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Polyester polycarbonates of particular diphenols

5 The present invention relates to novel polyester polycarbonates of particular diphenols, to a process for their preparation, to their use in the production of moulded bodies and extrudates, to the moulded bodies and extrudates obtainable therefrom, especially substrates containing them for optical data carriers, as well as to particular diphenols themselves and to their preparation and to their use in the preparation of polycarbonates.

10 In the course of new developments of optical data carriers, the requirements made of the carrier material are becoming increasingly more demanding and require the targeted development of new materials, for example with the aim of achieving lower birefringence and lower water absorption, especially for the shorter writing and reading wavelengths which are to be expected in the future and which represent new
15 challenges.

Low birefringence and low water absorption are not the only important properties for the substrate materials of optical data carriers, however; a combination of further properties that is as optimum as possible is required, such as high transparency,
20 dimensional stability under heat, flowability, strength, high purity, low density, low inhomogeneities or particulate contents and, especially, low raw material and production costs.

The materials at present proposed for such applications fail to meet one or more of
25 those requirements, and there is therefore a need for new materials for higher storage densities.

Polyester polycarbonates of linear or cyclic difunctional aliphatic carboxylic acids, diphenols and carbonate precursors are described, for example, in EP-A 433 716,
30 US-A 4 983 706 and US-A 5 274 068, which describe various processes for their synthesis. It is known to the person skilled in the art that the incorporation of



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- dicarboxylic acids leads to a lowering of the glass transition temperature and to an increase in flowability. For use as substrate materials, however, the reduction in the glass transition temperature means a limitation on the usability of the disks, because their climate resistance is reduced thereby. In addition, owing to the polar ester groups, such products have a high water absorption, which is disadvantageous for use in optical data storage media. As EP-A 433 716 teaches, the carboxylic acids known for polyester polycarbonates can be incorporated in a significant amount in the interfacial process only by means of a complex, multi-stage procedure.
- 10 Polyester polycarbonates of linear and longer-chain dicarboxylic acids in particular also exhibit an undesirable tendency to crystallise, which has a particularly adverse effect in the case of very slow cooling, which may be necessary for the forming of very fine structures and to reduce process-related birefringence.
- 15 Dimer fatty acids as possible acid components in polyester polycarbonates are listed, for example, in DE-A 43 06 961, US-A 5 134 220 and EP-A 443 058. A more precise definition of the acids to be used is not given. However, thermooxidative problems occur with non-hydrogenated dimer fatty acids. In addition, the customary commercial products contain more than 3 mol% of carboxylic acids having a
- 20 basicity of three or more, which leads to a high viscosity at zero rate of shear, which is undesirable in the forming of microstructures such as pits or grooves. For that reason, such polyester polycarbonates have generally been regarded hitherto as unsuitable for substrates for optical data storage media.
- 25 Particular copolycarbonates based on spirobischromans and other diphenols are described in JP-A 10251395 and JP-A 08123050 as binders for photoreceptors. Spirobischroman-based polymers, for example polyethers or polycarbonates, are disclosed in JP-A 3162413, the latter spirochroman types are composed solely of hydroquinone and acetone, that is to say they have a strict 1,4 linkage.

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The products described in the prior art are polymers that have too high a glass transition temperature for use as the substrate material for optical data storage media.

- 5 Accordingly, the object underlying the invention is to provide polyester polycarbonates that do not have the disadvantages mentioned above but, in particular, have improved optical properties and can readily be prepared.

10 Surprisingly, that object is achieved by polyester carbonates which are prepared by one of the conventional preparation processes for polycarbonates, characterised in that there are used in the preparation, in addition to the conventional carbonic acid derivatives, also dicarboxylic acids of formula (I)

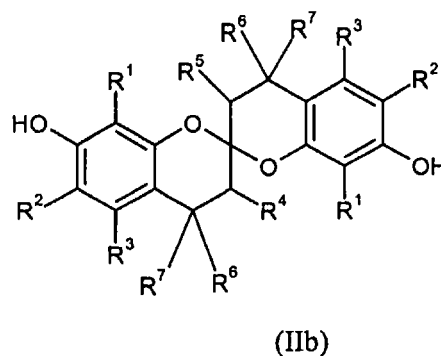
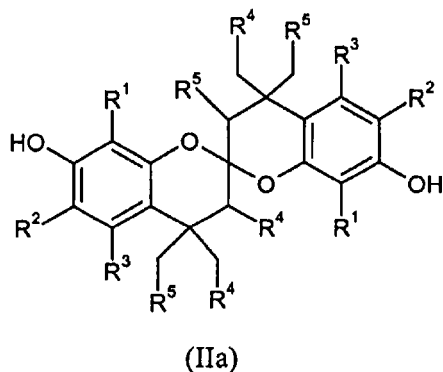


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wherein T represents a branched or linear, saturated or unsaturated alkyl, arylalkyl or cycloalkyl moiety of from 8 to 40 carbons, preferably saturated linear alkyldicarboxylic acids having from 8 to 40 carbons, particularly preferably having from 12 to 36 carbons,

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and, optionally proportionately in addition to the conventional diphenols, particular diphenols of formula (IIa) and/or (IIb)



in which

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5 R₁ to R₇ each independently of the others represents hydrogen, halogen, a C₁- to C₁₂-alkyl radical, preferably a C₁- to C₃-alkyl radical, particularly preferably methyl, a C₆- to C₁₉-aryl radical, preferably a phenyl radical, a C₇- to C₁₂-aralkyl radical, preferably phenyl-C₁- to C₄-alkyl, particularly preferably hydrogen, halogen, preferably chlorine or bromine.

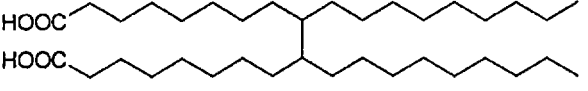
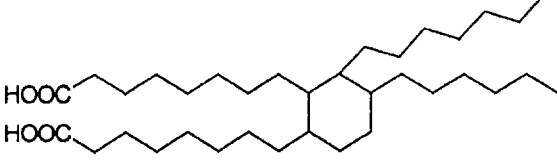
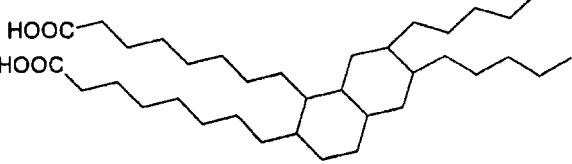
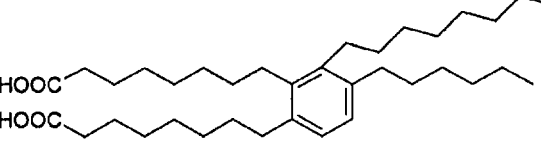
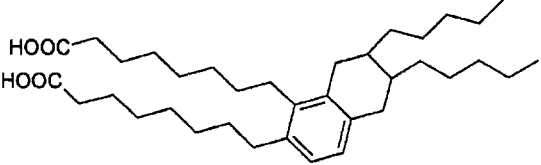
"Proportionately" in this context means that the particular diphenols of formulae IIa and IIb represent a proportion > 0 % of the total amount of diphenols used.

10 If no further conventional diphenols are used, the proportion of diphenols of formulae IIa and IIb is 100 % of the diphenols used. In all other cases, the sum of the molar amounts of each of the individual diphenols is 100 %. In such mixtures of diphenols, the proportion of diphenols of formulae IIa and IIb is preferably > 10 mol%, particularly preferably > 20 mol% and most particularly preferably
15 > 25 mol%. All conventional diphenols are suitable as diphenols used additionally in combination with the diphenols of formulae IIa and IIb.

Suitable dicarboxylic acids according to the invention are fatty acids, particularly preferably hydrogenated dimer fatty acids.
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Examples of dicarboxylic acids of formula (I), or mixtures of such fatty acids, are sebacic acid,
dodecanedioic acid,
hydrogenated dimer fatty acids, such as, for example, Pripol 1009 from Uniqema.

25 Pripol 1009 from Uniqema is a mixture of hydrogenated dimer fatty acids which, according to Uniqema, has approximately the following composition:

Structure (different isomers in each case)	Data Uniqema
Linear 	ca. 30%
Cyclic 	ca. 50%
Bicyclic 	
Aromatic 	ca. 15-20%
Aromatic bicyclic 	

Dodecanedioic acid and Pripol 1009 are particularly preferred.

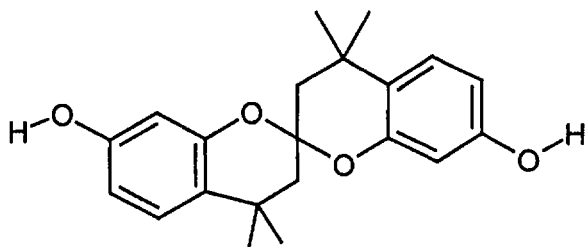
- A small amount of mono- and poly-functionalised fatty acids may also be present.
- 5 Products having very small contents of such components, especially having small contents of acids having a functionality of three or more, are especially suitable for the preparation of the polyester polycarbonates according to the invention. Preference is given, therefore, to dimer fatty acids having a content of less than approximately 1.5 %, determined by gas chromatography, of acids having a
- 10 functionality of three or more. The invention also includes mixtures of dimer fatty acids with other difunctional carboxylic acids having from 4 to 40 carbon atoms,

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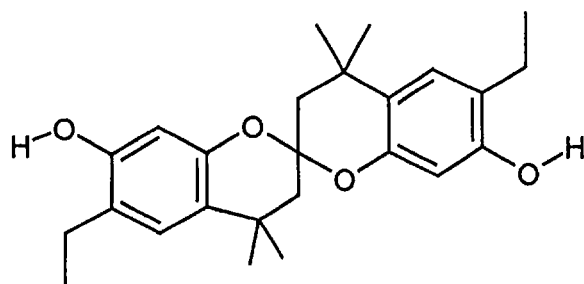
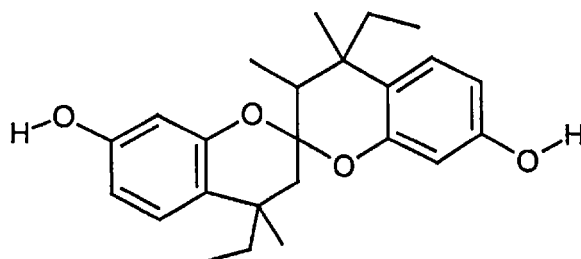
such as adipic acid, sebacic acid, α,ω -dodecanedicarboxylic acid, terephthalic acid, cis- or trans-9-octadecene- α,ω -dicarboxylic acid, or hydroxycarboxylic acids having from 4 to 40 carbon atoms, such as salicylic acid or p-hydroxybenzoic acid.

- 5 Within the scope of the invention, the dimer fatty alcohols obtained from dimer fatty acids by reduction, or mixtures of esters of dimer fatty alcohols with dimer fatty acids, can also be used and reacted to polyester polycarbonates.

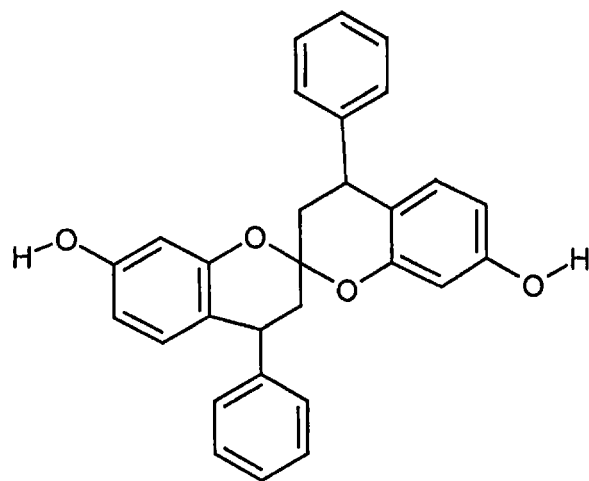
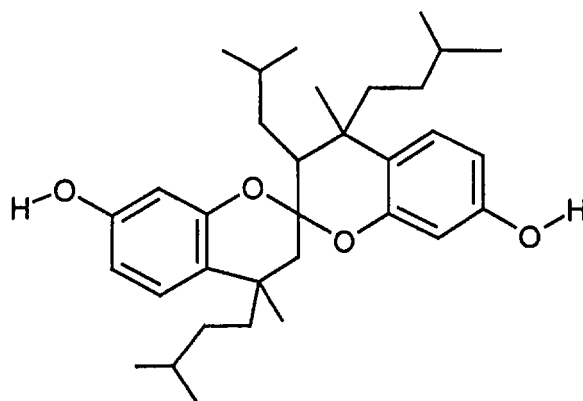
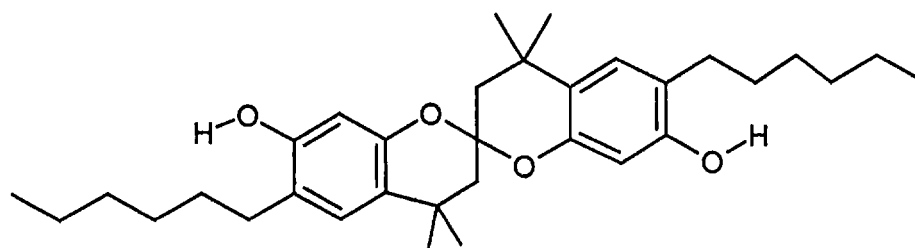
Particularly preferred diphenols of formulae (IIa) and (IIb) are:



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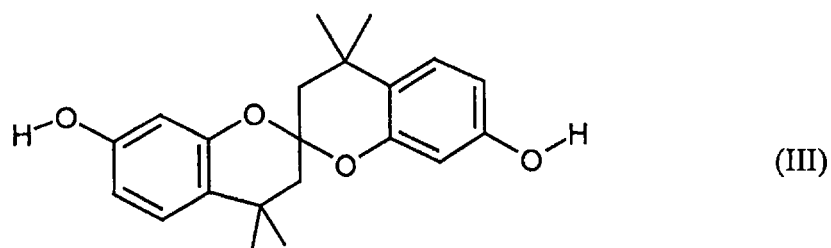


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Most particularly preferred is the diphenol (III), which is obtained from resorcinol
5 and acetone.

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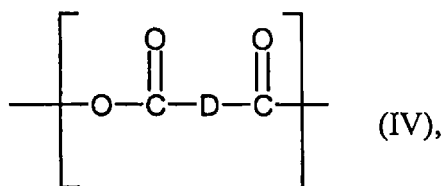


The compounds of formulae IIa, IIb and III can be used either individually or in mixtures with one another.

5 With the exception of the compounds in which R^1 to R^5 in formula IIa are hydrogen and R^6 and R^7 in formula IIb are simultaneously methyl groups, the diphenols of formulae IIa, IIb and III are novel, and the present Application relates thereto and to their preparation and their use in the preparation of polyester carbonates.

10 The polyester polycarbonates according to the invention are to be illustrated, by way of example and preference, but in a non-limiting manner, by the following structural description of the polyester carbonates:

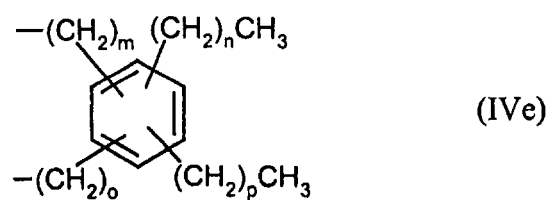
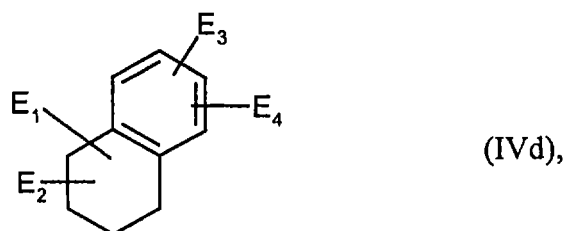
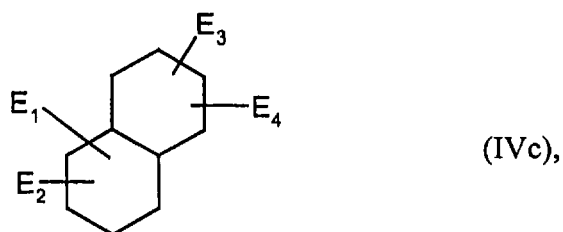
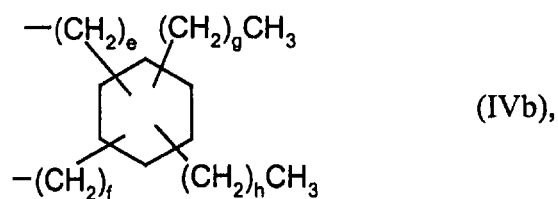
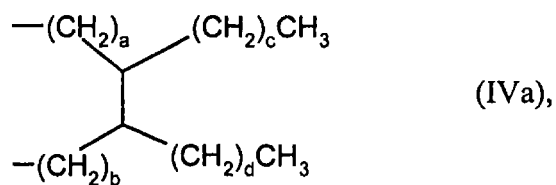
15 Polyester carbonates containing repeating bifunctional structural units A according to formula (IV)



wherein the square brackets characterise an optionally repeating structural unit,

20 D represents a mixture of divalent hydrocarbon radicals which contain from 30 to 42 carbon atoms, preferably from 32 to 38 carbon atoms, particularly preferably 34 carbon atoms. D corresponds substantially to formula IVa and/or IVb and/or IVc and/or IVd and/or IVe.

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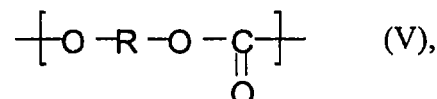
wherein

E_1 , E_2 , E_3 and E_4 in formulae Ic and Id each represents one of the substituents $-(CH_2)_i-$, $-(CH_2)_j-$, $-(CH_2)_kCH_3$ and $-(CH_2)_lCH_3$ and a , b , c , d , e , f , g , h , i , j , k , l ,

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m, n, o and p each independently of the others represents an integer from 1 to 10,

and at least one of the further bifunctional structural units B, which are different from A, according to formula (V)



wherein the square brackets here characterise an optionally repeating structural unit, and formulae A and B may optionally overlap in the region of the carbonyl group,

wherein the radical -O-R-O- represents diphenolate radicals derived from the above-mentioned diphenols of formulae (IIa) and (IIb) or from conventional diphenols, such as bisphenol A or bisphenol TMC.

In the present context, "conventional diphenols" means the diphenols that can conventionally be used for the preparation of polycarbonates, see, for example, US-A 3 028 635, 2 999 835, 3 148 172, 2 991 273, 3 271 367, 4 982 014 and 2 999 846, DE-A 1 570 703, 2 063 050, 2 036 052, 2 211 956 and 3 832 396, French Patent Specification 1 561 518, the monograph "H. Schnell, Chemistry and Physics of Polycarbonates, Interscience Publishers, New York 1964", p. 77 ff, and JP-A 62039/1986, 62040/1986 and 105550/1986.

There may be mentioned by way of illustration, but without being limited thereto, 2,2-bis(4-hydroxyphenyl)propane (bisphenol A), 1,1-bis(4-hydroxyphenyl)-3,3,5-trimethylcyclohexane (bisphenol TMC), 1,3-bis[2-(4-hydroxyphenyl)-2-propyl]benzene, 1,1-bis(4-hydroxyphenyl)-1-phenylethane, 1,1-bis(4-hydroxyphenyl)-cyclohexane (bisphenol Z), especially 2,2-bis(4-hydroxyphenyl)propane (bisphenol A) and 1,1-bis(4-hydroxyphenyl)-3,3,5-trimethylcyclohexane (bisphenol TMC), most particularly preferably 2,2-bis(4-hydroxyphenyl)propane (bisphenol A).

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In addition, there may be used for the preparation of the polyester polycarbonates according to the invention also bifunctional monophenols, such as resorcinol, hydroquinone or their derivatives mono- or poly-substituted by C₁- to C₁₂-alkyl, C₆- to C₁₉-aryl or C₇- to C₁₉-aralkyl.

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It has been found that substrates of the polyester polycarbonates according to the invention are distinguished by a surprisingly particularly low water absorption, astonishingly low birefringence, a very low tendency to crystallise, a low refractive index, good flowability and a low density, as well as a low glass transition temperature.

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The substrates for data carriers of the novel polyester polycarbonates also possess high transparency, good mechanical properties, especially at low temperatures, and high flowability.

15

Within the context of this invention, hydrogenated dimer fatty acids are to be understood as being acids that can be obtained by dimerisation of unsaturated monobasic fatty acids having from 16 to 22 carbon atoms and subsequent hydrogenation. The required acids can be obtained, for example, from vegetable or animal sources. Synthesis and properties are described, for example, in Encyclopedia of Chemical Technology, Vol. 8, 4th ed., John Wiley & Sons: 1993, page 223-237.

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Such hydrogenated dimer fatty acids can still contain small amounts of unsaturated aliphatic groups. Dimer fatty acids having an iodine number less than approximately 15 are preferred.

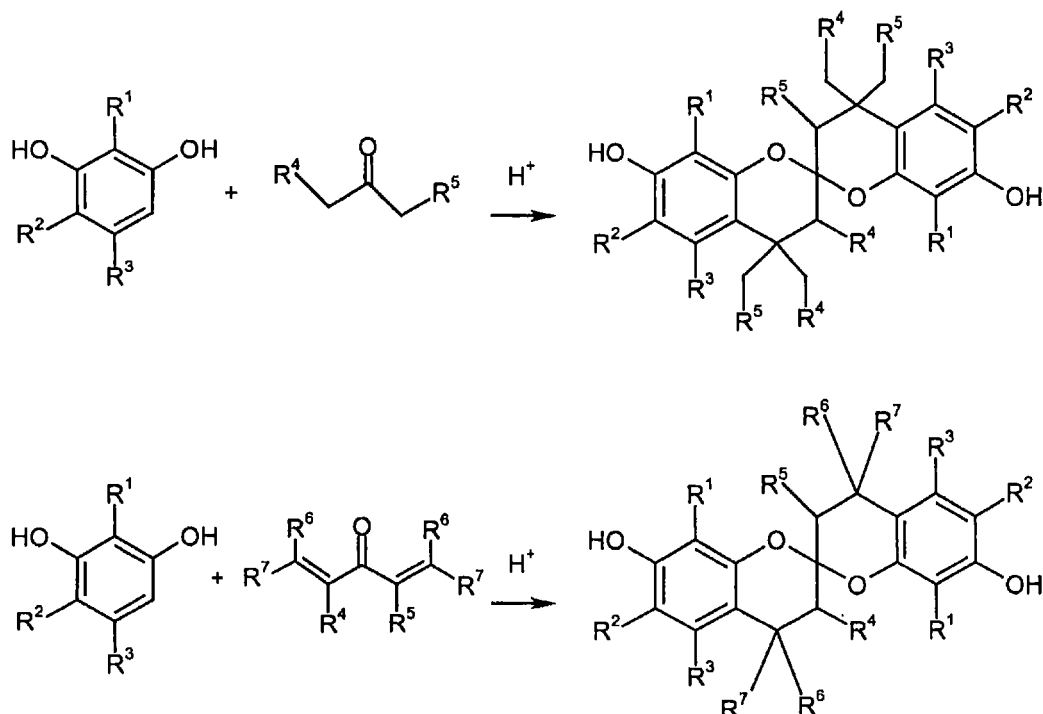
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The diphenols of formulae (IIa) and (IIb) can be prepared according to the reaction sequences shown in Schemes 1 and 2.

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Scheme 1:



The diphenols prepared according to Scheme 1 are obtained after condensation of ketones (e.g. acetone, methyl ethyl ketone, etc., Aldrich) and optionally substituted resorcinol derivatives (e.g. 4-hexylresorcinol, Aldrich) with removal of water under acid conditions. Alternatively, phorone (2,6-dimethyl-2,5-heptadien-4-one) (Aldrich) or substituted phorones may also be used as starting materials for the condensation. Suitable acids are inorganic acids, such as, for example, sulfuric acid. Acid cation exchangers, such as, for example, Lewatite[®], are also possible.

Corresponding condensation methods for the preparation of spiro components by reaction of resorcinol with ketones are described in JP-A 10265476. The condensations are conventionally carried out in customary solvents, such as, for example, hydrocarbons, toluene, NMP or chlorobenzene, at temperatures of from 20 to 200°C, preferably from 30 to 180°C, particularly preferably from 50 to 150°C and most particularly preferably from 60 to 130°C.

Preferred polyester polycarbonates according to the invention are those which contain from 0.5 to 49 mol%, preferably from 2 to 40 mol%, particularly preferably

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from 5 to 20 mol%, based on 100 mol% of the bifunctional structural units A and B, of structural units A.

5 Compounds and embodiments that fall within the definitions mentioned as being preferred, particularly preferred or most particularly preferred, or that use the definitions or explanations and parameters mentioned within the scope of preferences, are preferred, particularly preferred or most particularly preferred.

10 The definitions or explanations and parameters mentioned above in general or within the scope of preferences can, however, also be combined with one another as desired, that is to say between the respective ranges and scope of preferences.

15 The polyester polycarbonates according to the invention are distinguished in particular by a glass transition temperature of from 120 to 195°C, preferably from 125 to 180°C, particularly preferably from 130 to 170°C and most particularly preferably from 135 to 165°C.

20 The polyester polycarbonates according to the invention are further distinguished by a low water absorption of < 0.40 %, preferably < 0.38 %, particularly preferably < 0.36 %, most particularly preferably < 0.35 % at saturation.

"Saturation" in this context is to be understood as being the value achieved after 14 days' humid storage at 94 % relative humidity and 30°C. The water content is then determined by means of quantitative Karl-Fischer titration.

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The substrates according to the invention can be prepared by the three known methods (see H. Schnell, "Chemistry and Physics of Polycarbonates", Polymer Review, Volume IX, page 27 ff; Interscience Publishers, New York 1964, and DE 1495 626 A, DE 22 32 877 A, DE 27 03 376 A, EP 274 544 A, DE 30 00 610 A, DE 30 38 32 396 A).

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1. By the solution process in disperse phase, the so-called "two-phase interfacial process"

In this process, the diphenols and bifunctional acids to be used are dissolved in an aqueous alkaline phase. To that end, the chain terminators required for the preparation of the polyester polycarbonates according to the invention are optionally dissolved in amounts of from 1.0 to 20 mol%, based on moles of diphenols plus acid to be used according to the invention, in an aqueous alkaline phase, preferably sodium hydroxide solution, or are added thereto and to an inert organic phase, without a solvent. The whole is then reacted with phosgene in the presence of an inert organic phase which is preferably a solvent for polycarbonate. The reaction temperature is from 0°C to 50°C.

The addition of the necessary chain terminators, branching agents and acids according to the invention can also take place during the phosgenation or as long as chlorocarbonic acid esters are present in the synthesis mixture, without a solvent, in the form of a melt, in the form of a solution in alkali or inert organic solvents.

The reaction can be accelerated by means of catalysts, such as tertiary amines or onium salts. Preference is given to tributylamine, triethylamine and N-ethylpiperidine, as well as to tetrabutylammonium, tetraethylammonium and N-ethylpiperidinium salts.

In addition to or instead of the diphenols, their chlorocarbonic acid esters and/or bischlorocarbonic acid esters can also be used or metered in during the synthesis. Instead of the dimer fatty acids, it is also possible to use their acid chlorides. Suitable solvents are, for example, methylene chloride, chlorobenzene, toluene and mixtures thereof.

2. By the solution process in homogeneous phase, also called the "pyridine process"

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In this process, the diphenols and acids according to the invention are dissolved in organic bases such as pyridine, optionally with the addition of further organic solvents, and then, as described under 1., the chain terminators and branching agents
5 required for the preparation of the polyester polycarbonates according to the invention are optionally added.

The whole is then reacted with phosgene. The reaction temperature is from 10 to 50°C. Suitable organic bases, other than pyridine, are, for example, triethylamine, tributylamine, N-ethylpiperidine, as well as N,N-dialkyl-substituted anilines, such as
10 N,N-dimethylaniline. Suitable solvents are, for example, methylene chloride, chlorobenzene, toluene, tetrahydrofuran, 1,3-dioxolane and mixtures thereof.

In addition to the diphenols, up to 50 mol%, based on the phenols used, of their
15 bischlorocarbonic acid esters may also be used. Some or all of the fatty acids according to the invention can be replaced by their acid chlorides. The addition of the necessary chain terminators, branching agents and acids according to the invention can also take place during the phosgenation or as long as chlorocarbonic acid esters are present in the synthesis mixture, without a solvent, in the form of a
20 melt or in the form of a solution in inert organic solvents.

Isolation of the polyester polycarbonates according to the invention in processes 1 and 2 takes place in a known manner. Suitable processes for working up are especially precipitation, spray-drying, and evaporation of the solvent *in vacuo*.
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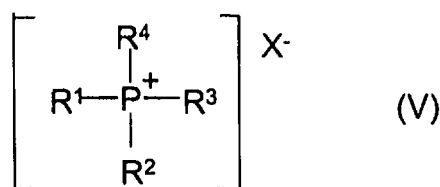
3. By the melt transesterification process

In the melt transesterification process, condensation is carried out, with the addition of diphenyl carbonate in stoichiometric amounts or in an excess of up to 40 %, to
30 diphenol melt/fatty acids, with the continuous removal by distillation of phenol and optionally of excess diphenyl carbonate, until a suitable molecular weight is reached

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or the reaction comes to a standstill. This is usually carried out under inert conditions, at approximately 280°C and under an oil-pump vacuum. This process is carried out using conventional catalysts, such as alkali metal ions, for example Li, Na, K, transition metal compounds, for example those based on Sn, Zn, Ti or
 5 nitrogen or phosphorus bases, preferably ammonium and phosphonium salts, as a single-stage or two-stage process, that is to say with the optional separate condensation of the oligomers and of the polymer.

Phosphonium salts within the context of the invention are those of formula (V)



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wherein R¹⁻⁴ may be the same or different C₁-C₁₀-alkyl radicals, C₆-C₁₀-aryl radicals, C₇-C₁₀-aralkyl radicals or C₅-C₆-cycloalkyl radicals, preferably methyl or C₆-C₁₄-aryl radicals, particularly preferably methyl or phenyl, and X⁻ may be an anion, such as hydroxide, sulfate, hydrogen sulfate, hydrogen carbonate, carbonate, a halide,
 15 preferably chloride, or an alcoholate of the formula OR, wherein R may be C₆-C₁₄-aryl or C₇-C₁₂-aralkyl, preferably phenyl.

Preferred catalysts are

tetraphenylphosphonium chloride,

tetraphenylphosphonium hydroxide,

20 tetraphenylphosphonium phenolate,

particularly preferably tetraphenylphosphonium phenolate.

Instead of the acids to be used according to the invention it is possible to employ their aromatic or aliphatic esters, for example methyl, ethyl, isopropyl or phenyl
 25 esters.

In a known manner, chain terminators and/or branching agents can be used concomitantly for the preparation of the polyester polycarbonates according to the

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invention. The corresponding chain terminators and/or branching agents are known *inter alia* from EP-A 335 214 (pages 3-5) and DE-A 30 07 934 (pages 8-9), and EP-A 411 433 (pages 4 and 5) and EP-A 691 361 (page 5). In addition, some or all of the branching agents and/or chain terminators can be replaced by dimer fatty acids having a higher content of tri- and/or mono-functional carboxylic acids.

It is also possible for the substrates of the polyester polycarbonates according to the invention to be mixed with different thermoplastic polymers in a weight ratio of from 2:98 to 98:2 and to be used in the form of blends.

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The polyester polycarbonates according to the invention have mean molecular weights M_w (weight average, determined by gel chromatography (Merck column combination consisting of PS4000, PS400 and PS40) after previous calibration on bisphenol A PC (calibration based on absolute values determined by means of light scattering and MALDI) of at least 6000, preferably from 7000 to 45,000, particularly preferably from 7000 to 40,000, most particularly preferably from 9000 to 40,000, especially from 9000 to 30,000.

It is possible to add to the polyester polycarbonates for the production of the data carriers according to the invention, before, during or after their processing, the additives conventional for thermoplastic polycarbonates, such as stabilisers, for example heat stabilisers, organic phosphites, optionally in combination with monomeric or oligomeric epoxides; UV stabilisers, especially those based on nitrogen-containing heterocycles, such as triazoles; optical brightening agents, flameproofing agents, especially fluorine-containing, such as perfluorinated salts of organic acids, polyperfluoroethylene, salts of organic sulfonic acids and combinations thereof; mould release agents; flow auxiliaries; flame retardants; colourants; pigments; antistatics; fillers and reinforcing agents, comminuted minerals, fibrous materials, for example alkyl and aryl phosphites, phosphates, phosphanes, low molecular weight carboxylic acid esters, halogen compounds, salts, chalk, quartz, inorganic or organic nanoparticles, glass and carbon fibres, in the

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conventional amounts. Examples of such additives will be found described, for example, in WO 99/55772, p. 15-25, and in "Plastics Additives", R. Gächter and H. Müller, Hanser Publishers 1983.

- 5 The data carriers or other moulded bodies according to the invention can be produced in a known manner by injection moulding or injection stamping on known machines.

10 In addition to the described polyester polycarbonates, the invention relates also to extrudates and moulded bodies containing them, such as optical lenses, disks and films which contain the polyester polycarbonates according to the invention, and to the use of those polyester polycarbonates in the production of such moulded bodies and extrudates. The excellent properties of these polyester polycarbonates are shown to advantage especially in the case of optical lenses and data storage media.

15

The following are mentioned as examples of possible applications of the polyester carbonate according to the invention, this list not being limiting:

- 20 1. Safety glazing, which, as is known, is required in many areas of buildings, motor vehicles and aircraft, as well as the visors of helmets.
2. Production of films, especially ski films.
3. Production of blow-moulded bodies (see, for example, US Patent 2 964 794), for example 1 to 5 gallon water bottles.
- 25 4. Production of transparent sheets, especially of hollow-chamber sheets, for example for covering buildings such as railway stations, greenhouses and lighting installations.
5. Production of optical data storage media.
6. For the production of traffic light housings or road signs.
7. For the production of foamed materials (see, for example, DE-AS 1 031 507).
- 30 8. For the production of threads and wires (see, for example, DE-AS 1 137 167 and DE-OS 1 785 137).

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9. As translucent plastics having a content of glass fibres for lighting purposes (see, for example, DE-OS 1 554 020).
10. As translucent plastics having a content of barium sulfate, titanium dioxide and or zirconium oxide or organic polymeric acrylate rubbers (EP-A 634 445, EP-A 269324) for the production of transparent and light-scattering mouldings.
11. For the production of precision injection-moulded parts, such as, for example, lens holders. To that end, polycarbonates having a content of glass fibres are used, which optionally contain in addition approximately from 1 to 10 wt.% MoS₂, based on the total weight.
12. For the production of parts for optical devices, especially lenses for photographic and film cameras (see, for example, DE-OS 2 701 173).
13. As light transmission carriers, especially as fibre-optic cables (see, for example, EP-A1 0 089 801).
14. As electrical insulating materials for electrical conductors and for plug housings as well as plug connectors.
15. Production of mobile phone casings having improved resistance to perfume, aftershave and perspiration.
16. Network interface devices.
17. As carrier material for organic photoconductors.
18. For the production of lamps, for example in the form of headlamps, headlight lenses or internal lenses.
19. For medical applications, for example oxygenators, dialysers.
20. For foodstuffs applications, such as, for example, bottles, kitchenware and chocolate moulds.
21. For applications in the automotive sector, where contact with fuels and lubricants can occur, such as, for example, bumpers, optionally in the form of suitable blends with ABS or suitable rubbers.
22. For sports articles, such as, for example, slalom poles or ski boot buckles.
23. For domestic articles, such as, for example, kitchen sinks and letter box casings.

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- 24. For casings, such as, for example, electrical distribution cabinets.
- 25. Casings for electric toothbrushes and hairdryer casings.
- 26. Transparent washing machines - bull's-eyes having improved resistance to the washing solution.
- 5 27. Safety goggles, optical corrective spectacles.
- 28. Lamp covers for kitchen appliances having improved resistance to cooking steam, especially oil vapours.
- 29. Packaging films for medicaments.
- 30. Chip boxes and chip carriers.
- 10 31. For other applications, such as, for example, stable doors or animal cages.

Polyester polycarbonates according to the invention containing structural units A and B in which the structural unit B is derived from the compounds of formulae IIa and IIb, but especially from formula III, and containing from 0.5 to 49 mol%,
15 preferably from 2 to 40 mol%, particularly preferably from 10 to 25 mol%, based on 100 mol% of the bifunctional structural units A and B, of bifunctional ester structural units A, are especially suitable owing to their low rheo-optical constant C_R for the production of the data carriers according to the invention.

20 For the production of data carriers according to the invention in particular, the substrates must have a high degree of purity. That is achieved by reducing the content of residual monomers, solvents, foreign particles (of inorganic or organic nature, especially salts and dust) and of chlorine to the lowest possible values during working up and isolation of the substrate resin. That is described, for example, in
25 EP-A 380 002 (pages 4 to 6) or EP-A 691 361 (pages 10 to 14), to the disclosure of which reference is therefore made.

The data carriers according to the invention can take various forms. Particular preference is given to known forms such as optical cards or cylindrical perforated
30 disks such as in the case of compact disks (CD), CD recordables (CD-R), CD rewritables (CD-RW), digital versatile disks (DVD) or minidisks (MD).

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Information storage layers (e.g. phase-change layers, magneto-optical layers, colourants, fluorescent colourants, photopolymers), dielectric (e.g. Si/N), reflective (e.g. silver, gold or aluminium), semi-reflective (e.g. Si, Ge), protective layers (e.g. acrylic lacquers) and further functional layers can be applied to the substrate. Various sequences of such layers are possible.

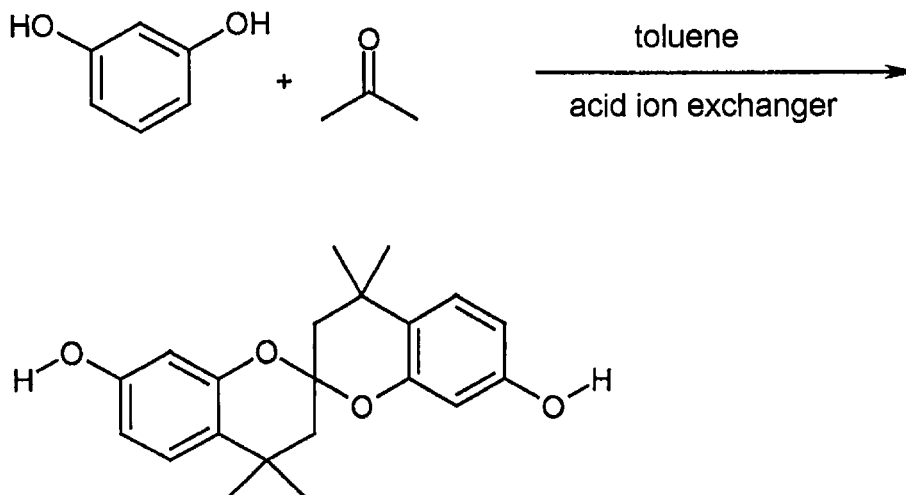
Several layers of the substrate or layers with other substrates can be laminated over one another. The stored information can be impressed into the surface (e.g. as a pit structure) or can be deposited in separate information layers. The information can be read through the transparent substrate or from the information side.

The invention relates also to optical information storage media in which the substrate material according to the invention is used in the form of films, for example for covering the information layer in DVR (direct video recording), or as the substrate of multi-layer systems (optionally with impressed information).

The Examples which follow are intended to illustrate the invention, but without limiting it.

20

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Example 1

30 g (0.27 mol) of resorcinol and 23.5 g (0.405 mol) of acetone are dissolved in 300 ml of dry toluene. 50 g of anhydrous ion exchanger SC 104 (Bayer AG) are added as catalyst. Condensation to the product is carried out by boiling at reflux for 5.5 hours. When the reaction is complete, the ion exchanger is separated off and then washed with toluene. The toluene fractions are combined and concentrated to dryness. Drying *in vacuo* at 50°C yields 33.3 g of crude product, which is purified further by column chromatography.

There is obtained a white solid having the following analytical data:

- Melting point: 200°C
- GC-MS: as TMS mass 484 (M=340)
- HPLC-MS: M=340
- ¹H-NMR (400 MHz, D₆-DMSO, room temperature, TMS): δ = 1.21-1.47 (d, 12H; CH₃); 1.92-2.06 (dd, 4H; -CH₂-); 5.96 (s, 2H; Ar-H); 6.35-6.37 (d, 2H; Ar-H); 7.12-7.17 (d, 2H; Ar-H); 9.02 (s, 2H; Ar-OH)

Preparation of polyester polycarbonates from the diphenol of Example 1 and dimer fatty acid Pripol 1009.

A. 10 wt.% Pripol 1009

- 5 The hydrogenated fatty acid used (Pripol 1009 from Uniqema) has the following specifications: iodine number < 10, monomer content < 0.1 %, trimer content < 1 %.

0.42 g of phosgene is introduced at room temperature into a mixture of 1.22 g of Pripol 1009, 0.169 g of NaOH, 87.6 g of water and 175.1 ml of methylene chloride.

- 10 The mixture is stirred briefly. A mixture of 10.21 g of diphenol of Example 1, 0.09 g of tert-butylphenol, 2.64 g of NaOH, 87.6 g of water and 0.04 ml of N-ethylpiperidine from a receiver vessel is then added. For the purposes of condensation, 5.93 g of phosgene are introduced, the pH value being maintained in the range from 12.5 to 12.8 by the occasional addition of sodium hydroxide solution.

15

After 30 minutes' stirring, the batch is acidified with dilute phosphoric acid and then washed free of electrolytes with distilled water. The organic phase is separated off and concentrated in a rotary evaporator. The product is precipitated by introduction into methanol, isolated by filtration and dried under a water-jet vacuum.

20

Yield: 10.14 g of white polymer

Glass transition temperature (DSC, 2 heating steps): 160.8°C

Molecular weight (BPA-PC calibration): Mw 10,340 g/mol

- 25 **B. 13 wt.% Pripol 1009**

A polyester polycarbonate was prepared in an analogous manner from the diphenol of Example 1 and Pripol 1009 using 13 wt.% Pripol 1009. For isolation of the polymer, the organic phase was concentrated to dryness (no precipitation).

- 30 Molecular weight (BPA-PC calibration): Mw 43,860 g/mol

Glass transition temperature (DSC, 2 heating steps): 137.8°C

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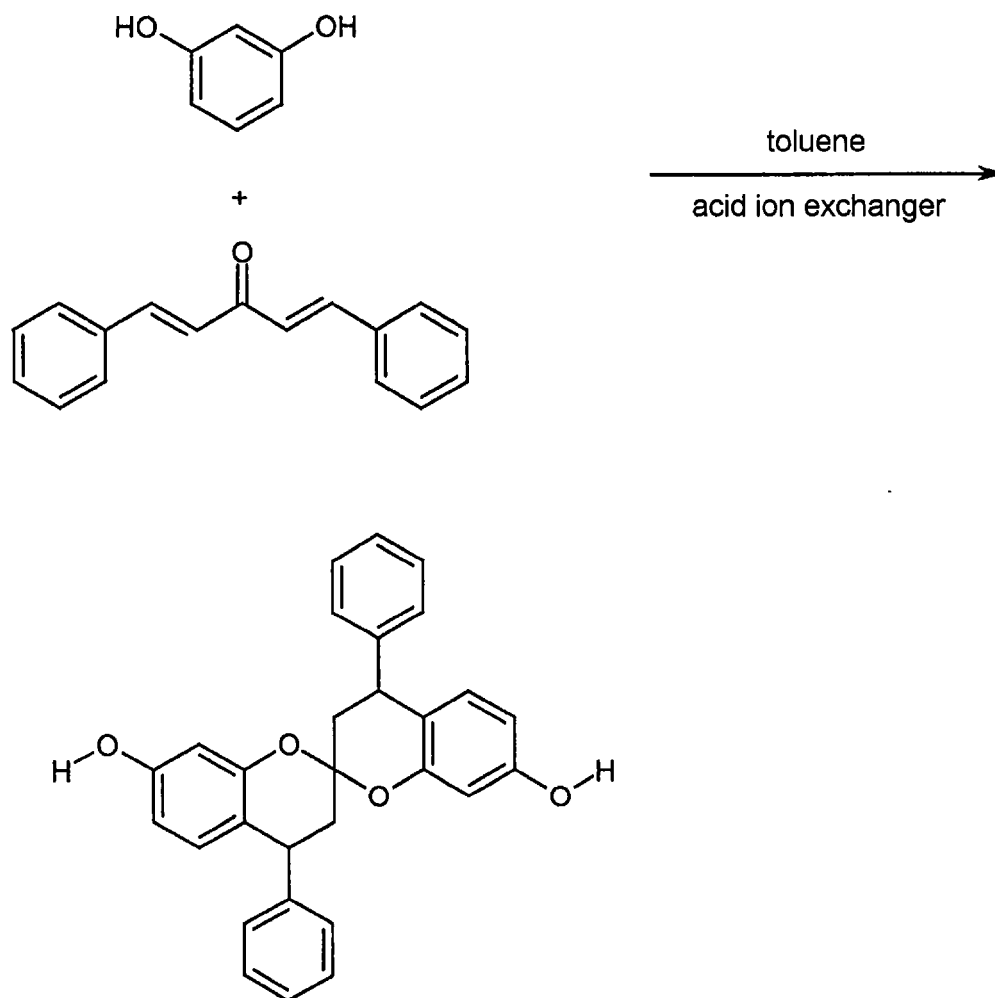
Water content: 0.32 %

0.31 % (1st repetition)

0.32 % (2nd repetition)

0.29 % (3rd repetition)

5

Examples of substituted spirochromans according to the invention**Example 2:**

10

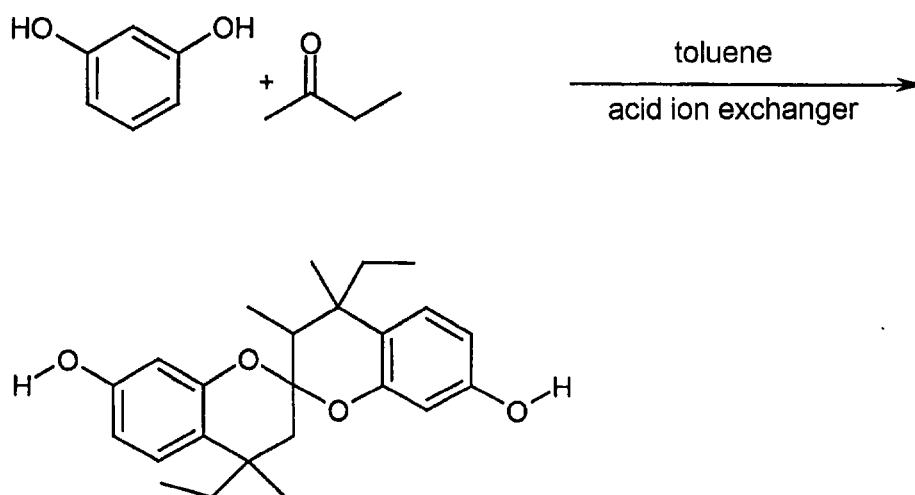
10 g (0.09 mol) of resorcinol and 10.64 g (0.045 mol) of trans,trans-1,5-diphenyl-1,4-pentadien-3-one (Aldrich) are dissolved in 150 ml of dry toluene. 25 g of anhydrous ion exchanger SC 104 (Bayer AG) are added as catalyst. Condensation to

- 25 -

the product is carried out by boiling at reflux for 6 hours. When the reaction is complete, the ion exchanger is separated off and then washed with toluene. The toluene fractions are combined and concentrated to dryness. Drying *in vacuo* at 50°C yields 17.4 g of crude product, which is purified further by column chromatography. There is obtained a yellowish solid having the following analytical data:

- GC-MS: as TMS mass 580 (M=436, cis, trans)

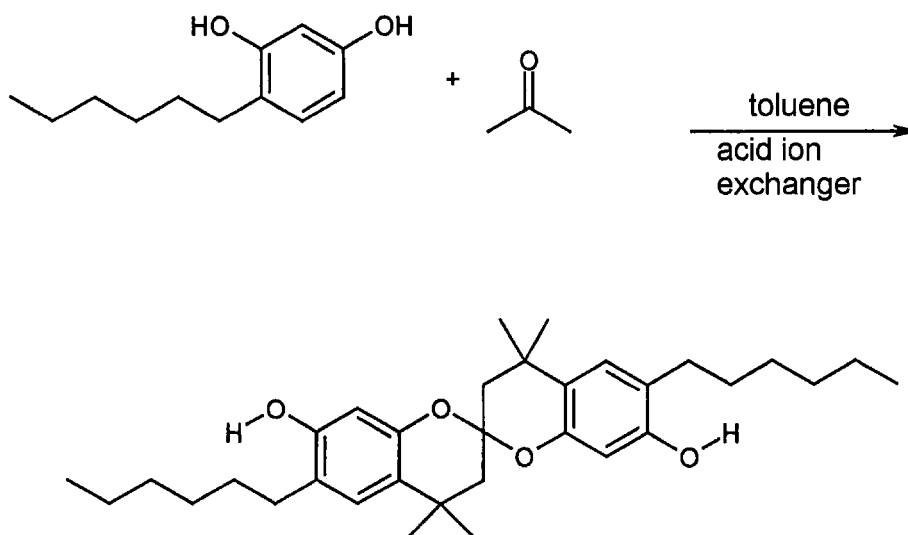
10 **Example 3:**



30 g (0.27 mol) of resorcinol and 29.2 g (0.405 mol) of methyl ethyl ketone (MEK) are dissolved in 300 ml of dry toluene. 50 g of anhydrous ion exchanger K1221 (Bayer AG) are added as catalyst. Condensation to the product is carried out by boiling at reflux for 6 hours. When the reaction is complete, the ion exchanger is separated off and then washed with toluene. The toluene fractions are combined and concentrated to dryness. Drying *in vacuo* at 50°C yields 50.4 g of crude product, which is purified further by column chromatography. There is obtained a white solid having the following analytical data:

- GC-MS: as TMS mass 526 (M=382, stereoisomers)
- HPLC-MS: M=382

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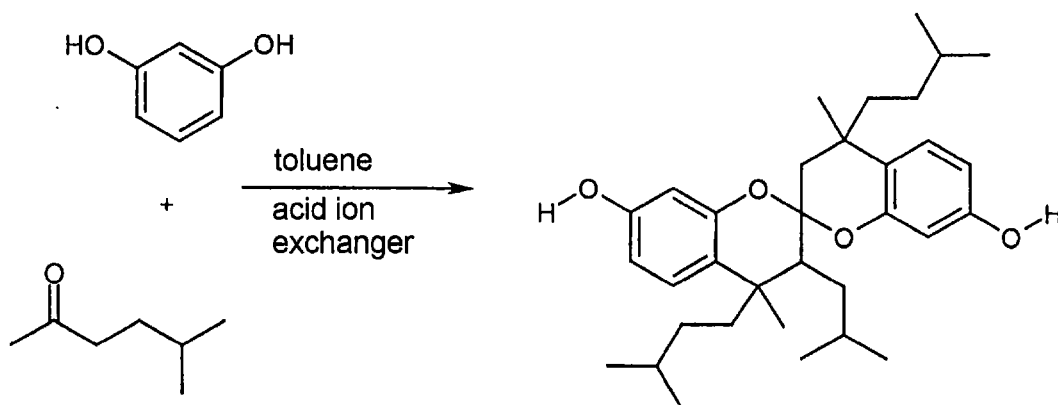
Example 4:

5 52.45 g (0.27 mol) of 4-hexylresorcinol and 23.5 g (0.405 mol) of acetone are dissolved in 300 ml of dry toluene. 50 g of anhydrous ion exchanger K1221 (Bayer AG) are added as catalyst. Condensation to the product is carried out by boiling at reflux for 6 hours. When the reaction is complete, the ion exchanger is separated off and then washed with toluene. The toluene fractions are combined and concentrated to dryness. Drying *in vacuo* at 50°C yields 61.6 g of crude product,
10 which is purified further by column chromatography.

There is obtained a white solid having the following analytical data:

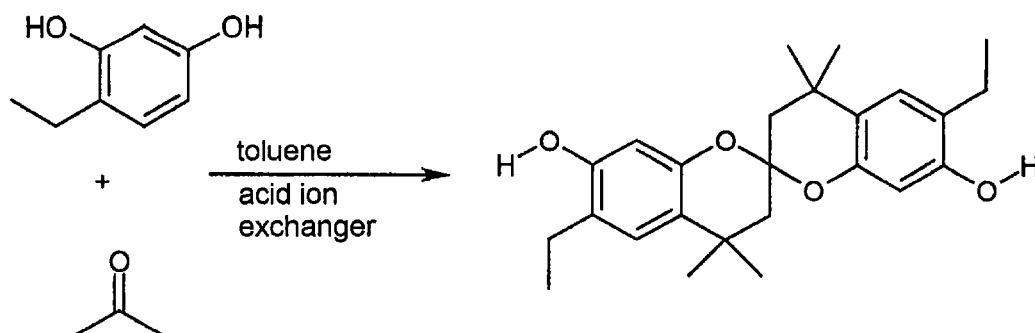
- GC-MS: as TMS mass 652 (M=508)

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Example 5:

30 g (0.27 mol) of resorcinol and 46.25 g (0.405 mol) of 5-methyl-2-hexanone are dissolved in 300 ml of dry toluene. 50 g of anhydrous ion exchanger K1221 (Bayer AG) are added as catalyst. Condensation to the product is carried out by boiling at reflux for 6 hours. When the reaction is complete, the ion exchanger is separated off and then washed with toluene. The toluene fractions are combined and concentrated to dryness. Drying *in vacuo* at 50°C yields 63.4 g of crude product (still contains toluene), which is purified further by column chromatography.

There is obtained a yellowish-white solid having the following analytical data:
HPLC-MS: M=508

Example 6:

37.31 g (0.27 mol) of 4-ethylresorcinol and 23.5 g (0.405 mol) of acetone are dissolved in 300 ml of dry toluene. 50 g of anhydrous ion exchanger SC 104

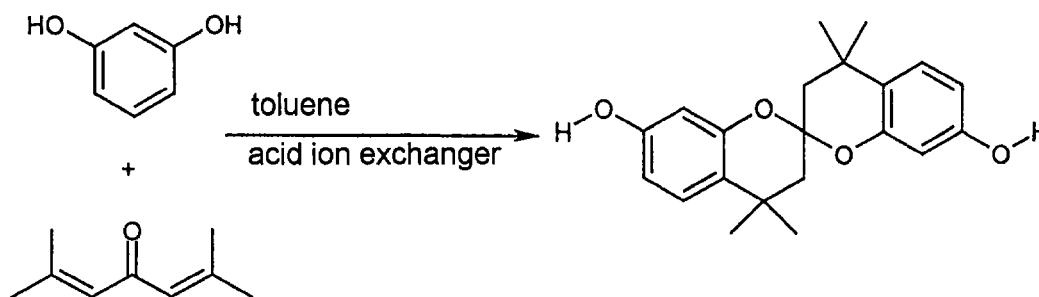
- 28 -

(Bayer AG) are added as catalyst. Condensation to the product is carried out by boiling at reflux for 2 days. When the reaction is complete, the ion exchanger is separated off and then washed with toluene. The resulting precipitate is dried *in vacuo* at 50°C, yielding 3.35 g of product, which did not require further purification by column chromatography.

There is obtained a light-beige solid having the following analytical data:

- GC-MS: as TMS mass 540 (M=396)
- HPLC-MS: M=396
- 10 - ¹H-NMR (400 MHz, D₆-DMSO, room temperature, TMS): δ = 1.07-1.11 (t, 6H; CH₂-CH₃); 1.22-1.46 (d, 12H; CH₃); 1.85-2.03 (dd, 4H; -CH₂-); 2.42-2.5 (q, 4H, -CH₂-CH₃); 6.0 (s, 2H; Ar-H); 7.0 (s, 2H; Ar-H); 8.86 (s, 2H; Ar-OH)

Example 7:



30 g (0.27 mol) of resorcinol and 18.66 g (0.135 mol) of phorone (Aldrich) are dissolved in 300 ml of dry toluene. 50 g of anhydrous ion exchanger SC 104 (Bayer AG) are added as catalyst. Condensation to the product is carried out by boiling at reflux for 8 hours, with water separation. When the reaction is complete, the ion exchanger is separated off and then washed with toluene. The resulting precipitate is dried *in vacuo* at 50°C, yielding 40.1 g of crude product (still contains toluene), which is purified further by column chromatography.

There is obtained a white solid having the following analytical data:

- 29 -

- GC-MS: as TMS mass 484 (M=340)
- HPLC-MS: M=340
- NMR characterisation see also Example 1

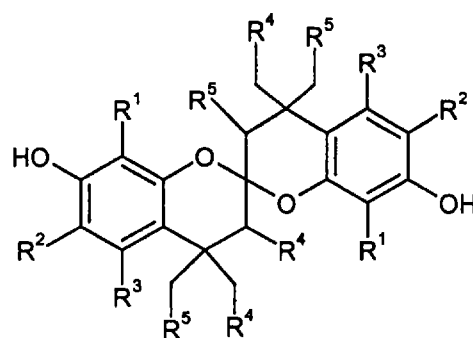
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Patent claims

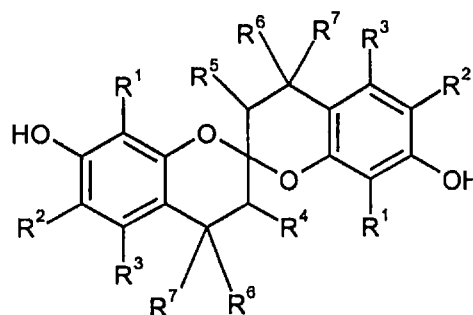
1. Polyester carbonates, characterised in that there are used as monomers, in addition to the conventional carbonic acid derivatives, also dicarboxylic acids of formula (I)



wherein T represents a branched or linear, saturated or unsaturated alkyl, arylalkyl or cycloalkyl moiety of from 8 to 40 carbons, and, at least proportionately in addition to the conventional diphenols, particular diphenols of formula (IIa) and/or (IIb)



(IIa)



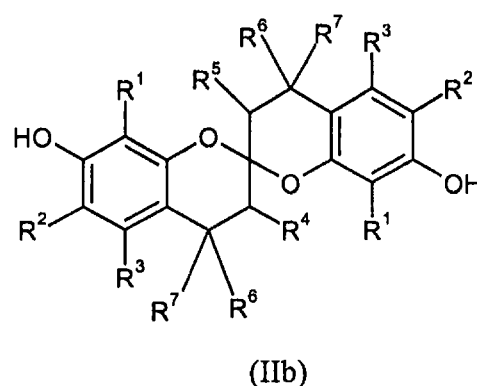
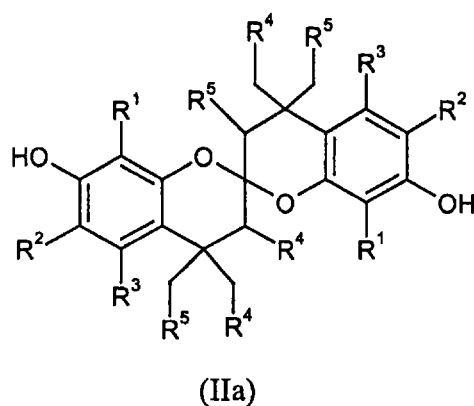
(IIb)

in which

R_1 to R_7 each independently of the others represents hydrogen, halogen, a C_1 - to C_{12} -alkyl radical, a C_6 - to C_{19} -aryl radical, a C_7 - to C_{12} -aralkyl radical.

2. Polyester carbonates according to claim 1, characterised in that only the compounds of formulae IIa and IIb are used as the diphenol component.
3. Diphenols of formula (IIa) and/or (IIb)

- 31 -



in which

5 R_1 to R_7 each independently of the others represents hydrogen, halogen, a C_1 - to C_{12} -alkyl radical, a C_6 - to C_{19} -aryl radical, a C_7 - to C_{12} -aralkyl radical, with the exception of compounds in which R^1 to R^5 in formula IIa are hydrogen and R^6 and R^7 in formula IIb are simultaneously methyl groups.

- 10 4. Polyester polycarbonate according to claim 1, characterised in that the mean molecular weight M_w is from 7000 to 40,000.
5. Moulded bodies containing a polyester polycarbonate according to claim 1, especially optical lenses, disks and films.
- 15 6. Machine-readable data carrier, characterised in that it is based on a substrate of a polyester polycarbonate according to claim 1.
7. Process for the preparation of polyester polycarbonates according to claim 1, by one of the conventional processes for the preparation of polycarbonates, characterised in that diphenols of formula IIa and/or IIb as well as dicarboxylic acids of formula I are reacted with carbonic acid derivatives.
- 20

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8. Use of the compounds according to claim 2 in the preparation of polyester polycarbonates and polycarbonates.
- 5 9. Process for the preparation of compounds according to claim 3 by acid condensation of ketones or phorones with substituted or unsubstituted resorcinols.