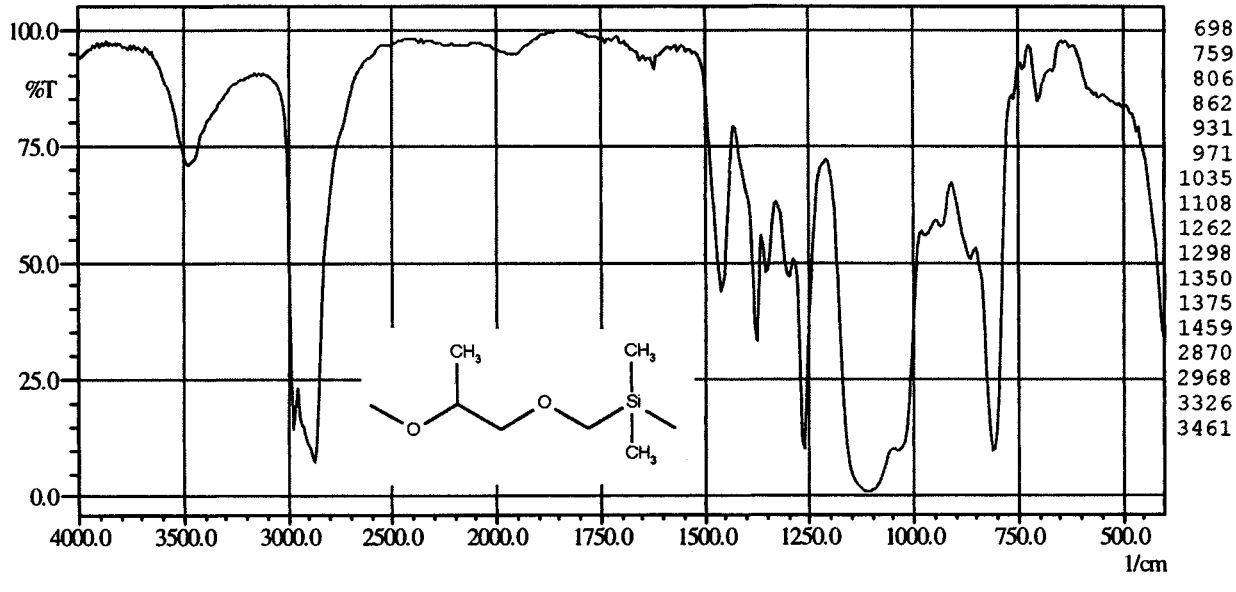
(1) **mixture of polyglycol ether and phthalate ester**
(2) Atepas U
(3) Dr. Th. Boehme
(5) viscosity modifier, plasticiser
(6) yellowish, clear, viscous liquid
(7) -10 °C
(13) layer btw KBr

451



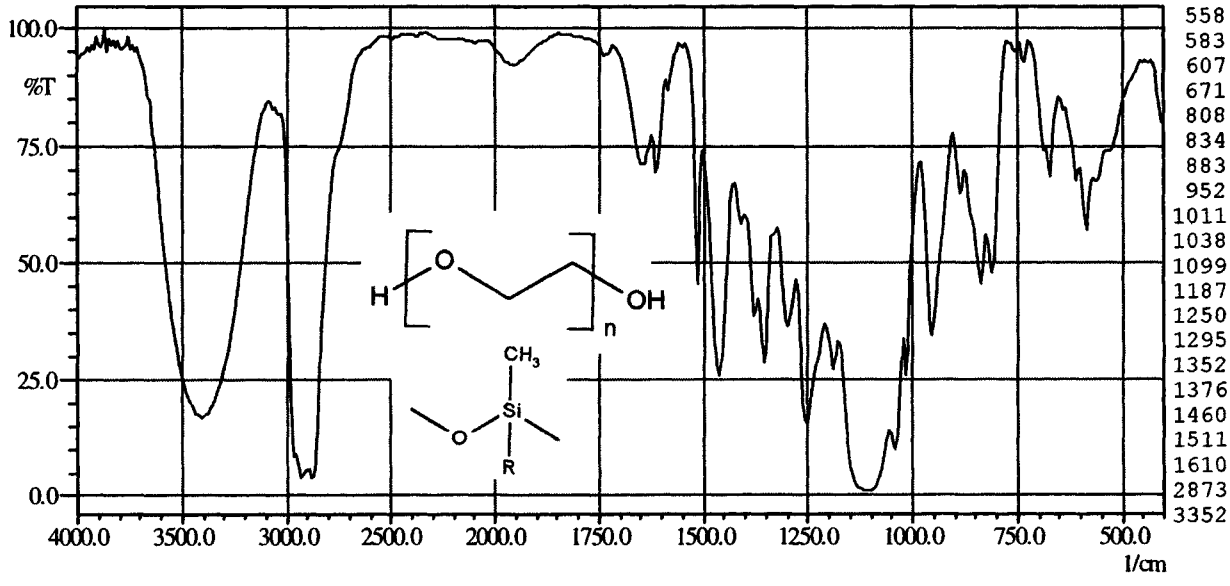
(1) **ethoxylated fatty amine**
(2) Hostastat FA 18
(3) Hoechst
(5) antistatic
(6) yellowish solid
(13) recrystallised film from melt

451



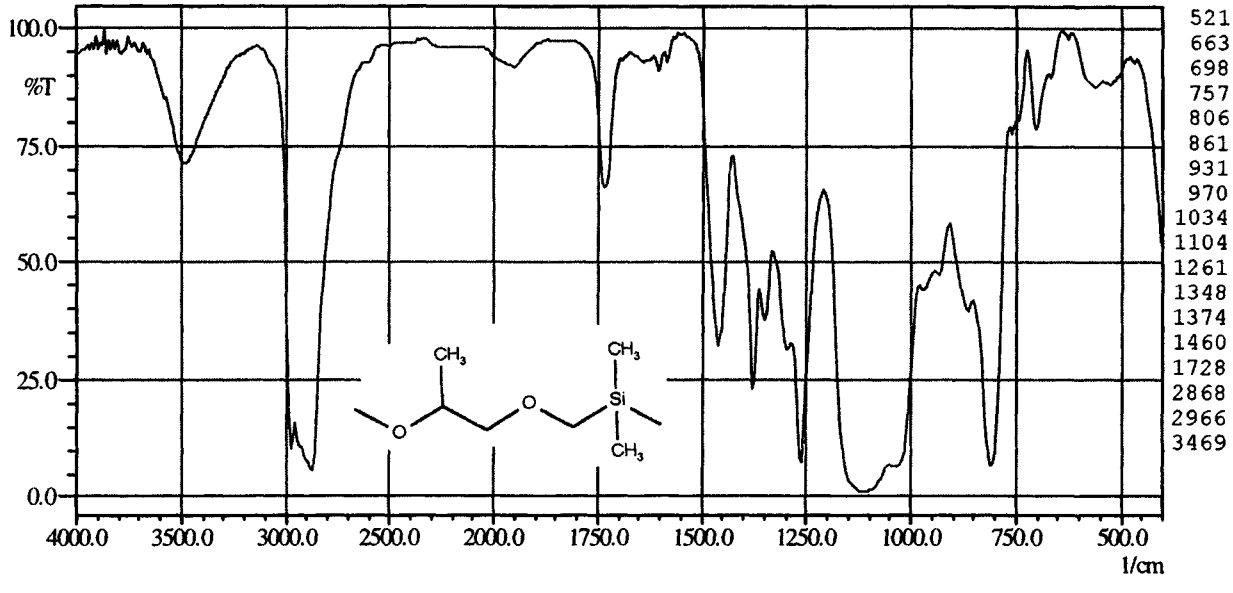
(1) **poly(oxyalkylene)-polysiloxane blockcopolymer**
(2) Tegostab B 1048
(3) Th. Goldschmidt
(5) foam stabiliser
(6) yellowish, clear liquid
(9) 1.04 g cm^{-3}
(13) layer btw KBr

451



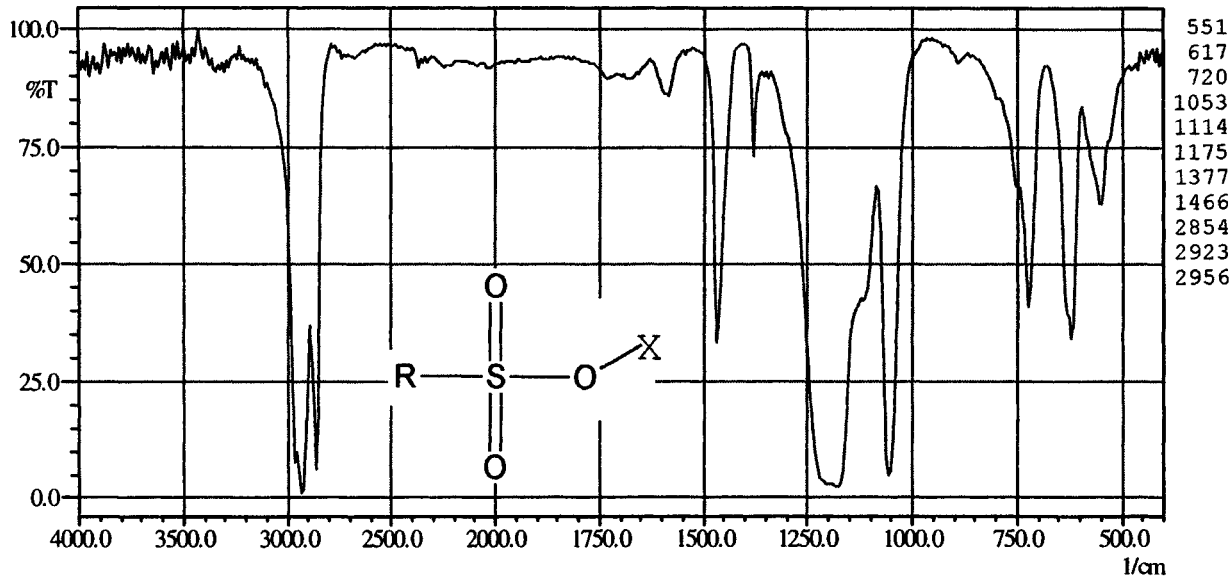
(1) **mixture of polyether-modified polysiloxane and surfactant**
(2) Tegostab B 5055
(3) Th. Goldschmidt
(5) foam stabiliser
(6) yellowish, clear liquid
(7) –20 °C
(9) 1.07 g cm^{-3}
(13) layer btw KBr

451



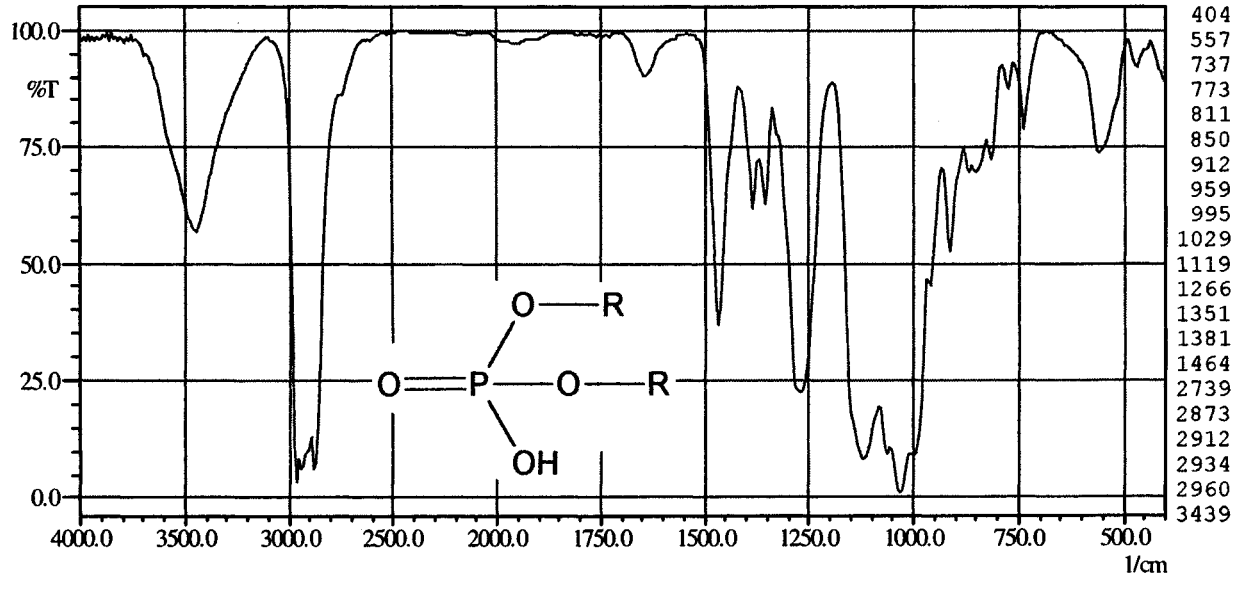
(1) **poly(oxyalkylene)-polysiloxane blockcopolymer**
(2) Tegostab B 1400 A
(3) Th. Goldschmidt
(5) foam stabiliser
(6) yellowish, clear liquid
(9) 1.04 g cm^{-3}
(13) layer btw KBr

451



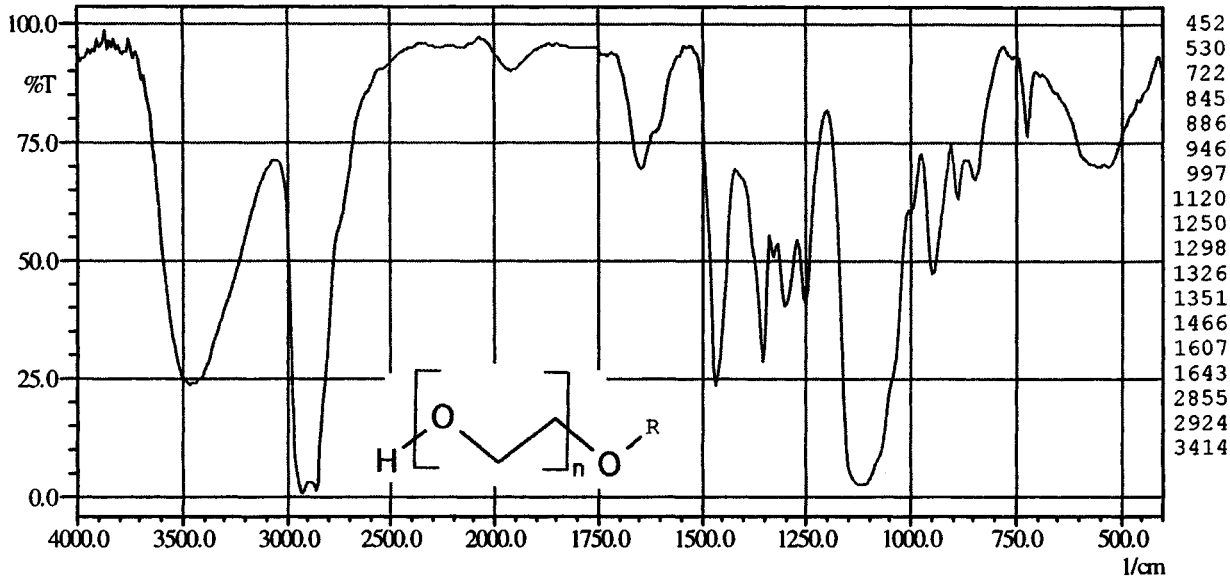
(1) **alkane sulfonate**
(2) Hostastat HS 1
(3) Hoechst
(5) antistatic
(6) colourless solid
(13) KBr pellet

451



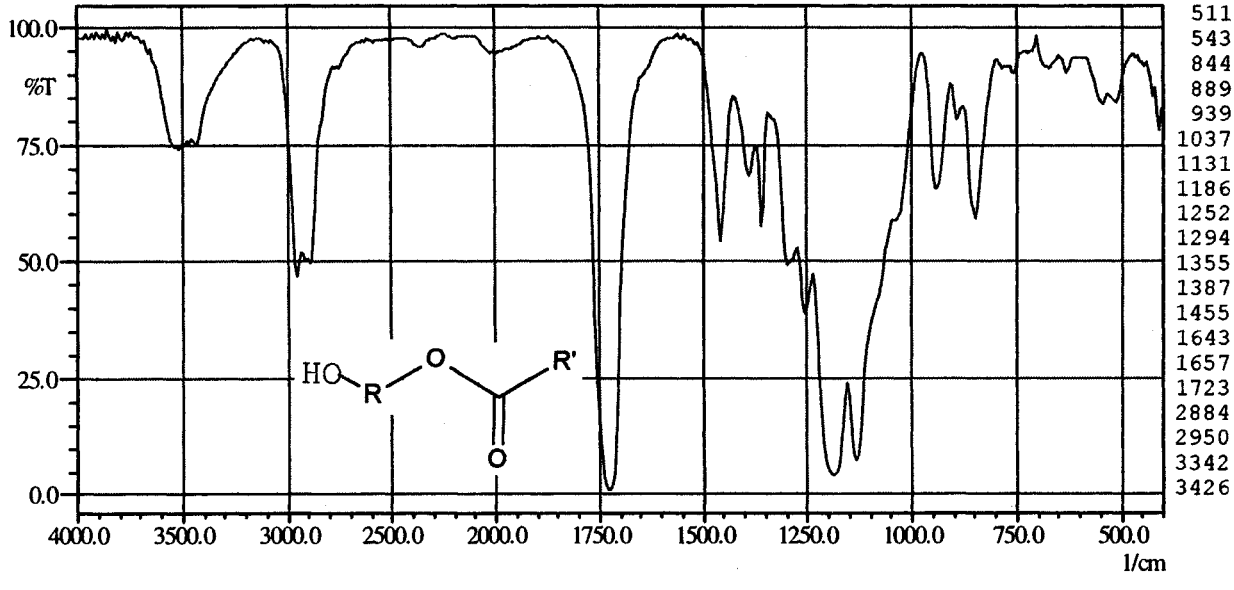
(1) **phosphoric acid ester and ethoxylated fatty alcohol**
(2) Ruco-Netzer VF
(3) Rudolf Chemie
(5) wetting agent for textile dyeing
(6) colourless, clear liquid
(13) layer btw KBr

452



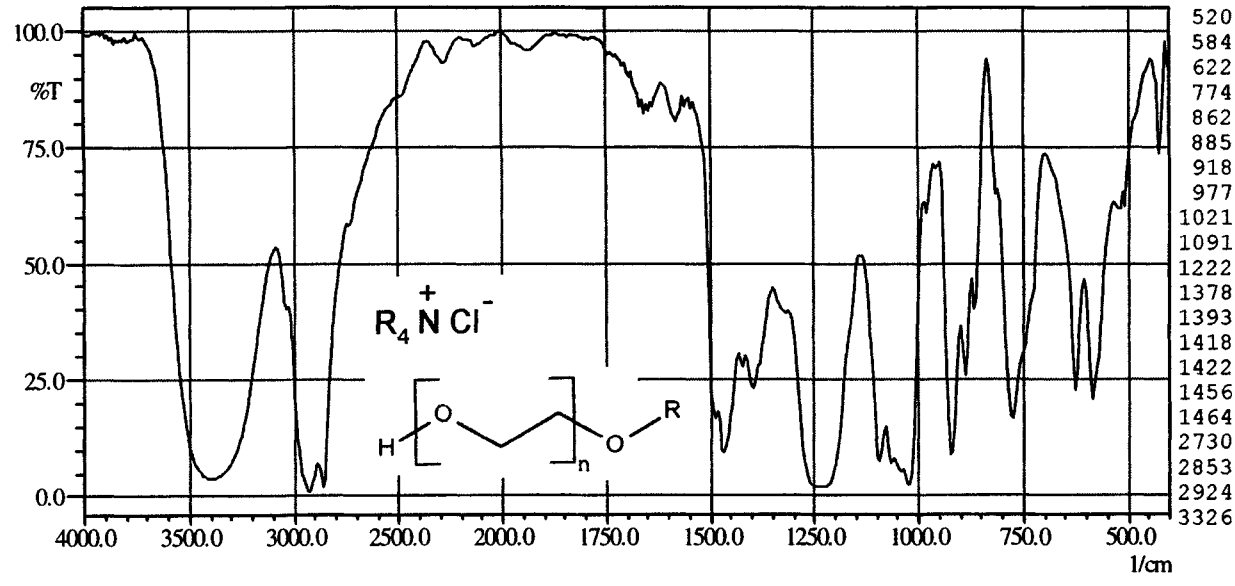
(1) **alkylpolyglycolether and ethoxylated fatty alcohol**
(2) Ruco-Egalisierer RF
(3) Rudolf Chemie
(5) leveling agent for textile dyeing
(6) yellowish, clear liquid
(13) layer btw KBr

452



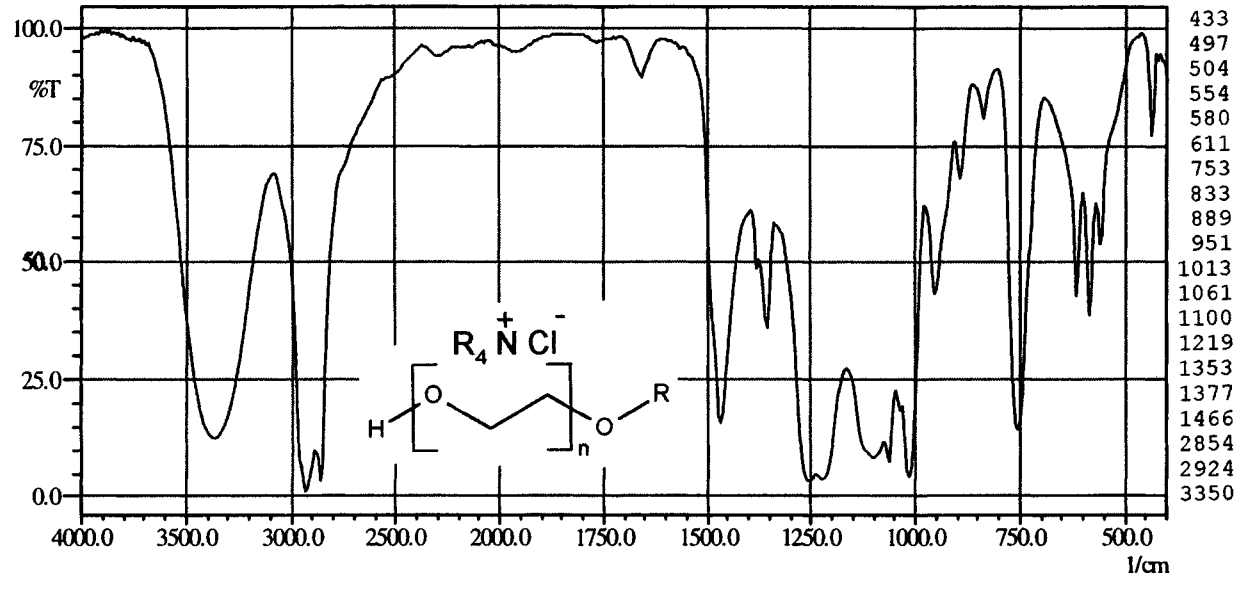
(1) **aliphatic esteralcohol**
(2) Verolan GBK
(3) Rudolf Chemie
(5) acid-producing component for acid-dyeing
(6) colourless, clear liquid
(13) layer btw KBr

453



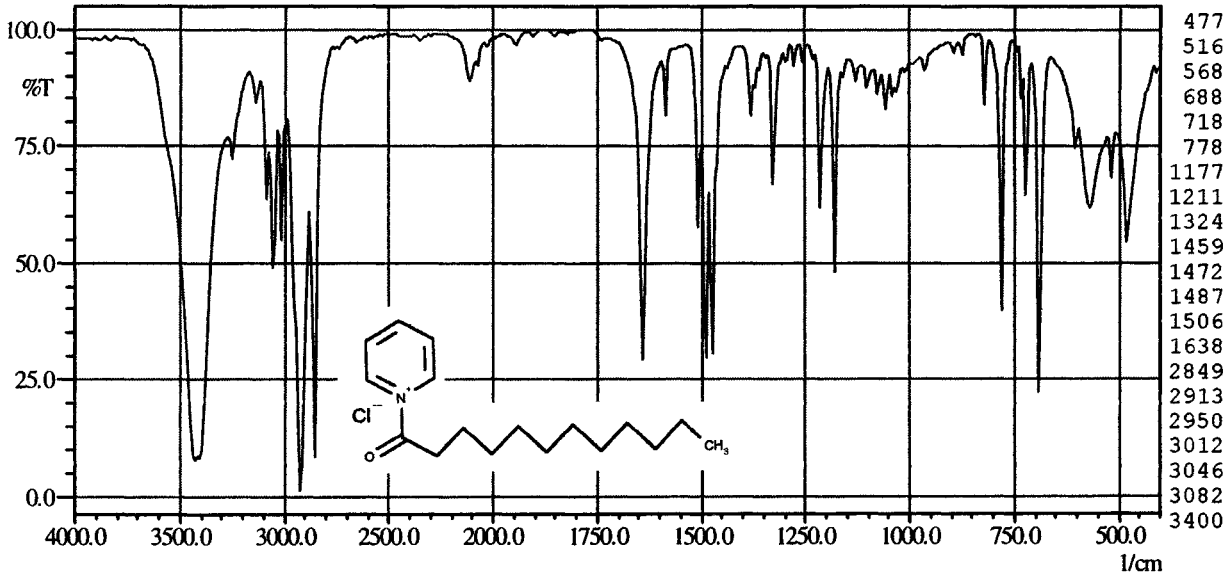
(1) **quaternary ammonium compound**
(2) Tebestat BK
(3) Dr. Th. Boehme
(5) antistatic
(6) yellow, clear liquid
(13) layer btw KBr
(14) contains ethyleneglycol

453



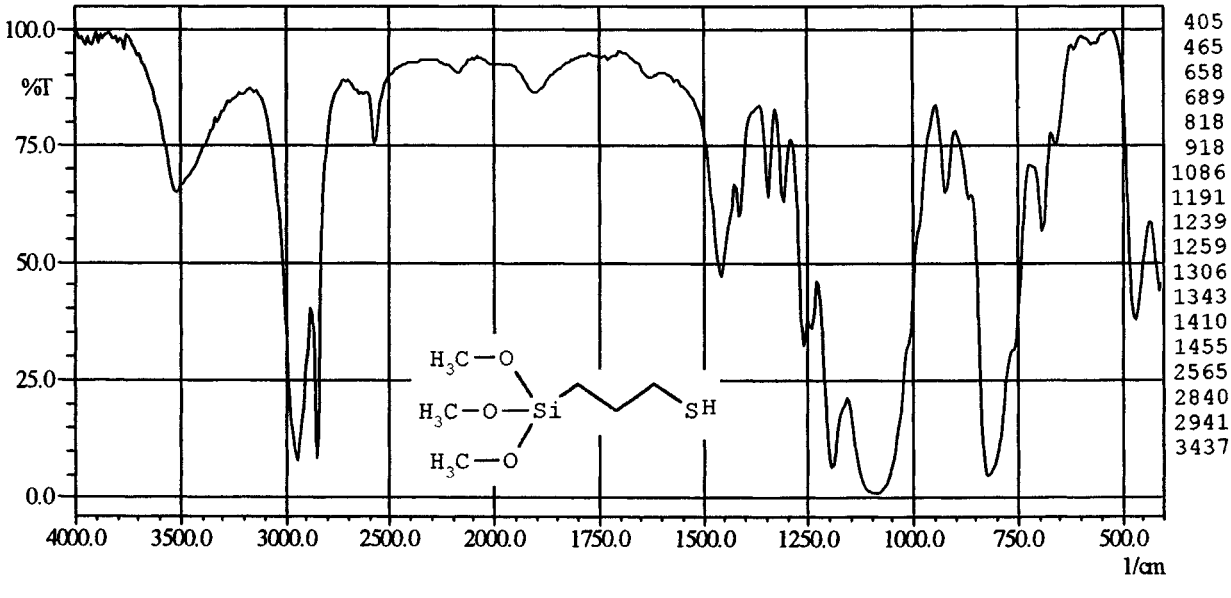
(1) **modified quaternary ammonium compound with ethyleneoxide adduct**
(2) Tebestat IK 39
(3) Dr. Th. Boehme
(5) antistatic
(6) darkyellow, clear liquid
(7) -7.5 °C
(13) layer btw KBr

453 $C_{17}H_{30}ClN$



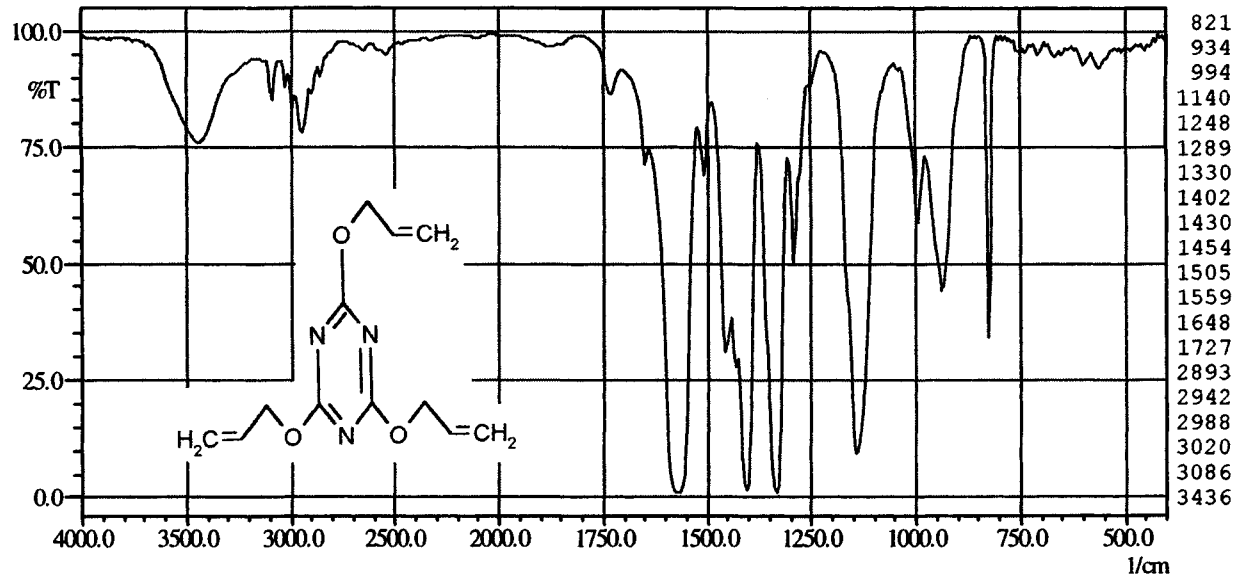
(1) **laurylpyridiniumchloride**
(2) Dehydat C krist.
(3) Henkel
(4) 283.9 g mol^{-1}
(5) antistatic
(6) colourless solid
(13) KBr pellet

454 $SiC_6H_{16}O_3S$



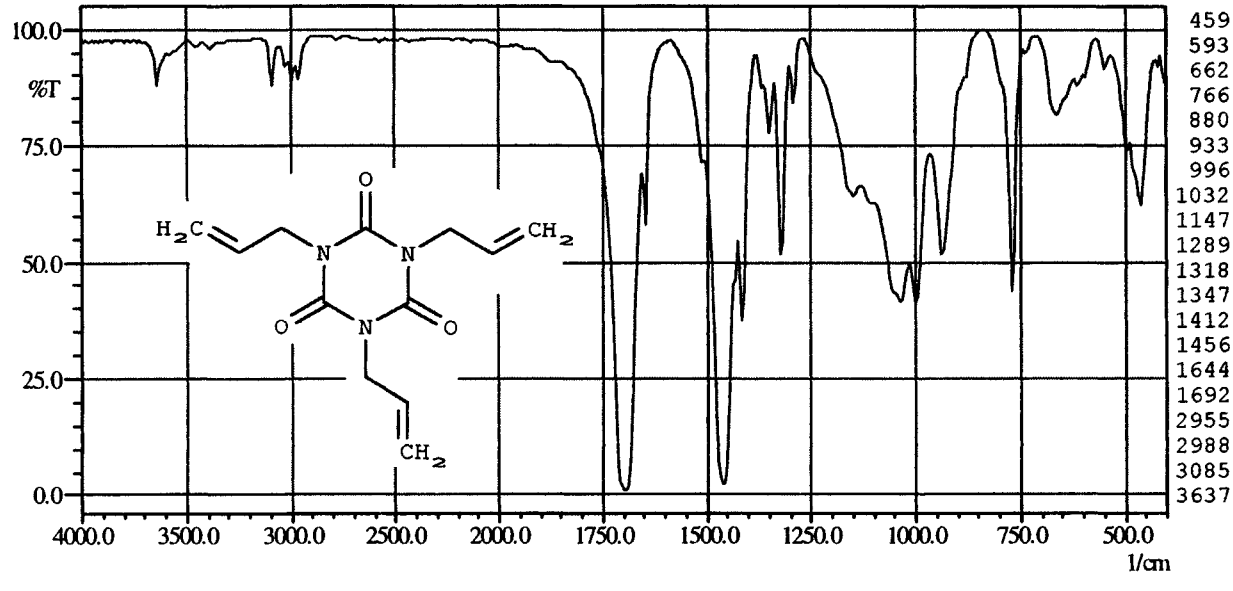
(1) **3-mercaptopropyltrimethoxysilane**
(2) Silane A 189
(3) Freudenberg (Brunne collection)
(4) 196.3 g mol^{-1}
(5) hydrophobing and adhesive agent
(6) colourless, clear liquid
(13) layer btw KBr

461 $C_{12}H_{15}N_3O_3$



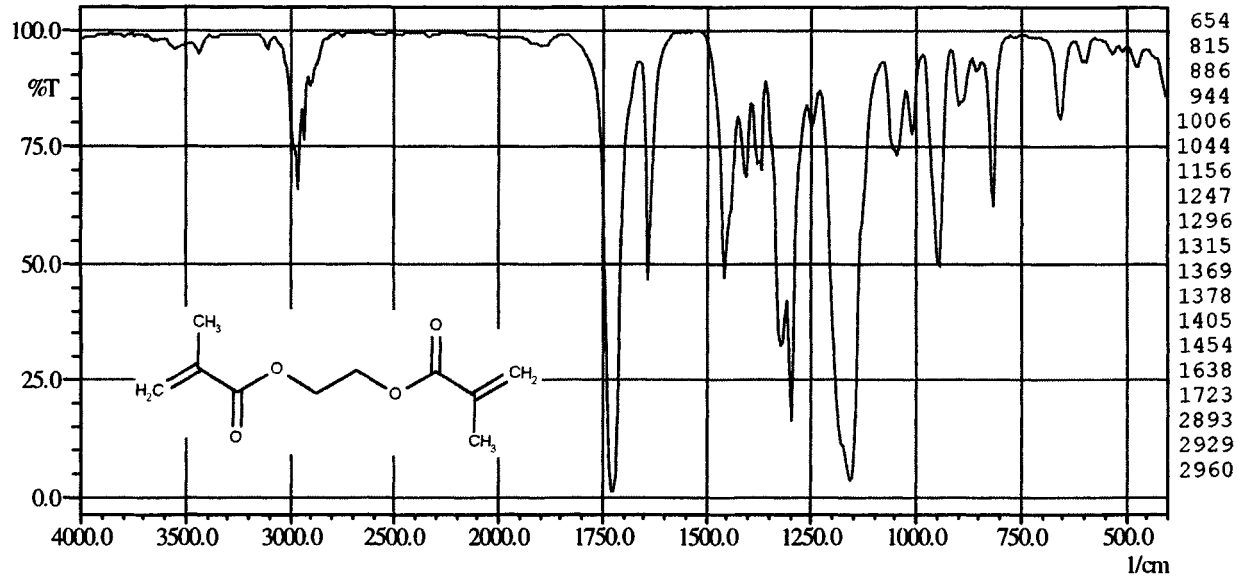
(1) **triallylcyanurate**
(2) Perkalink 300
(3) Akzo Chemie
(4) 249.3 g mol^{-1}
(5) crosslinking agent, co-reactant
(6) colourless solid
(13) KBr pellet

461 $C_{12}H_{15}N_3O_3$



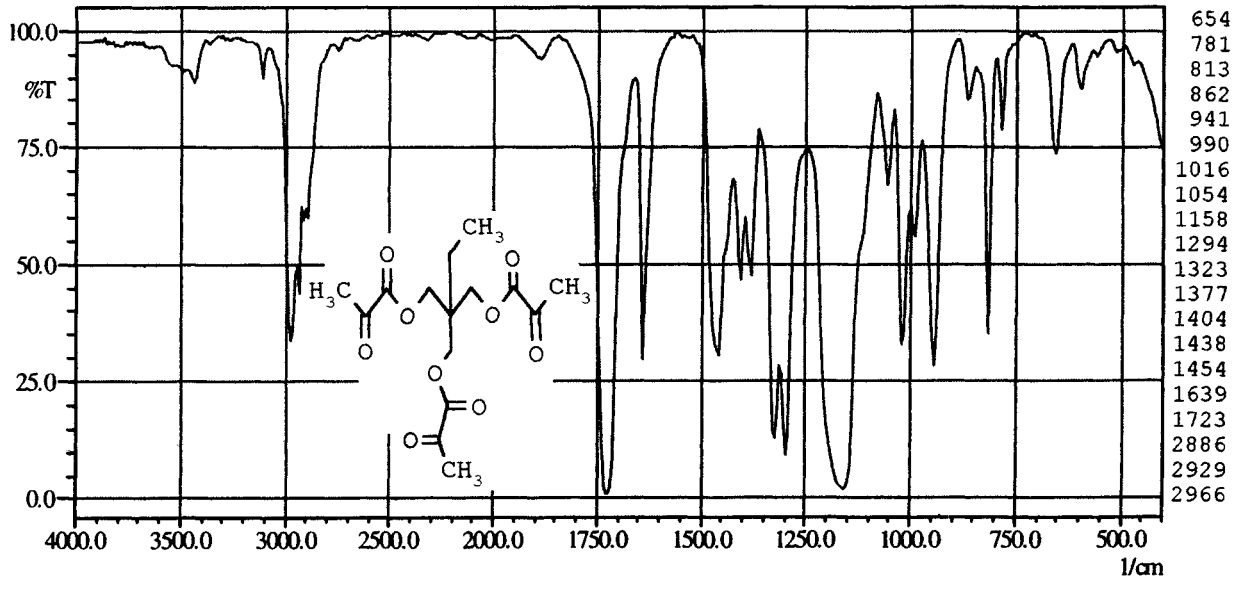
(1) **triallylisocyanurate**
(2) TAIC DL 70
(3) Freudenberg (Brunne collection)
(4) 249.3 g mol^{-1}
(5) crosslinking agent, co-reactant
(6) colourless, clear liquid
(13) layer on KBr

461 $C_{10}H_{14}O_4$



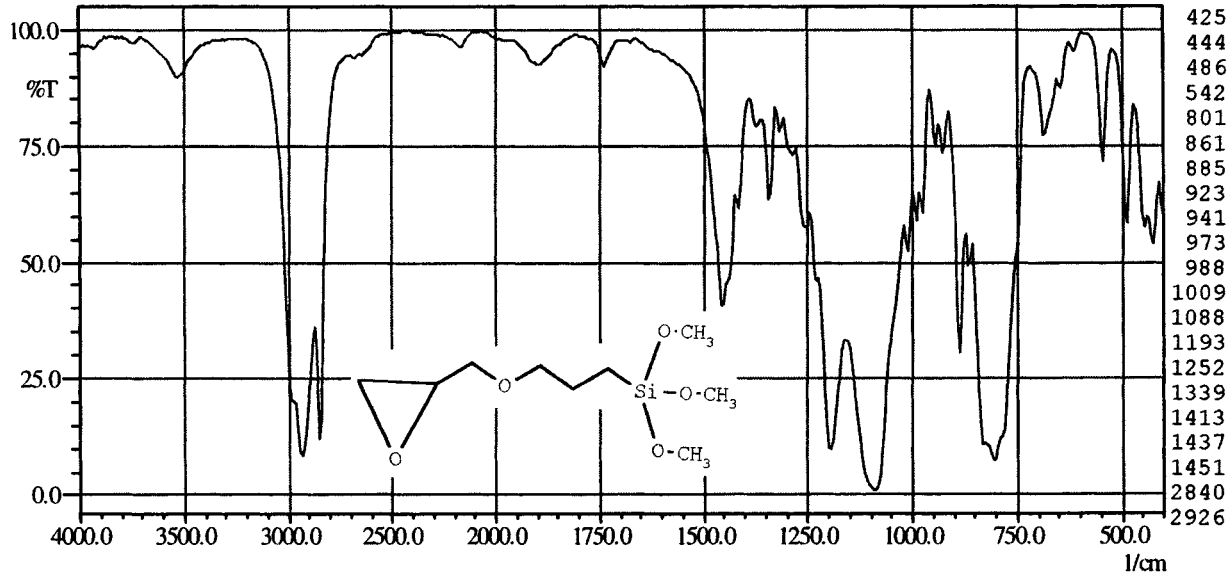
(1) **ethyleneglycoldimethacrylate**
(2) Perkalink 401
(3) Akzo Chemie
(4) 198.2 g mol^{-1}
(5) crosslinking agent, co-reactant
(6) colourless, clear liquid
(13) layer btw KBr

461 $C_{18}H_{26}O_6$



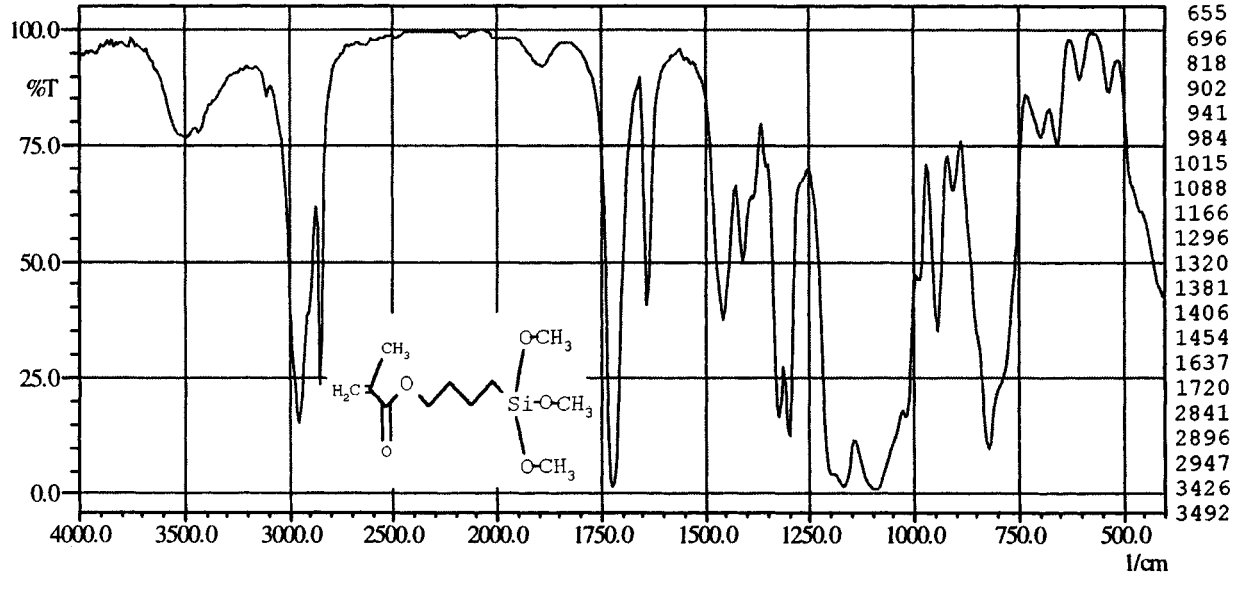
(1) **2-ethyl-2-hydroxymethyl-1,3-propanedioltrimethacrylate, trimethylolpropanetrimethacrylate**
(2) Perkalink 400
(3) Akzo Chemie
(4) 338.4 g mol^{-1}
(5) crosslinking agent, co-reactant
(6) colourless, clear liquid
(13) layer btw KBr

461 $SiC_9H_{20}O_5$



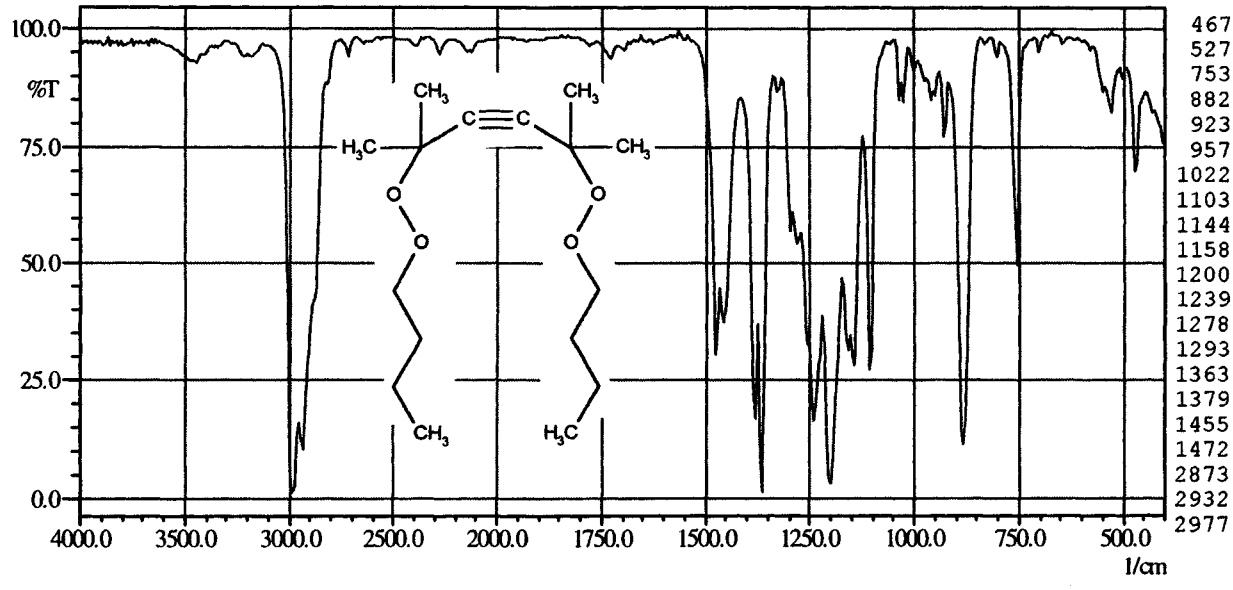
(1) **3-glycidyloxypropyltrimethoxysilane**
(2) Silane A 186
(3) Freudenberg (Brunne collection)
(4) 236.3 g mol^{-1}
(5) hydrophobing and adhesive agent
(6) colourless, clear liquid
(8) 256 °C
(9) 1.045 g cm^{-3}
(10) 1.431
(13) layer btw KBr

461 $SiC_{10}H_{20}O_5$



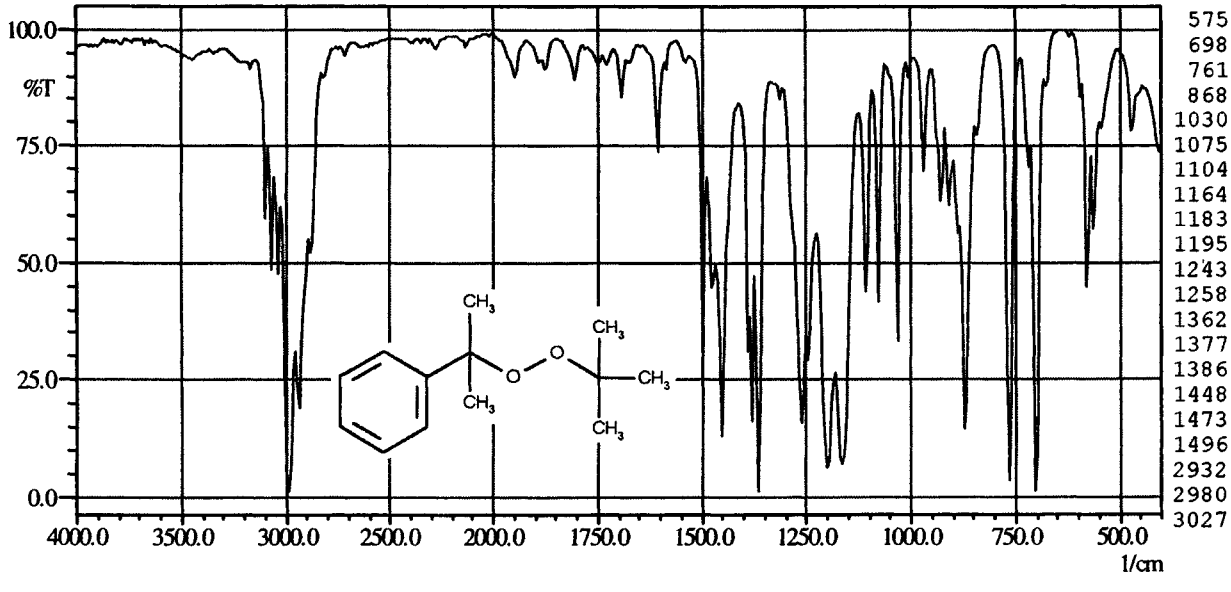
(1) **methacrylic acid 3-trimethoxysilylpropylester**
(2) Silane A 174, 3-trimethoxysilylpropylmethacrylate
(3) Freudenberg (Brunne collection)
(4) 248.4 g mol^{-1}
(5) crosslinking and adhesive agent
(6) colourless, clear liquid
(8) 256 °C
(9) 1.045 g cm^{-3}
(10) 1.431
(13) layer btw KBr

46222 $C_{16}H_{40}O_4$



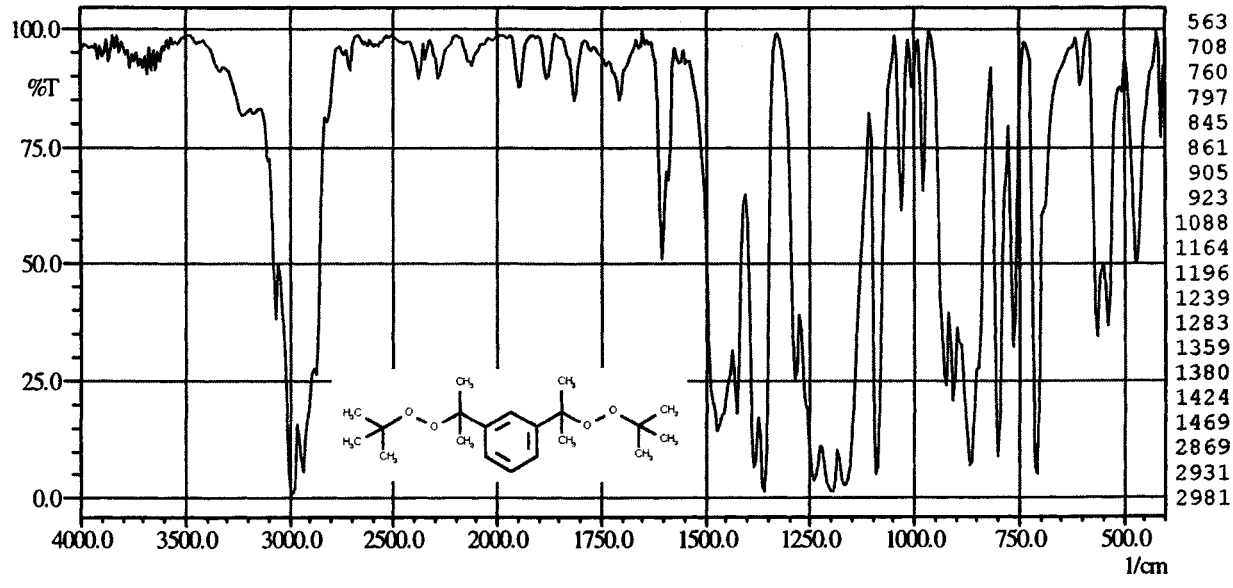
(1) **2,5-dimethyl-2,5-di-*t*-butylperoxyhexyne-3**
(2) Trigonox 145
(3) Akzo Chemie
(4) 296.5 g mol^{-1}
(5) crosslinking agent
(6) light-yellowish, clear liquid
(13) layer btw KBr

46223 $C_{13}H_{20}O_2$



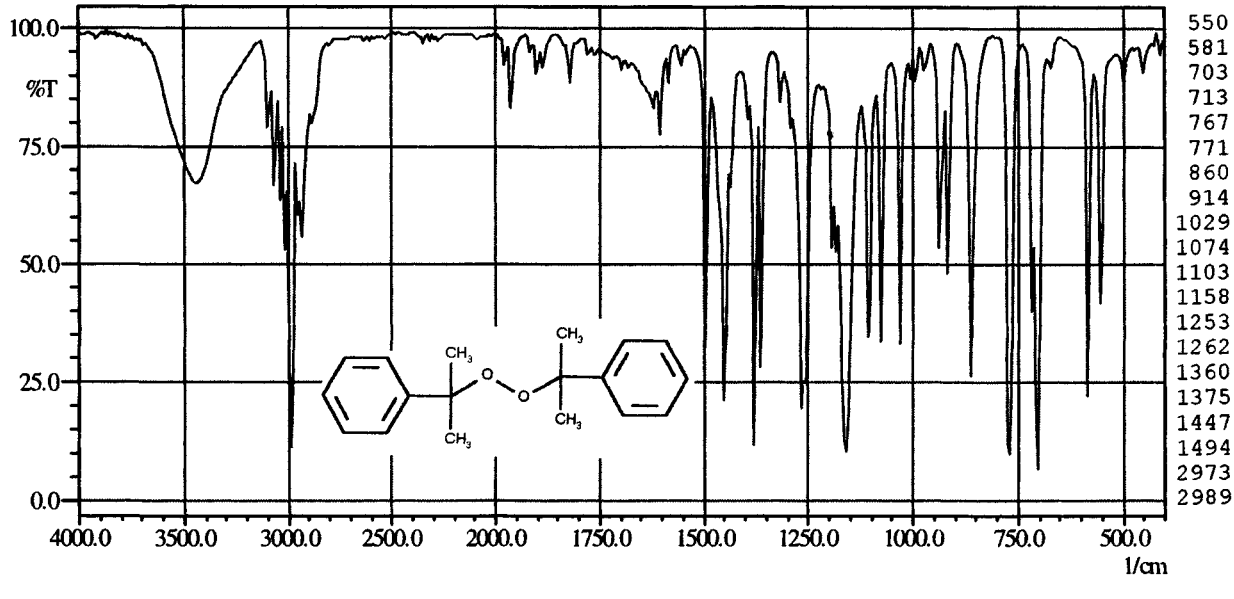
(1) ***t*-butylcumylperoxide**
(2) Trigonox T
(3) Akzo Chemie
(4) 208.3 g mol^{-1}
(5) crosslinking agent
(6) colourless, clear liquid
(13) layer btw KBr

46223 $C_{20}H_{34}O_4$



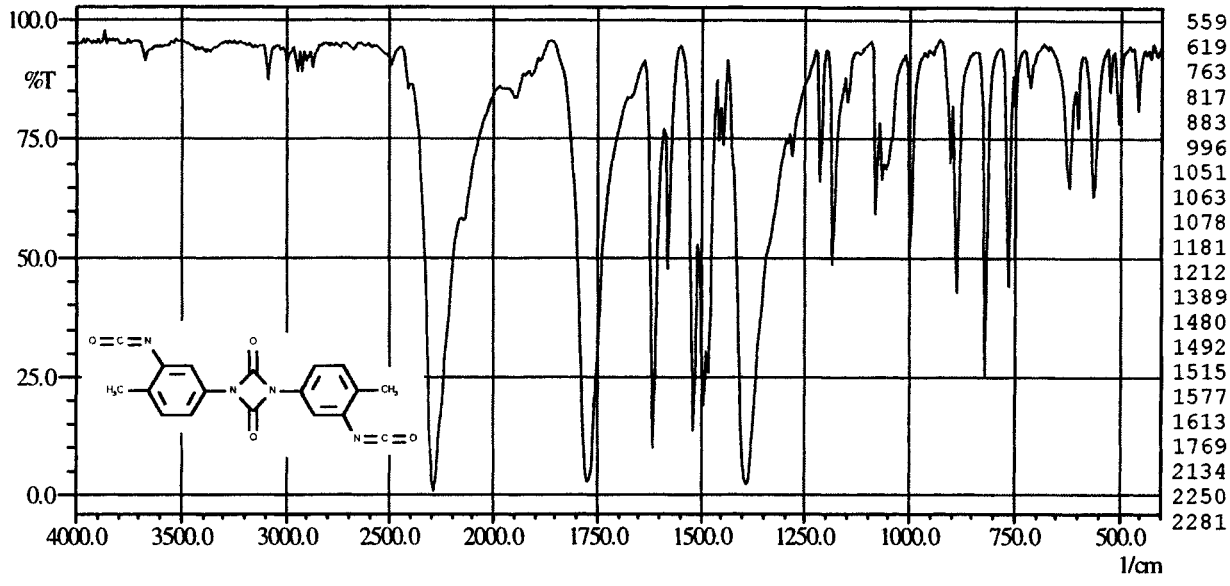
(1) **1,3-*bis*(*t*-butylperoxy-2-propyl)benzene**
(2) Perkadox-14 S
(3) Akzo Chemie
(4) 338.5 g mol^{-1}
(5) crosslinking agent
(6) colourless solid
(13) KBr pellet

46223 $C_{18}H_{22}O_2$



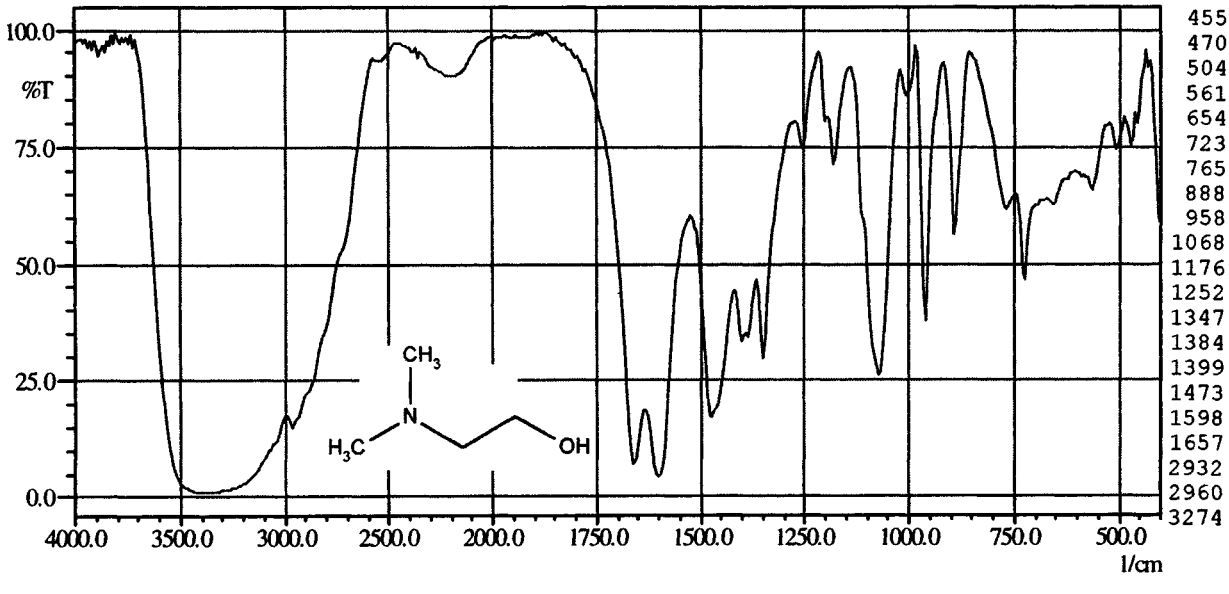
(1) **dicumylperoxide**
(2) Perkadox BC
(3) Akzo Chemie
(4) 270.4 g mol^{-1}
(5) crosslinking agent
(6) colourless granules
(13) KBr pellet

463 $C_{18}H_{12}N_4O_4$



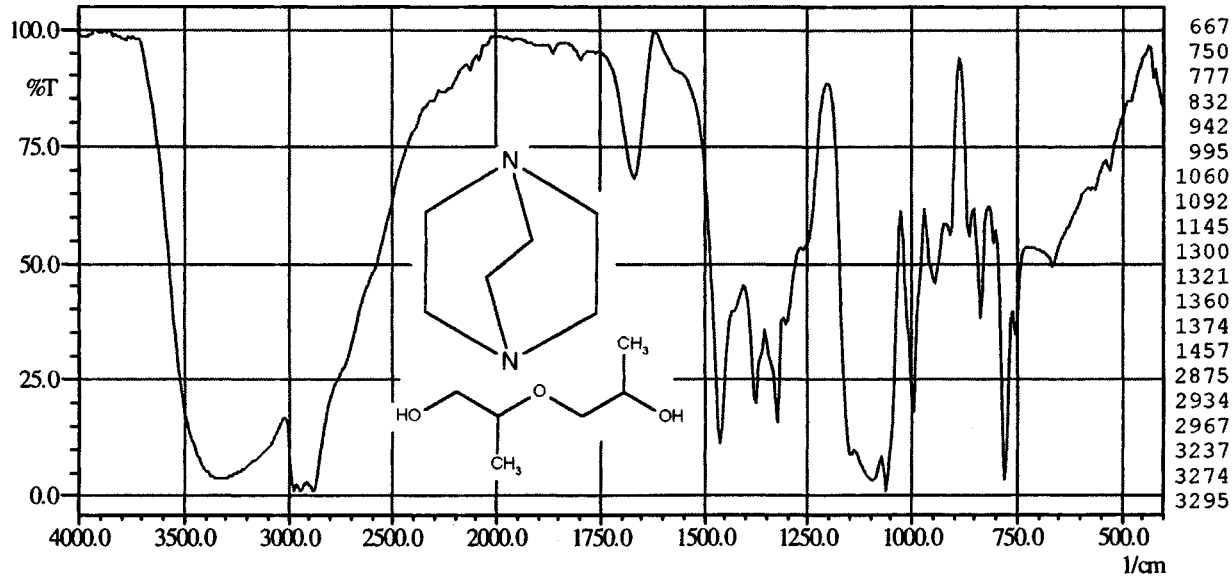
(1) **isocyanate with carbodiimide**
(2) Desmodur TT
(3) Bayer
(4) 348.3 g mol^{-1}
(5) peptizer, crosslinking agent
(6) yellowish solid
(13) KBr pellet

465 $C_4H_{11}NO$



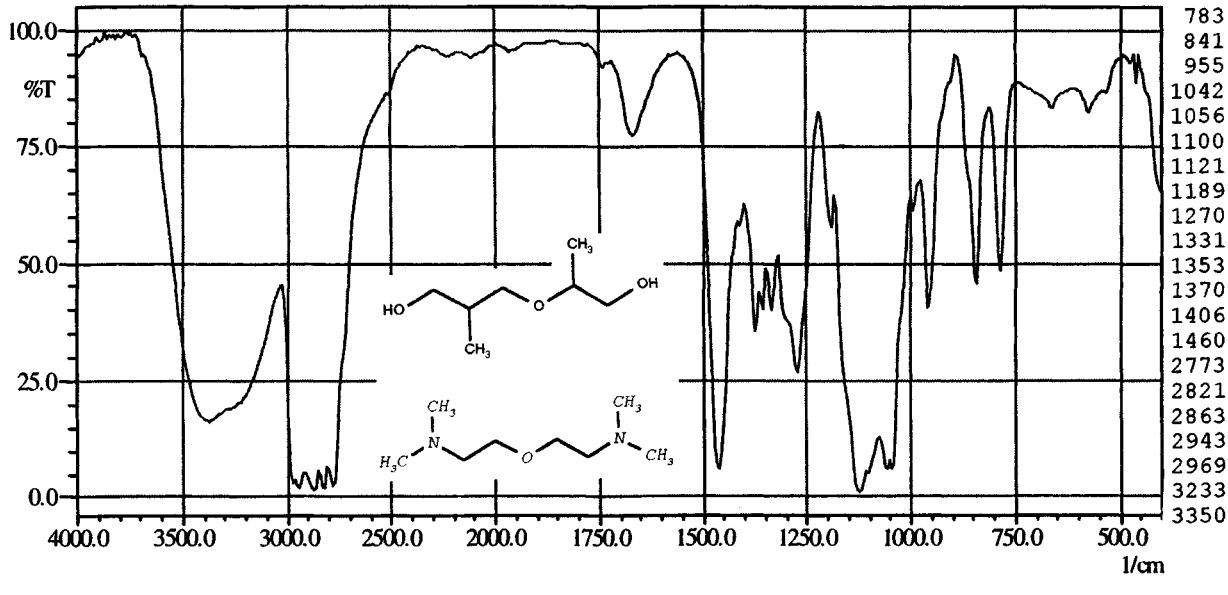
(1) **N,N-dimethylethanolamine**
(2) Tegoamin DMEA
(3) Th. Goldschmidt
(4) 89.13 g mol^{-1}
(5) curing agent/activator
(6) colourless, clear liquid
(7) -70 °C
(8) 133–135 °C
(9) 0.887 g cm^{-3}
(13) layer btw KBr

465 $C_6H_{15}N$



(1) **solution of triethylenediamine in dipropyleneglycol**
(2) Tegoamin 33
(3) Th. Goldschmidt
(4) 101.2 g mol^{-1}
(9) 1.033 g cm^{-3}
(5) curing agent/activator, catalyst
(6) yellowish, clear liquid
(7) –31 °C
(8) 216.5 °C
(13) layer btw KBr

465 $C_8H_{20}N_2O$



(1) ***bis*(2-dimethylaminoethyl)ether in dipropyleneglycol**
(2) Tegoamin BDE
(3) Th. Goldschmidt
(4) 160.3 g mol^{-1}
(5) curing agent/activator, catalyst
(6) colourless, clear liquid
(7) –80 °C
(8) 206 °C
(9) 0.902 g cm^{-3}
(13) layer btw KBr

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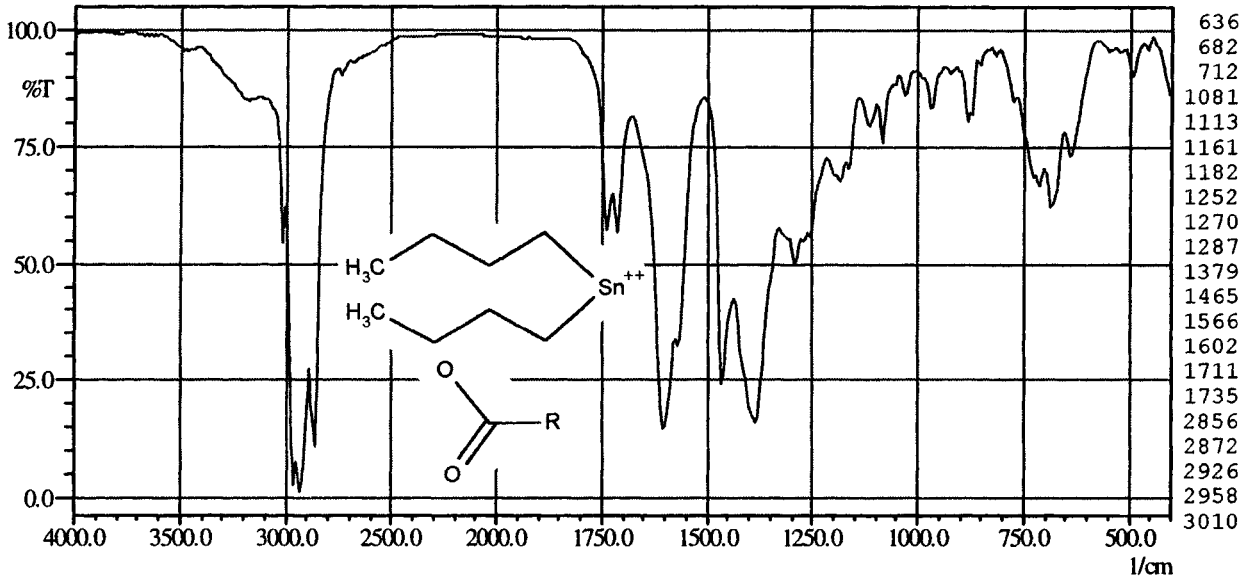
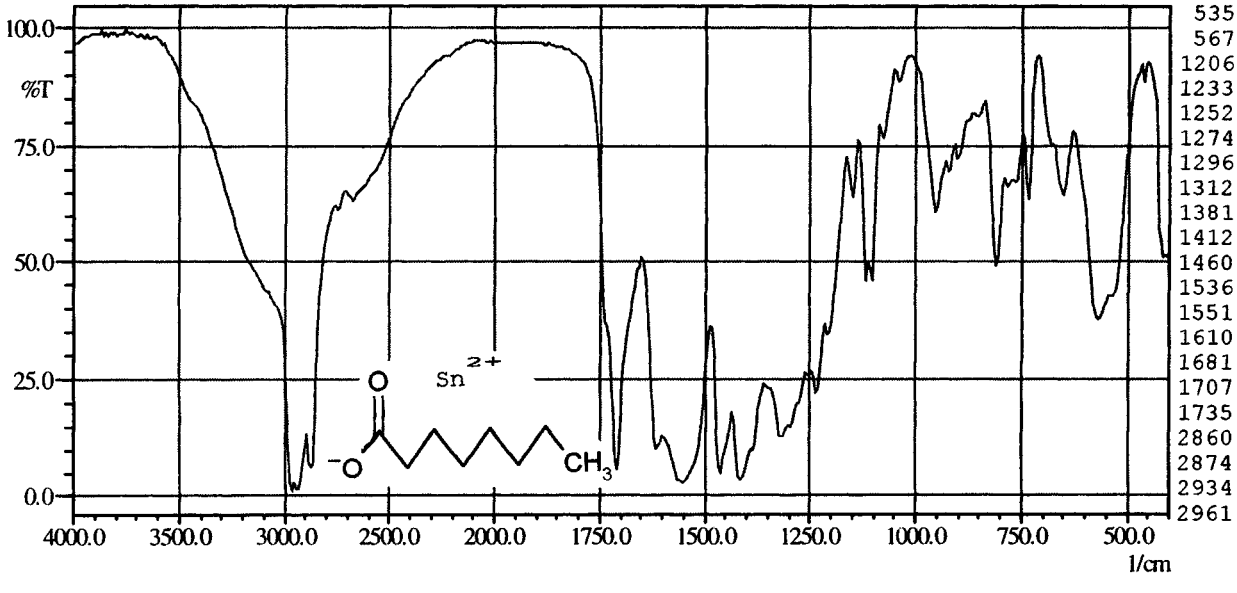
465



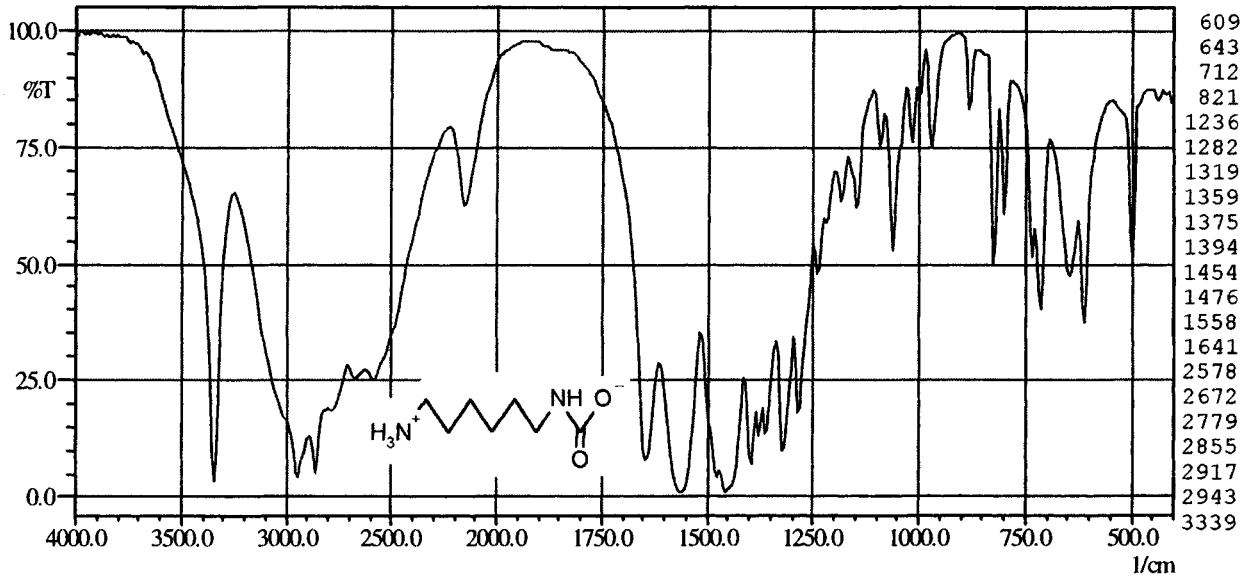
(1) **dibutyltin carboxylate**
(2) Kosmos 19
(3) Th. Goldschmidt
(5) curing agent/activator, catalyst
(6) yellow, clear liquid
(7) 0 °C
(8) 250 °C
(9) 1.07 g cm^{-3}
(13) layer btw KBr

465 **$C_{16}H_{30}O_4Sn$**



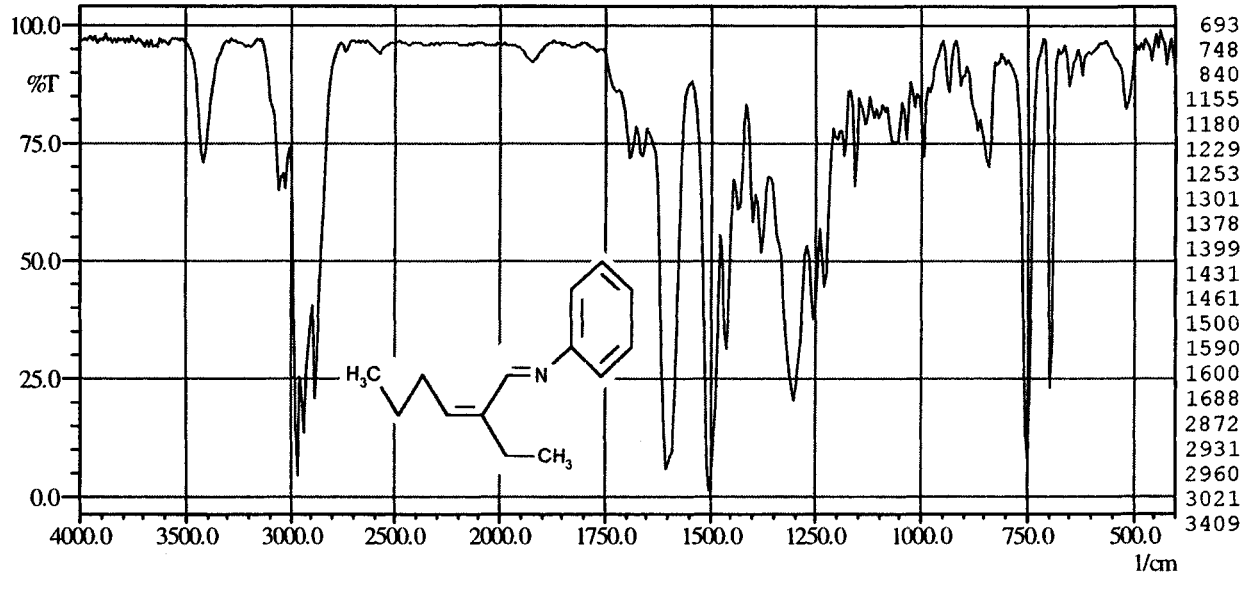
(1) **Sn(II) octoate**
(2) Kosmos 29
(3) Th. Goldschmidt
(4) 405.1 g mol^{-1}
(5) curing agent/activator, catalyst
(6) pale yellowish, clear liquid
(7) –20 °C
(8) 200 °C
(9) 1.25 g cm^{-3}
(10) 1.4955
(13) layer btw KBr

5123 $C_7H_{16}N_2O_2$



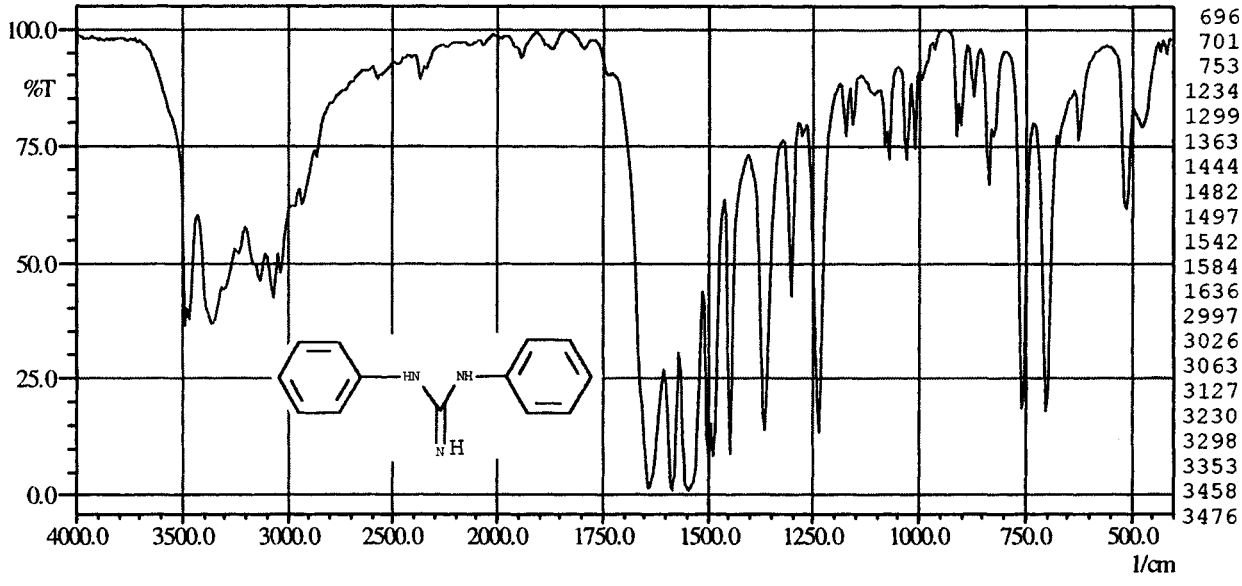
(1) **hexamethylenediamine carbamate**
(2) Diak 1
(3) Du Pont Dow Elastomers
(4) 160.2 g mol^{-1}
(5) co-agens for crosslinking of Viton A, B, and E
(6) colourless solid
(7) 25 °C
(9) 1.28 g cm^{-3}
(13) KBr pellet

5215 $C_{14}H_{19}N$



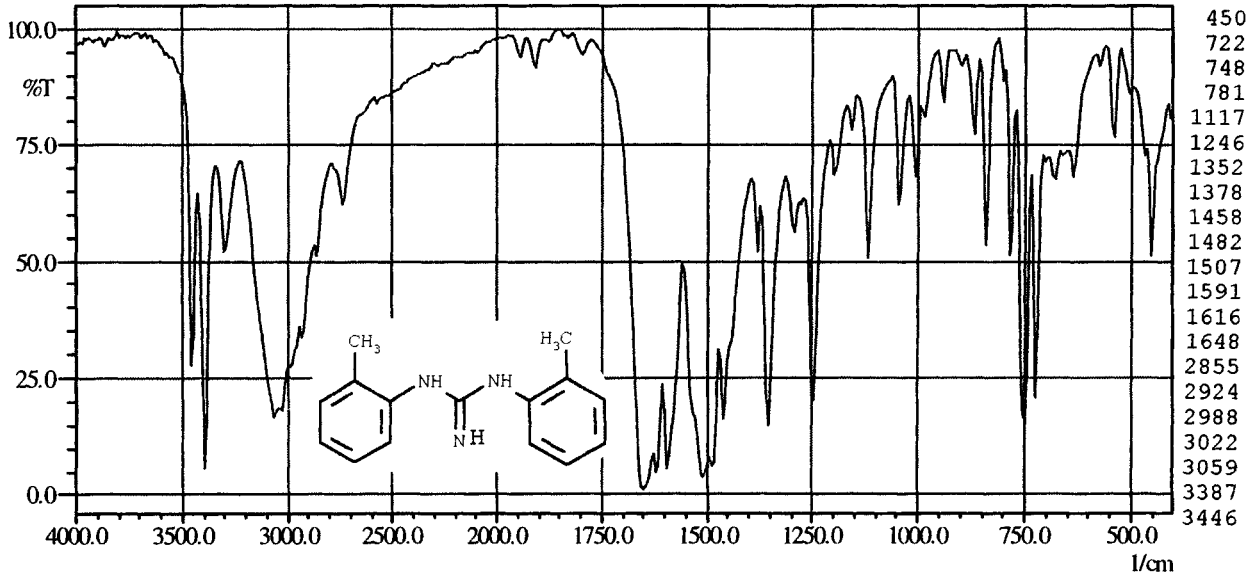
(1) **cond. product of α-ethyl-β-propylacrolein and aniline**
(2) Vulkacit 576
(3) Bayer
(4) 201.3 g mol^{-1}
(5) vulcanisation accelerator
(6) red-brown liquid
(9) 0.99 g cm^{-3}
(13) layer btw KBr

15221 $C_{13}H_{13}N_3$



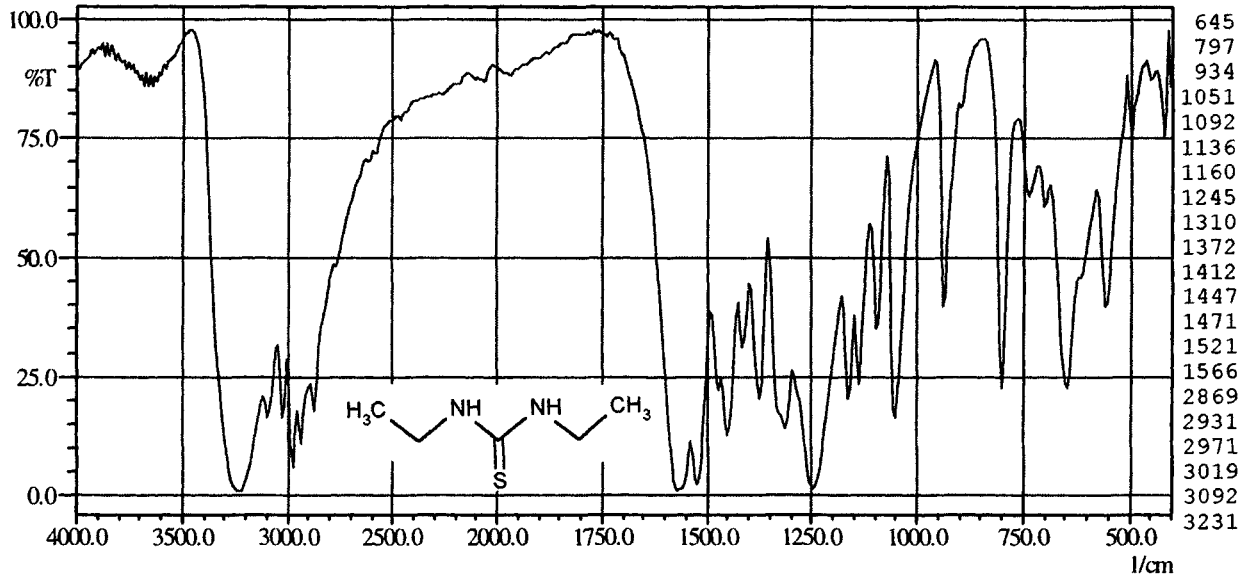
(1) **N,N'-diphenylguanidine**
(2) Vulkasit DC
(3) Bayer
(4) 211.2 g mol^{-1}
(5) vulcanisation accelerator
(6) colourless solid
(13) KBr pellet

15221 $C_{15}H_{17}N_3$



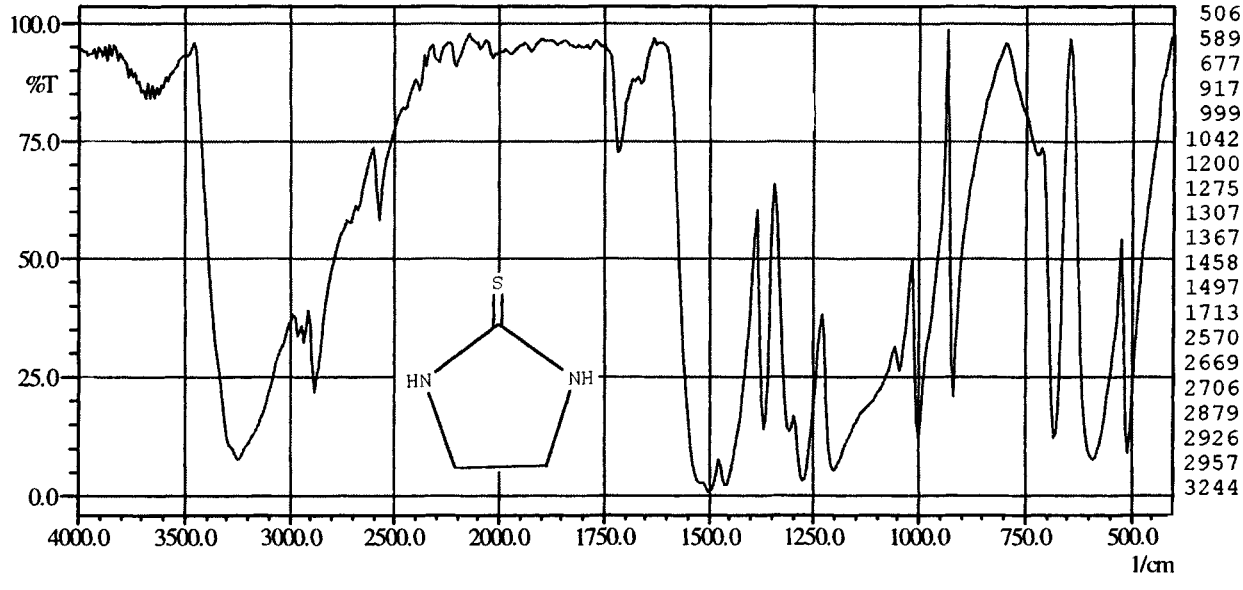
(1) **1,3-di-*o*-tolylguanidine**
(2) Vulkacit DOTG
(3) Bayer
(4) 239.3 g mol^{-1}
(5) vulcanisation accelerator
(6) greyish solid
(13) KBr pellet

5222 $C_5H_{12}N_2S$



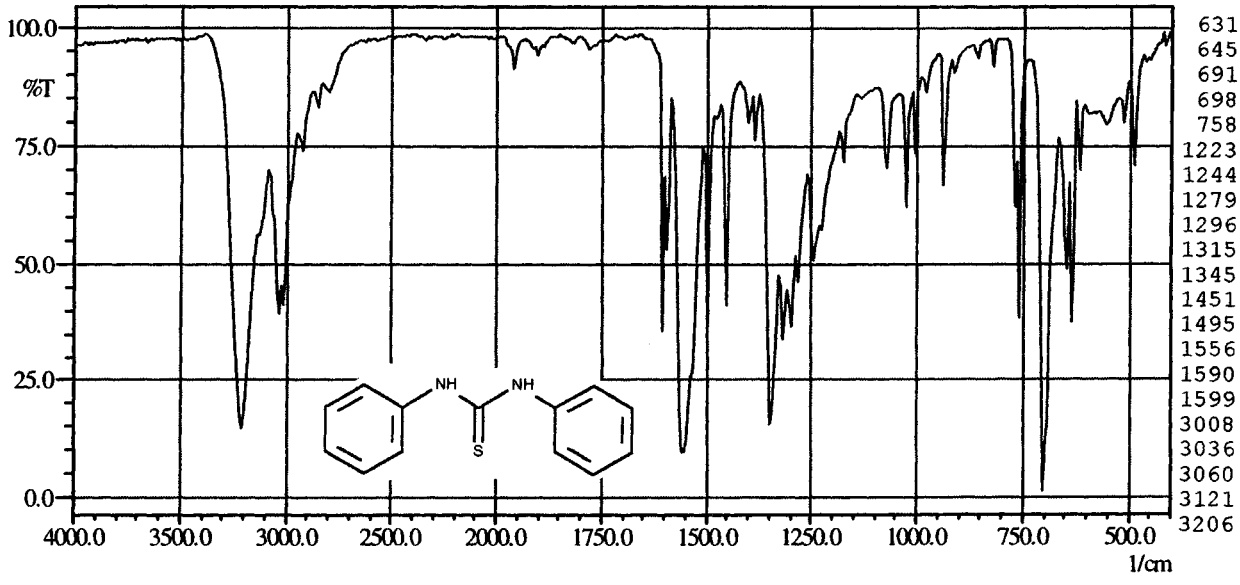
(1) **N,N'-diethylthiourea**
(2) Perkacit DETU
(3) Akzo Chemie
(4) 132.2 g mol^{-1}
(5) accelerator
(6) colourless, crystalline solid
(13) KBr pellet

5222 $C_3H_6N_2S$



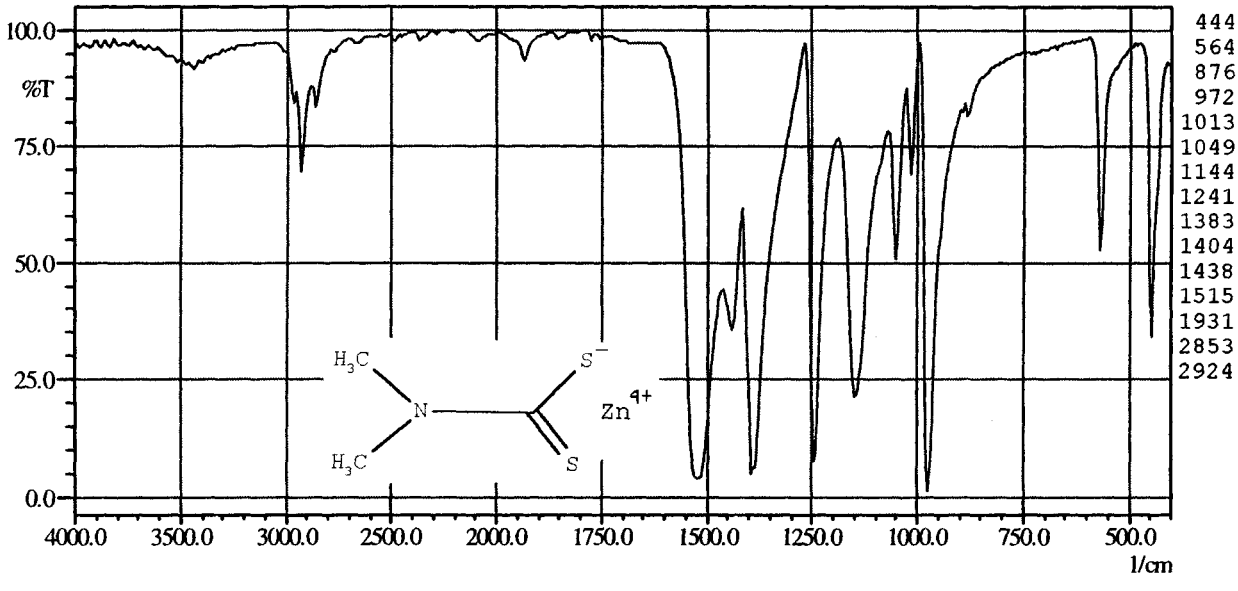
(1) **2-imidazolidinethione, ethylenethiourea**
(2) Perkacit ETU
(3) Akzo Chemie
(4) 102.2 g mol^{-1}
(5) accelerator
(6) colourless solid
(13) KBr pellet

5222 $C_{13}H_{12}N_2S$



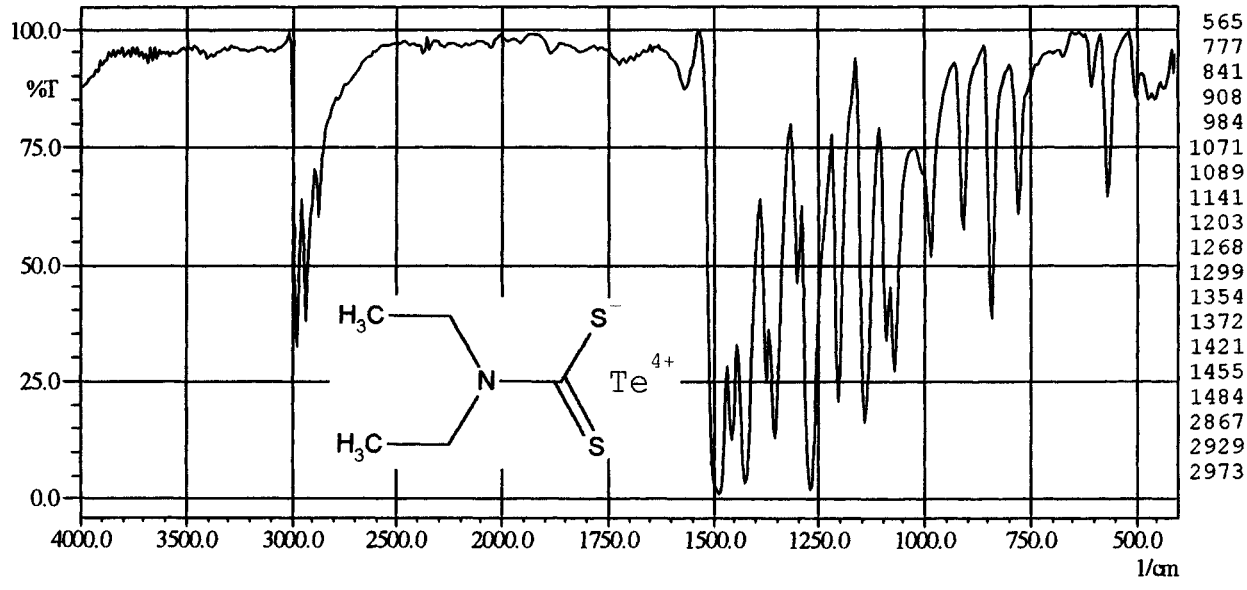
(1) **N,N'-diphenylthiourea**
(2) Rhenocure CA
(3) Rhein Chemie
(4) 228.3 g mol^{-1}
(5) antioxidant, accelerator
(6) colourless solid
(7) 155 °C
(9) 1.32 g cm^{-3}
(13) KBr pellet

52231 $C_6H_{12}N_2S_4Zn$



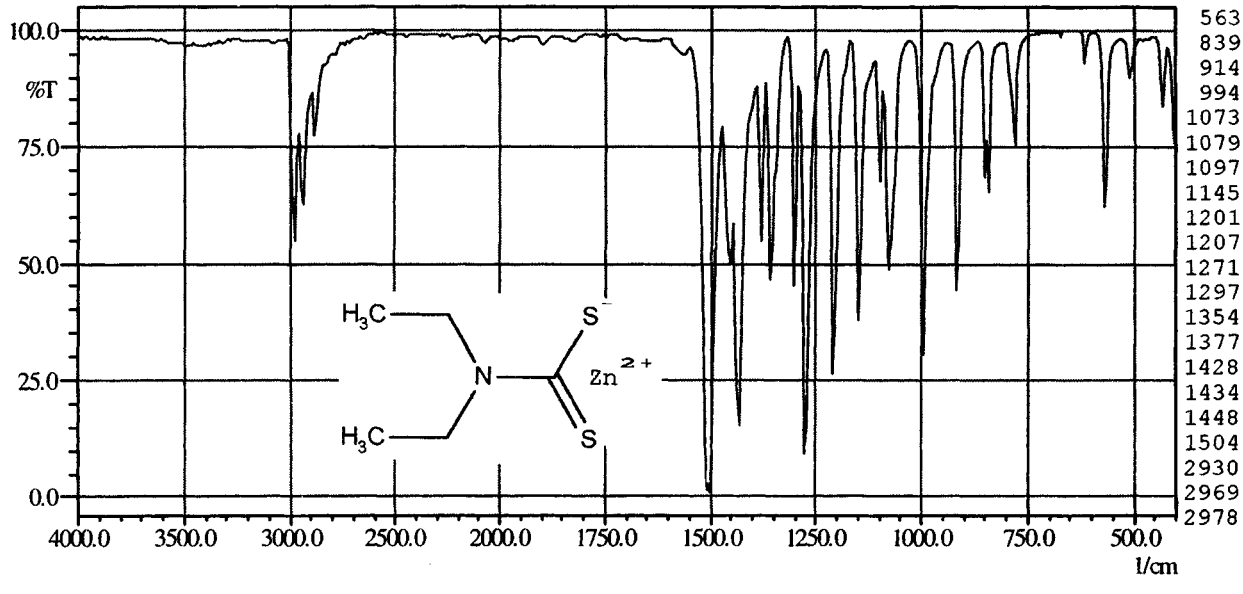
(1) **Zn dimethyldithiocarbamate**
(2) Vulkacit L
(3) Bayer
(4) 305.8 g mol^{-1}
(5) vulcanisation accelerator
(6) colourless solid
(13) KBr pellet, H_2O subtr.

52231 $C_{20}H_{40}N_4S_8Te$



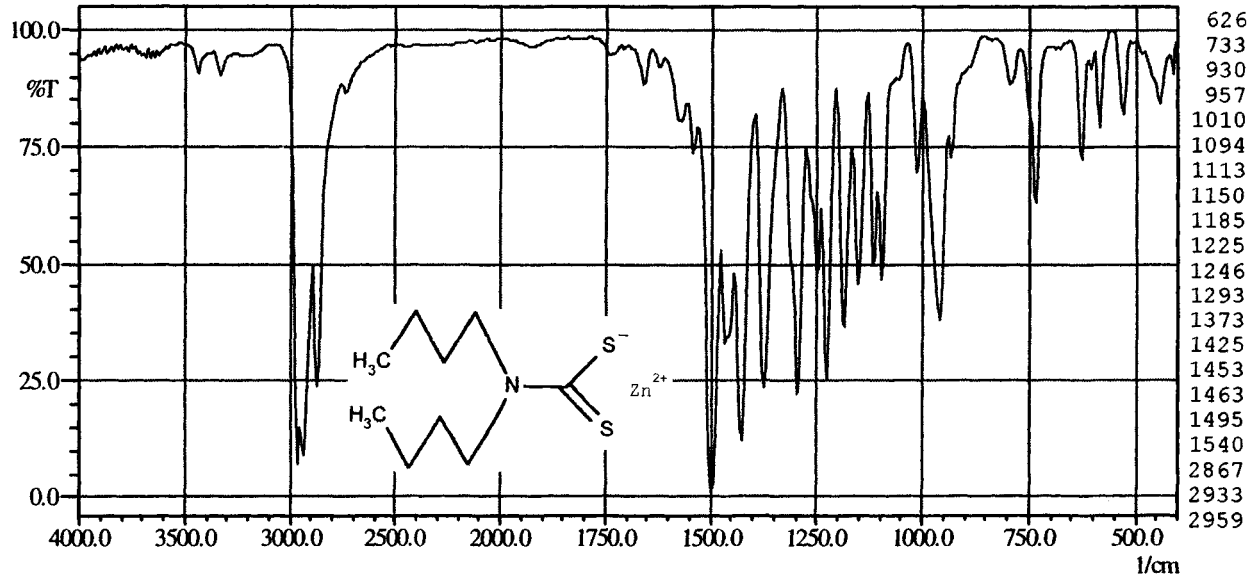
(1) **Te diethyldithiocarbamate**
(2) Perkacit TDEC
(3) Akzo Chemie
(4) 720.6 g mol^{-1}
(5) accelerator
(6) yellowish, soft granules
(13) KBr pellet

52231 $C_{10}H_{20}N_2S_4Zn$



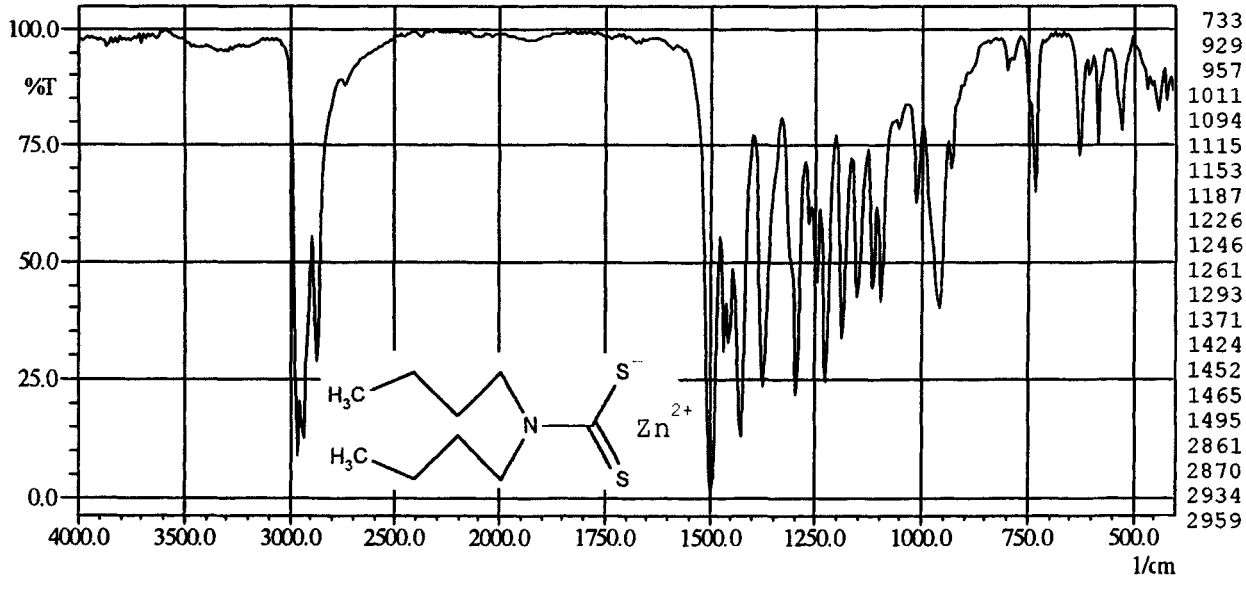
(1) **Zn diethyldithiocarbamate**
(2) Vulkacit LDA
(3) Bayer
(4) 361.9 g mol^{-1}
(5) vulcanisation accelerator
(6) colourless solid
(13) KBr pellet, H_2O subtr.

52231 $C_{18}H_{36}N_2S_4Zn$



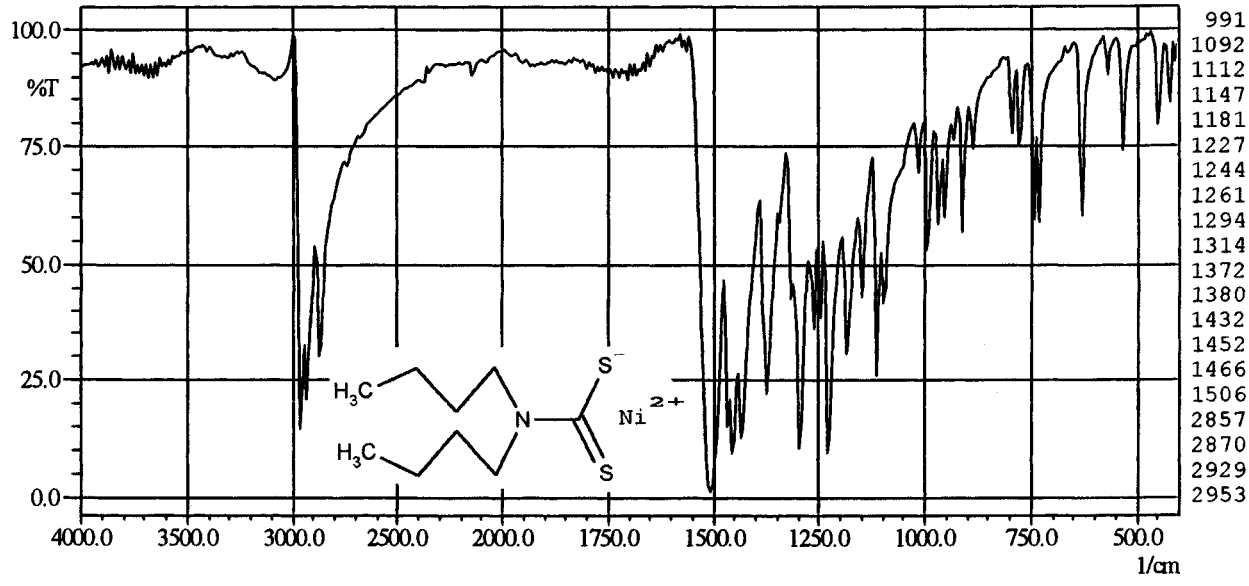
(1) **Zn-dibutyldithiocarbamate**
(2) Perkacit ZDBC
(3) Akzo Chemie
(4) 474.1 g mol^{-1}
(5) accelerator
(6) colourless solid
(13) KBr pellet

52231 $C_{18}H_{36}N_2S_4Zn$



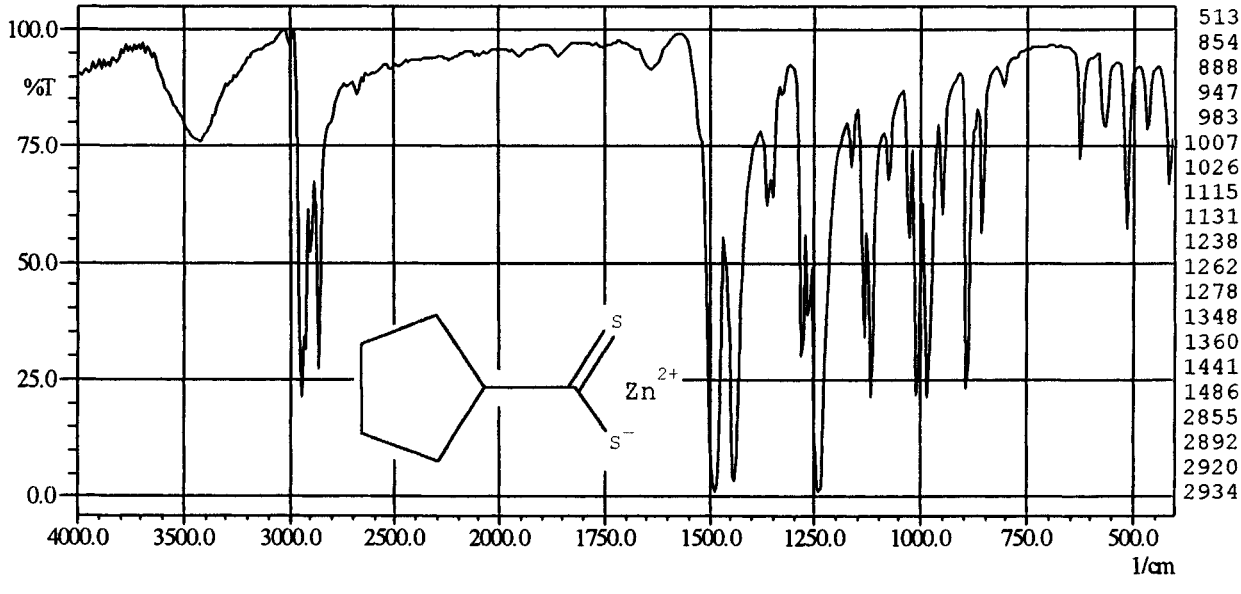
(1) **Zn N-dibutydithiocarbamate**
(2) Vulkacit LDB/C
(3) Bayer
(4) 474.1 g mol^{-1}
(5) accelerator
(6) light-grey solid
(7) 104 °C
(9) 1.26 g cm^{-3}
(13) KBr pellet

52231 $C_{18}H_{36}N_2S_4Ni$



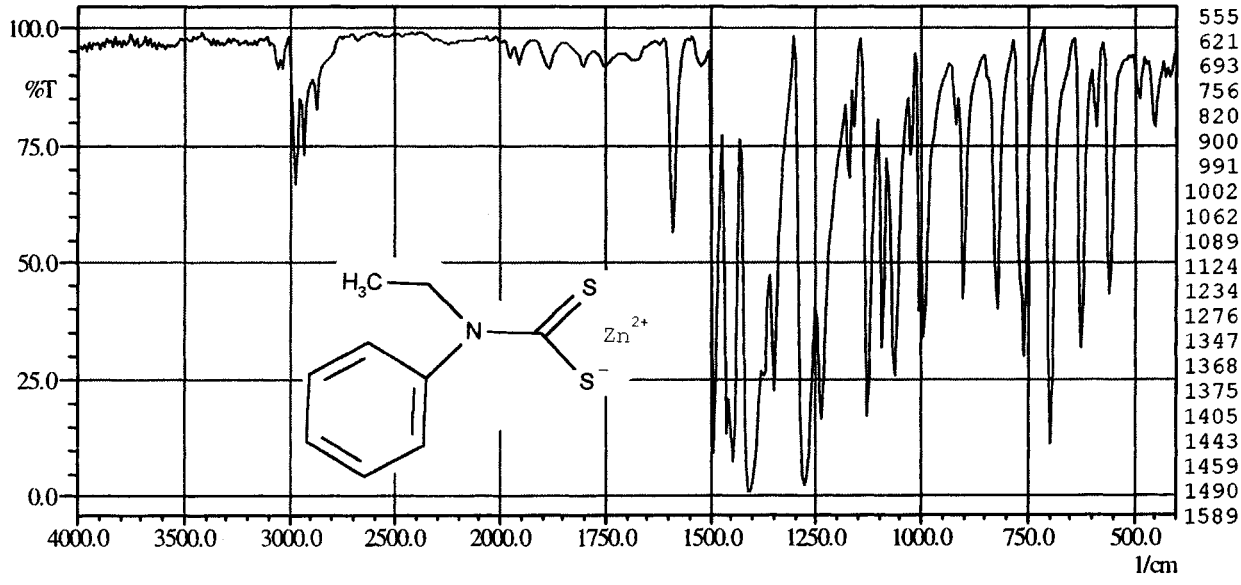
(1) **Ni dibutyldithiocarbamate**
(2) Perkacit NDBC
(3) Akzo Chemie GmbH
(4) 467.4 g mol^{-1}
(5) accelerator
(6) green, soft, granules
(13) KBr pellet

52231 $C_{12}H_{20}N_2S_4$



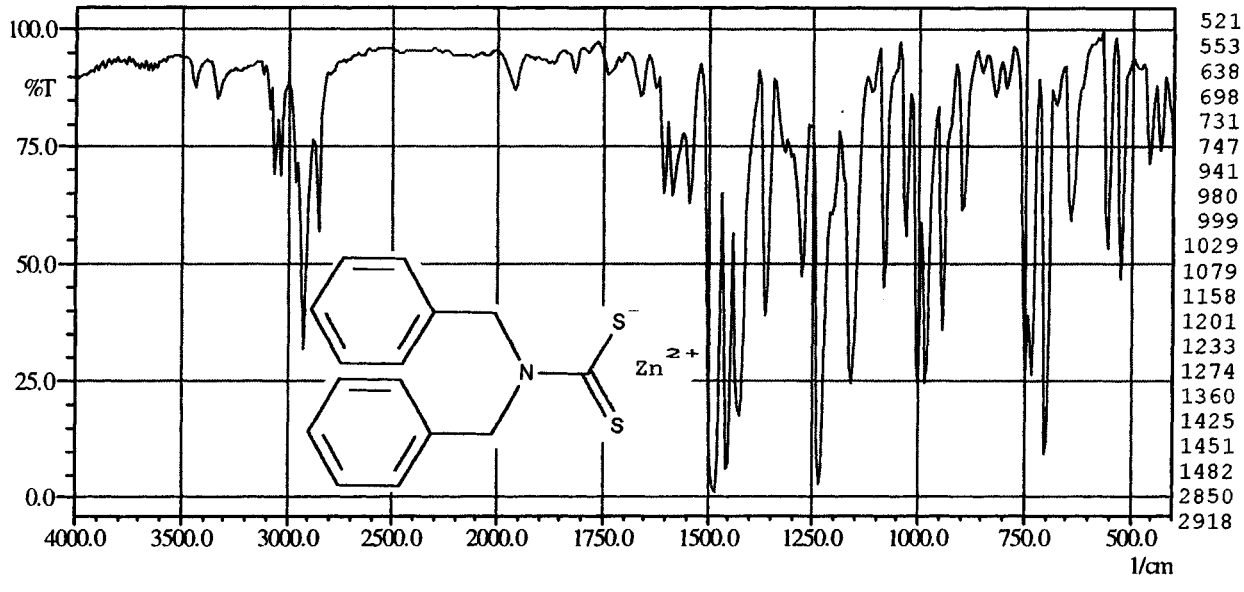
(1) **Zn pentamethylenedithiocarbamate**
(2) Vulkacit ZP
(3) Bayer
(4) 385.9 g mol^{-1}
(5) vulcanisation accelerator
(6) colourless solid
(13) KBr pellet

52231 $C_{18}H_{20}N_2S_4Zn$



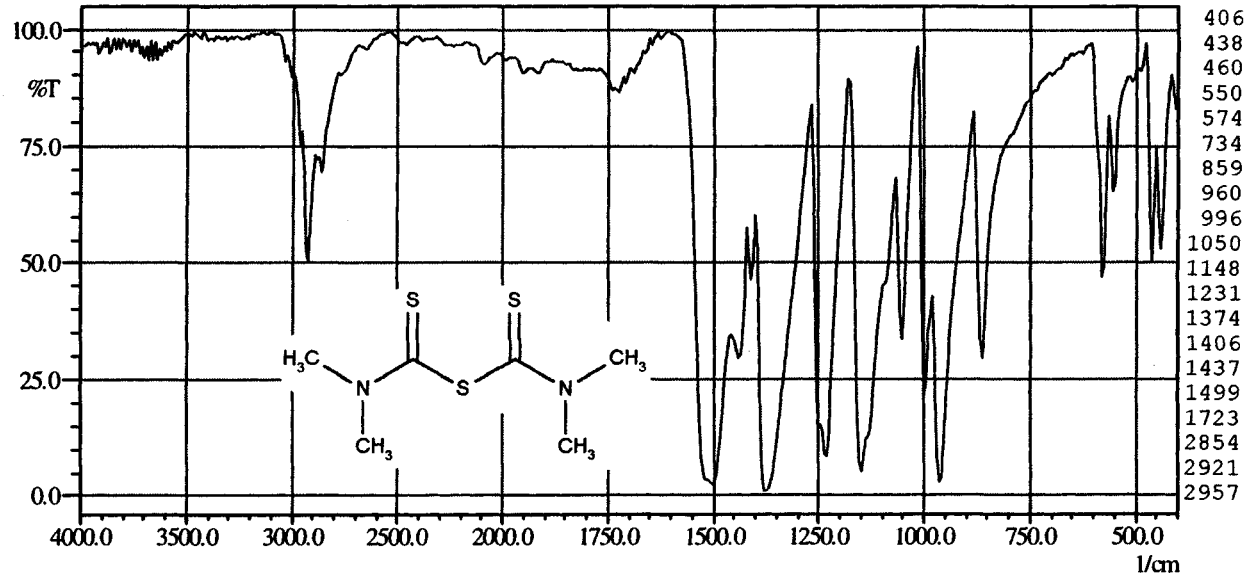
(1) **Zn ethylphenyldithiocarbamate**
(2) Desmorapid DA
(3) Bayer
(5) vulcanisation accelerator
(6) colourless solid
(13) KBr pellet
(14) Christiansen effect

52231 $C_{30}H_{28}N_2S_4Zn$



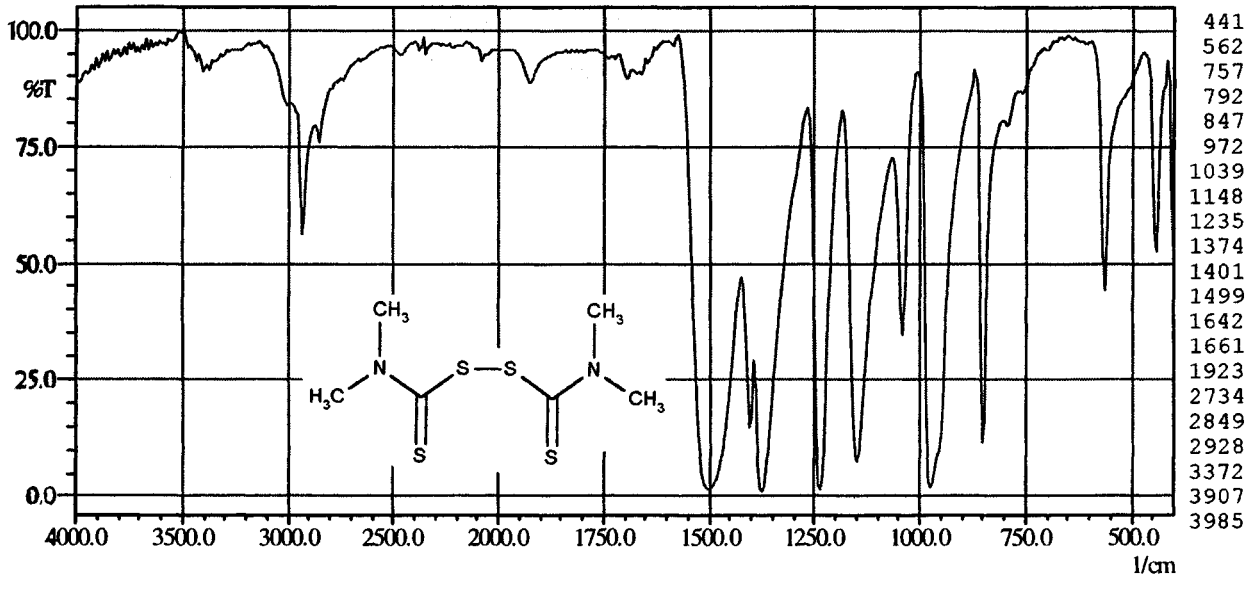
(1) **Zn-dibenzyldithiocarbamate**
(2) Perkacit ZBEC
(3) Akzo Chemie
(4) 610.2 g mol^{-1}
(5) accelerator
(6) colourless solid
(13) KBr pellet

52241 $C_6H_{12}N_2S_3$



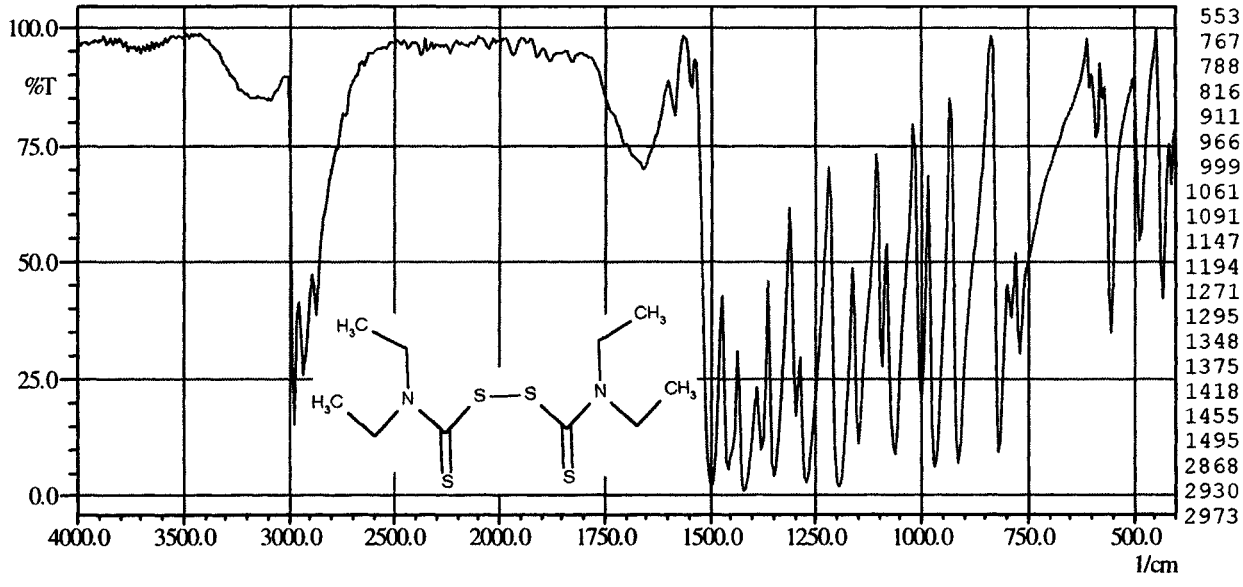
(1) **tetramethylthiurammonosulfide**
(2) Perkacit TMTM
(3) Akzo Chemie
(4) 208.3 g mol^{-1}
(5) accelerator
(6) yellowish, soft granules
(13) KBr pellet

52242 $C_6H_{12}N_2S_4$



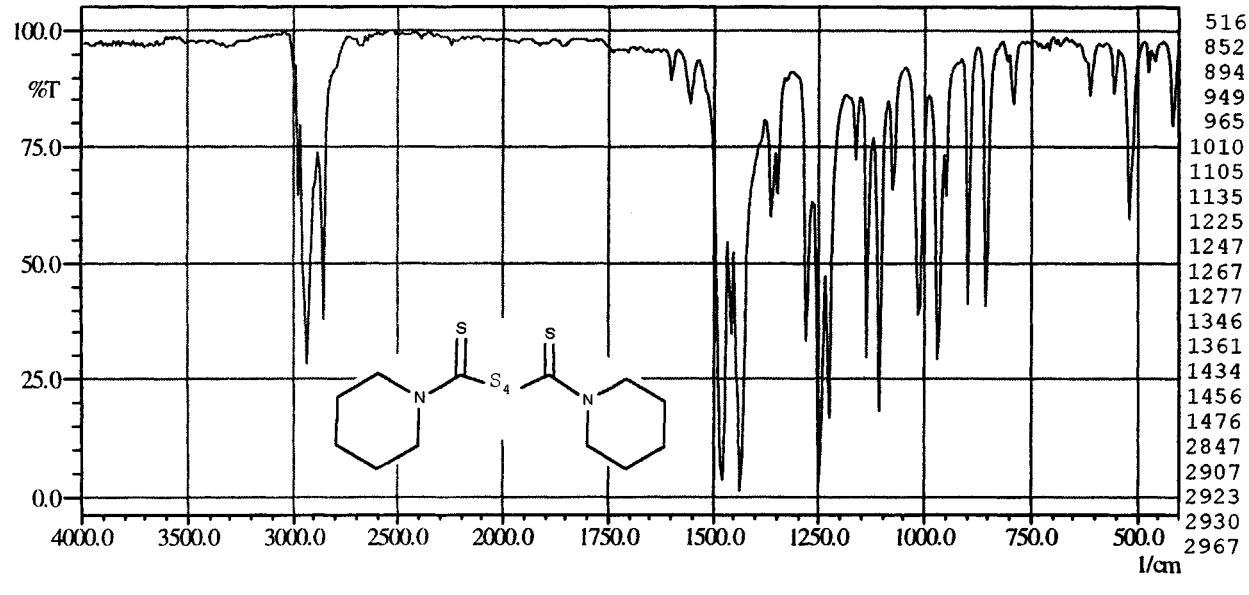
(1) **tetramethylthiuramdisulfide**
(2) Perkacit TMTD
(3) Akzo Chemie
(4) 240.4 g mol^{-1}
(5) accelerator
(6) colourless solid
(13) KBr pellet

52242 $C_{10}H_{20}N_2S_4$



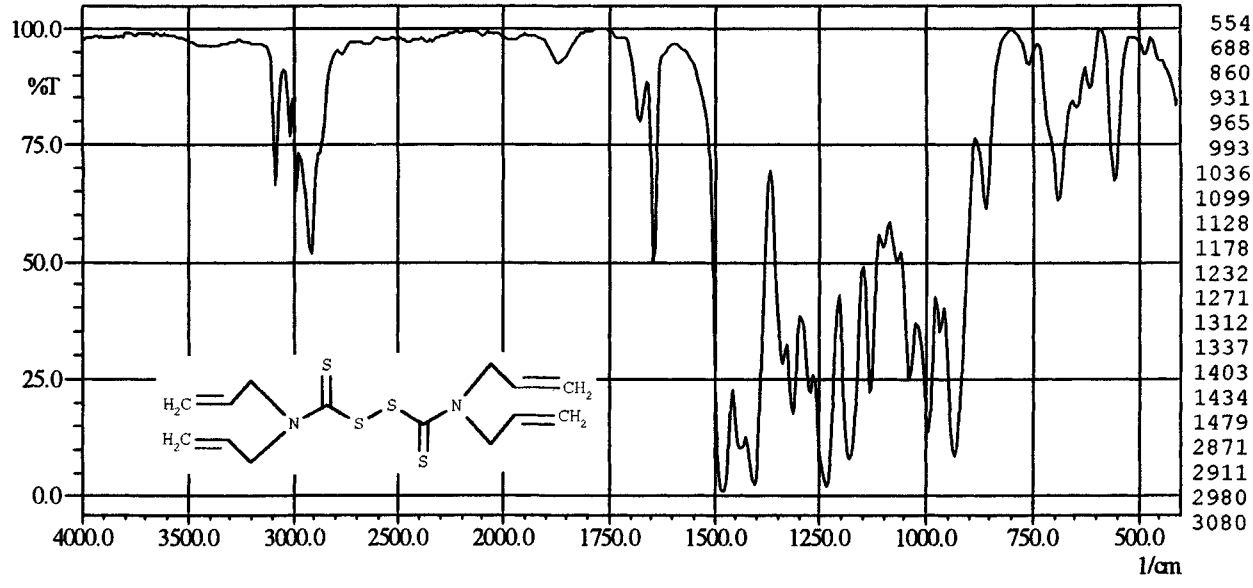
(1) **tetraethylthiuramdisulfide**
(2) Perkacit TETD
(3) Akzo Chemie
(4) 296.6 g mol^{-1}
(5) accelerator
(6) colourless solid
(13) KBr pellet
(14) Christiansen effect

52242 $C_{12}H_{20}N_2S_6$



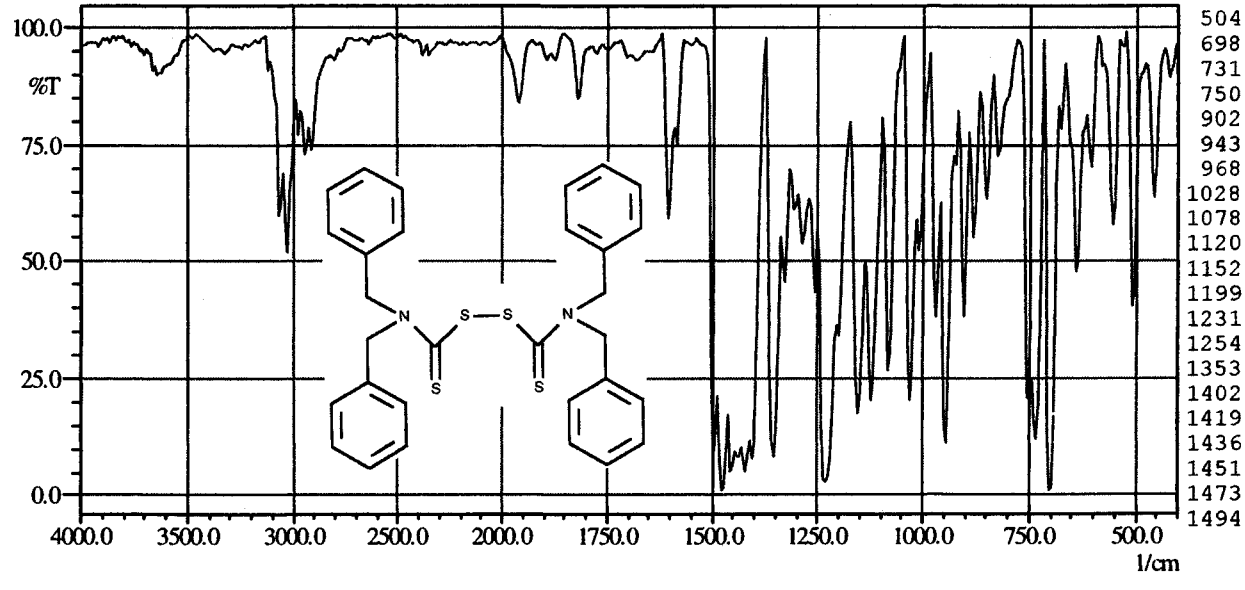
(1) **dipentamethylenethiuram tetrasulfide**
(2) Perkacit DPTT
(3) Akzo Chemie
(4) 384.6 g mol^{-1}
(5) accelerator
(6) colourless solid
(13) KBr pellet
(14) *bis*(N-piperidylthiocarbonyl)tetrasulfane

52242 $C_{14}H_{20}N_2S_4$



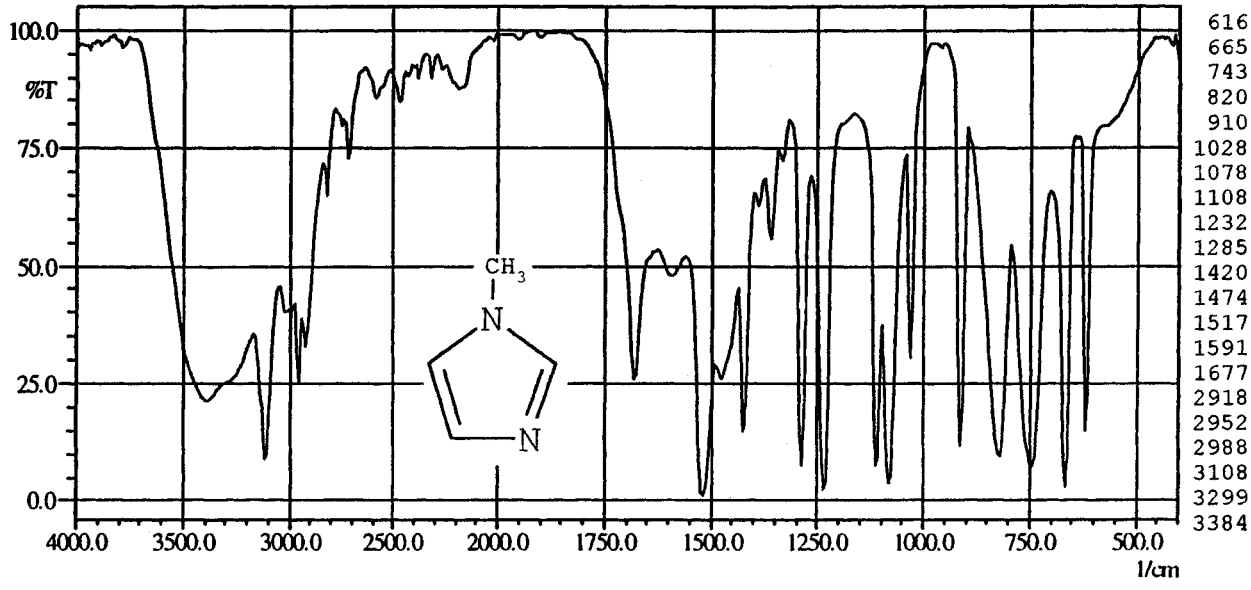
(1) **tetraallylthiuramdisulfide**
(3) Freudenberg (Brunne collection)
(4) 344.6 g mol^{-1}
(5) vulcanisation agent and accelerator
(6) yellowish, clear liquid
(13) layer btw KBr

52242 $C_{30}H_{28}N_2S_4$



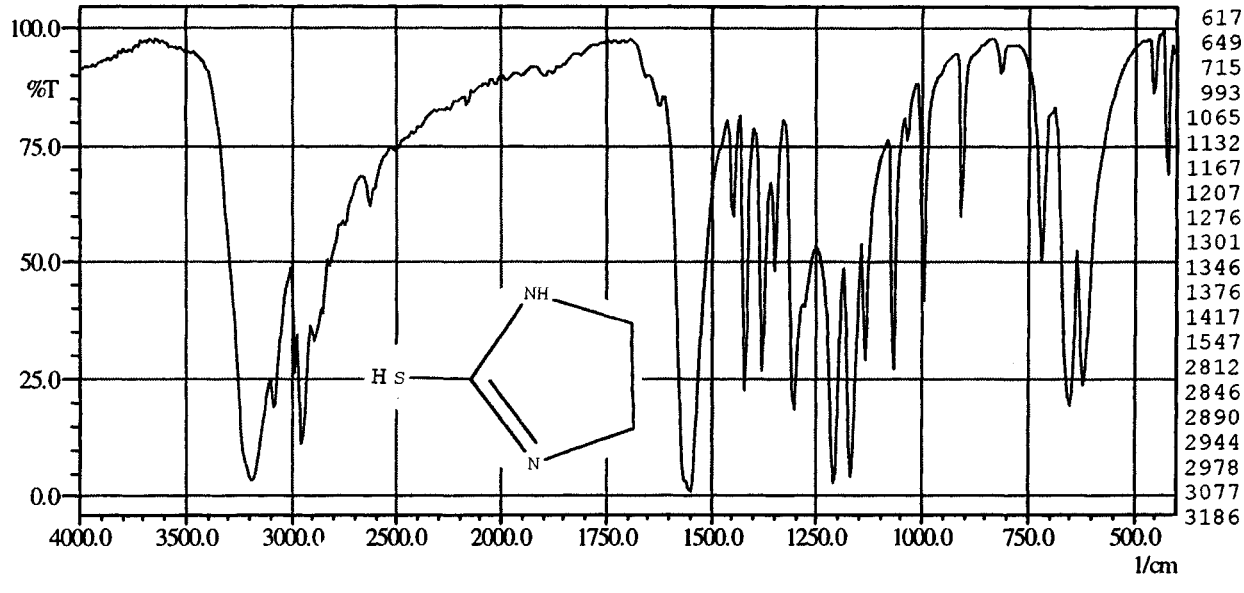
(1) **tetrabenzylthiuramdisulfide**
(2) Perkacit TBZTD
(3) Akzo Chemie
(4) 544.8 g mol^{-1}
(5) accelerator
(6) colourless solid
(13) KBr pellet

5234 $C_4H_6N_2$



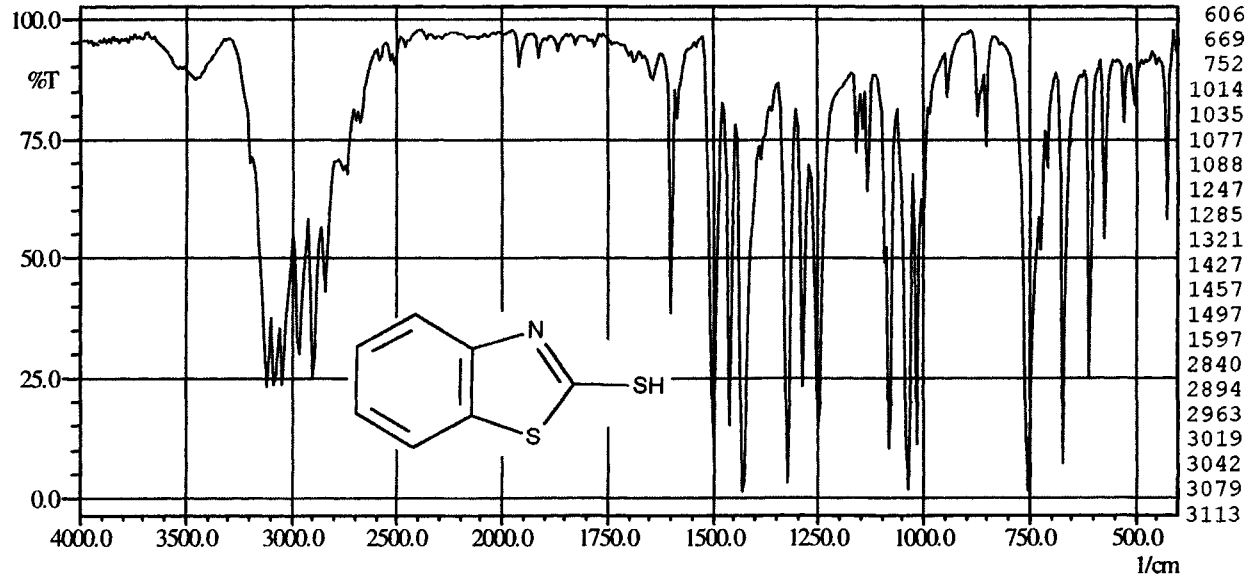
(1) **1-methylimidazol**
(2) Beschleuniger DY 070
(3) Ciba
(4) 82.09 g mol^{-1}
(5) vulcanisation accelerator
(6) colourless liquid
(8) 198 °C
(9) 1.035 g cm^{-3}
(10) 1.497
(13) layer btw. KBr

5234 $C_3H_6N_2S$



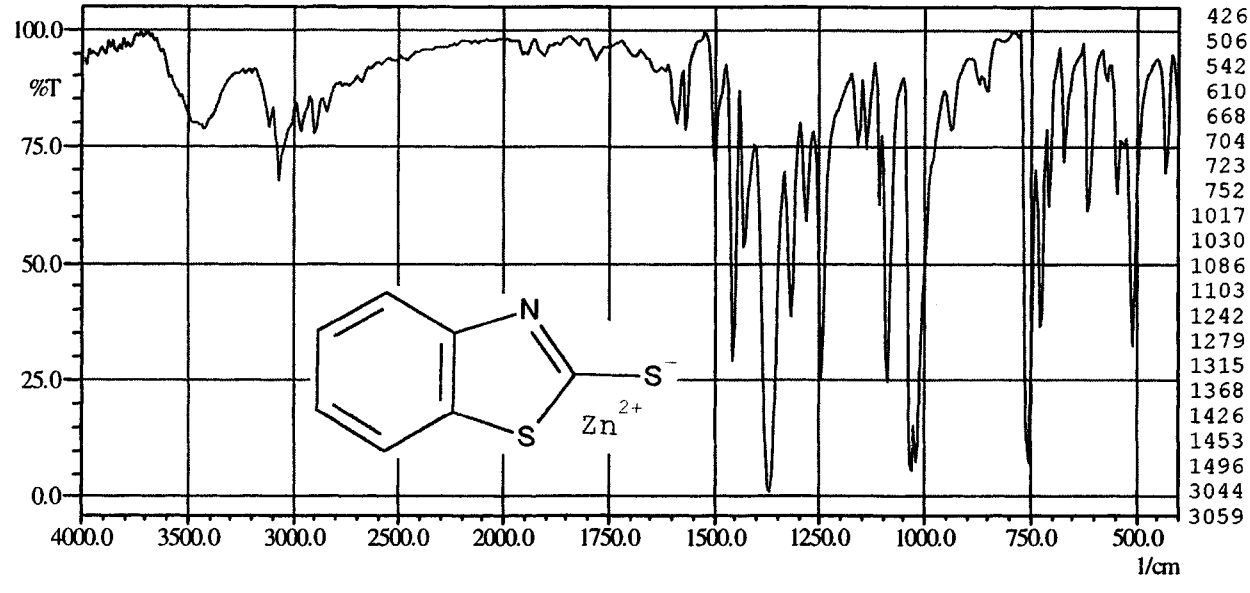
(1) **2-mercaptoimidazoline**
(2) Vulkacit NP
(3) Bayer
(4) 102.1 g mol^{-1}
(5) vulcanisation accelerator
(6) colourless solid
(13) KBr pellet

52351 $C_7H_5NS_2$



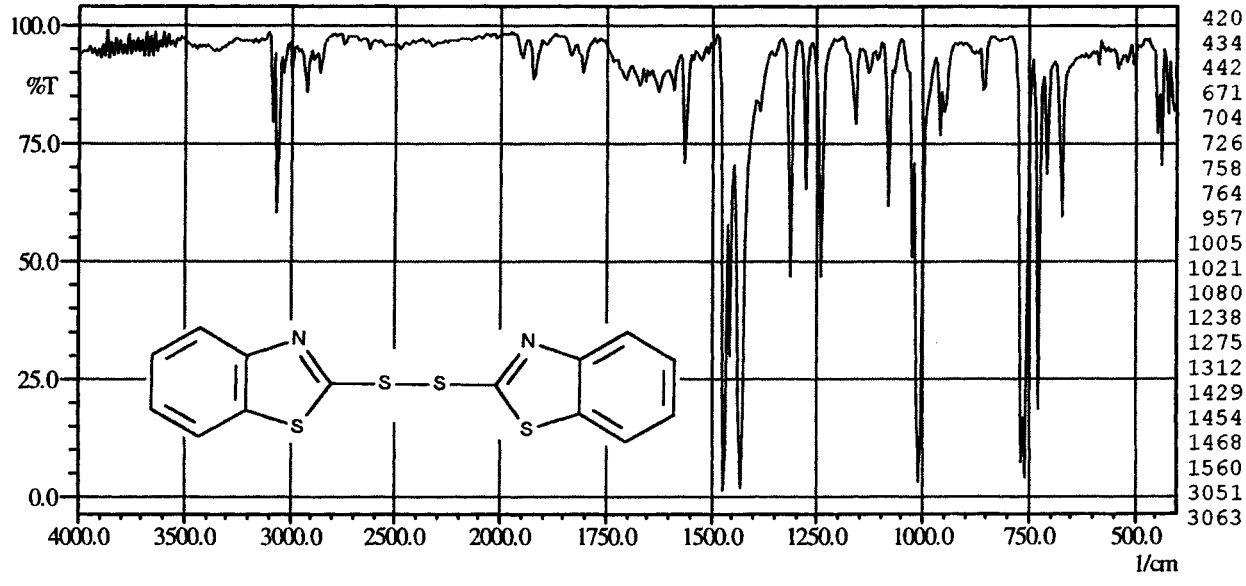
(1) **2-mercaptobenzothiazole**
(2) Perkacit MBT
(3) Akzo Chemie
(4) 167.2 g mol^{-1}
(5) accelerator
(6) colourless solid
(13) KBr pellet

52351 $C_{14}H_8NS_2Zn$



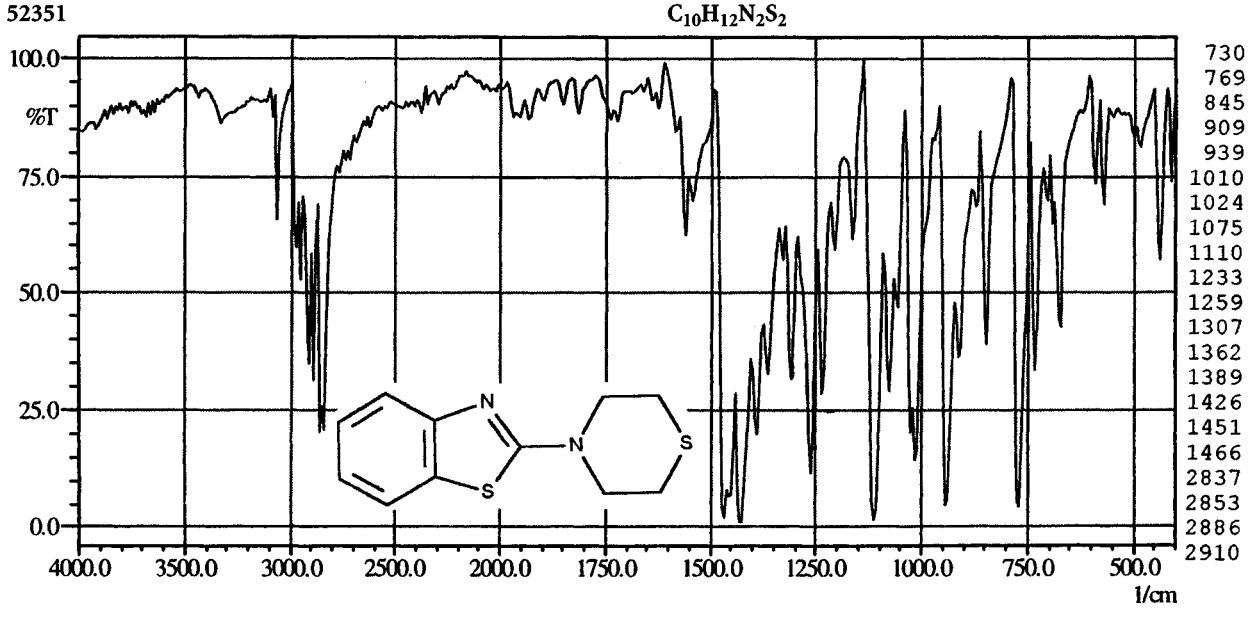
(1) **Zn benzothiazolemercaptide**
(2) Vulkacit ZM
(3) Bayer
(4) 319.7 g mol^{-1}
(5) vulcanisation accelerator
(6) colourless solid
(13) KBr pellet

52351 $C_{14}H_8N_2S_4$



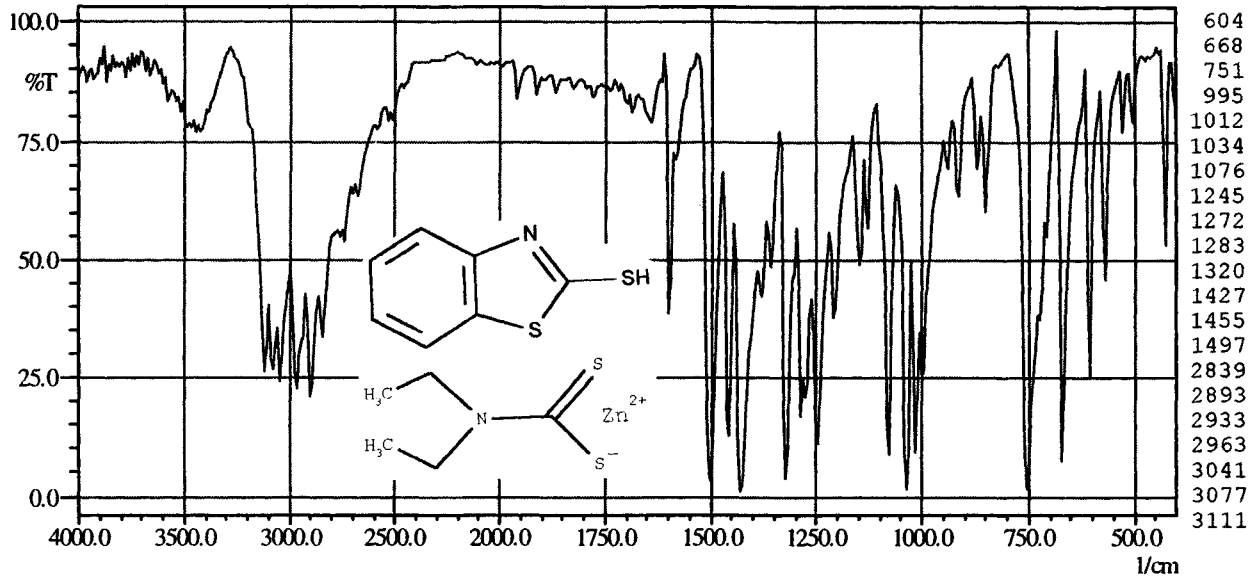
(1) **bis(2-benzothiazole)disulfide**
(2) Perkacit MBTS
(3) Akzo Chemie
(4) 332.5 g mol^{-1}
(5) accelerator
(6) slightly yellowish solid
(13) KBr pellet

52351 $C_{10}H_{12}N_2S_2$



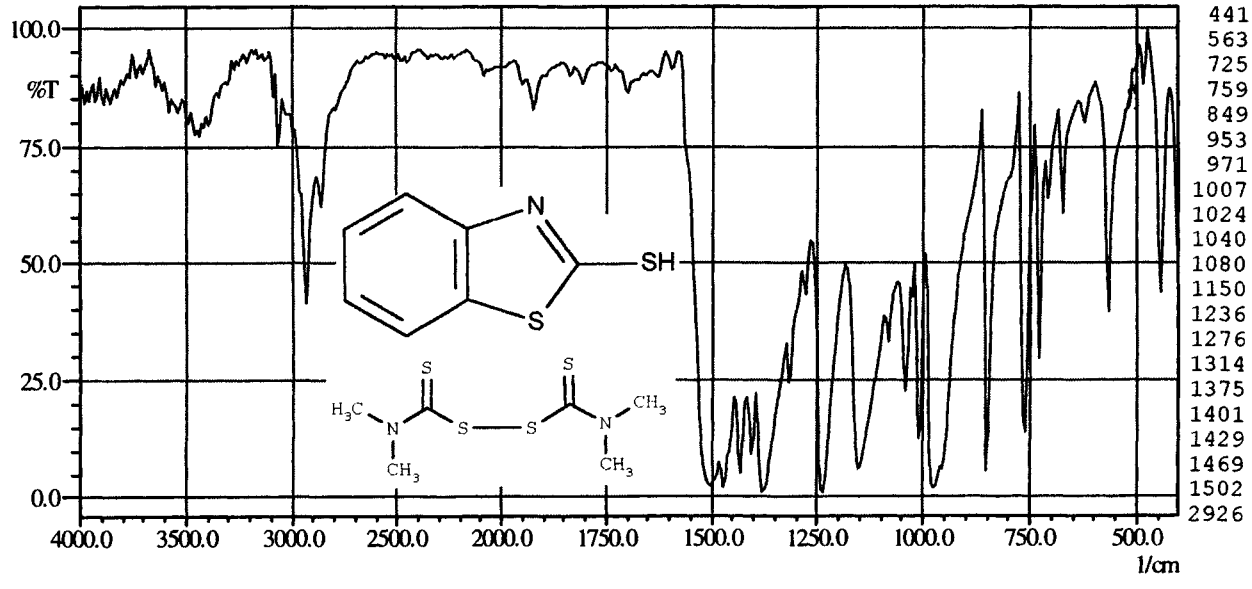
(1) **2-(thiomorpholino)benzothiazole**
(2) Perkacit MBS
(3) Akzo Chemie
(4) 224.4 g mol^{-1}
(5) accelerator
(6) yellowish, soft granules
(13) KBr pellet

52351+5223 $C_{10}H_{10}N_2S_4Zn + C_7H_5NS_2$



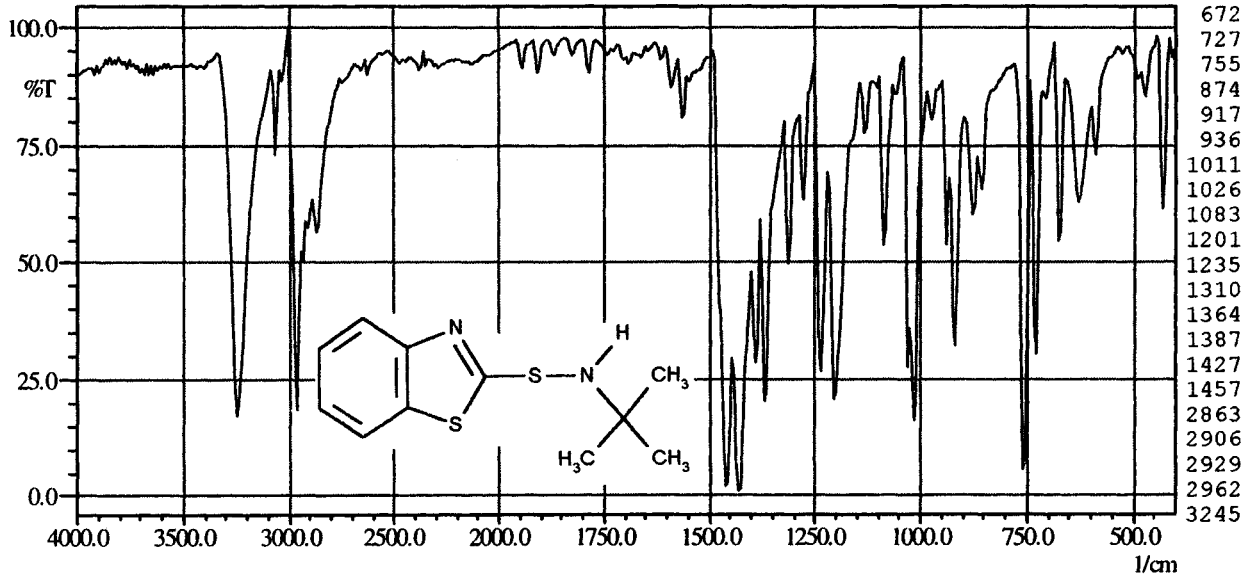
(1) **Zn diethyldithiocarbamate + mercaptobenzothiazole**
(2) Vulkacit MDA/C
(3) Bayer
(4) 351.8+167.2 g mol^{-1}
(5) vulcanisation accelerator
(6) greyish solid
(13) KBr pellet

52351+52242 $C_7H_5NS_2+C_6H_{12}N_2S_4$



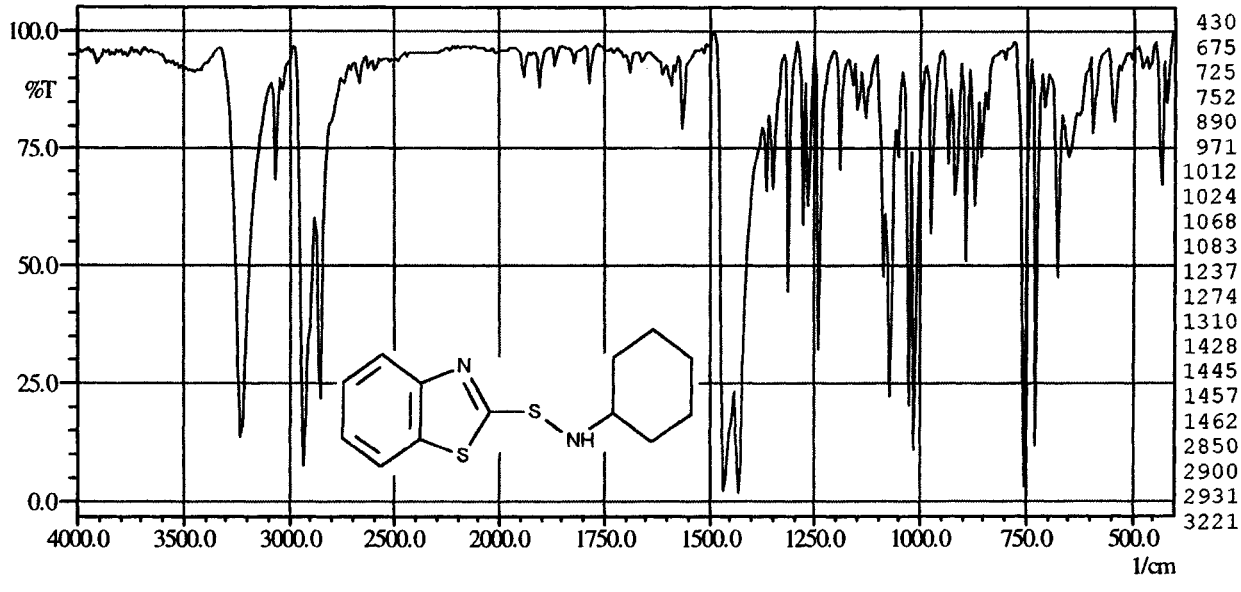
(1) **2-mercaptobenzothiazole + tetramethylthiuramdisulfide**
(2) Vulkacit MT/C
(3) Bayer
(4) 167.3+240.4 g mol^{-1}
(5) vulcanisation accelerator
(6) colourless solid
(13) KBr pellet

52352 $C_{11}H_{14}N_2S_2$



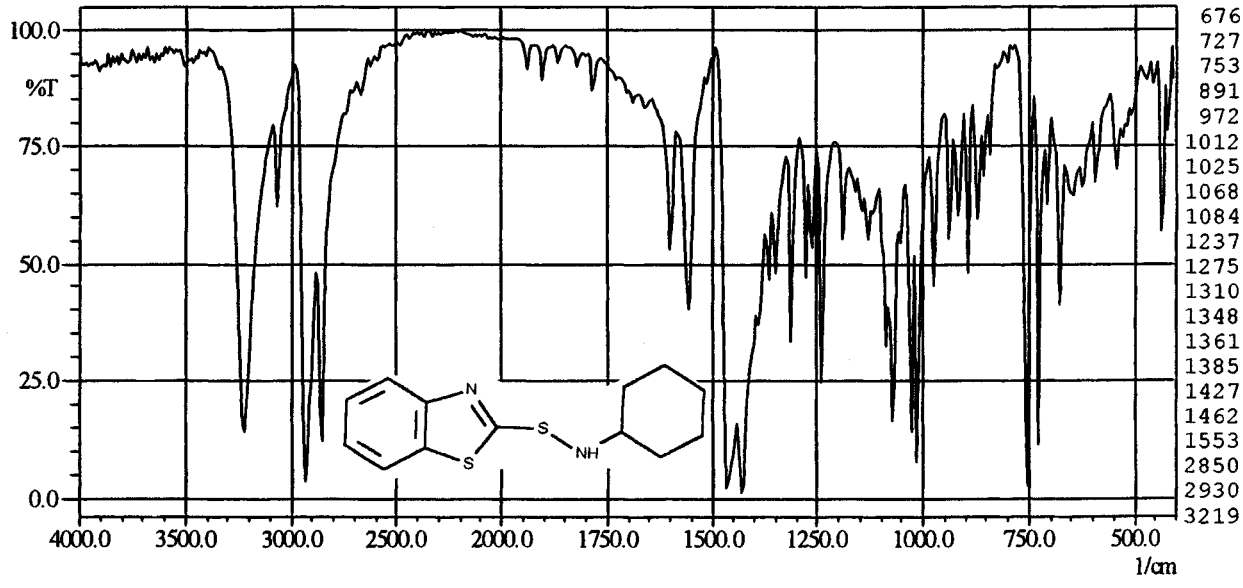
(1) **N-*t*-butyl-2-benzothiazolesulfenamide**
(2) Perkacit TBBS
(3) Akzo Chemie
(4) 238.3 g mol^{-1}
(5) accelerator
(6) colourless, soft granules
(13) KBr pellet

52352 $C_{13}H_{16}N_2S_2$



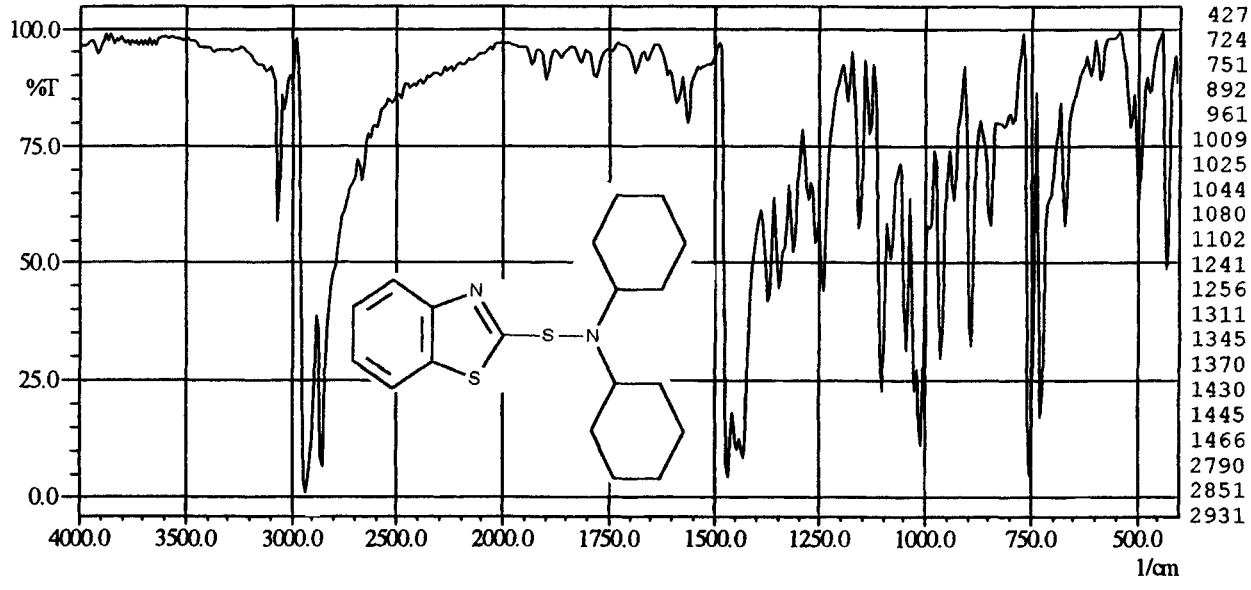
(1) **N-cyclohexyl-2-benzothiazolsulfenamide**
(2) Vulkacit CZ/EG-C
(3) Bayer
(4) 264.4 g mol^{-1}
(5) vulcanisation accelerator
(6) colourless solid
(13) KBr pellet

52352 $C_{13}H_{16}N_2S_2$



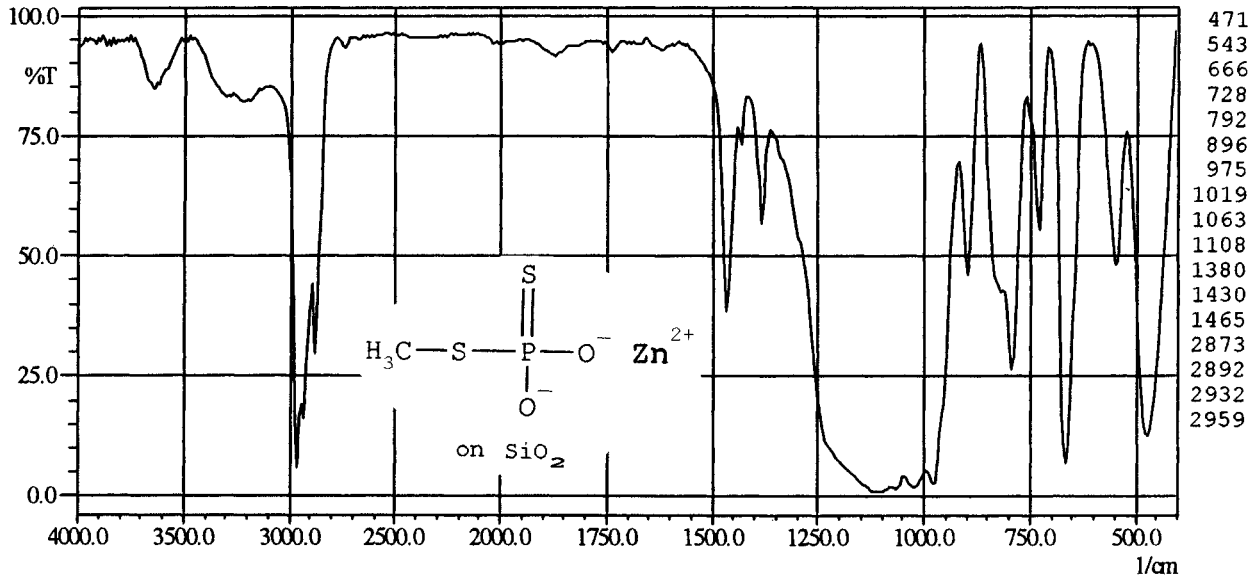
(1) **N-cyclohexyl-2-benzothiazole sulfenamide**
(2) Perkacit CBS
(3) Akzo Chemie
(4) 264.4 g mol^{-1}
(5) accelerator
(6) colourless granules
(13) KBr pellet

52352 $C_{19}H_{26}N_2S_2$



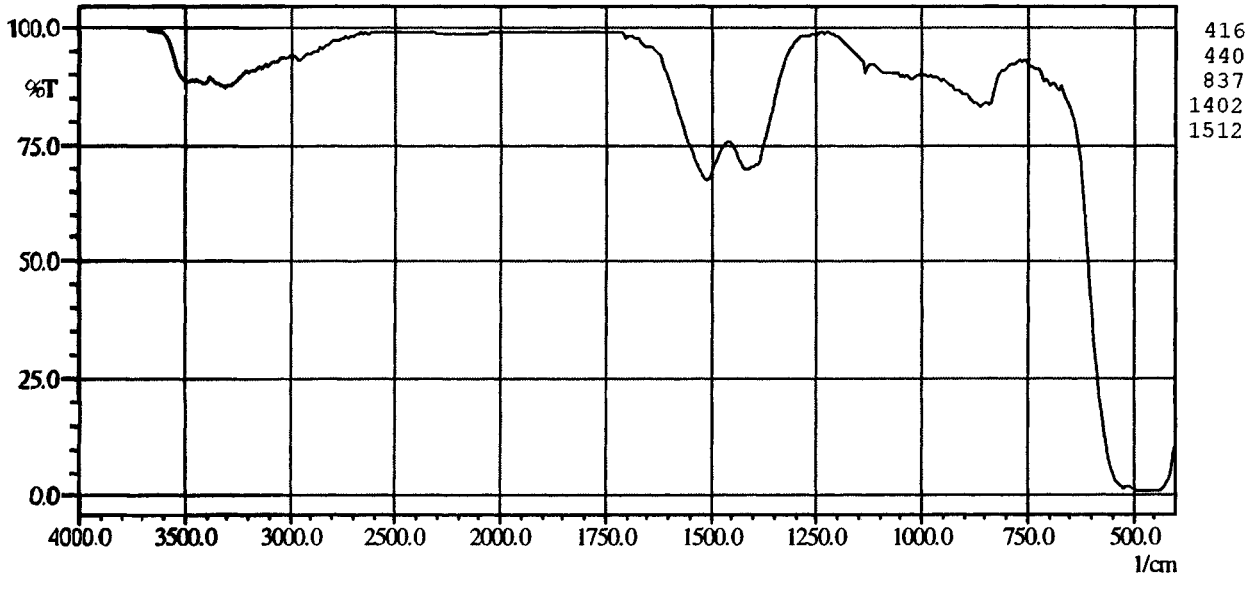
(1) **N,N'-dicyclohexyl-2-benzothiazolesulfenamide**
(2) Perkacit DCBS
(3) Akzo Chemie
(4) 346.6 g mol^{-1}
(5) accelerator
(6) colourless, soft granules
(13) KBr pellet

524



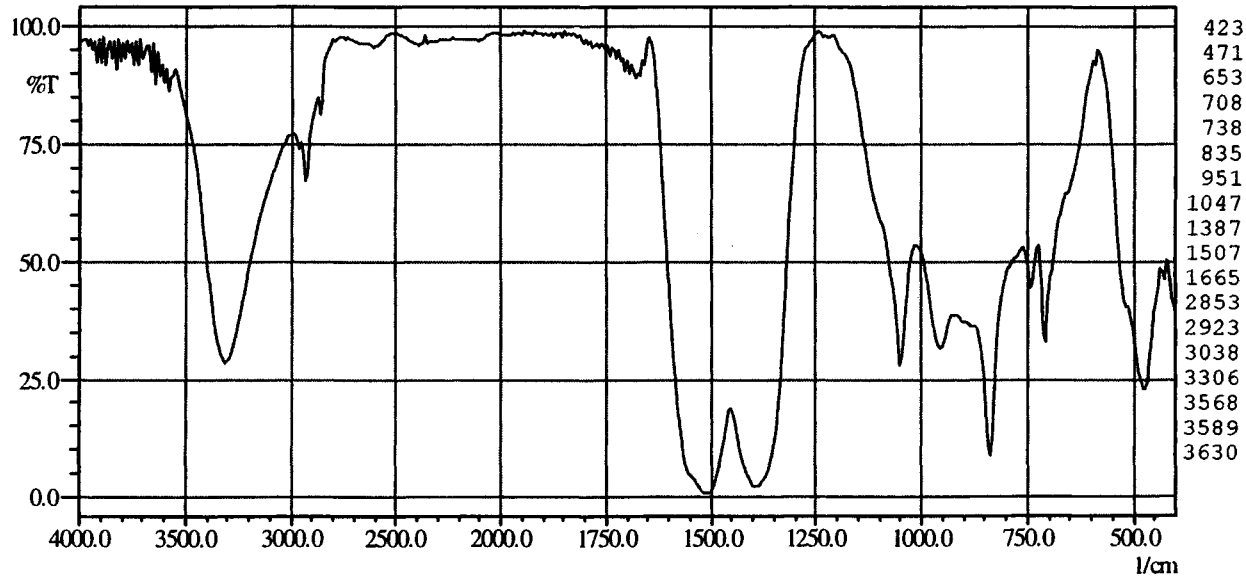
(1) **dithiophosphoric acid ester, Zn salt, on SiO2**
(2) Rhenocure TP/S (Rhenocure TP + SiO2 2:1)
(3) Rhein-Chemie
(5) vulcanisation accelerator
(6) colourless solid
(13) KBr pellet

5311 **ZnO**



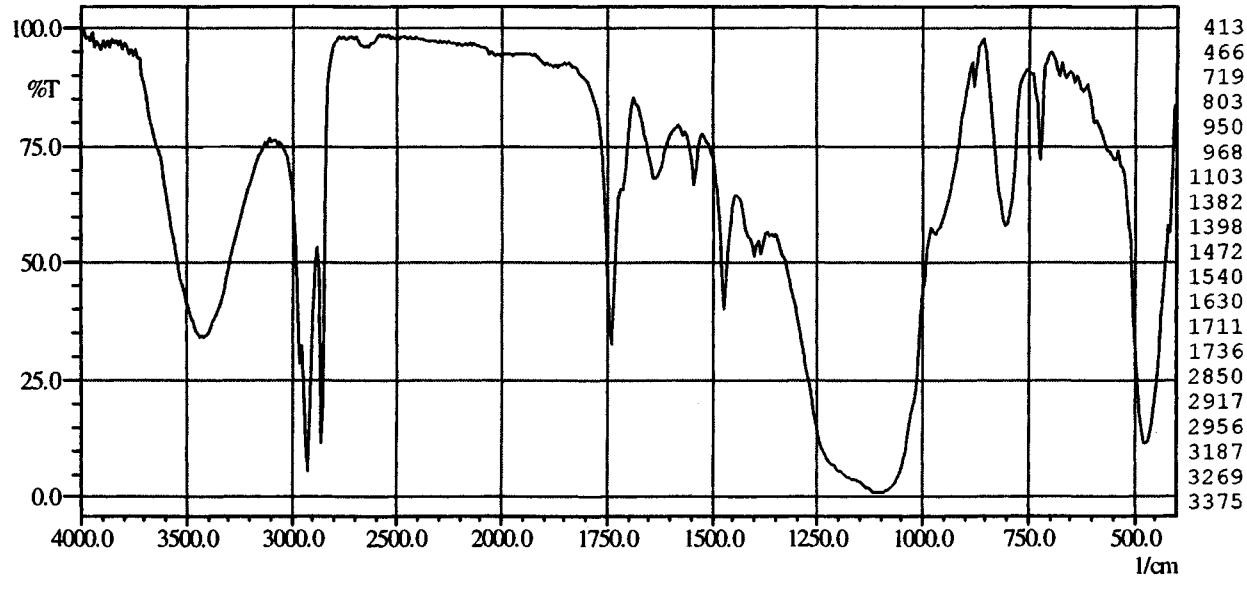
(1) **Zn oxide (93–95% ZnO, <10 ppm PbO)**
(2) Zinkoxid Aktiv
(3) Bayer
(4) 81.38 g mol^{-1}
(5) vulcanisation activator, filler
(6) colourless solid
(9) 5.5 g cm^{-3}
(13) KBr pellet

5311 $ZnCO_3$



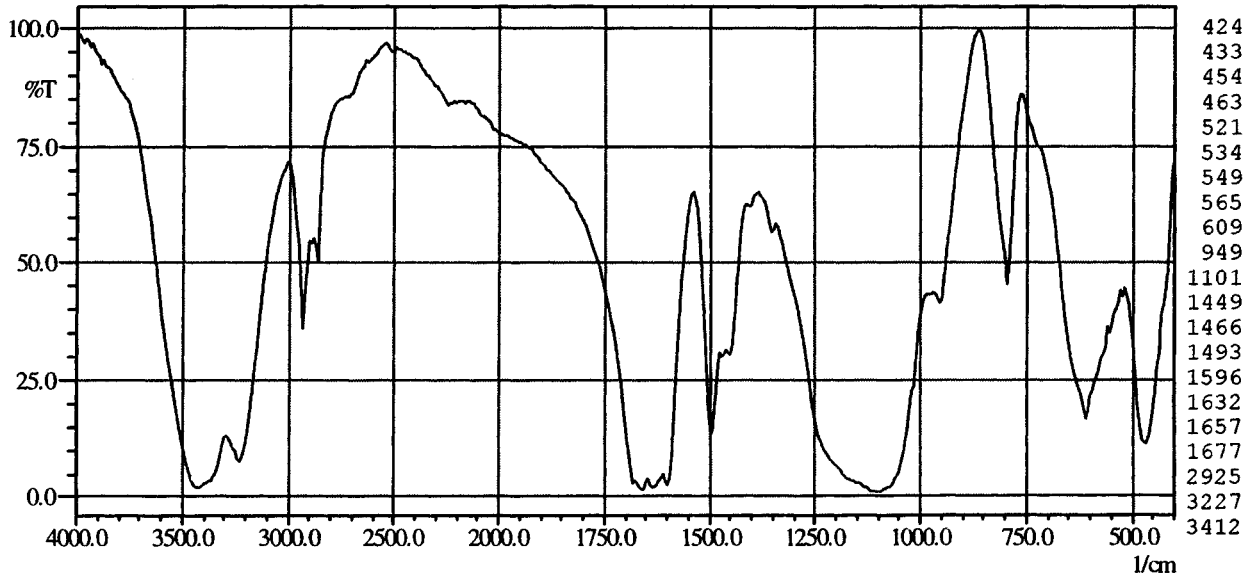
(1) **basic Zn carbonate (70–73% ZnO, <10 ppm PbO)**
(2) Zinkoxid transparent
(3) Bayer
(4) 125.4 g mol^{-1}
(5) vulcanisation activator, filler
(6) colourless solid
(13) KBr pellet

5314 SiO_2



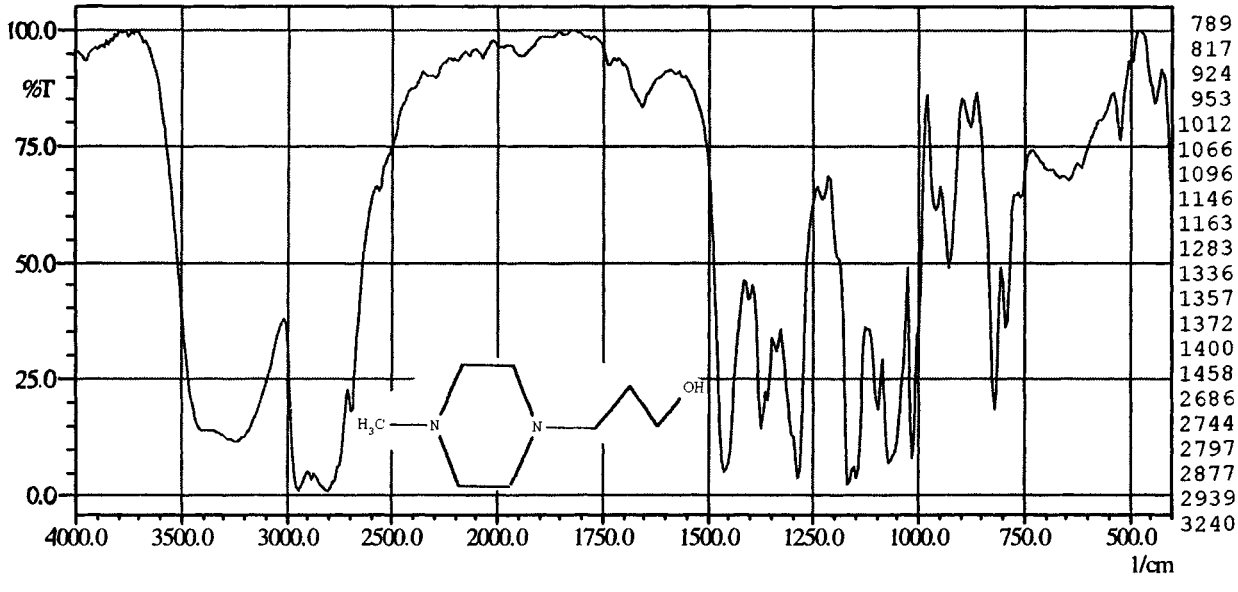
(1) **amorphous silicium dioxide with active organic substance**
(2) Aflux S
(3) Freudenberg (Brunne collection)
(4) 60.09 g mol^{-1}
(5) vulcanisation activator
(6) colorless solid
(13) KBr pellet

5314 SiO_2



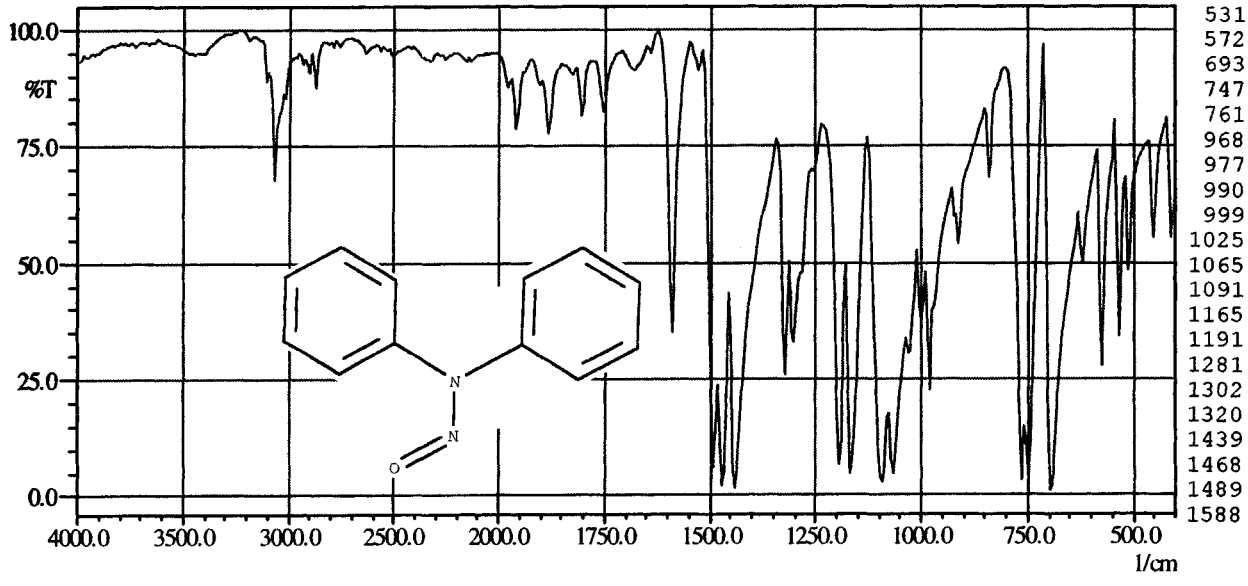
(1) **mixture of amorphous siliciumdioxide with surfactants**
(2) Rhenofit 1987
(3) Rhein-Chemie
(5) vulcanisation activator
(6) colourless solid
(13) KBr

5321 $C_8H_{18}N_2O$



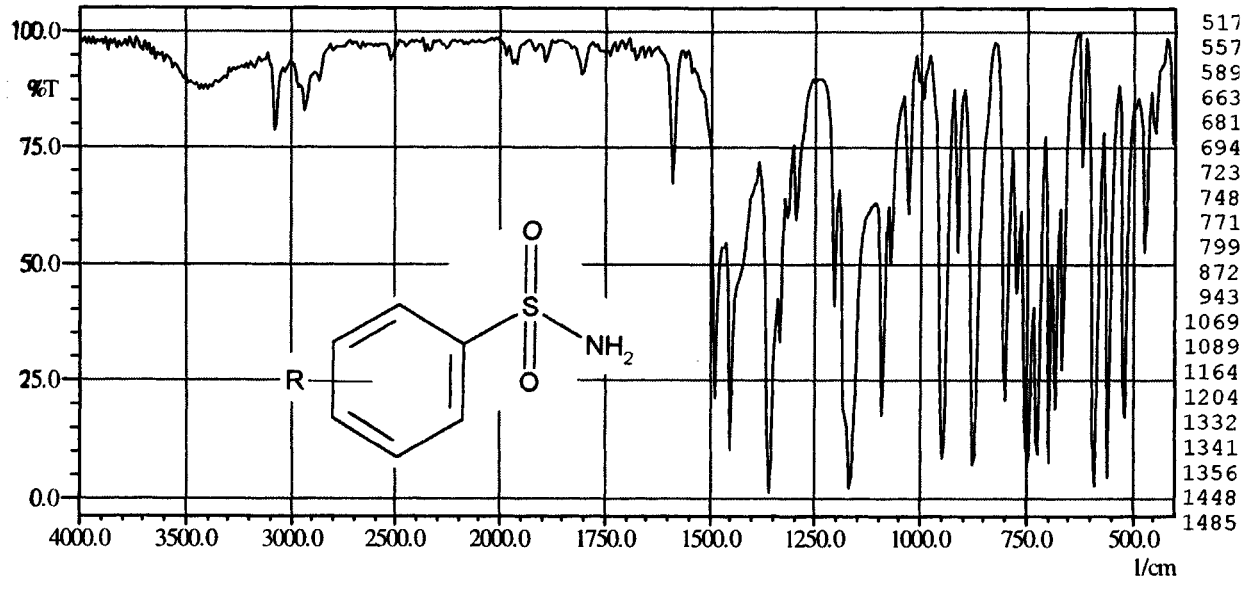
(1) **4-methyl-1-piperazinepropanol**
(3) Freudenberg (Brunne collection)
(4) 158.2 g mol^{-1}
(5) vulcanisation activator
(6) colourless, clear liquid
(13) layer on KBr

543 $C_{12}H_{10}N_2O$



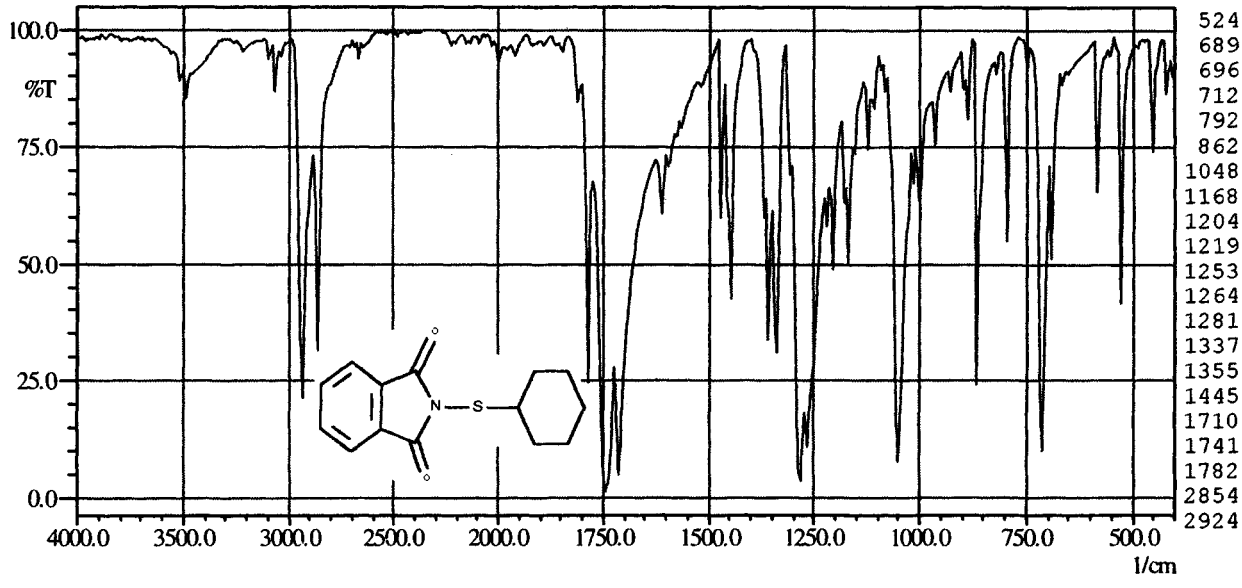
(1) **N-nitrosodiphenylamine**
(2) Vulkalent A
(3) Bayer
(4) 198.2 g mol^{-1}
(5) vulcanisation retarder
(6) solid
(13) KBr pellet

544



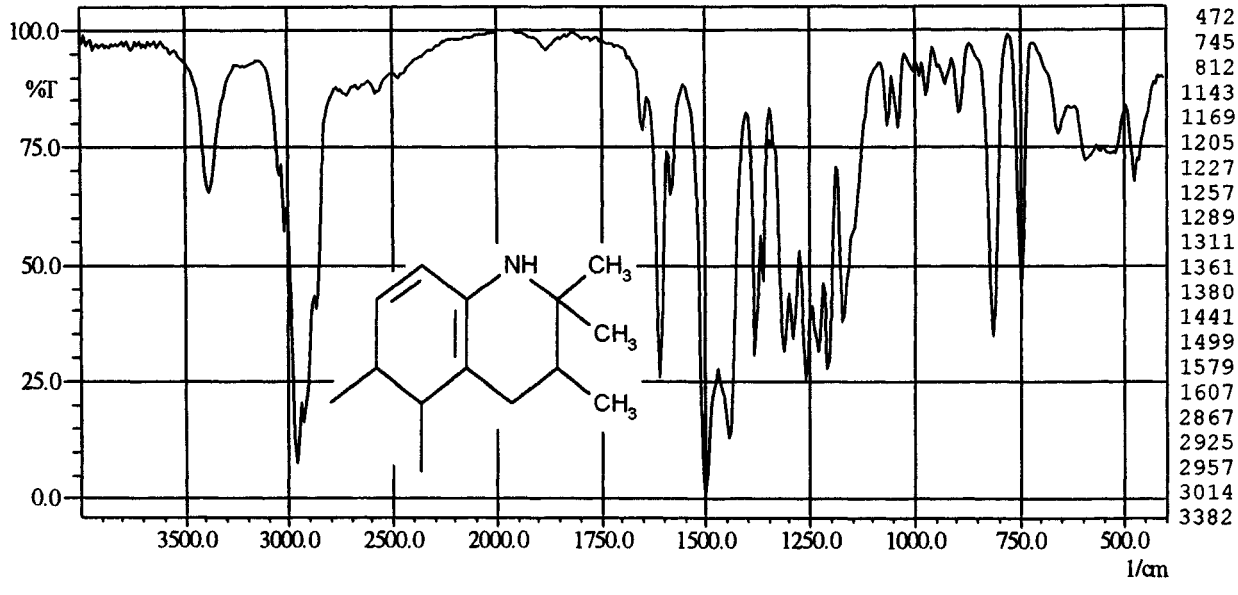
(1) **aromatic-aliphatic sulfonamide**
(2) Vulkalent E
(3) Bayer
(5) vulcanisation retarder
(6) colourless solid
(13) KBr pellet

545 $C_{14}H_{15}NO_2S$



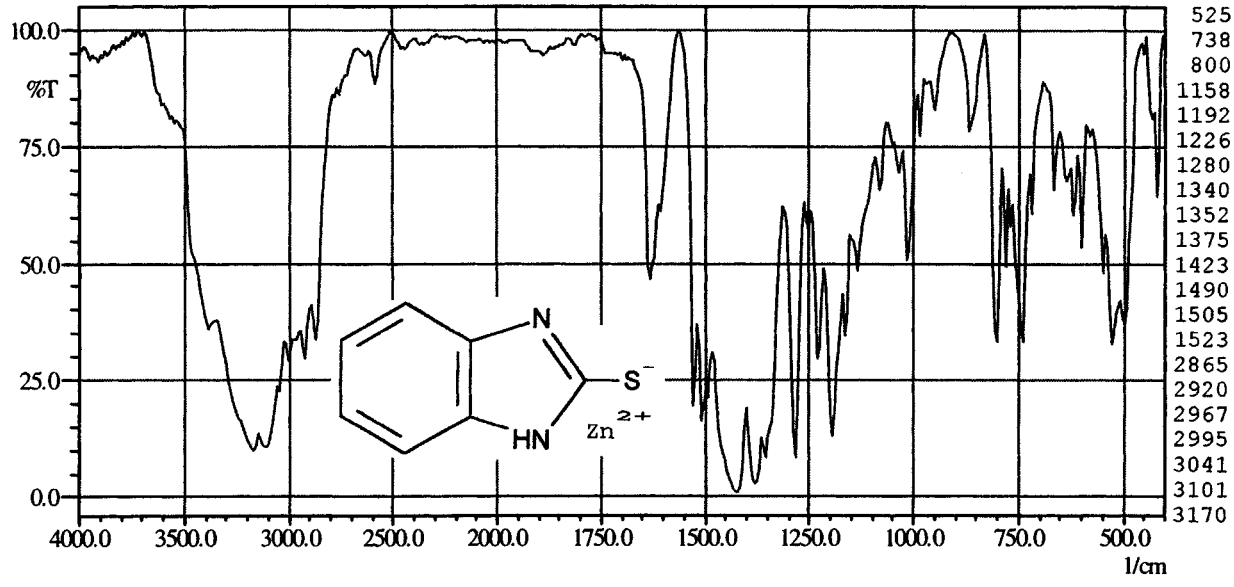
(1) **N-(cyclohexylthio)phthalimide**
(2) Santogard PVI DS
(3) Monsanto
(4) 261.3 g mol^{-1}
(5) vulcanisation retarder
(6) colourless solid
(13) KBr pellet

551112 $C_{12}H_{17}N$



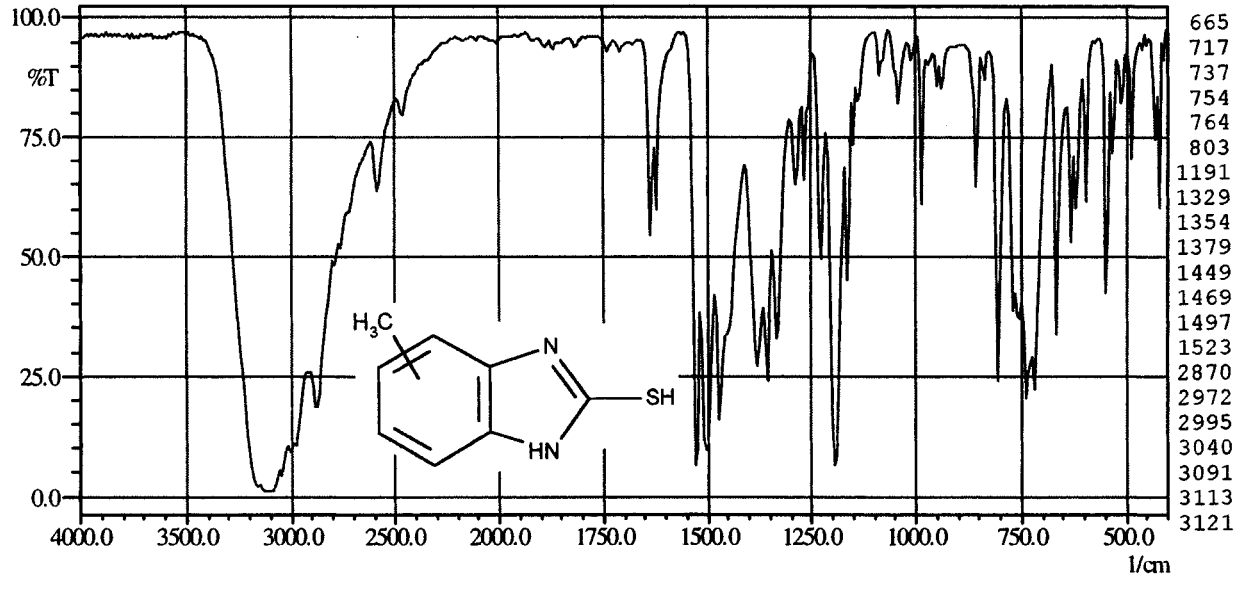
(1) **acetone-aniline condensation product, polymeric 1, 2-dihydro-2, 2, 4-trimethylquinoline**
(2) Flectol H
(3) Monsanto
(5) ageing inhibitor and antioxidant for vulcanisates
(6) light-brown solid
(13) film from the melt btw KBr

55131 $ZnC_{14}H_{10}N_4S_2$



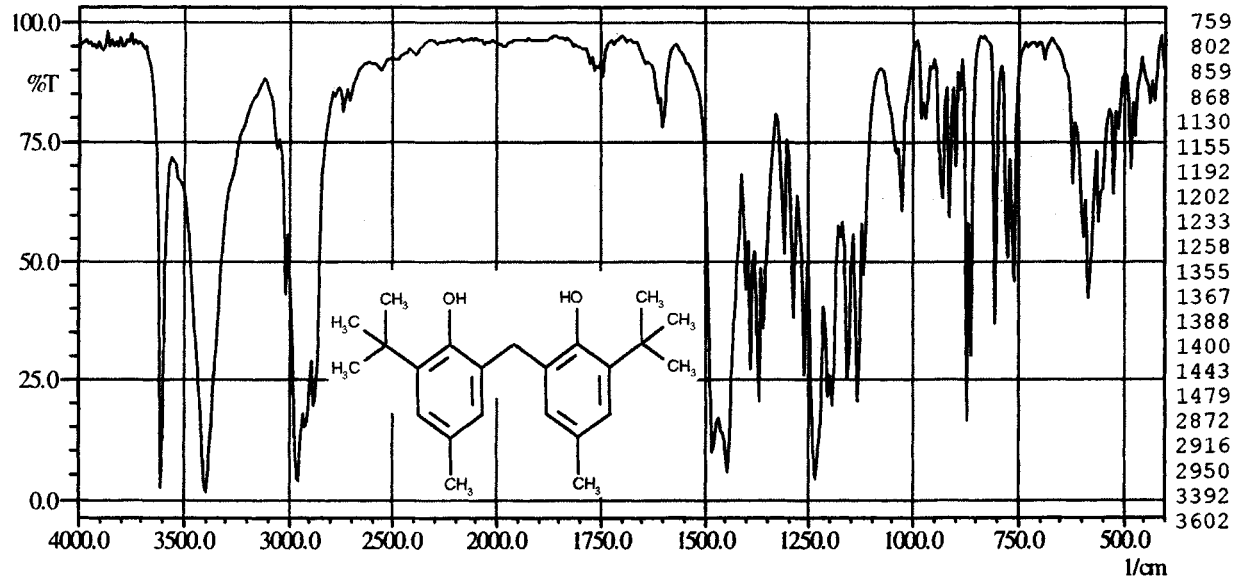
(1) **Zn 2-benzimidazole ethiolate**
(2) Vulkanox ZMB 2
(3) Bayer
(4) 363.6 g mol^{-1}
(5) antioxidant
(6) colourless solid
(13) KBr pellet

5523 $C_8H_8N_2S$



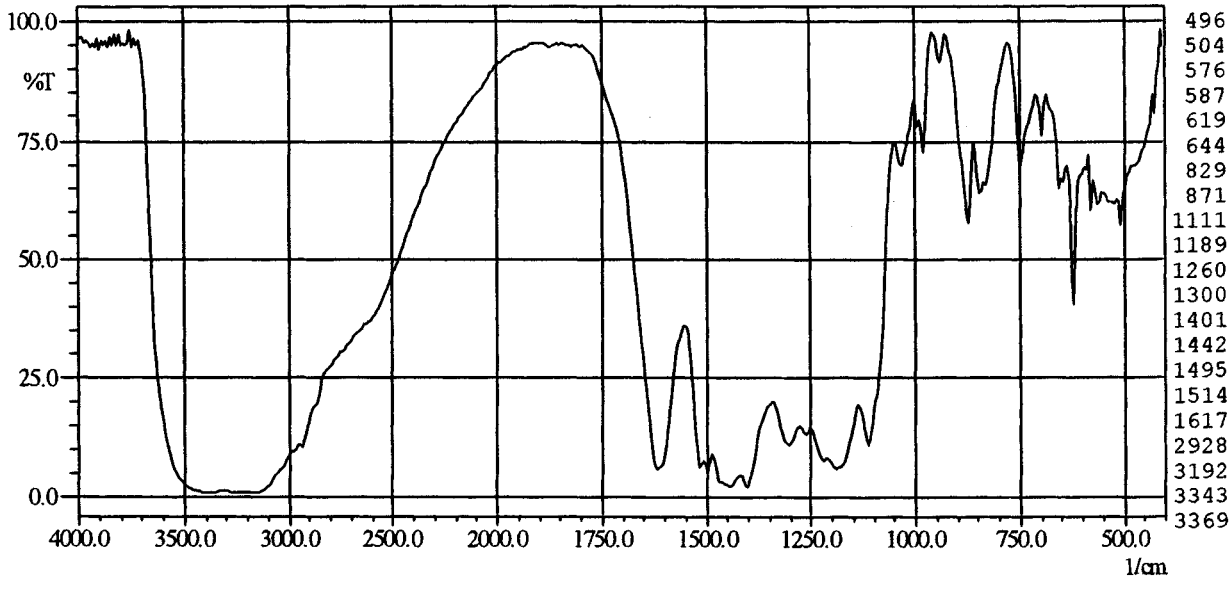
(1) **4- or 5-methylmercaptobenzimidazole**
(2) Vulkanox MB2/MG
(3) Bayer
(4) 164.2 g mol^{-1}
(5) antioxidant
(6) yellowish-white solid
(7) 290 °C
(9) 1.25 g cm^{-3}
(13) KBr pellet

56 $C_{23}H_{32}O_2$



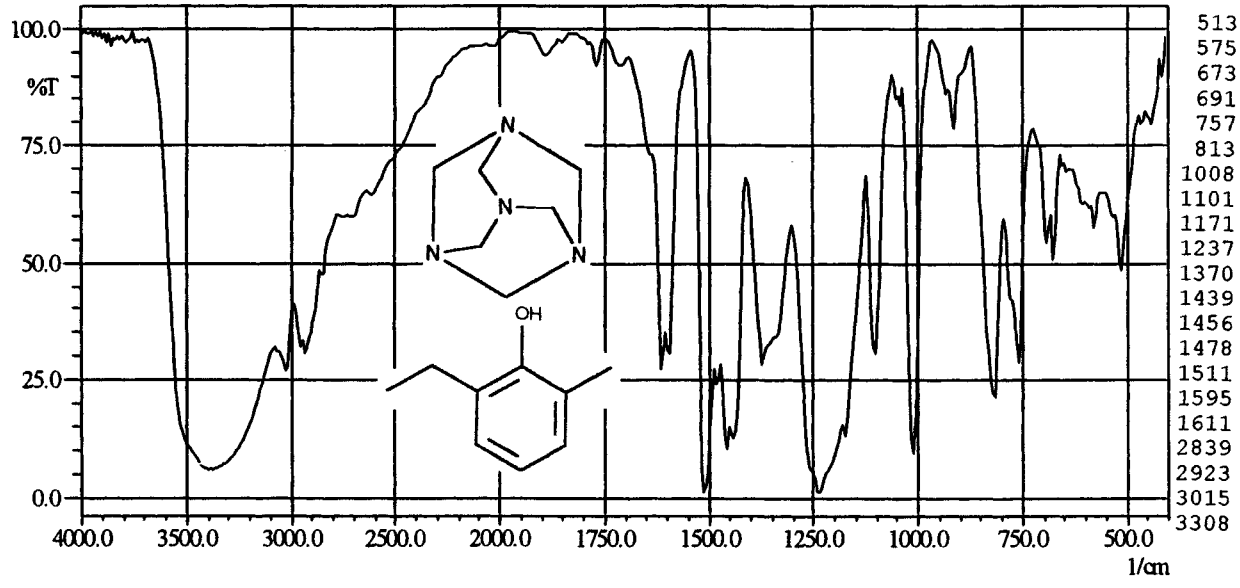
(1) **2,2'-methylene-*bis*(6-*t*-butyl-4-methylphenol)**
(2) Vulkadur RB
(3) Bayer
(4) 340.5 g mol^{-1}
(5) reinforcing resin
(6) red flakes
(7) 85 °C
(9) 1.15 g cm^{-3}
(13) KBr pellet

56



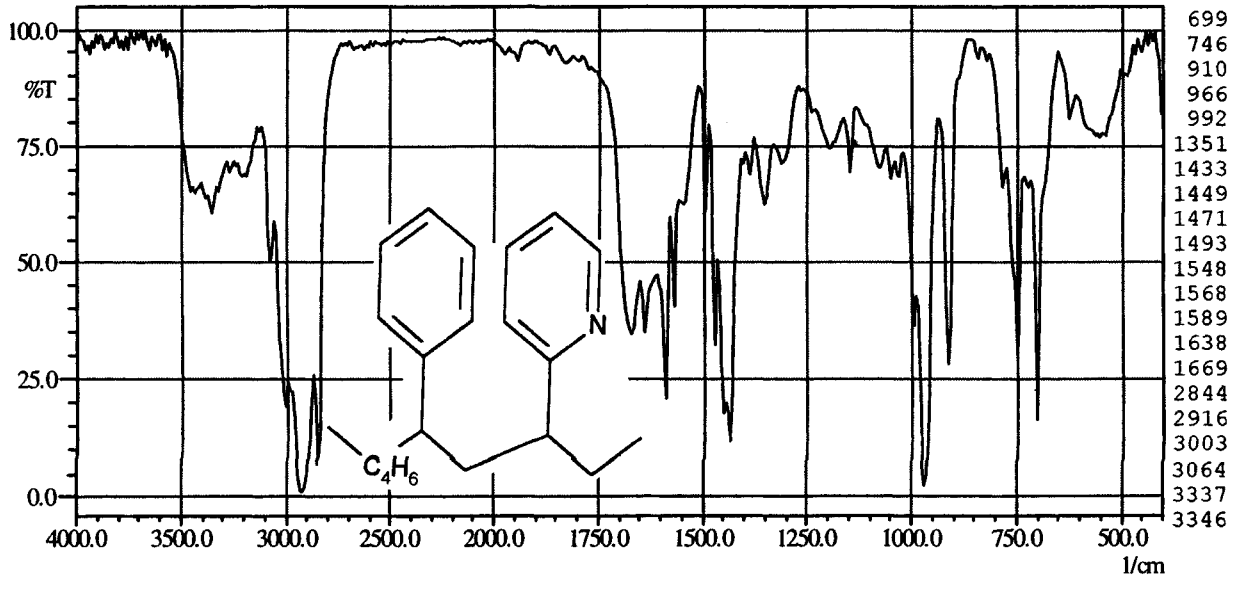
(1) **H-active mixture, phenol-formaldehyde resin (resol)**
(2) Vulcabond E
(3) Akzo Chemie
(5) adhesion agent
(6) black liquid, dried (solid residue)
(13) KBr pellet

56



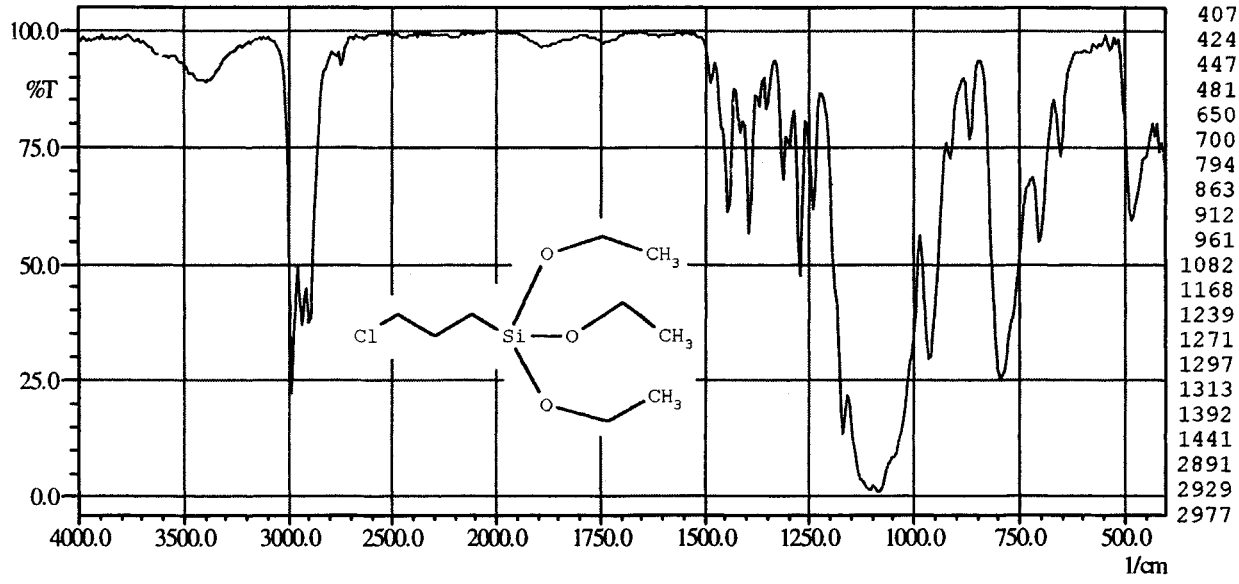
(1) **phenol-formaldehyde novolac with 10% hexamethylenetetramine**
(2) Vulkadur A
(3) Bayer
(5) intensifier
(6) ochre solid
(7) 82.5 °C
(9) 1.3 g cm^{-3}
(13) KBr pellet

56



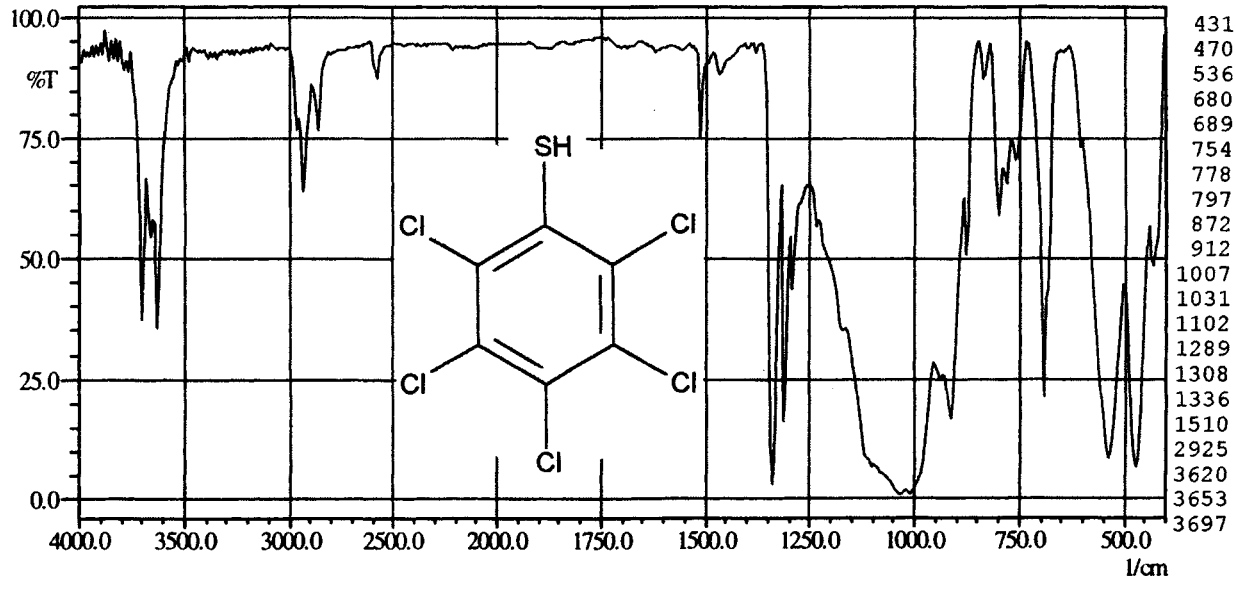
(1) **poly(butadiene-*co*-styrene-*co*-2-vinylpyridine-*co*-amide/acid)**
(2) Pyratex 240
(3) Bayer
(5) adhesion agent, adhesion improver
(6) yellowish, clear liquid
(13) layer on KRS-5

56 $SiC_9H_{21}ClO_3$



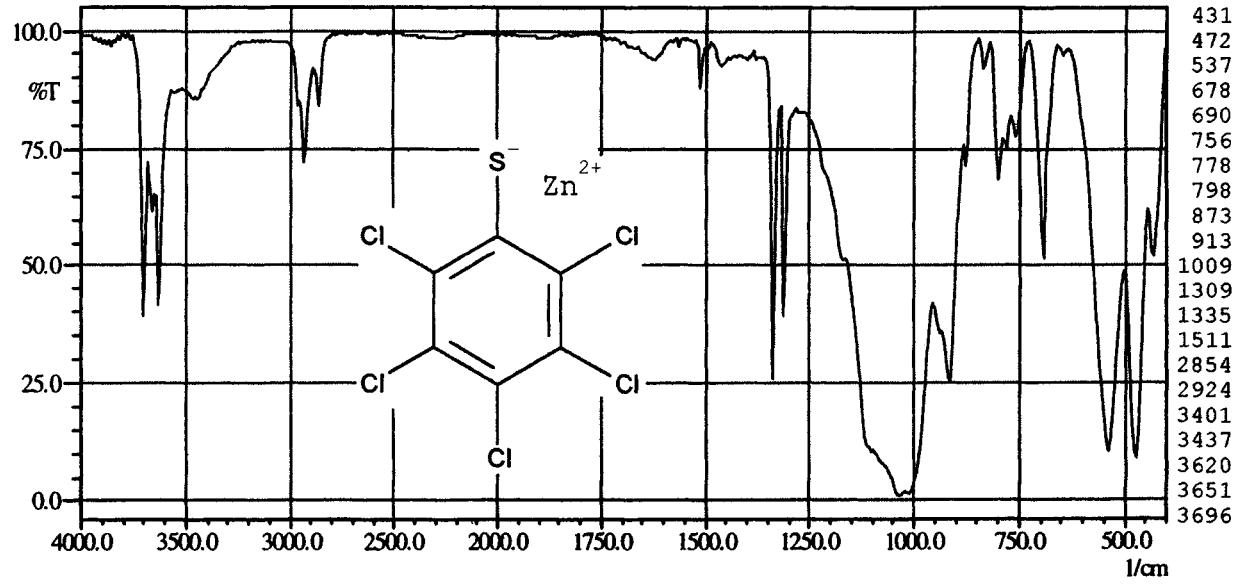
(1) **3-chloropropyltriethoxysilane**
(2) Dynasylan CPTEO
(3) Dynamit Nobel
(4) 240.8 g mol^{-1}
(5) promoter between inorganics, adhesion-improving agent
(6) colourless, clear liquid
(13) layer btw KBr

57 C_6HCl_5S



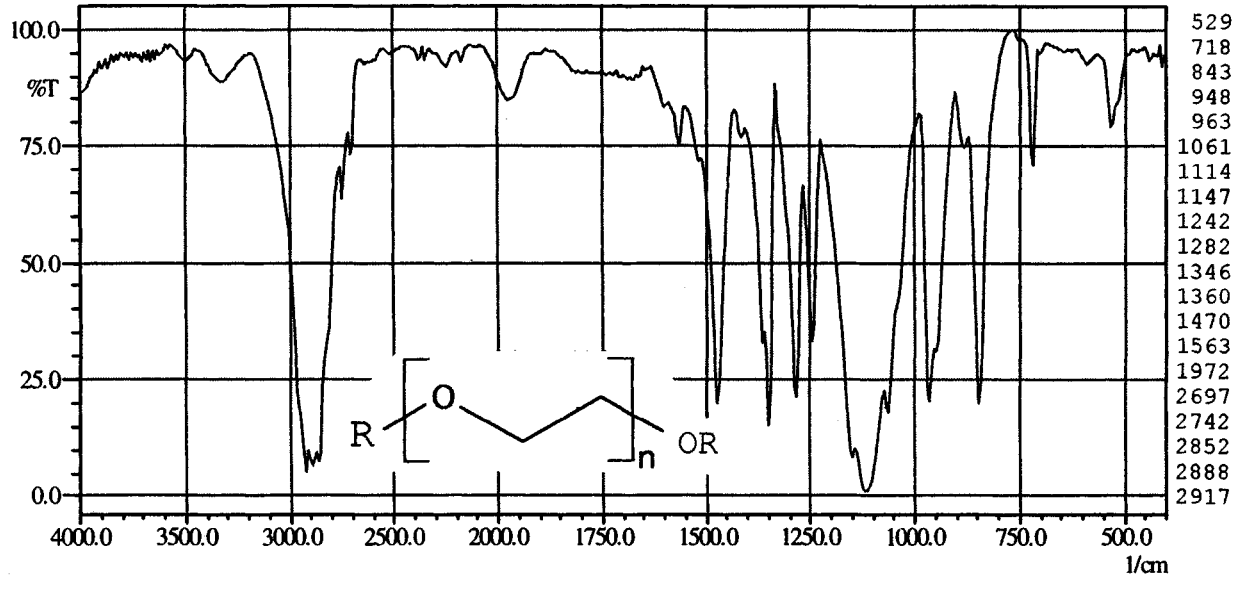
(1) **pentachlorothiophenol on kaolin**
(2) Renacit 7
(3) Bayer
(4) 282.4 g mol^{-1}
(5) peptiser, plastificator
(6) light-grey solid
(9) 2.3 g cm^{-3}
(13) KBr pellet

57 C_6HCl_5S



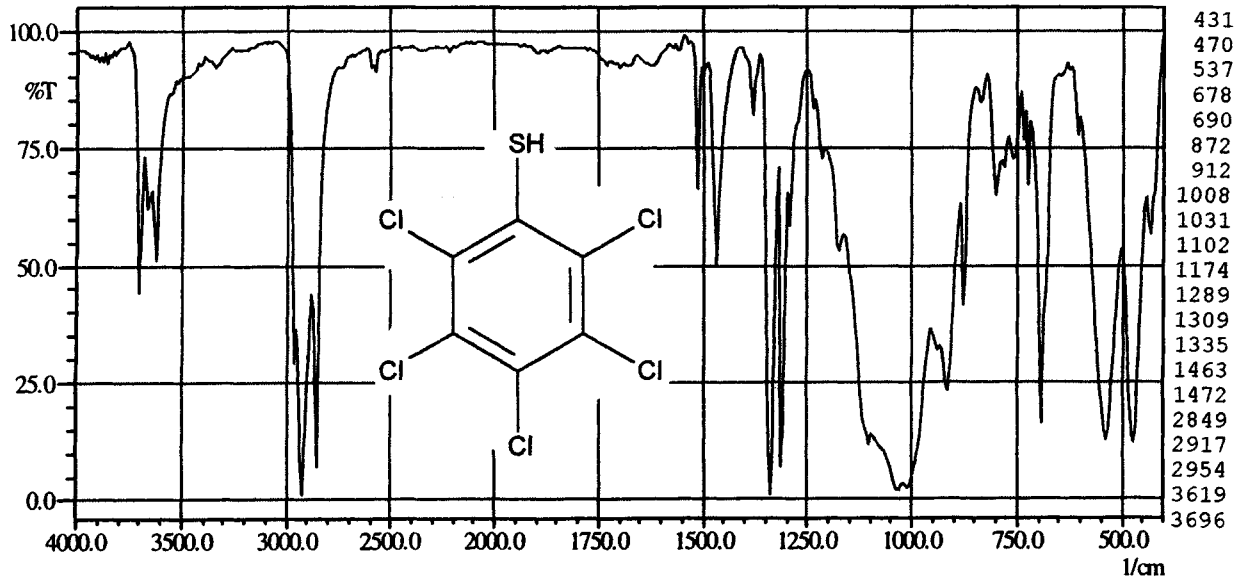
(1) **Zn pentachlorothiophenolate on kaolin with other ingredients**
(2) Renacit 9
(3) Bayer
(4) 282.4 g mol^{-1}
(5) peptiser
(6) colourless solid
(9) 2.3 g cm^{-3}
(13) KBr pellet

57



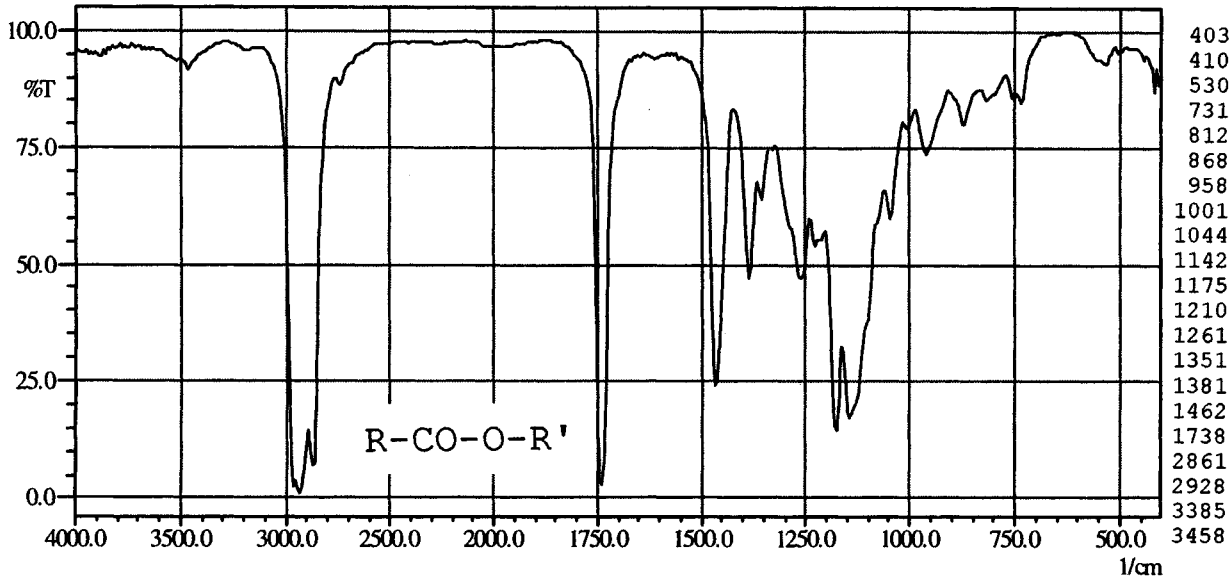
(1) **poly(oxyethylene)dialkylether**
(2) Vulcastab LW
(3) Akzo Chemie
(5) stabiliser for latex
(6) colourless solid
(13) KBr pellet

57 C_6HCl_5S



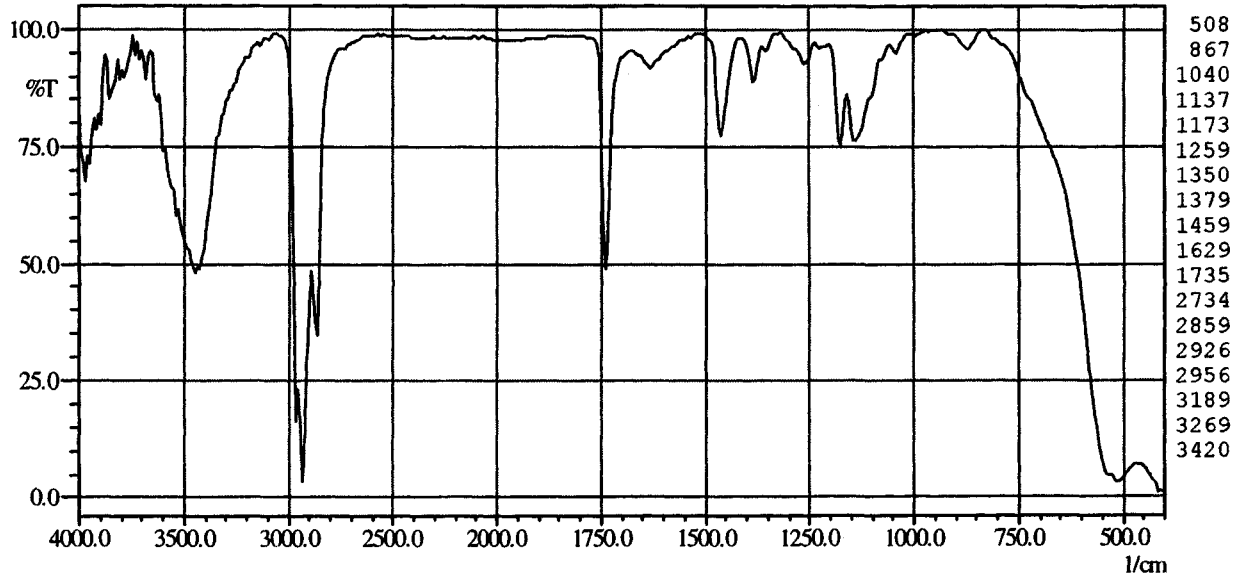
(1) **pentachlorothiophenol on kaolin with other ingredients**
(2) Renacit 7/WG
(3) Bayer
(4) 282.4 g mol^{-1}
(5) peptiser
(6) grey sticks
(9) 2.1 g cm^{-3}
(13) KBr pellet

57



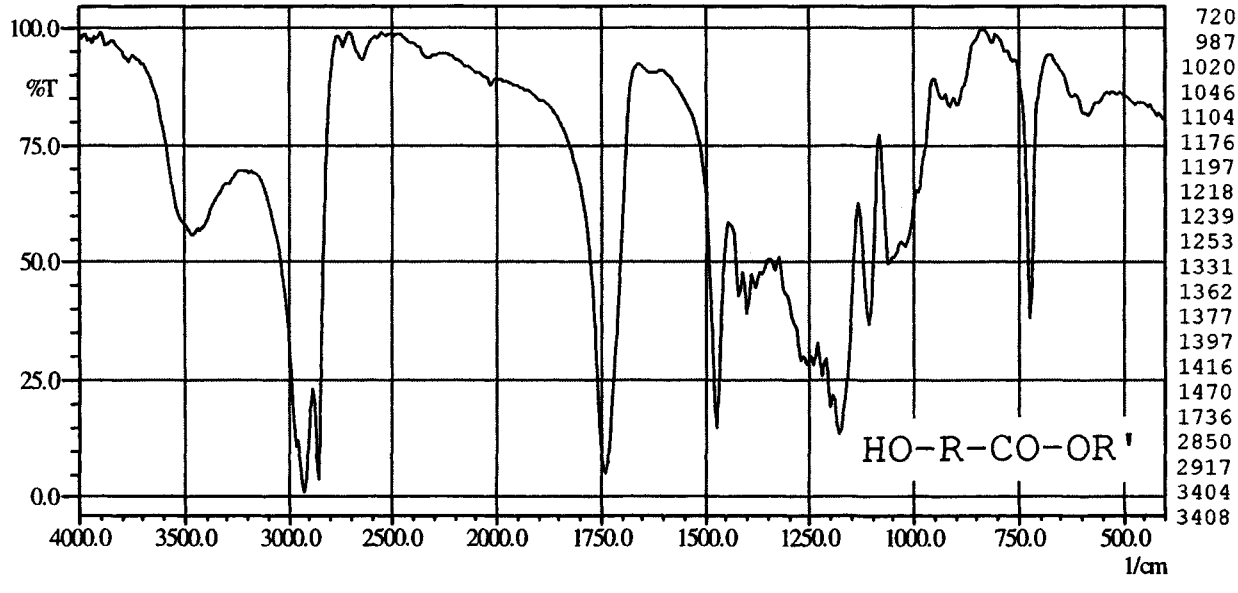
(1) **fatty acid ester + mineral oil + dispersant**
(2) Struktol WB 700, extract
(3) Schill & Seilacher
(5) emulsion plasticiser for rubber processing
(6) colourless, oily liquid
(13) solution dried on KBr

57



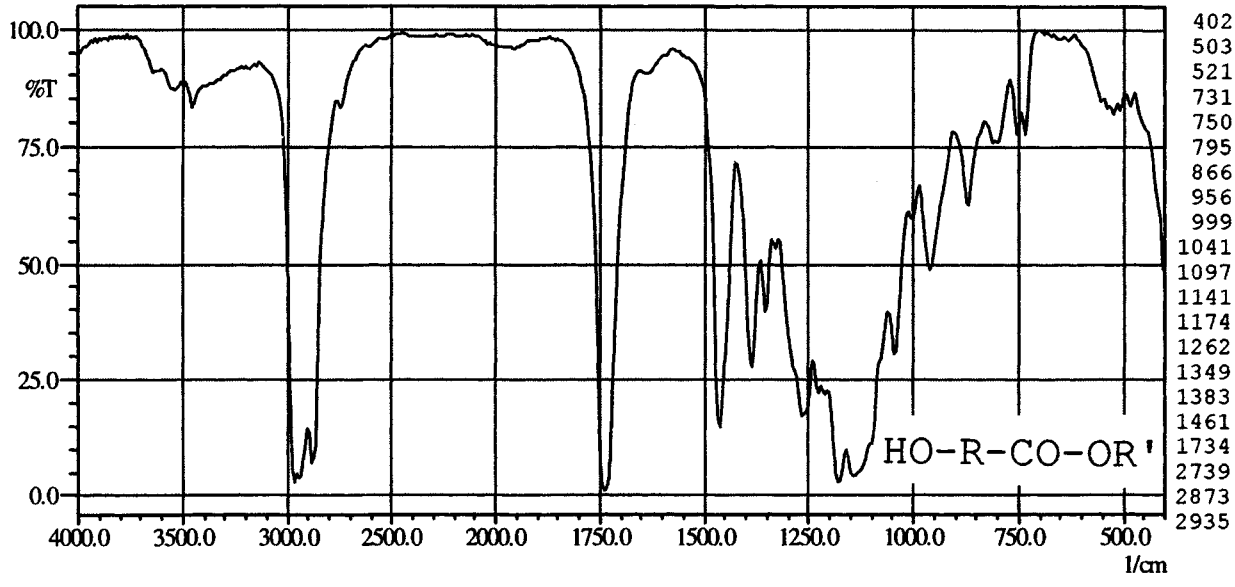
(1) **fatty acid ester + mineral oil + dispersant on ZnO**
(2) Struktol WB 700
(3) Schill & Seilacher
(5) emulsion plasticiser for rubber processing
(6) colourless solid
(13) KBr pellet

57



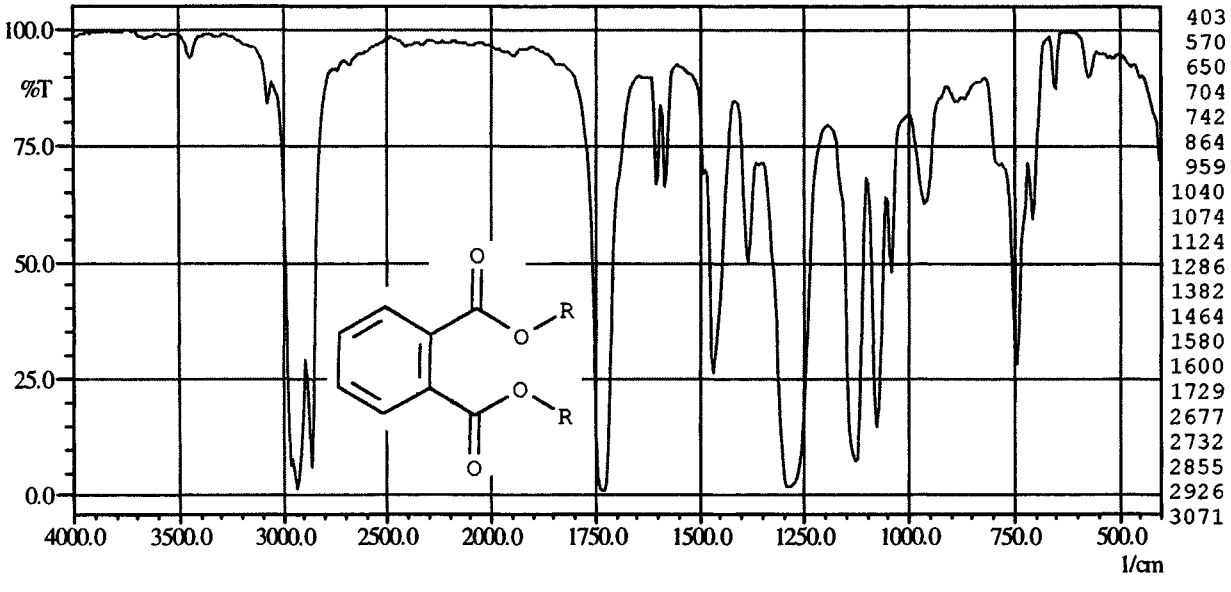
(1) **hydrophilised fatty acid ester**
(2) Struktol WB 222
(3) Schill & Seilacher
(5) emulsion plastificator for rubber processing
(6) colourless, soft waxy material
(13) KBr pellet

57



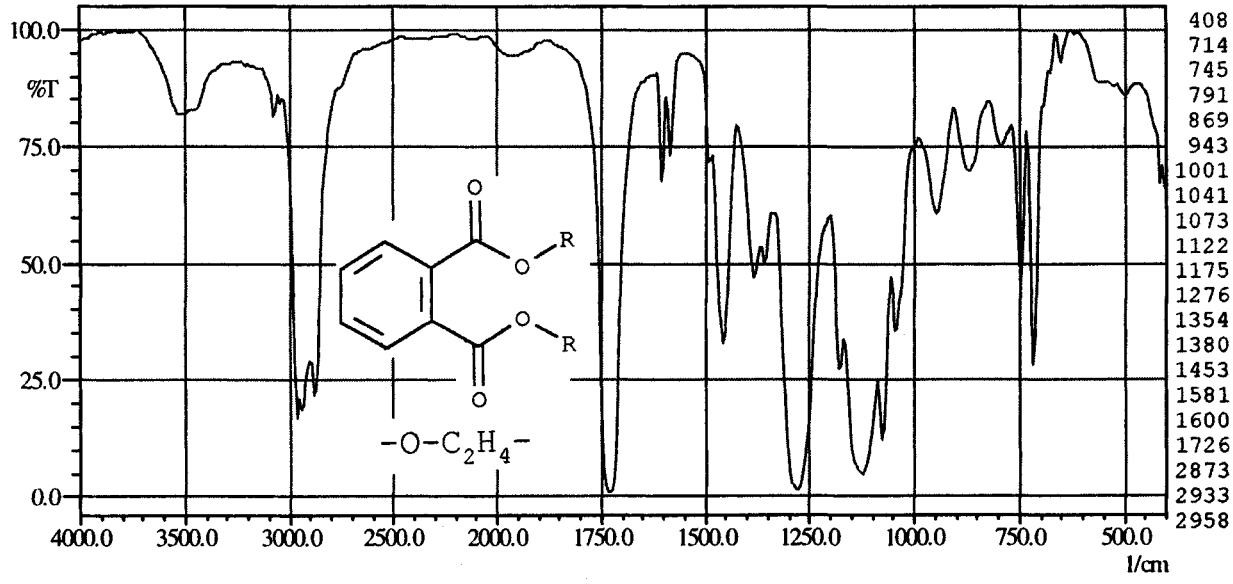
(1) **hydrophilised aliphatic ester on carrier**
(2) Struktol KW 400
(3) Schill & Seilacher
(5) plastificator for rubber processing
(6) colourless solid
(13) KBr pellet

57



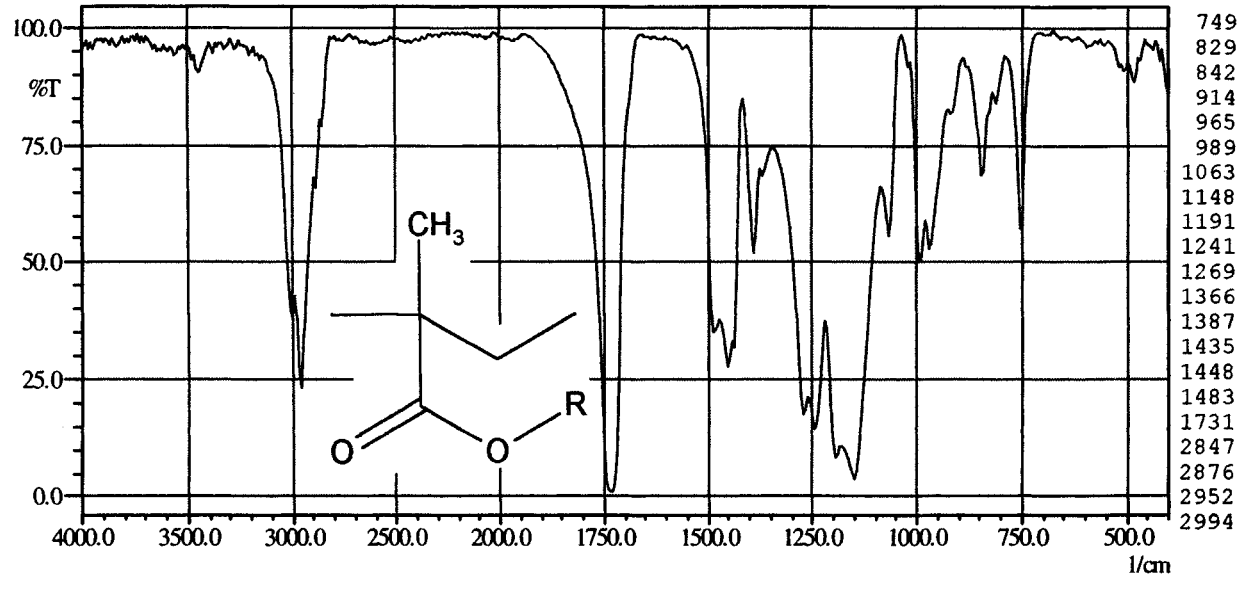
(1) **phthalic acid ester**
(2) Struktol KW 500
(3) Schill & Seilacher
(5) plastificator for rubber processing
(6) colourless liquid
(13) layer on KBr

57



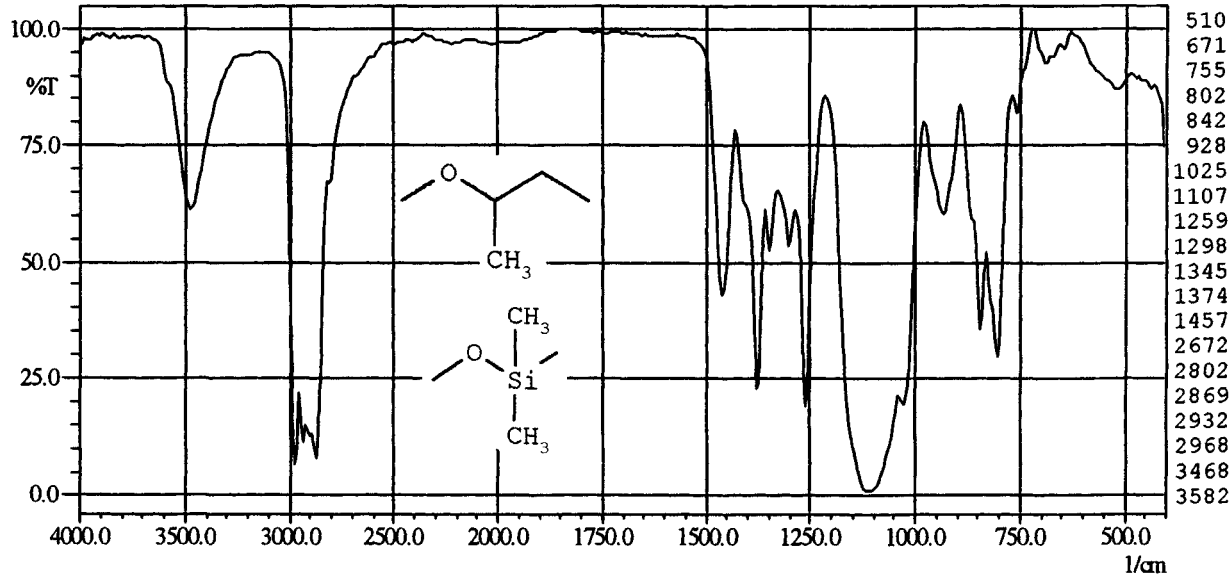
(1) **aliphatic-aromatic polyester based on phthalic acid**
(2) Struktol WB 300
(3) Schill & Seilacher
(5) plastificator for rubber processing, additive to nitrile rubber
(6) colourless, viscous liquid
(13) layer on KBr

57



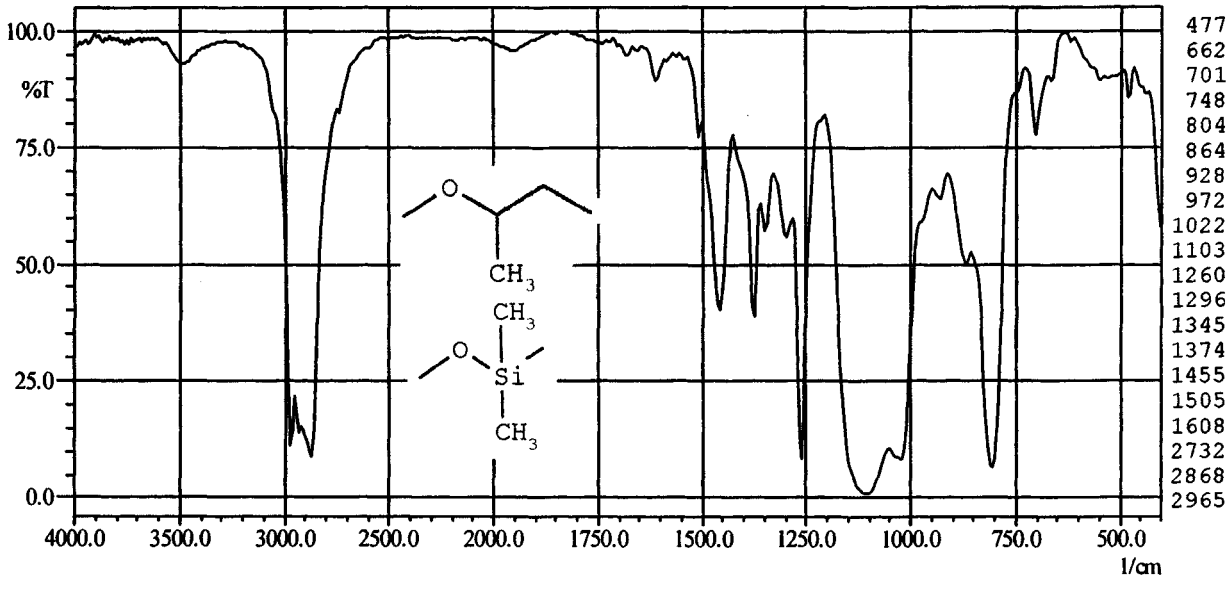
(1) **methacrylate copolymer**
(2) Baerorapid 10 F
(3) Baerlocher
(5) acrylate-modifier
(6) white powder, free flowing
(9) 1.2 g cm^{-3}
(13) KBr pellet

57 $C_3H_6O\text{-}SiC_2H_6O$ M



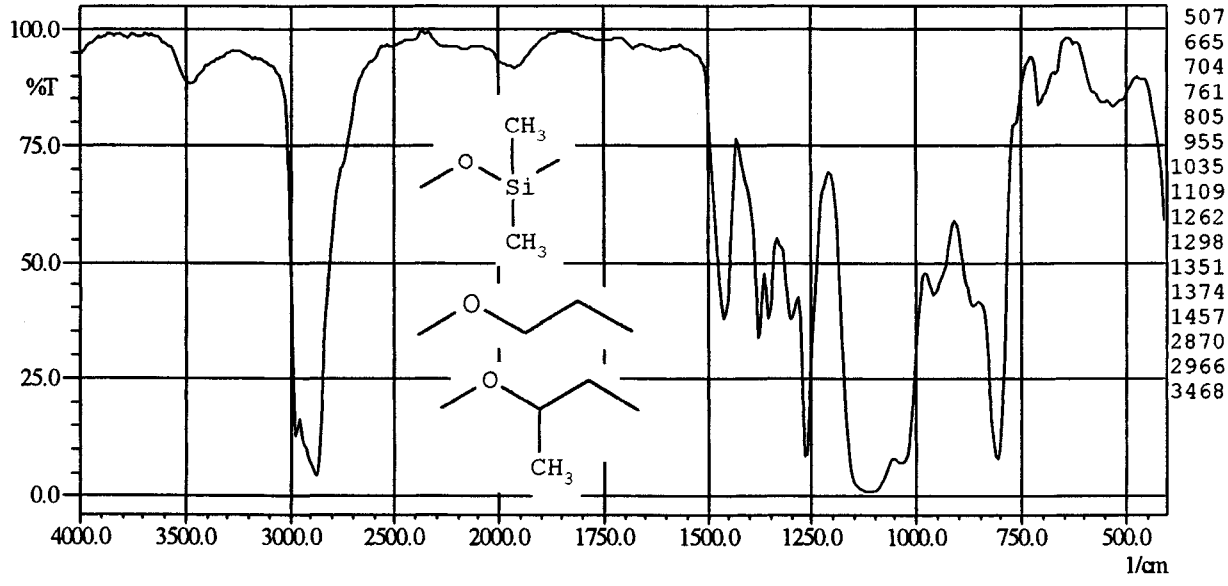
(1) **poly(oxypropylene)-*b*-poly(dimethylsiloxane)**
(2) Tegostab B 8680
(3) Goldschmidt
(5) foam-stabiliser during the production of highly elastic polyurethane expanded rubber
(6) colourless, clear liquid
(13) layer btw KBr

57 $C_3H_6O\text{-}SiC_2H_6O$ M



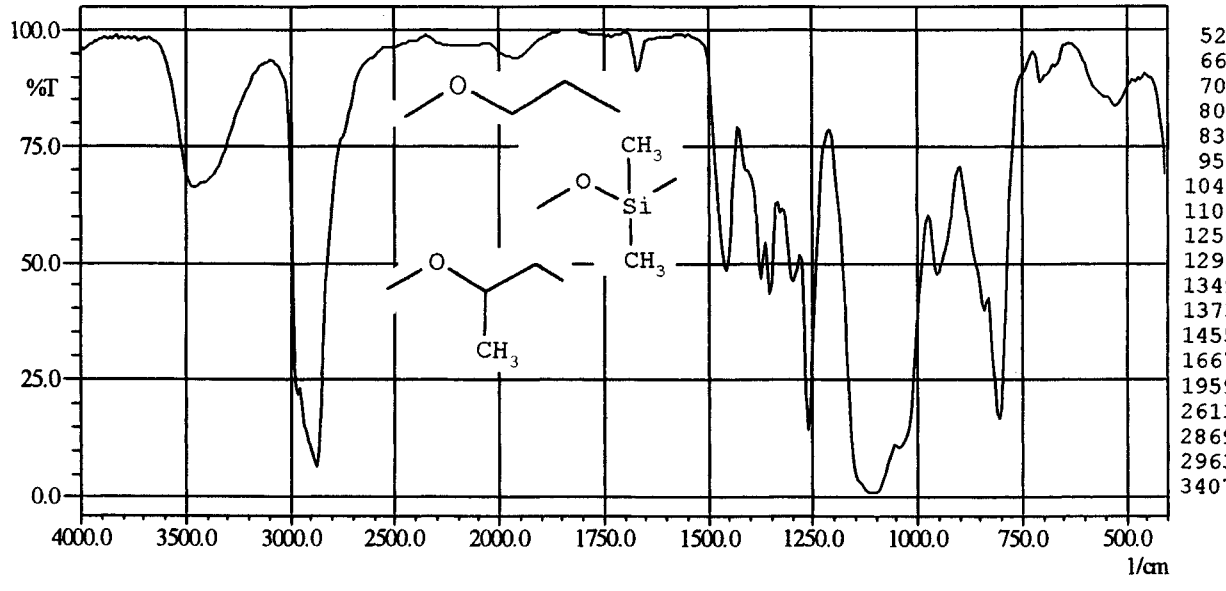
(1) **poly(oxypropylene)-*b*-poly(dimethylsiloxane)**
(2) Tegostab B 1651
(3) Goldschmidt
(5) stabiliser for the production of polyether-urethane expanded rubber
(6) colourless, clear liquid
(13) layer btw KBr

57 $C_3H_6O\text{-}C_2H_4O\text{-}SiC_2H_6O$ M



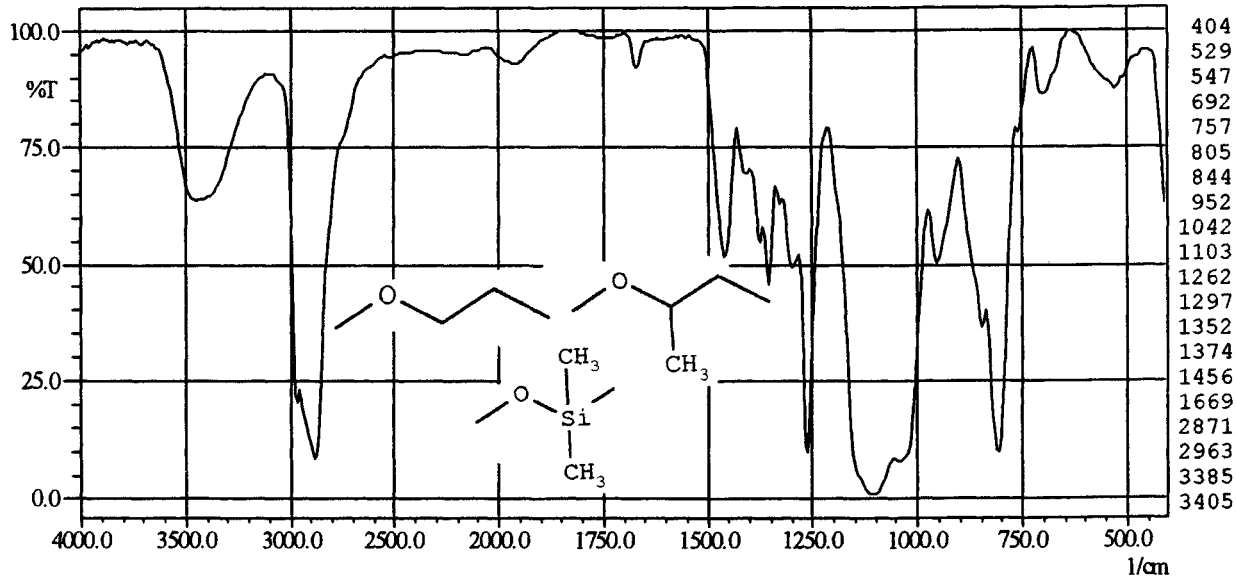
(1) **poly(oxypropylene)-*b*-poly(oxyethylene)-*b*-poly(dimethylsiloxane)**
(2) Tegostab B 2219
(3) Goldschmidt
(5) foam-stabiliser for the production of polyurethane expanded hard-rubber
(6) colourless, clear liquid
(13) layer btw KBr

57 $C_2H_4O\text{-}C_3H_6O\text{-}SiC_2H_6O$ M



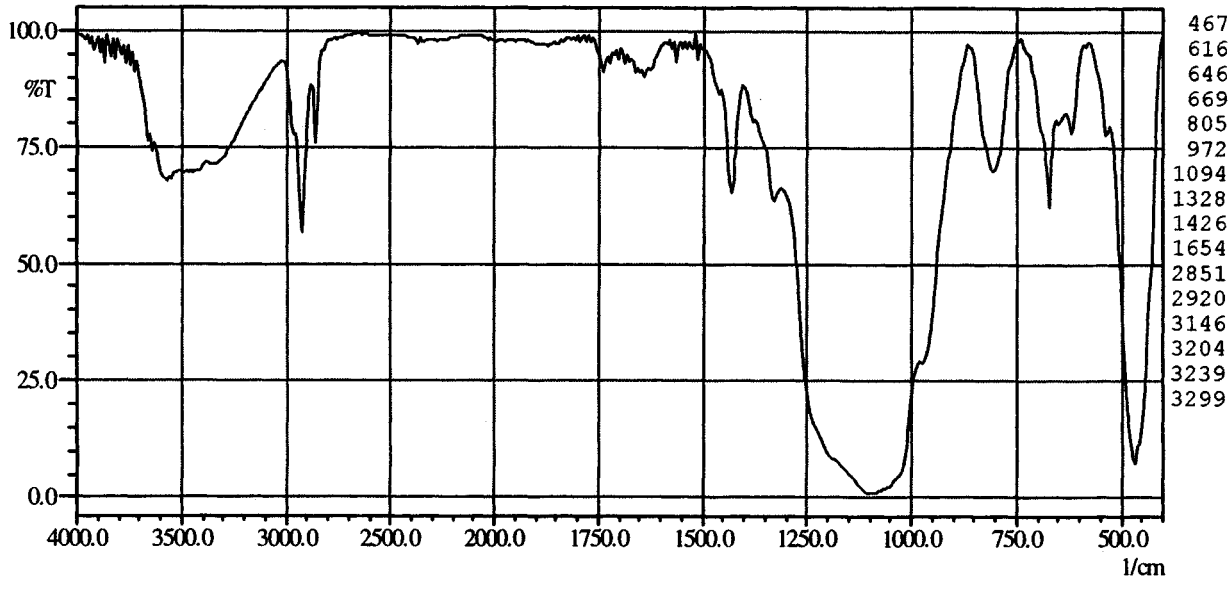
(1) **poly(oxyethylene)-*b*-poly(oxypropylene)-*b*-poly(dimethylsiloxane)**
(2) Tegostab B 8425
(3) Goldschmidt
(5) foam-stabiliser during the production of polyurethane expanded hard-rubbers
(6) colourless, clear, viscous liquid
(13) layer btw KBr

57 C_2H_4O-C_3H_6O-SiC_2H_6O M



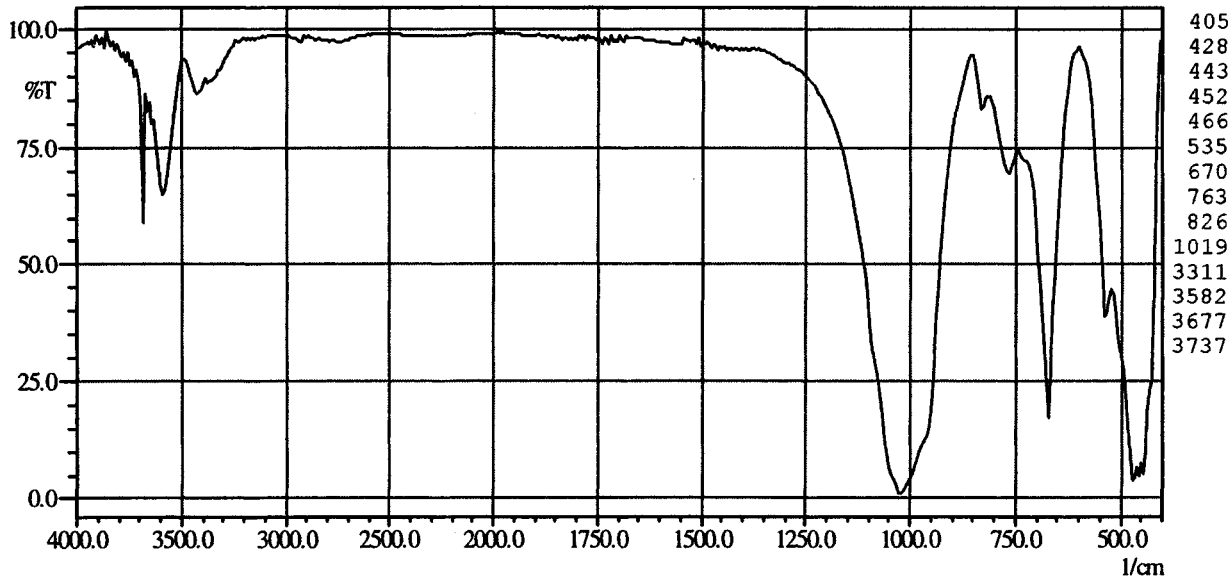
(1) **poly(oxyethylene)-*b*-poly(oxypropylene)-*b*-poly(dimethylsiloxane)**
(2) Tegostab B 8404
(3) Goldschmidt
(5) additive for the production of polyurethane expanded hard-rubber, stable against hydrolysis
(6) colourless, clear, viscous liquid
(13) layer btw KBr

57



(1) **modified silicate complex**
(2) Antiblocking 7831
(3) Baerlocher
(5) antiblocking agent
(6) colourless solid
(9) 1.7 g cm^{-3}
(13) KBr pellet

418



(1) **modified silicate complex**
(2) Antiblocking 3780
(3) Baerlocher
(5) antiblocking agent
(6) grey-white solid
(9) 2.8 g cm^{-3}
(13) KBr pellet

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