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(54) **COMPOSITION AND PROCESS FOR PREPARING MOISTURE-CROSSLINKING POLYMERS AND USE THEREOF**

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(57) **ABSTRACT**

The invention relates to a composition and to a process for preparing moisture-crosslinking polymers under catalysis by at least one metal-siloxane-silanol(ate) compound, and to the use of the composition in the CASE sector (coatings, adhesives, sealants and elastomers), especially in the field of adhesives and sealants.

COMPOSITION AND PROCESS FOR PREPARING MOISTURE-CROSSLINKING POLYMERS AND USE THEREOF

CROSS REFERENCE TO RELATED APPLICATIONS

[0001] This application is a National Stage of International Application No. PCT/EP2020/057868, filed Mar. 20, 2020, claiming priority based on European Patent Application No. 19 165 363.3 filed Mar. 26, 2019 and European Patent Application No. 19 191 330.0 filed Aug. 12, 2019.

[0002] The present invention relates to compositions comprising moisture-crosslinking polymers and to processes for preparation thereof, especially of silane-functional hybrid polymers, and to the moisture-crosslinking polymers as such. In a further aspect, the present invention relates to the use of these compositions in CASE sectors (coatings, adhesives, sealants and elastomers), for example in adhesives and sealants.

[0003] Polymers such as silylated polyurethanes, for example, that condense ("crosslink") on contact with water or air humidity and at room temperature have long been known. They are also referred to as moisture-crosslinking polymers. Depending on factors including the content of silane groups and the structure thereof, it is possible for long-chain polymers, wide-mesh three-dimensional networks or highly crosslinked systems to form.

[0004] Moisture-crosslinking polymers, especially silylated polyurethanes, have long found various uses as adhesives and sealants. For instance, the field of traditional silicone adhesives and sealants based on dimethylpolysiloxanes and of polyurethane adhesives and sealants having free isocyanate groups has developed to include silane-terminated adhesives and sealants.

[0005] Typically, methoxy-substituted silanes are used. The use of these compounds has become generally established since these have good reactivity. However, methoxysilane-substituted polymers have the disadvantage of eliminating methanol on curing. This is a matter of toxicological concern.

[0006] It is therefore an object of the invention to achieve an improvement in this regard.

[0007] The object is achieved in accordance with the invention by the provision of a composition obtainable according to claim **1**. Advantageous developments are the subject of the dependent claims or of the further independent claims.

[0008] The core of the invention is accordingly that of providing a composition comprising at least two catalysts A and B and at least one silylated polymer (SiP), wherein catalyst A is selected from the group of the metal-siloxane-silanol(ate) compounds. The silylated polymer (SiP) has preferably been prepared from a metal-siloxane-silanol(ate) compound-catalysed synthesis of at least one hydroxy-functionalized polymer (also "hydroxy-functional polymer"), and a compound having at least one isocyanate group.

[0009] It has been found that, surprisingly, the composition according to claim **1** permits the use of ethoxy-substituted silanes. The curing of the SiP accordingly eliminates not methanol but ethanol, which is of no toxicological concern. In the curing of the polymers, it is possible to achieve acceptable fibre times and tack-free times (similarly to the case of methoxy-functional hybrid polymers).

[0010] The invention therefore permits provision of formulations, for example for the adhesives and sealants sectors, in which it is possible to dispense with the methanol-eliminating hybrid polymers.

[0011] Very particular preference is given according to the invention to the use of heptaisobutyl POSS-titanium(IV) ethoxide (TiPOSS) as catalyst A. In further particularly preferred embodiments, catalyst B is likewise a metal-siloxane-silanol(ate) compound. Catalyst B may advantageously also be an organometallic compound.

[0012] According to the invention, it is advantageously possible to reduce the total amount of the catalysts used for curing of moisture-crosslinking polymers, especially of catalyst A. Accordingly, a composition according to the invention advantageously comprises moisture-curing silylated polymers (SiP) and at least one metal-siloxane-silanol(ate) compound, wherein the metal-siloxane-silanol(ate) compound is present with a proportion by weight in the range from 0.001% to 5%, preferably from 0.002% to 1%, based in each case on the total weight of the composition. The compositions according to the invention preferably comprise silylated polymers that have been prepared by means of catalysis by metal-siloxane-silanol(ate) compounds in molar concentrations in the range from 0.000001 to 0.0001 mol/kg or 0.0001 to 0.1 mol/kg, especially from 0.00001 to 0.00005 mol/kg or 0.001 to 0.01 mol/kg, based in each case on the total weight of the composition.

[0013] The term "catalyst" relates to a substance that lowers the activation energy of a particular reaction and hence increases the reaction rate.

[0014] The term "metal-siloxane-silanol(ate)" refers to all metal-siloxane compounds that contain either one or more silanol and/or silanolate groups. In one embodiment of the invention, it is likewise possible that there are exclusively metal-siloxane-silanolates. If no specific differentiation is made between these different configurations, all combinations are included. The metal-siloxane-silanol(ate) compounds (=metal-siloxane-silanol/silanolate compounds) just described are also referred to hereinafter as oligomeric metallosilsesquioxanes, "POMS", metal silsesquioxanes or metallized silsesquioxanes. The terms are used interchangeably hereinafter.

[0015] In one embodiment of the present invention, the metal-siloxane-silanol(ate) compound may take the form of a monomer, oligomer and/or polymer for preparation of the silylated polymers (SiP) of the composition according to the invention, the transition from oligomers to polymers being fluid according to the general definition.

[0016] The metal(s) was/were preferably present terminally and/or within the chain in the oligomeric and/or polymeric metal-siloxane-silanol(ate) compound.

[0017] In the composition according to the invention and in the preparation of the silylated polymers (SiP), the catenated metal-siloxane-silanol(ate) compound is linear, branched and/or a cage.

[0018] In a preferred embodiment, the catenated metal-siloxane-silanol(ate) compound in the composition according to the invention and/or in the preparation of the silylated polymers (SiP) in the composition according to the invention has a cage structure.

[0019] A "cage" or an oligomeric or polymeric "cage structure" for the purposes of the present invention is a three-dimensional arrangement of the catenated metal-siloxane-silanol(ate) compound, wherein individual atoms in the chain form the vertices of a multifaceted base structure of the compound. In this case, the mutually linked atoms form at least two surfaces, giving rise to a common intersection. In one embodiment of the compound, for example, a cubic base structure of the compound is formed. A one-cage structure or else a cage structure in singular form, i.e. a compound that has an isolated cage, is the structure (IVc). Compounds having multiple cages within the compound may be described by the compounds (I) and (Ia) to (Id). According to the invention, a cage may be "open" or else "closed", depending on whether all vertices are bonded, joined or coordinated so as to form a closed cage structure. One example of a closed cage is the structures (II), (IV), (IVb), (IVc).

[0020] According to the invention, the term "-nuclear" gives the nuclearity of a compound, how many metal atoms are present therein. A mononuclear compound has one metal atom, whereas a dinuclear compound has two metal atoms within a compound. The metals may be bonded directly to one another or linked via their substituents. One example of a mononuclear compound according to the invention is, for example, the structures (IV), (IVb), (IVc), (Ia), (Ib) or (Ic); a dinuclear compound is represented by structure (Id).

[0021] A mononuclear one-cage structure is represented by the metal-siloxane-silanol(ate) compounds (IV), (IVb) and (IVc). Mononuclear two-cage structures are, for example, the structures (Ia), (Ib) or (Ic).

[0022] The metal-siloxane-silanol(ate) compound in the preparation of the silylated polymers (SiP) of the composition according to the invention preferably comprises an oligomeric metal silsesquioxane.

[0023] The metal-siloxane-silanol(ate) compound in the preparation of the silylated polymers (SiP) of the composition according to the invention especially comprises a polyhedral metal silsesquioxane.

[0024] In one embodiment, the metal-siloxane-silanol(ate) compound in the composition according to the invention and/or in the preparation of the silylated polymers (SiP) has the general formula $R^*_qSi_rO_sM_t$ where each R* is independently selected from the group consisting of optionally substituted C1- to C20-alkyl, optionally substituted C3- to C8-cycloalkyl, optionally substituted C2- to C20-alkenyl, optionally substituted C5- to C10-aryl, —OH and —O—(C1- to C10-alkyl), each M is independently selected from the group consisting of s- and p-block metals, d- and f-block transition metals, lanthanide and actinide metals and semimetals, especially from the group consisting of metals from transition group 1, 2, 3, 4, 5, 8, 10 and 11 and metals from main group 1, 2, 3, 4 and 5, preferably from the group consisting of Na, Zn, Sc, Nd, Ti, Zr, Hf, V, Fe, Pt, Cu, Ga, Sn and Bi; especially preferably from the group consisting of Zn, Ti, Zr, Hf, V, Fe, Sn and Bi,

[0025] q is an integer from 4 to 19,

[0026] r is an integer from 4 to 10,

[0027] s is an integer from 8 to 30, and

[0028] t is an integer from 1 to 8.

[0029] In a further embodiment, the metal-siloxane-silanol(ate) compound in the composition according to the invention and/or in the preparation of the silylated polymers (SiP) has the general formula $R^{\#}_4Si_4O_{11}Y_2Q_2X_4Z_3$ where each X is independently selected from the group consisting of Si, M^1, $-M^3L^1_\Delta$, M^3, or $—Si(R^8)—O-M^3L^1_\Delta$, where M^1 and M^3 are independently selected from the group consisting of s- and p-block metals, d- and f-block transition metals, lanthanide and actinide metals and semimetals, especially from the group consisting of metals from transition group 1, 2, 3, 4, 5, 8, 10 and 11 and metals from main group 1, 2, 3, 4 and 5, preferably from the group consisting of Na, Zn, Sc, Nd, Ti, Zr, Hf, V, Fe, Pt, Cu, Ga, Sn and Bi; especially preferably from the group consisting of Zn, Ti, Zr, Hf, V, Fe, Sn and Bi, and

[0030] where L^1 is selected from the group consisting of —OH and —O—(C1- to C10-alkyl), especially —O—(C1- to C8-alkyl) or —O—(C1- to C6-alkyl), or where L^1 is selected from the group consisting of —OH, —O-methyl, —O-ethyl, —O-propyl, —O-butyl, —O-octyl, —O-isopropyl, and —O-isobutyl, and where R^8 is selected from the group consisting of optionally substituted C1- to C20-alkyl, optionally substituted C3- to C8-cycloalkyl, optionally substituted C2- to C20-alkenyl and optionally substituted C5- to C10-aryl;

[0031] each Z is independently selected from the group consisting of L^2, R^5, R^6 and R^7, where L^2 is selected from the group consisting of —OH and —O—(C1- to C10-alkyl), especially —O—(C1- to C8-alkyl) or —O—(C1- to C6-alkyl), or where L^2 is selected from the group consisting of —OH, —O-methyl, —O-ethyl, —O-propyl, —O-butyl, —O-octyl, —O-isopropyl, and —O-isobutyl;

[0032] each $R^{\#}$, R^5, R^6 and R^7 is independently selected from the group consisting of optionally substituted C1- to C20-alkyl, optionally substituted C3- to C8-cycloalkyl, optionally substituted C2- to C20-alkenyl and optionally substituted C5- to C10-aryl; each Y is independently $—O-M^2-L^3_\Delta$, or two Y are associated and together are $—O-M^2(L^3_\Delta)-O—$ or —O—, where L^3 is selected from the group consisting of —OH and —O—(C1- to C10-alkyl), especially —O—(C1- to C8-alkyl) or —O—(C1- to C6-alkyl), or where L^3 is selected from the group consisting of —OH, —O-methyl, —O-ethyl, —O-propyl, —O-butyl, —O-octyl, —O-isopropyl, and —O-isobutyl, and each M^2 is independently selected from the group consisting of s- and p-block metals, d- and f-block transition metals, lanthanide and actinide metals and semimetals, especially from the group consisting of metals from transition group 1, 2, 3, 4, 5, 8, 10 and 11 and metals from main group 1, 2, 3, 4 and 5, preferably from the group consisting of Na, Zn, Sc, Nd, Ti, Zr, Hf, V, Fe, Pt, Cu, Ga, Sn and Bi; especially preferably from the group consisting of Zn, Ti, Zr, Hf, V, Fe, Sn and Bi,

[0033] each Q is independently H, $M^4L^4_\Delta$, $—SiR^8$, $-M^3L^1_\Delta$, a single bond joined to M^3 of X or a single bond joined to the silicon atom of the $—Si(R^8)—O-M^3L^1_\Delta$ radical, where M^3, R^8 and L^1 are as defined for X, where M^4 is selected from the group consisting of s- and p-block metals, d- and f-block transition metals, lanthanide and actinide metals and semimetals, especially from the group consisting of metals from transition group 1, 2, 3, 4, 5, 8, 10 and 11 and metals from main group 1, 2, 3, 4 and 5, preferably from the group consisting of Na, Zn, Sc, Nd, Ti, Zr, Hf, V, Fe, Pt, Cu, Ga, Sn and Bi; especially preferably from the group consisting of Zn, Ti, Zr, Hf, V, Fe, Sn and Bi, and where L^4 is selected from the group consisting of —OH and —O—(C1- to C10-alkyl), especially —O—(C1- to C8-alkyl) or —O—(C1- to C6-alkyl), or where L^4 is selected from the group consisting of —OH, —O-methyl, —O-ethyl, —O-propyl, —O-butyl, —O-octyl, —O-isopropyl, and —O-isobutyl,

[0034] with the proviso that at least one X is M^3, $-M^3L^1_\Delta$ or $—Si(R^8)—O-M^3L^1_\Delta$.

[0035] It is known to the person skilled in the art that the number (Δ) of possible ligands for L^1_Δ, L^2_Δ, L^3_Δ, L^4_Δ results directly from the number of free valences of the metal atom used, where the valence number describes the valency of the metal.

[0036] In a further embodiment, the metal-siloxane-silanol(ate) compound in the composition according to the invention and/or in the preparation of the silylated polymers (SiP) has the general formula $(Y_{0.25}R^{\#}SiO_{1.25})_4(Z_{0.75}Y_{0.25}XO)_4(OQ)_2$ where each X is independently selected from the group consisting of Si, M^1, $-M^3L^1_\Delta$, M^3, or —Si(R^8)—O-$M^3L^1_\Delta$, where M^1 and M^3 are independently selected from the group consisting of s- and p-block metals, d- and f-block transition metals, lanthanide and actinide metals and semimetals, especially from the group consisting of metals from transition group 1, 2, 3, 4, 5, 8, 10 and 11 and metals from main group 1, 2, 3, 4 and 5, preferably from the group consisting of Na, Zn, Sc, Nd, Ti, Zr, Hf, V, Fe, Pt, Cu, Ga, Sn and Bi; especially preferably from the group consisting of Zn, Ti, Zr, Hf, V, Fe, Sn and Bi, and where L^1 is selected from the group consisting of —OH and —O—(C1- to C10-alkyl), especially —O—(C1- to C8-alkyl) or —O—(C1- to C6-alkyl), or where L^1 is selected from the group consisting of —OH, —O-methyl, —O-ethyl, —O-propyl, —O-butyl, —O-octyl, —O-isopropyl, and —O-isobutyl, and where R^8 is selected from the group consisting of optionally substituted C1- to C20-alkyl, optionally substituted C3- to C6-cycloalkyl, optionally substituted C2- to C20-alkenyl and optionally substituted C6- to C10-aryl;

[0037] each Z is independently selected from the group consisting of L^2, R^5, R^6 and R^7, where L^2 is selected from the group consisting of —OH and —O—(C1- to C10-alkyl), especially —O—(C1- to C8-alkyl) or —O—(C1- to C6-alkyl), or where L^2 is selected from the group consisting of —OH, —O-methyl, —O-ethyl, —O-propyl, —O-butyl, —O-octyl, —O-isopropyl, and —O-isobutyl;

[0038] each $R^{\#}$, R^5, R^6 and R^7 is independently selected from the group consisting of optionally substituted C1- to C20-alkyl, optionally substituted C3- to C6-cycloalkyl, optionally substituted C2- to C20-alkenyl and optionally substituted C6- to C10-aryl;

[0039] each Y is independently —O-M^2-L^3_Δ, or two Y are associated and together are —O-M^2(L^3_Δ)-O— or —O—, where L^3 is selected from the group consisting of —OH and —O—(C1- to C10-alkyl), especially —O—(C1- to C8-alkyl) or —O—(C1- to C6-alkyl), or where L^3 is selected from the group consisting of —OH, —O-methyl, —O-ethyl, —O-propyl, —O-butyl, —O-octyl, —O-isopropyl, and —O-isobutyl, and each M^2 is independently selected from the group consisting of s- and p-block metals, d- and f-block transition metals, lanthanide and actinide metals and semimetals, especially from the group consisting of metals from transition group 1, 2, 3, 4, 5, 8, 10 and 11 and metals from main group 1, 2, 3, 4 and 5, preferably from the group consisting of Na, Zn, Sc, Nd, Ti, Zr, Hf, V, Fe, Pt, Cu, Ga, Sn and Bi; especially preferably from the group consisting of Zn, Ti, Zr, Hf, V, Fe, Sn and Bi,

[0040] each Q is independently H, $M^4L^4_\Delta$, —SiR^8, $-M^3L^1_\Delta$, a single bond joined to M^3 of X or a single bond joined to the silicon atom of the —Si(R^8)—O-$M^3L^1_\Delta$ radical, where M^3, R^8 and L^1 are as defined for X, where M^4 is selected from the group consisting of s- and p-block metals, d- and f-block transition metals, lanthanide and actinide metals and semimetals, especially from the group consisting of metals from transition group 1, 2, 3, 4, 5, 8, 10 and 11 and metals from main group 1, 2, 3, 4 and 5, preferably from the group consisting of Na, Zn, Sc, Nd, Ti, Zr, Hf, V, Fe, Pt, Cu, Ga, Sn and Bi; especially preferably from the group consisting of Zn, Ti, Zr, Hf, V, Fe, Sn and Bi, and where L^4 is selected from the group consisting of —OH and —O—(C1- to C10-alkyl), especially —O—(C1- to C8-alkyl) or —O—(C1- to C6-alkyl), or where L^4 is selected from the group consisting of —OH, —O-methyl, —O-ethyl, —O-propyl, —O-butyl, —O-octyl, —O-isopropyl, and —O-isobutyl,

[0041] with the proviso that at least one X is M^3, $-M^3L^1_\Delta$ or —Si(R^8)—O-$M^3L^1_\Delta$.

[0042] The metal-siloxane-silanol(ate) compound in the composition according to the invention and/or the preparation of the silylated polymers (SiP) preferably has the general formula $Si_4O_9R^1R^2R^3R^4X^1X^2X^3X^4OQ^1OQ^2Y^1Y^2Z^1Z^2Z^3$ where X^1, X^2 and X^3 are independently selected from Si and M^1, where M^1 is selected from the group consisting of s- and p-block metals, d- and f-block transition metals, lanthanide and actinide metals and semimetals, especially from the group consisting of metals from transition group 1, 2, 3, 4, 5, 8, 10 and 11 and metals from main group 1, 2, 3, 4 and 5, preferably from the group consisting of Na, Zn, Sc, Nd, Ti, Zr, Hf, V, Fe, Pt, Cu, Ga, Sn and Bi; especially preferably from the group consisting of Zn, Ti, Zr, Hf, V, Fe, Sn and Bi,

[0043] Z^1, Z^2 and Z^3 are independently selected from the group consisting of L^2, R^5, R^6 and R^7, where L^2 is selected from the group consisting of —OH and —O—(C1- to C10-alkyl), especially —O—(C1- to C8-alkyl) or —O—(C1- to C6-alkyl), or where L2 is selected from the group consisting of —OH, —O-methyl, —O-ethyl, —O-propyl, —O-butyl, —O-octyl, —O-isopropyl, and —O-isobutyl;

[0044] R^1, R^2, R^3, R^4, R^5, R^6 and R^7 are independently selected from the group consisting of optionally substituted C1- to C20-alkyl, optionally substituted C3- to C8-cycloalkyl, optionally substituted C2- to C20-alkenyl and optionally substituted C5- to C10-aryl;

[0045] Y^1 and Y^2 are independently —O-M^2-L^3_Δ, or Y^1 and Y^2 are associated and together are —O-M^2(L^3_Δ)-O— or —O—, where L^3 is selected from the group consisting of —OH and —O—(C1- to C10-alkyl), especially —O—(C1- to C8-alkyl) or —O—(C1- to C6-alkyl), or where L^3 is selected from the group consisting of —OH, —O-methyl, —O-ethyl, —O-propyl, —O-butyl, —O-octyl, —O-isopropyl, and —O-isobutyl, and M^2 is selected from the group consisting of s- and p-block metals, d- and f-block transition metals, lanthanide and actinide metals and semimetals, especially from the group consisting of metals from transition group 1, 2, 3, 4, 5, 8, 10 and 11 and metals from main group 1, 2, 3, 4 and 5, preferably from the group consisting of Na, Zn, Sc, Nd, Ti, Zr, Hf, V, Fe, Pt, Cu, Ga, Sn and Bi; especially preferably from the group consisting of Zn, Ti, Zr, Hf, V, Fe, Sn and Bi, and

[0046] X^4 is $-M^3L^1_\Delta$ or M^3 and Q^1 and Q^2 are each H or a single bond joined to M^3, where L^1 is selected from the group consisting of —OH and —O—(C1- to C10-alkyl), especially —O—(C1- to C8-alkyl) or —O—(C1- to C6-alkyl), or where L^1 is selected from the group consisting of —OH, —O-methyl, —O-ethyl, —O-propyl, —O-butyl, —O-octyl, —O-isopropyl, and —O-isobutyl, and where M^3 is selected from the group consisting of s- and p-block metals, d- and f-block transition metals, lanthanide and actinide metals and semimetals, especially from the group consisting of metals from transition group 1, 2, 3, 4, 5, 8, 10 and 11 and metals from main group 1, 2, 3, 4 and 5, preferably from the group consisting of Na, Zn, Sc, Nd, Ti, Zr, Hf, V, Fe, Pt, Cu, Ga, Sn and Bi; especially preferably from the group consisting of Zn, Ti, Zr, Hf, V, Fe, Sn and Bi, or

[0047] X^4 is -$M^3L^1_\Delta$ and Q^2 is H or a single bond joined to M^3 and Q^1 is H, $M^4L^4_\Delta$ or —SiR^8, where M^4 is selected from the group consisting of s- and p-block metals, d- and f-block transition metals, lanthanide and actinide metals and semimetals, especially from the group consisting of metals from transition group 2, 3, 4, 5 and 8 and metals from main group 1, 2, 3, 4 and 5, especially from the group consisting of Zn, Sc, Ti, Zr, Hf, V, Pt, Ga, Sn and Bi, where L^4 is selected from the group consisting of —OH and —O—(C1- to C10-alkyl), especially —O—(C1- to C8-alkyl) or —O—(C1- to C6-alkyl), or where L^4 is selected from the group consisting of —OH, —O-methyl, —O-ethyl, —O-propyl, —O-butyl, —O-octyl, —O-isopropyl, and —O-isobutyl, and where R^8 is selected from the group consisting of optionally substituted C1- to C20-alkyl, optionally substituted C3- to C8-cycloalkyl, optionally substituted C2- to C20-alkenyl and optionally substituted C5- to C10-aryl, or

[0048] X^4, Q^1 and Q^2 are independently -$M^3L^1_\Delta$, or

[0049] X^4 is —Si(R^8)—O-M^3L^1, Q^2 is a single bond joined to the silicon atom of X^4 and Q^1 is -$M^4L^4_\Delta$, or

[0050] X^4 is —Si(R^8)—O-$M^3L^1_\Delta$, Q^2 is a single bond joined to the silicon atom of X^4 and Q^1 is a single bond joined to the M^3 atom of X^4.

[0051] In a further embodiment, the metal silsesquioxane in the composition according to the invention and/or in the preparation of the silylated polymers (SiP) has the general formula $(X^4)(Z^1Y^1X^2O)(Z^2X^1O_2)(Z^3X^3O_2)(R^1Y^2SiO)(R^3SiO)(R^4SiO_2)(R^2SiO_2)(Q^1)(Q^2)$ where X^1, X^2 and X^3 are independently selected from Si and M^1, where M^1 is selected from the group consisting of s- and p-block metals, d- and f-block transition metals, lanthanide and actinide metals and semimetals, especially from the group consisting of metals from transition group 1, 2, 3, 4, 5, 8, 10 and 11 and metals from main group 1, 2, 3, 4 and 5, preferably from the group consisting of Na, Zn, Sc, Nd, Ti, Zr, Hf, V, Fe, Pt, Cu, Ga, Sn and Bi; especially preferably from the group consisting of Zn, Ti, Zr, Hf, V, Fe, Sn and Bi,

[0052] Z^1, Z^2 and Z^3 are independently selected from the group consisting of L^2, R^5, R^6 and R^7, where L^2 is selected from the group consisting of —OH and —O—(C1- to C10-alkyl), especially —O—(C1- to C8-alkyl) or —O—(C1- to C6-alkyl), or where L^2 is selected from the group consisting of —OH, —O-methyl, —O-ethyl, —O-propyl, —O-butyl, —O-octyl, —O-isopropyl, and —O-isobutyl;

[0053] R^1, R^2, R^3, R^4, R^5, R^6 and R^7 are independently selected from the group consisting of optionally substituted C1- to C20-alkyl, optionally substituted C3- to C6-cycloalkyl, optionally substituted C2- to C20-alkenyl and optionally substituted C6- to C10-aryl;

[0054] Y^1 and Y^2 are independently —O-M^2-L^3_Δ, or Y^1 and Y^2 are associated and together are —O-$M^2(L^3_\Delta)$-O— or —O—, where L^3 is selected from the group consisting of —OH and —O—(C1- to C10-alkyl), especially —O—(C1- to C8-alkyl) or —O—(C1- to C6-alkyl), or where L^3 is selected from the group consisting of —OH, —O-methyl, —O-ethyl, —O-propyl, —O-butyl, —O-octyl, —O-isopropyl, and —O-isobutyl, and M^2 is selected from the group consisting of s- and p-block metals, d- and f-block transition metals, lanthanide and actinide metals and semimetals, especially from the group consisting of metals from transition group 1, 2, 3, 4, 5, 8, 10 and 11 and metals from main group 1, 2, 3, 4 and 5, preferably from the group consisting of Na, Zn, Sc, Nd, Ti, Zr, Hf, V, Fe, Pt, Cu, Ga, Sn and Bi; especially preferably from the group consisting of Zn, Ti, Zr, Hf, V, Fe, Sn and Bi, and

[0055] X^4 is -$M^3L^1_\Delta$ or M^3 and Q^1 and Q^2 are each H or a single bond joined to M^3, where L^1 is selected from the group consisting of —OH and —O—(C1- to C10-alkyl), especially —O—(C1- to C8-alkyl) or —O—(C1- to C6-alkyl), or where L^1 is selected from the group consisting of —OH, —O-methyl, —O-ethyl, —O-propyl, —O-butyl, —O-octyl, —O-isopropyl, and —O-isobutyl, and where M^3 is selected from the group consisting of s- and p-block metals, d- and f-block transition metals, lanthanide and actinide metals and semimetals, especially from the group consisting of metals from transition group 1, 2, 3, 4, 5, 8, 10 and 11 and metals from main group 1, 2, 3, 4 and 5, preferably from the group consisting of Na, Zn, Sc, Nd, Ti, Zr, Hf, V, Fe, Pt, Cu, Ga, Sn and Bi; especially preferably from the group consisting of Zn, Ti, Zr, Hf, V, Fe, Sn and Bi, or

[0056] X^4 is -$M^3L^1_\Delta$ and Q^2 is H or a single bond joined to M^3 and Q^1 is H, $M^4L^4_\Delta$ or —SiR^8, where M4 is selected from the group consisting of s- and p-block metals, d- and f-block transition metals, lanthanide and actinide metals and semimetals, especially from the group consisting of metals from transition group 2, 3, 4, 5 and 8 and metals from main group 1, 2, 3, 4 and 5, especially from the group consisting of Zn, Sc, Ti, Zr, Hf, V, Pt, Ga, Sn and Bi, where L^4 is selected from the group consisting of —OH and —O—(C1- to C10-alkyl), especially —O—(C1- to C8-alkyl) or —O—(C1- to C6-alkyl), or where L^4 is selected from the group consisting of —OH, —O-methyl, —O-ethyl, —O-propyl, —O-butyl, —O-octyl, —O-isopropyl, and —O-isobutyl, and where R^8 is selected from the group consisting of optionally substituted C1- to C20-alkyl, optionally substituted C3- to C6-cycloalkyl, optionally substituted C2- to C20-alkenyl and optionally substituted C6- to C10-aryl, or

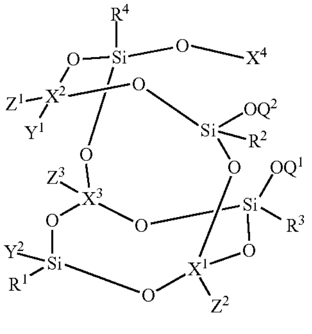
[0057] X^4, Q^1 and Q^2 are independently -$M^3L^1_\Delta$, or

[0058] X^4 is —Si(R^8)—O-$M^3L^1_\Delta$, Q^2 is a single bond joined to the silicon atom of X^4 and Q^1 is -$M^4L^4_\Delta$, or

[0059] X^4 is —Si(R^8)—O-$M^3L^1_\Delta$, Q^2 is a single bond joined to the silicon atom of X^4 and Q^1 is a single bond joined to the M^3 atom of X^4.

[0060] In a further aspect of the invention, the catalyst used in accordance with the invention and based on a metal-siloxane-silanol(ate) compound may be described by the structure (I)

(I)



[0061] where

[0062] X^1, X^2 and X^3 are independently selected from Si and M^1, where M^1 is selected from the group consisting of s- and p-block metals, d- and f-block transition metals, lanthanide and actinide metals and semimetals, especially from the group consisting of metals from transition group 1, 2, 3, 4, 5, 8, 10 and 11 and metals from main group 1, 2, 3, 4 and 5, preferably from the group consisting of Na, Zn, Sc, Nd, Ti, Zr, Hf, V, Fe, Pt, Cu, Ga, Sn and Bi; especially preferably from the group consisting of Zn, Ti, Zr, Hf, V, Fe, Sn and Bi,

[0063] Z^1, Z^2 and Z^3 are independently selected from the group consisting of L^2, R^5, R^6 and R^7, where L^2 is selected from the group consisting of —OH and —O—(C1- to C10-alkyl), especially —O—(C1- to C8-alkyl) or —O—(C1- to C6-alkyl), or where L^2 is selected from the group consisting of —OH, —O-methyl, —O-ethyl, —O-propyl, —O-butyl, —O-octyl, —O-isopropyl, and —O-isobutyl;

[0064] R^1, R^2, R^3, R^4, R^5, R^6 and R^7 are independently selected from the group consisting of optionally substituted C1- to C20-alkyl, optionally substituted C3- to C8-cycloalkyl, optionally substituted C2- to C20-alkenyl and optionally substituted C5- to C10-aryl;

[0065] Y^1 and Y^2 are independently —O-M^2-L^3_{Δ}, or Y^1 and Y^2 are associated and together are —O-$M^2(L^3_{\Delta})$-O— or —O—, where L^3 is selected from the group consisting of —OH and —O—(C1- to C10-alkyl), especially —O—(C1- to C8-alkyl) or —O—(C1- to C6-alkyl), or where L^3 is selected from the group consisting of —OH, —O-methyl, —O-ethyl, —O-propyl, —O-butyl, —O-octyl, —O-isopropyl, and —O-isobutyl, and where M^2 is selected from the group consisting of s- and p-block metals, d- and f-block transition metals, lanthanide and actinide metals and semimetals, especially from the group consisting of metals from transition group 1, 2, 3, 4, 5, 8, 10 and 11 and metals from main group 1, 2, 3, 4 and 5, preferably from the group consisting of Na, Zn, Sc, Nd, Ti, Zr, Hf, V, Fe, Pt, Cu, Ga, Sn and Bi; especially preferably from the group consisting of Zn, Ti, Zr, Hf, V, Fe, Sn, Bi,

[0066] and X^4 is -$M^3L^1_{\Delta}$ or M^3 and Q^1 and Q^2 are each H or a single bond joined to M^3, where L^1 is selected from the group consisting of —OH and —O—(C1- to C10-alkyl), especially —O—(C1- to C8-alkyl) or —O—(C1- to C6-alkyl), or where L^1 is selected from the group consisting of —OH, —O-methyl, —O-ethyl, —O-propyl, —O-butyl, —O-octyl, —O-isopropyl, and —O-isobutyl, and where M^3 is selected from the group consisting of s- and p-block metals, d- and f-block transition metals, lanthanide and actinide metals and semimetals, especially from the group consisting of metals from transition group 1, 2, 3, 4, 5, 8, 10 and 11 and metals from main group 1, 2, 3, 4 and 5, preferably from the group consisting of Na, Zn, Sc, Nd, Ti, Zr, Hf, V, Fe, Pt, Cu, Ga, Sn and Bi; especially preferably from the group consisting of Zn, Ti, Zr, Hf, V, Fe, Sn, Bi, or

[0067] X^4 is -M^3L^1 and Q^2 is H or a single bond joined to M^3 and Q^1 is H, $M^4L^4_{\Delta}$ or —SiR^8, where M^4 is selected from the group consisting of s- and p-block metals, d- and f-block transition metals, lanthanide and actinide metals and semimetals, especially from the group consisting of metals from transition group 1, 2, 3, 4, 5, 8, 10 and 11 and metals from main group 1, 2, 3, 4 and 5, preferably from the group consisting of Na, Zn, Sc, Nd, Ti, Zr, Hf, V, Fe, Pt, Cu, Ga, Sn and Bi; especially preferably from the group consisting of Zn, Ti, Zr, Hf, V, Fe, Sn and Bi, and where L^4 is selected from the group consisting of —OH and —O—(C1- to C10-alkyl), especially —O—(C1- to C8-alkyl) or —O—(C1- to C6-alkyl), or where L^4 is selected from the group consisting of —OH, —O-methyl, —O-ethyl, —O-propyl, —O-butyl, —O-octyl, —O-isopropyl, and —O-isobutyl, and where R^8 is selected from the group consisting of optionally substituted C1- to C20-alkyl, optionally substituted C3- to C6-cycloalkyl, optionally substituted C2- to C20-alkenyl and optionally substituted C6- to C10-aryl, or

[0068] X^4, Q^1 and Q^2 are independently -$M^3L^1_{\Delta}$, or

[0069] X^4 is —Si(R^8)—O-$M^3L^1_{\Delta}$, Q^2 is a single bond joined to the silicon atom of X^4 and Q^1 is -$M^4L^4_{\Delta}$, or

[0070] X^4 is —Si(R^8)—O-$M^3L^1_{\Delta}$, Q^2 is a single bond joined to the silicon atom of X^4 and Q^1 is a single bond joined to the M^3 atom of X^4.

[0071] In a further preferred embodiment, the metal-siloxane-silanol(ate) compound in the preparation of the silylated polymers has the general formula (I) where X^1, X^2 and X^3 are independently Si,

[0072] X^4 is -$M^3L^1_{\Delta}$ and Q^1 and Q^2 are each a single bond joined to M^3, where L^1 is selected from the group consisting of —OH and —O—(C1- to C10-alkyl), especially —O—(C1- to C8-alkyl) or —O—(C1- to C6-alkyl), or where L^1 is selected from the group consisting of —OH, —O-methyl, —O-ethyl, —O-propyl, —O-butyl, —O-octyl, —O-isopropyl, and —O-isobutyl, and where M^3 is selected from the group consisting of s- and p-block metals, d- and f-block transition metals, lanthanide and actinide metals and semimetals, especially from the group consisting of metals from transition group 1, 2, 3, 4, 5, 8, 10 and 11 and metals from main group 1, 2, 3, 4 and 5, preferably from the group consisting of Na, Zn, Sc, Nd, Ti, Zr, Hf, V, Fe, Pt, Cu, Ga, Sn and Bi; especially preferably from the group consisting of Zn, Ti, Zr, Hf, V, Fe, Sn and Bi,

[0073] Z^1, Z^2 and Z^3 are each independently selected from optionally substituted C1- to C20-alkyl, optionally substituted C3- to C8-cycloalkyl, optionally substituted C2- to C20-alkenyl and optionally substituted C5- to C10 aryl,

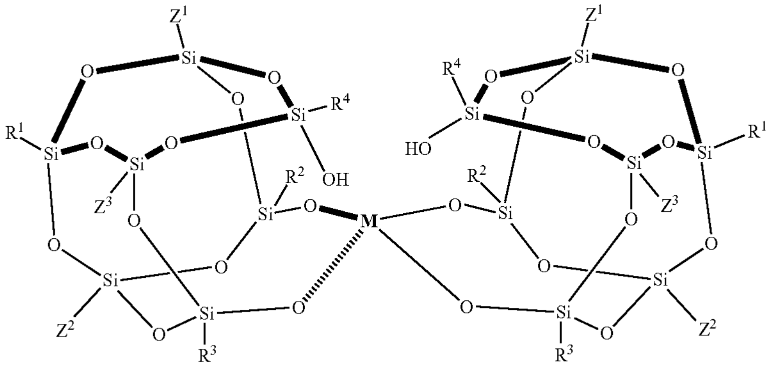
[0074] R^1, R^2 and R^3 are each independently optionally substituted C1- to C20-alkyl, optionally substituted C3- to C8-cycloalkyl, optionally substituted C2- to C20-alkenyl and optionally substituted C5- to C10-aryl,

[0075] Y^1 and Y^2 are associated and together form —O—.

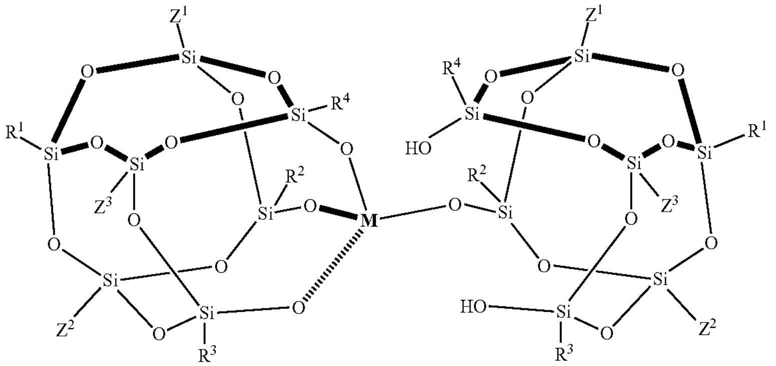
[0076] In one embodiment, the metal-siloxane-silanol(ate) compound of formula (I) in the composition according to the invention and/or in the preparation of the silylated polymers (SiP), depending on the equivalents of metal present, may be in mononuclear form as a monomer or in polynuclear form as a dimer (dinuclear), trimer (trinuclear), multimer (multinuclear) and/or mixtures thereof, such that, for example, structures of the formulae (Ia) to (Id) are possible.

[0077] Further polynuclear metal-siloxane-silanol(ate) compounds usable in accordance with the invention are the structures (Ia), (Ib), (Ic) and (Id)

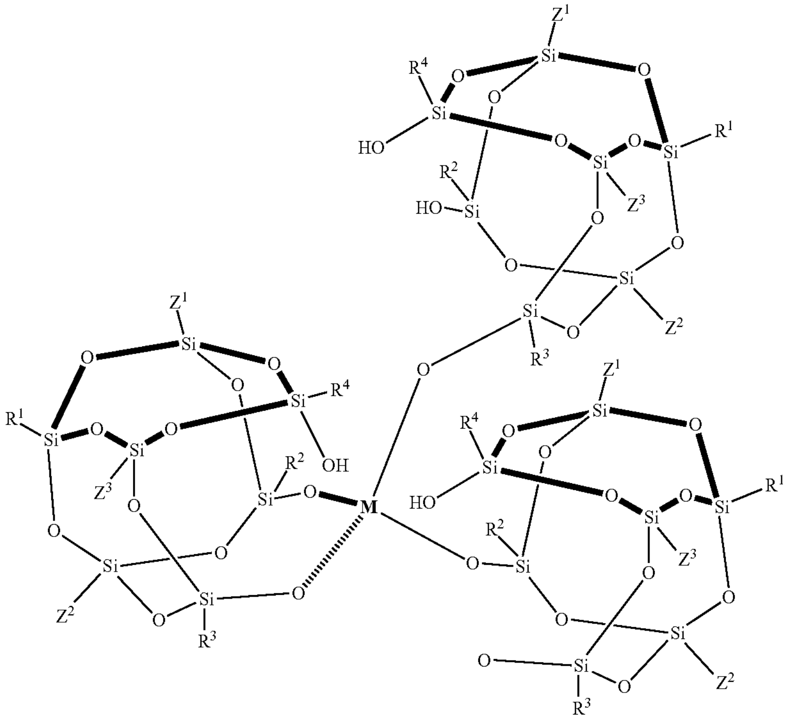
(Ia)



(Ib)



(Ic)



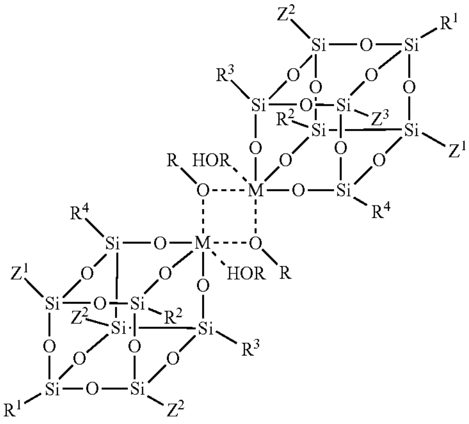
[0078] where

[0079] M is selected from the group consisting of s- and p-block metals, d- and f-block transition metals, lanthanide and actinide metals and semimetals, especially from the group consisting of metals from transition group 1, 2, 3, 4, 5, 8, 10 and 11 and metals from main group 1, 2, 3, 4 and 5, preferably from the group consisting of Na, Zn, Sc, Nd, Ti, Zr, Hf, V, Fe, Pt, Cu, Ga, Sn and Bi; especially preferably from the group consisting of Zn, Ti, Zr, Hf, V, Fe, Sn and Bi, and each R (R^1 to R^4) is independently selected from the group consisting of optionally substituted C1- to C20-alkyl, optionally substituted C3- to C8-cycloalkyl, optionally substituted C2- to C20-alkenyl, optionally substituted C5- to C10-aryl, —OH and —O—(C1- to C10-alkyl). The tetravalent metal M here is a shared part of multiple cages. It is known here to the person skilled in the art that the number of bonds to the metal M depends on the valency of the metal M. The structural formulae (Ia) to (Ic) should be adjusted correspondingly if necessary.

[0080] In one embodiment of the composition according to the invention, a mixture of the metal-siloxane-silanol(ate) compounds of formula (I), (Ia), (Ib) and (Ic) is used therein and/or in the preparation of the silylated polymers (SiP).

[0081] In addition, the polynuclear metal-siloxane-silanol (ate) compound of formula (Id) in the composition according to the invention and/or in the preparation of the silylated polymers (SiP) may have hexacoordinated metal centres, enabling structures of formula (Id)

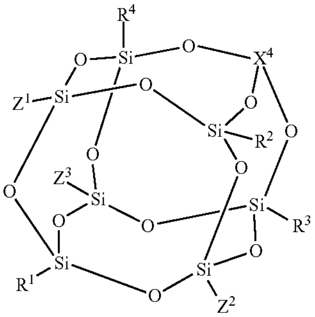
(Id)



[0082] where each M is independently selected from the group consisting of s- and p-block metals, d- and f-block transition metals, lanthanide and actinide metals and semimetals, especially from the group consisting of metals from transition group 1, 2, 3, 4, 5, 8, 10 and 11 and metals from main group 1, 2, 3, 4 and 5, preferably from the group consisting of Na, Zn, Sc, Nd, Ti, Zr, Hf, V, Fe, Pt, Cu, Ga, Sn and Bi; especially preferably from the group consisting of Zn, Ti, Zr, Hf, V, Fe, Sn and Bi, and each R is independently selected from the group consisting of optionally substituted C1- to C20-alkyl, optionally substituted C3- to C8-cycloalkyl, optionally substituted C2- to C20-alkenyl, optionally substituted C5- to C10-aryl, —OH and —O—(C1- to C10-alkyl).

[0083] In the context of the invention, the term "mononuclear" refers to the isolated cage structure, i.e. present in singular form, of the catalyst according to the invention based on a metal-siloxane-silanol(ate) compound. Mononuclear catalysts based on a metal-siloxane-silanol(ate) compound may be encompassed by the structure (IV) and likewise by the structures (I) and (II)

(II)



[0084] where

[0085] X^4 is $-M^3L^1_\Delta$ where L^1 is selected from the group consisting of —OH and —O—(C1- to C10-alkyl), especially —O—(C1- to C8-alkyl) or —O—(C1- to C6-alkyl), or where L^1 is selected from the group consisting of —OH, —O-methyl, —O-ethyl, —O-propyl, —O-butyl, —O-octyl, —O-isopropyl, and —O-isobutyl, and where M^3 is selected from the group consisting of s- and p-block metals, d- and f-block transition metals, lanthanide and actinide metals and semimetals, especially from the group consisting of metals from transition group 1, 2, 3, 4, 5, 8, 10 and 11 and metals from main group 1, 2, 3, 4 and 5, preferably from the group consisting of Na, Zn, Sc, Nd, Ti, Zr, Hf, V, Fe, Pt, Cu, Ga, Sn and Bi; especially preferably from the group consisting of Zn, Ti, Zr, Hf, V, Fe, Sn and Bi,

[0086] Z^1, Z^2 and Z^3 are independently selected from the group consisting of optionally substituted C1- to C20-alkyl, optionally substituted C3- to C8-cycloalkyl, optionally substituted C2- to C20-alkenyl and optionally substituted C5- to C10-aryl;

[0087] R^1, R^2, R^3 and R^4 are each independently selected from the group consisting of optionally substituted C1- to C20-alkyl, optionally substituted C3- to C8-cycloalkyl, optionally substituted C2- to C20-alkenyl and optionally substituted C5- to C10-aryl.

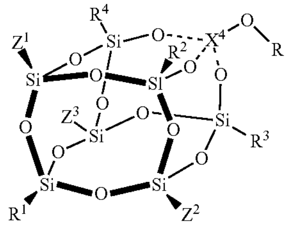
[0088] The invention further relates to the metal-siloxane-silanol(ate) compounds of the general structural formula (II) that are used for preparation of the silylated polymers according to the invention where X^4 is $-M^3L^1_\Delta$ where L^1 is selected from the group consisting of —OH and —O—(C1- to C10-alkyl), especially —O—(C1- to C8-alkyl) or —O—(C1- to C6-alkyl), or where L^1 is selected from the group consisting of —OH, —O-methyl, —O-ethyl, —O-propyl, —O-butyl, —O-octyl, —O-isopropyl, and —O-isobutyl, and where M^3 is selected from the group consisting of s- and p-block metals, d- and f-block transition metals, lanthanide and actinide metals and semimetals, especially from the group consisting of metals from transition group 1, 2, 3, 4, 5, 8, 10 and 11 and metals from main group 1, 2, 3, 4 and 5, preferably from the group consisting of Na, Zn, Sc, Nd, Ti, Zr, Hf, V, Fe, Pt, Cu, Ga, Sn and Bi; especially preferably from the group consisting of Zn, Ti, Zr, Hf, V, Fe, Sn and Bi,

[0089] Z^1, Z^2 and Z^3 are independently selected from the group consisting of L^2, R^5, R^6 and R^7, where L^2 is selected from the group consisting of —OH and —O—(C1- to C10-alkyl), especially —O—(C1- to C8-alkyl) or —O—(C1- to C6-alkyl), or where L^2 is selected from the group consisting of —OH, —O-methyl, —O-ethyl, —O-propyl, —O-butyl, —O-octyl, —O-isopropyl, and —O-isobutyl, and

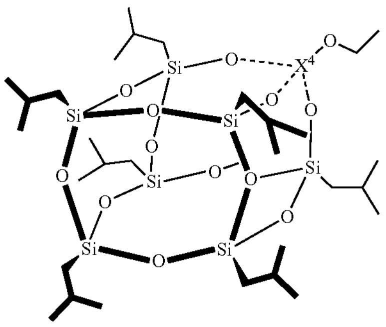
[0090] R^1, R^2, R^3, R^4, R^5, R^6 and R^7 are independently selected from the group consisting of optionally substituted C1- to C20-alkyl, optionally substituted C3- to C8-cycloalkyl, optionally substituted C2- to C20-alkenyl and optionally substituted C5- to C10-aryl.

[0091] In a particularly advantageous embodiment, the silylated polymers (SiP) of the composition according to the invention may have been prepared by a catalysed reaction with heptaisobutyl POSS-titanium(IV) ethoxide (TiPOSS) as a metal-siloxane-silanol(ate) compound and/or the composition may include the latter. The abbreviation "TiPOSS" here represents the monovalent titanium-metallized silsesquioxane of the structural formula (IV) and can be used in an equivalent manner to "heptaisobutyl POSS-titanium(IV) ethoxide" for the purposes of the invention.

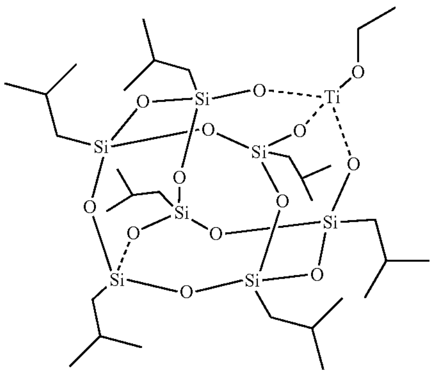
(IV)



(IVb)



(IVc)



[0092] In the composition according to the invention and/or in the preparation of the silylated polymers (SiP), the metal-siloxane-silanol(ate) compound may be a mixture comprising structures (I), (Ia), (Ib), (Ic), (Id), (II), (IV), (IVb), (IVc).

[0093] In a preferred embodiment, the metal in the metal-siloxane-silanol(ate) compound is a titanium.

[0094] Very particularly preferred catalysts from the group of the metal-siloxane-silanol(ate) compounds are heptaisobutyl POSS-titanium(IV) ethoxide (TiPOSS) and heptaisobutyl POSS-tin(IV) ethoxide (SnPOSS). Among these, preference is given to heptaisobutyl POSS-titanium(IV) ethoxide (TiPOSS).

[0095] If catalyst B is not selected from the group of the metal-siloxane-silanol(ate) compounds, it preferably comprises organometallic compounds. Particular preference is given to organotin, organobismuth, organozinc, organozirconium, organoaluminium or organotitanium compounds. Very particular preference is given to organotin or organotitanium compounds.

[0096] In that case, catalyst B may be selected from the group consisting of tetraalkyl titanates, such as tetramethyl titanate, tetraethyl titanate, tetra-n-propyl titanate, tetraisopropyl titanate, tetra-n-butyl titanate, tetraisobutyl titanate, tetra-sec-butyl titanate, tetraoctyl titanate, tetra(2-ethylhexyl) titanate, dialkyl titanates ($(RO)_2TiO_2$ in which R is, for example, isopropyl, n-butyl, isobutyl), such as isopropyl n-butyl titanate; titanium acetylacetonate chelates, such as diisopropoxybis(acetylacetonate) titanate, diisopropoxybis(ethylacetylacetonate) titanate, di-n-butylbis(acetylacetonate) titanate, di-n-butylbis(ethylacetoacetate) titanate, triisopropoxidebis(acetylacetonate) titanate, zirconium tetraalkoxides, such as zirconium tetraethoxide, zirconium tetrabutoxide, zirconium tetrabutyrate, zirconium tetrapropoxide, zirconium carboxylates, such as zirconium diacetate; zirconium acetylacetonate chelates, such as zirconium tetra(acetylacetonate), tributoxyzirconium acetylacetonate, dibutoxyzirconium bisacetylacetonate, aluminium trisalkoxides, such as aluminium triisopropoxide, aluminium trisbutoxide; aluminium acetylacetonate chelates, such as aluminium tris(acetylacetonate) and aluminium tris(ethylacetylacetonate), organotin compounds such as dibutyltin dilaurate (DBTL), dibutyltin maleate, dibutyltin diacetate, tin(II) 2-ethylhexanoate (tin octoate), tin naphthenate, dimethyltin dineodecanoate, dioctyltin dineodecanoate, dimethyltin dioleate, dioctyltin dilaurate, dimethyl mercaptides, dibutyl mercaptides, dioctyl mercaptides, dibutyltin dithioglycolate, dioctyltin glycolate, dimethyltin glycolates, a solution of dibutyltin oxide, reaction products of zinc salts and organic carboxylic acids (carboxylates) such as zinc(II) 2-ethylhexanoate or zinc(II) neodecanoate, mixtures of bismuth carboxylates and zinc carboxylates, reaction products of bismuth salts and organic carboxylic acids, such as bismuth (III) tris(2-ethylhexanoate) and bismuth(III) tris(neodecanoate) and bismuth complexes, organolead compounds such as lead octoxide, organovanadium compounds, amine compounds such as butylamine, octylamine, dibutylamine, monoethanolamine, diethanolamine, triethanolamine, diethylenetriamine, oleylamine, cyclohexylamine, benzylamine, diethylaminopropylamine, xylylenediamine, triethylenediamine, guanidine, diphenylguanidine, 2,4,6-tris(dimethylaminomethyl)phenol, morpholine, N-methylmorpholine, 2-ethyl-4-methylimidazole and 1,8-diazabicyclo(5.4.0)undecene-7 (DBU), salts of these amines with carboxylic acids or other acids or mixtures thereof.

[0097] Catalyst B may preferably be selected from the group consisting of dibutyltin dilaurate (DBTL), tin(II) 2-ethylhexanoate (tin octoate), zinc(II) 2-ethylhexanoate, zinc(II) neodecanoate, bismuth(III) tris(2-ethylhexanoate), bismuth(III) tris(neodecanoate) or mixtures thereof.

[0098] Catalyst B is more preferably dibutyltin dilaurate (DBTL).

[0099] The catalysts are preferably present in a relative ratio between 1:10 and 10:1; catalysts A and B are further preferably present in a relative ratio between 1:8 and 8:1; catalysts A and B are especially preferably present in a relative ratio between 1:5 and 5:1; catalysts A and B are more especially preferably present in a relative ratio between 1:2 and 2:1, most preferably in a relative ratio of 0.9:1.1 to 1.1:0.9, based on percent by weight.

[0100] In a preferred composition according to the invention, the total amount of catalyst, composed of at least one catalyst A and one catalyst B, is between 5 and 30 000 ppm, further preferably between 15 and 20 000 ppm, more preferably between 20 and 15 000 ppm, most preferably between 20 and 10 000 ppm, based on the total weight of the composition.

[0101] "Polymers" are chemical compounds composed of chain or branched molecules (macromolecules) that in turn consist of a number of identical/equivalent or else different units, called the monomers. Polymers also include oligomers. Oligomers are polymers having a smaller number of units. Unless explicitly defined differently, oligomers are included in the concept of polymers in accordance with the invention. Polymers may occur as homopolymers (=consisting only of one monomer unit), copolymers (=consisting of two or more monomer units) or as a polymer mixture (=polymer alloy, polymer blends, i.e. mixtures of different polymers and copolymers).

[0102] In the context of the invention, "silylated polymers" are silane-modified, silane-functional or silane-terminated polymers that are also referred to interchangeably as SMP, STP or SiP. The definition includes polymers, polycondensates or polyadducts.

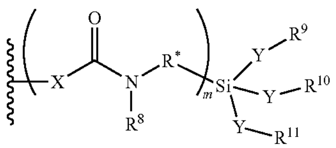
[0103] This also includes moisture-crosslinking polymers that can cure under the influence of water, either via addition or mixture constituents of or including water or by contacting with air humidity, preferably with additional use of a catalyst.

[0104] Silane-functional polymers are also referred to as hybrid polymers in general use and in accordance with the invention. These polymers can combine the curing chemistry of alkoxysilane groups with the chemistry of the polyols or polyurethanes. Alkoxysilane groups are known from silicone chemistry; the isocyanate-functional polymers, especially hydroxy-functional polymers, contribute at least parts of the polymer backbone of the hybrid polymer. Crosslinking ("curing") takes place via the reactive silane end groups through ingress of air humidity, for example. The curing mechanism of these systems is preferably neutral.

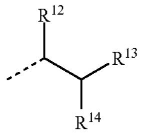
[0105] "Alkoxy" refers to an alkyl group joined via an oxygen atom to the main carbon chain or the main skeleton of the compound.

[0106] Silane-functional polymers (SiP) include a polymer backbone (P) and at least two end groups or functional groups or modifications of the following general formula (V)

(V)



(Vb)



[0107] where

[0108] X is C, Si or a heteroatom and these, according to their valency, optionally have one or more R^8 radicals, preferably C, N, O, P, S, more preferably C, N or O, most preferably N or O, and each is bonded to a carbon in the polymer backbone,

[0109] R* is 0 or an optionally substituted straight-chain or branched C1- to C25-alkyl group or an optionally substituted C4- to C18-cycloalkyl group or an optionally substituted C4- to C18-aryl group and, when R*=0, the silicon atom is bonded directly to the nitrogen atom,

[0110] each Y is independently either O or a direct bond of the silicon atom to the respective R^9, R^{10} or R^{11} radical, and preferably at least one Y is O,

[0111] R^8 is H, an optionally substituted straight-chain or branched C1- to C25-alkyl group, an optionally substituted straight-chain or branched C2- to C25-alkenyl group or an optionally substituted straight-chain or branched C2- to C18-alkynyl group, an optionally substituted C4- to C18-cycloalkyl group or an optionally substituted C4- to C18-aryl group, or a radical of the general structure (Vb),

[0112] R^{12} and R^{14} are each independently H or a radical from the group consisting of $—R^{15}$, $—COOR^{15}$ and —CN,

[0113] R^{13} is H or a radical from the group consisting of $—CH_2—COOR^{15}$, $—COOR^{15}$, $—CONHR^{15}$, $—CON(R^{15})$, —CN, $—NO_2$, $—PO(OR^{15})_2$, $—SOR^{15}$ and $—SO_2OR^{15}$,

[0114] R^{15} is a hydrocarbyl radical having 1 to 20 carbon atoms and optionally having at least one heteroatom,

[0115] R^9, R^{10} and R^{11} are independently H, an optionally substituted straight-chain or branched C1- to C20-alkyl group, an optionally substituted straight-chain or branched C2- to C20-alkenyl group or an optionally substituted C4- to C14-cycloalkyl group or an optionally substituted C4- to C14-aryl group, preferably at least R^9 is a C2-alkyl group, more preferably at least R^9 and R^{10} are a C2-alkyl group, and

[0116] m is 0 or 1 and, when m=0, the silicon atom is bonded directly to a carbon in the polymer backbone (P).

[0117] Unless stated otherwise, N especially denotes nitrogen. In addition, O especially denotes oxygen, unless stated otherwise. S especially denotes sulfur, unless stated otherwise. P especially denotes phosphorus, unless stated otherwise. C especially denotes carbon, unless stated otherwise.

H especially denotes hydrogen, unless stated otherwise. Si especially denotes silicon, unless stated otherwise.

[0118] "Optionally substituted" means that hydrogen atoms in the corresponding group or in the corresponding radical may be replaced by substituents. Substituents may especially be selected from the group consisting of C1- to C4-alkyl, methyl, ethyl, propyl, butyl, phenyl, benzyl, halogen, fluorine, chlorine, bromine, iodine, hydroxy, amino, alkylamino, dialkylamino, C1- to C4-alkoxy, phenoxy, benzyloxy, cyano, nitro, and thio. If a group is referred to as optionally substituted, it is possible for 0 to 50, especially 0 to 20, hydrogen atoms of the group to be replaced by substituents. If a group is substituted, at least one hydrogen atom is replaced by a substituent.

[0119] The term "alkyl group" means a saturated hydrocarbyl chain. Alkyl groups especially have the general formula $—C_nH_{2n+1}$. The term "C1- to C16-alkyl group" especially denotes a saturated hydrocarbyl chain having 1 to 16 carbon atoms in the chain. Examples of C1- to C16-alkyl groups are methyl, ethyl, propyl, butyl, isopropyl, isobutyl, sec-butyl, tert-butyl, n-pentyl and ethylhexyl. Correspondingly, a "C1- to C8-alkyl group" especially denotes a saturated hydrocarbyl chain having 1 to 8 carbon atoms in the chain. Alkyl groups may especially also be substituted even if this is not stated specifically.

[0120] "Straight-chain alkyl groups" denote alkyl groups containing no branches. Examples of straight-chain alkyl groups are methyl, ethyl, n-propyl, n-butyl, n-pentyl, n-hexyl, n-heptyl and n-octyl.

[0121] "Branched alkyl groups" denote alkyl groups that are not straight-chain, i.e. in which the hydrocarbyl chain especially has a fork. Examples of branched alkyl groups are isopropyl, isobutyl, sec-butyl, tert-butyl, sec-pentyl, 3-pentyl, 2-methylbutyl, isopentyl, 3-methylbut-2-yl, 2-methylbut-2-yl, neopentyl, ethylhexyl, and 2-ethylhexyl.

[0122] "Alkenyl groups" denote hydrocarbyl chains containing at least one double bond along the chain. For example, an alkenyl group having a double bond especially has the general formula —CnH2n−1. However, alkenyl groups may also have more than one double bond. The term "C2- to C16-alkenyl group" especially denotes a hydrocarbyl chain having 2 to 16 carbon atoms in the chain. The number of hydrogen atoms varies according to the number of double bonds in the alkenyl group. Examples of alkenyl groups are vinyl, allyl, 2-butenyl and 2-hexenyl.

[0123] "Straight-chain alkenyl groups" denote alkenyl groups containing no branches. Examples of straight-chain alkenyl groups are vinyl, allyl, n-2-butenyl and n-2-hexenyl.

[0124] "Branched alkenyl groups" denote alkenyl groups that are not straight-chain, i.e. in which the hydrocarbyl chain especially has a fork. Examples of branched alkenyl groups are 2-methyl-2-propenyl, 2-methyl-2-butenyl and 2-ethyl-2-pentenyl.

[0125] "Aryl groups" denote monocyclic (for example phenyl), bicyclic (for example indenyl, naphthalenyl, tetrahydronapthyl or tetrahydroindenyl) and tricyclic (for example fluorenyl, tetrahydrofluorenyl, anthracenyl or tetrahydroanthracenyl) ring systems in which the monocyclic ring system or at least one of the rings in a bicyclic or tricyclic ring system is aromatic. More particularly, a C4- to C14-aryl group denotes an aryl group having 4 to 14 carbon atoms. Aryl groups may especially also be substituted even if this is not stated specifically.

[0126] For example, it is possible to use silylated polymers that are moisture-curing in the compositions according to the invention, especially silylated polyethers and/or silylated polyurethane polymers (SPURs). Silylated polymers or silane-terminated polymers that may be used in the composition according to the invention include at least two or more reactive silane groups, for example alkoxysilanes.

[0127] One example of possible silylated polymers usable in accordance with the invention is that of oxyalkylene polymers having at least one reactive silane group at each end of the polymer molecule. The backbone of the silane-terminated oxyalkylene polymer according to the invention has repeating units of the general formula (1):

$$—R—O— \tag{1}$$

[0128] where R is a divalent organic group, preferably a straight or branched alkylene group including 1 to 14 carbon atoms, more preferably a straight or branched alkylene group including 2 to 4 carbon atoms, or mixtures thereof. Most preferably polypropylene oxide backbones, polyethylene oxide backbones and copolyethylene oxide/copolypropylene oxide backbones are or mixtures thereof. Other repeating units may include, but are not limited to, the following units:

[0129] $—CH_2—O—$, $—CH_2CH(CH_3)O—$, $—CH_2CH(C_2H_5)O—$, $—CH_2C(CH_3)O—$, $—CH_2CH_2CH_2CH_2O—$ and others of similar structure.

[0130] The reactive silane groups in the silylated polymers (SiP) may be described by the following formula (2):

$$—Si(R^2)_{3-a}(G)_a \tag{2}$$

[0131] where each R^2 is independently a C1- to C20-alkyl group, a C6- to C20-aryl group, a C7- to C20-aralkyl group or a mixture thereof,

[0132] G may represent a hydrolysable group or a hydroxyl group, and when two or more G are present, these may be the same or different, and

[0133] a is an integer from 1 to 3.

[0134] In a reactive silane group described by the formula (2), at least one hydrolysable or hydroxy group is represented by G.

[0135] According to the invention, "hydrolysable groups" are those that can enter into hydrolysis reactions through the influence of water, for example from air humidity or through the addition of water or aqueous constituents, and can form silanols as a result thereof. Hydrolysable groups may, for example, be alkoxy groups, and less commonly also —Cl. In a similar manner, these groups (or the silanols formed thereby) may react with OH or COOH groups on surfaces and form a composite.

[0136] In the context of the invention, "silanols" are organic silicon compounds in which at least one hydroxyl group (OH) is bonded to the silicon atom (—Si—OH).

[0137] In the context of the invention, "silanolates" are organic silicon compounds in which at least one deprotonated hydroxy function (R—O—) is bonded to the silicon atom (—Si—O—), where this negatively charged oxygen atom may also be chemically covalently bonded and/or coordinated to further compounds, for example metals.

[0138] According to the invention, isocyanate-reactive compounds are those that can react with an isocyanate. These compounds may have one or more NH, OH or SH functions.

[0139] The isocyanate-reactive compounds especially include the class of the hydroxy-functional compounds.

Polyols are hydroxy-functional compounds, especially hydroxy-functional polymers. Suitable polyols for the preparation of polyurethane polymers are especially polyether polyols, polyester polyols and polycarbonate polyols, and mixtures of these polyols.

[0140] "Polyethers" are a class of polymers. They are long-chain compounds comprising at least two identical or different ether groups. According to the invention, polyethers also include those where the polymeric ether groups are interrupted by another group (for example by copolymerized/incorporated isocyanates or further polymer or oligomer units of a different monomer origin).

[0141] Suitable polyether polyols, also called polyoxyalkylene polyols or oligoetherols, are especially those that are polymerization products of ethylene oxide, 1,2-propylene oxide, 1,2- or 2,3-butylene oxide, oxetane, tetrahydrofuran or mixtures thereof, optionally polymerized with the aid of a starter molecule having two or more active hydrogen atoms, for example water, ammonia or compounds having multiple OH or NH groups, for example ethane-1,2-diol, propane-1,2- or -1,3-diol, neopentyl glycol, diethylene glycol, triethylene glycol, the isomeric dipropylene glycols and tripropylene glycols, the isomeric butanediols, pentanediols, hexanediols, heptanediols, octanediols, nonanediols, decanediols, undecanediols, cyclohexane-1,3- and -1,4-dimethanol, bisphenol A, hydrogenated bisphenol A, 1,1,1-trimethylolethane, 1,1,1-trimethylolpropane, glycerol, aniline, and mixtures of the compounds mentioned.

[0142] It is possible to use either polyoxyalkylene polyols having a low degree of unsaturation (measured in accordance with ASTM D-2849-69 and expressed in milliequivalents of unsaturation per gram of polyol (meq/g)), produced for example using so-called double metal cyanide complex catalysts (DMC catalysts), or polyoxyalkylene polyols having a relatively high degree of unsaturation, produced for example using anionic catalysts such as NaOH, KOH, CsOH or alkali metal alkoxides. Polyoxyethylene polyols and polyoxypropylene polyols are particularly suitable, especially polyoxyethylene diols, polyoxypropylene diols, polyoxyethylene triols, and polyoxypropylene triols.

[0143] Especially suitable are polyoxyalkylene diols or polyoxyalkylene triols having a degree of unsaturation lower than 0.02 meq/g and having a molecular weight within a range from 1000 g/mol to 30 000 g/mol, as are polyoxyethylene diols, polyoxyethylene triols, polyoxypropylene diols, and polyoxypropylene triols having a molecular weight of 200 to 20 000 g/mol. Likewise particularly suitable are so-called ethylene oxide-terminated ("EO-endcapped", ethylene oxide-endcapped) polyoxypropylene polyols. The latter are special polyoxypropylene polyoxyethylene polyols that are obtained for example when pure polyoxypropylene polyols, in particular polyoxypropylene diols and triols, are at the end of the polypropoxylation reaction further alkoxylated with ethylene oxide and thus have primary hydroxyl groups. Preference in this case is given to polyoxypropylene polyoxyethylene diols and polyoxypropylene polyoxyethylene triols. Also suitable are hydroxyl-terminated polybutadiene polyols, for example those produced by polymerization of 1,3-butadiene and allyl alcohol or by oxidation of polybutadiene and also the hydrogenation products thereof. Also suitable are styrene-acrylonitrile grafted polyether polyols such as those commercially available for example under the trade name Lupranol® from Elastogran GmbH, Germany.

[0144] Suitable polyester polyols include in particular polyesters that bear at least two hydroxyl groups and are produced by known processes, in particular polycondensation of hydroxycarboxylic acids or polycondensation of aliphatic and/or aromatic polycarboxylic acids with dihydric or polyhydric alcohols.

[0145] Especially suitable are polyester polyols produced from dihydric to trihydric alcohols such as ethane-1,2-diol, diethylene glycol, propane-1,2-diol, dipropylene glycol, butane-1,4-diol, pentane-1,5-diol, hexane-1,6-diol, neopentyl glycol, glycerol, 1,1,1-trimethylolpropane or mixtures of the abovementioned alcohols with organic dicarboxylic acids or the anhydrides or esters thereof, for example succinic acid, glutaric acid, adipic acid, trimethyladipic acid, suberic acid, azelaic acid, sebacic acid, dodecanedicarboxylic acid, maleic acid, fumaric acid, dimer fatty acid, phthalic acid, phthalic anhydride, isophthalic acid, terephthalic acid, dimethyl terephthalate, hexahydrophthalic acid, trimellitic acid and trimellitic anhydride or mixtures of the abovementioned acids, as are polyester polyols formed from lactones such as ε-caprolactone. Particularly suitable are polyester diols, in particular those produced from adipic acid, azelaic acid, sebacic acid, dodecanedicarboxylic acid, dimer fatty acid, phthalic acid, isophthalic acid and terephthalic acid as the dicarboxylic acid or from lactones such as ε-caprolactone and from ethylene glycol, diethylene glycol, neopentyl glycol, butane-1,4-diol, hexane-1,6-diol, dimer fatty acid diol, and cyclohexane-1,4-dimethanol as the dihydric alcohol.

[0146] Suitable polycarbonate polyols include in particular those obtainable by reaction for example of the abovementioned alcohols used to form the polyester polyols with dialkyl carbonates such as dimethyl carbonate, diaryl carbonates such as diphenyl carbonate, or phosgene. Polycarbonate diols, in particular amorphous polycarbonate diols, are particularly suitable. In addition, polycarbonate diols or polyether polycarbonate diols may be obtainable via polymerization of propylene oxide with CO_2.

[0147] Further suitable polyols are poly(meth)acrylate polyols.

[0148] Also suitable are polyhydroxy-functional fats and oils, for example natural fats and oils, in particular castor oil, or so-called oleochemical polyols obtained by chemical modification of natural fats and oils, the epoxy polyesters or epoxy polyethers obtained for example by epoxidation of unsaturated oils and subsequent ring opening with carboxylic acids or alcohols respectively, or polyols obtained by hydroformylation and hydrogenation of unsaturated oils. Also suitable are polyols obtained from natural fats and oils by degradation processes such as alcoholysis or ozonolysis and subsequent chemical linking, for example by transesterification or dimerization, of the thus obtained degradation products or derivatives thereof. Suitable breakdown products of natural fats and oils are in particular fatty acids and fatty alcohols and also fatty acid esters, in particular the methyl esters (FAME), which can be derivatized to hydroxy fatty acid esters, for example by hydroformylation and hydrogenation.

[0149] Likewise suitable are, in addition, polyhydrocarbon polyols, also referred to as oligohydrocarbonols, for example polyhydroxy-functional ethylene-propylene, ethylene-butylene or ethylene-propylene-diene copolymers, for example those produced by Kraton Polymers, USA, or polyhydroxy-functional copolymers of dienes, such as 1,3-

butadiene or diene mixtures, and vinyl monomers such as styrene, acrylonitrile or isobutylene, or polyhydroxy-functional polybutadiene polyols, for example those which are produced by copolymerization of 1,3-butadiene and allyl alcohol and which may also be hydrogenated. Also suitable are polyhydroxy-functional acrylonitrile/butadiene copolymers, such as those that can be produced for example from epoxides or amino alcohols and carboxyl-terminated acrylonitrile/butadiene copolymers that are commercially available under the Hypro® CTBN name from Emerald Performance Materials, LLC, USA.

[0150] These likewise particularly preferred polyols have an average molecular weight of 250 to 40 000 g/mol, especially of 1000 to 30 000 g/mol, and an average OH functionality in the range from 1.6 to 3.

[0151] Particularly suitable polyols are polyester polyols and polyether polyols, in particular polyoxyethylene polyol, polyoxypropylene polyol, and polyoxypropylene polyoxyethylene polyol, preferably polyoxyethylene diol, polyoxypropylene diol, polyoxyethylene triol, polyoxypropylene triol, polyoxypropylene polyoxyethylene diol, and polyoxypropylene polyoxyethylene triol.

[0152] In addition to these polyols mentioned, it is also possible to use small amounts of low molecular weight di- or polyhydric alcohols, for example ethane-1,2-diol, propane-1,2- and -1,3-diol, neopentyl glycol, diethylene glycol, triethylene glycol, the isomeric dipropylene glycols and tripropylene glycols, the isomeric butanediols, pentanediols, hexanediols, heptanediols, octanediols, nonanediols, decanediols, undecanediols, cyclohexane-1,3- and -1,4-dimethanol, hydrogenated bisphenol A, dimeric fatty alcohols, 1,1,1-trimethylolethane, 1,1,1-trimethylolpropane, glycerol, pentaerythritol, sugar alcohols such as xylitol, sorbitol or mannitol, sugars such as sucrose, other higher polyhydric alcohols, low molecular weight alkoxylation products of the aforementioned di- and polyhydric alcohols, and mixtures of the aforementioned alcohols in the preparation of the polymer having terminal isocyanate groups (for example in the AmSi route).

[0153] Isocyanate-containing compounds (Iso or Iso-Si) have at least one NCO group (=isocyanate group). A distinction may be made between the monoisocyanates (z=1) and the di- and polyisocyanates (z=2). The NCO groups may react, for example, with alcohols to give urethanes or with amines to give urea derivatives. The isocyanate-containing compounds of the invention may be described by the general formula (VI)

$$R^x\text{-}(\text{-N}{=}\text{C}{=}\text{O})_z \quad \text{(VI)}$$

[0154] where

[0155] R^x is a carbon-containing group, preferably at least one aromatic or aliphatic group or mixtures thereof, more preferably an optionally substituted straight-chain or branched C1- to C20-alkyl group, an optionally substituted straight-chain or branched C2- to C20-alkenyl group or an optionally substituted straight-chain or branched C2- to C20-alkynyl group, an optionally substituted C4- to C14-cycloalkyl group or an optionally substituted C4- to C14-aryl group, most preferably diphenylmethane, toluene, dicyclohexylmethane, hexane or methyl-3,5,5-trimethylcyclohexyl or

[0156] R^x is a —(R*)—Si($YR^{9/10/11}$)$_3$ group where R^9, R^{10} and R^{11} are independently H, an optionally substituted straight-chain or branched C1- to C25-alkyl group, an optionally substituted straight-chain or branched C2- to C25-alkenyl group or an optionally substituted C4- to C18-cycloalkyl group or an optionally substituted C4- to C18-aryl group,

[0157] R* is 0 or an optionally substituted straight-chain or branched C1- to C25-alkyl group or an optionally substituted C4- to C18-cycloalkyl group or an optionally substituted C4- to C18-aryl group and, when R*=0, the silicon atom is bonded directly to the nitrogen atom,

[0158] each Y is independently either O or a direct bond of the silicon atom to the respective R^9, R^{10} or R^{11} radical, and preferably at least one Y is O, and

[0159] z is at least 1, preferably at least 1 or 2, more preferably 1 or 2.

[0160] According to the invention, it is possible to prepare silylated polymers (SiP) by two routes by a metal-siloxane-silanol(ate) compound-catalysed synthesis of at least one isocyanate-reactive compound, especially a hydroxy-functionalized polymer, and a compound having at least one isocyanate group.

[0161] In one route according to the invention, the synthesis is effected via a metal-siloxane-silanol(ate) compound-catalysed synthesis of an isocyanate-reactive compound, especially a hydroxy-functionalized polymer, and a di- or polyisocyanate compound (Iso). Subsequently, the resultant isocyanate group-containing prepolymer is reacted with an aminosilane (AmSi) to give the silylated polymer (SiP) according to the invention. This synthesis route is referred to in accordance with the invention as the “AmSi route”.

[0162] Di- or polyisocyanates (Iso) used for the preparation of the polymer of the invention may be conventional isocyanates, especially di- or polyisocyanates of the general formula (VI)

$$R^x\text{-}(\text{-N}{=}\text{C}{=}\text{O})_z \quad \text{(VI)}$$

[0163] where

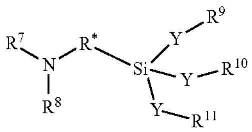
[0164] R^x is a carbon-containing group, preferably at least one aromatic or aliphatic group or mixtures thereof, more preferably an optionally substituted straight-chain or branched C1- to C20-alkyl group, an optionally substituted straight-chain or branched C2- to C20-alkenyl group or an optionally substituted straight-chain or branched C2- to C20-alkynyl group, an optionally substituted C4- to C14-cycloalkyl group or an optionally substituted C4- to C14-aryl group, most preferably diphenylmethane, toluene, dicyclohexylmethane, hexane or methyl-3,5,5-trimethylcyclohexyl and

[0165] z is at least 2, preferably 2 or >2.

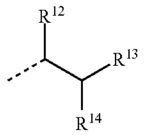
[0166] For example, suitable diisocyanates are hexamethylene 1,6-diisocyanate (HDI) or the trimer thereof (HDI trimer), methylene diphenyl isocyanate (MDI), especially 4,4'-methylene diphenyl isocyanate (4,4'-MDI), 2,4'-methylene diphenyl isocyanate (2,4'-MDI), 2,2'-methylene diphenyl isocyanate (2,2'-MDI), 4,4'-diisocyanatodicyclohexylmethane (H12MDI), 2-methylpentamethylene 1,5-diisocyanate, 2,2,4- and 2,4,4-trimethylhexamethylene 1,6-diisocyanate (TMDI), dodecamethylene 1,12-diisocyanate, lysine and lysine ester diisocyanate, cyclohexane 1,3-diisocyanate, cyclohexane 1,4-diisocyanate, 3-isocyanatomethyl-3,5,5-trimethylcyclohexyl isocyanate (=isophorone diisocyanate or IPDI), perhydro(diphenylmethane 2,4'-diisocyanate) and perhydro(diphenylmethane 4,4'-diisocyanate), 1,4-diisocyanato-2,2,6-trimethylcyclohexane (TMCDI), 2,2,4- and/or 2,4,4-trimethylhexamethylene 1,6-diisocyanate, 1,4-bis(isocyanato)cyclohexane, 1,4-bis(isocyanato)benzene (PPDI), 1,3- and/or 1,4-bis(isocyanatomethyl)cyclohexane, m- and/or p-xylylene diisocyanate (m- and/or p-XDI), m- and/or p-tetramethylxylylene 1,3-diisocyanate, m- and/or p-tetramethylxylylene 1,4-diisocyanate, bis(1-isocyanato-1-methylethyl)naphthalene, tolylene 2,4- and 2,6-diisocyanate (TDI), diphenylmethane 4,4'-, 2,4'- and 2,2'-diisocyanate (MDI), phenylene 1,3- and 1,4-diisocyanate, 1,3-bis(isocyanato-4-methylphenyl)-2,4-dioxo-1,3,5, 6-tetramethyl-1,4-diisocyanatobenzene, diazetidine, naphthalene 1,5-diisocyanate (NDI), 3,3'-dimethyl-4,4'-diisocyanatodiphenyl (TODD, 1,3-bis(isocyanatomethyl) benzene or mixtures thereof, preferably 4,4'-methylene diphenyl isocyanate (4,4'-MDI) or isophorone diisocyanate (IPDI), hexamethylene 1,6-diisocyanate (HDI) or the trimer thereof (HDI trimer) or mixtures thereof, most preferably 4,4'-methylene diphenyl isocyanate (4,4'-MDI) or isophorone diisocyanate (IPDI), oligomers and polymers of the aforementioned isocyanates, and any mixtures of the aforementioned isocyanates.

[0167] The subsequent reaction with an aminosilane (AmSi) of the formula (VIII) affords the silylated polymer (SiP)

(VIII)



(Vb)



[0168] where

[0169] R^7 is H,

[0170] R^8 is H, an optionally substituted straight-chain or branched C1- to C25-alkyl group, an optionally substituted straight-chain or branched C2- to C25-alkenyl group or an optionally substituted C4- to C18-cycloalkyl group or an optionally substituted C4- to C18-aryl group, or a radical of the general structure (Vb),

[0171] R* is 0 or an optionally substituted straight-chain or branched C1- to C25-alkyl group or an optionally substituted C4- to C18-cycloalkyl group or an optionally substituted C4- to C18-aryl group and, when R*=0, the silicon atom is bonded directly to the nitrogen atom,

[0172] R^{12} and R^{14} are each independently H or a radical from the group consisting of $—R^{15}$, $—COOR^{15}$ and —CN,

[0173] R^{13} is H or a radical from the group consisting of $—CH_2—COOR^{15}$, $—COOR^{15}$, $—CONHR^{15}$, $—CON(R^{15})$, —CN, $—NO_2$, $—PO(OR^{15})_2$, $—SOR^{15}$ and $—SO_2OR^{15}$,

[0174] R^{15} is a hydrocarbyl radical having 1 to 20 carbon atoms and optionally having at least one heteroatom,

[0175] R^9, R^{10} and R^{11} are independently H, an optionally substituted straight-chain or branched C1- to C25-alkyl group, an optionally substituted straight-chain or branched C2- to C25-alkenyl group or an optionally substituted C4- to C18-cycloalkyl group or an optionally substituted C4- to C18-aryl group, preferably at least R^9 is a C2-alkyl group, more preferably R^9 and R^{10} are a C2-alkyl group, and

[0176] each Y is independently either O or a direct bond of the silicon atom to the respective R^9, R^{10} or R^{11} radical, and preferably at least one Y is O.

[0177] "Aminosilanes" refer to organosilanes wherein the organic radical has an amino group. "Primary aminosilanes" refer to aminosilanes having a primary amino group, i.e. an NH2 group bonded to one organic radical. "Secondary aminosilanes" refer to aminosilanes having a secondary amino group, i.e. an NH group bonded to two organic radicals.

[0178] The silylated polymer (SiP) according to the invention can be obtained by a second route. This second synthesis route is referred to in accordance with the invention as "Iso-Si route" or "isocyanate route".

[0179] The reaction of an isocyanatosilane (Iso-Si) of the formula (VI), preferably of the formula (VII), with a polymer having functional end groups reactive toward isocyanate groups, especially hydroxyl groups, mercapto groups and/or amino groups. This reaction can be effected in a stoichiometric ratio of the isocyanate groups to the functional end groups reactive toward isocyanate groups of 0.9:1.1 to 1.1:0.9, or with a slight excess of the functional end groups reactive toward isocyanate groups, for example at temperatures of 20° C. to 100° C., with additional use of at least one metal-siloxane-silanol(ate) compound as catalyst.

$$R^x\!\!\left(\!-N{=}C{=}O\right)_z \qquad \text{(VI)}$$

[0180] where

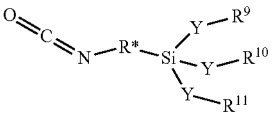
[0181] R^x is a $—(R^*)—Si(YR^{9/10/11})_3$ group where R^9, R^{10} and R^{11} are independently H, an optionally substituted straight-chain or branched C1- to C25-alkyl group, an optionally substituted straight-chain or branched C2- to C25-alkenyl group or an optionally substituted C4- to C18-cycloalkyl group or an optionally substituted C4- to C18-aryl group,

[0182] R* is 0 or an optionally substituted straight-chain or branched C1- to C25-alkyl group or an optionally substituted C4- to C18-cycloalkyl group or an optionally substituted C4- to C18-aryl group and, when R*=0, the silicon atom is bonded directly to the nitrogen atom,

[0183] each Y is independently either O or a direct bond of the silicon atom to the respective R^9, R^{10} or R^{11} radical, and preferably at least one Y is O, and

[0184] z is at least 1, preferably 1.

[0185] For the purposes of the invention, the isocyanatosilane (Iso-Si) is preferably selected from the group consisting of the following compounds of the general formula (VII):



(VII)

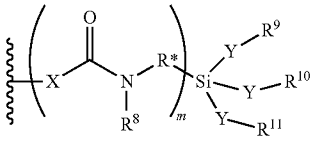
[0186] where

[0187] each Y is independently either O or a direct bond of the silicon atom to the respective R^9, R^{10} or R^{11} radical, and preferably at least one Y is O,

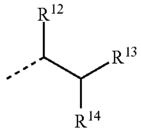
[0188] R^9, R^{10} and R^{11} are independently H, an optionally substituted straight-chain or branched C1- to C20-alkyl group, an optionally substituted straight-chain or branched C2- to C20-alkenyl group or an optionally substituted C4- to C14-cycloalkyl group or an optionally substituted C4- to C14-aryl group, preferably at least R^9 is a C2-alkyl group, more preferably R^9 and R^{10} are a C2-alkyl group, and

[0189] R* is 0 or an optionally substituted straight-chain or branched C1- to C25-alkyl group or an optionally substituted C4- to C18-cycloalkyl group or an optionally substituted C4- to C18-aryl group and, when R*=0, the silicon atom is bonded directly to the nitrogen atom.

[0190] End groups according to the invention in the silylated polymer (SiP) may be described by the general formula (V)



(V)



(Vb)

[0191] where

[0192] X is C, Si or a heteroatom and these, according to their valency, optionally have one or more R^9 radicals, preferably C, N, O, P, S, more preferably C, N or O, most preferably N or O, and is bonded to a carbon in the polymer backbone,

[0193] R* is 0 or an optionally substituted straight-chain or branched C1- to C25-alkyl group or an optionally substituted C4- to C18-cycloalkyl group or an optionally substituted C4- to C18-aryl group, preferably an optionally substituted straight-chain or branched C1- to C15-alkyl group, and, when R*=0, the silicon atom is bonded directly to the nitrogen atom,

[0194] each Y is independently either O or a direct bond of the silicon atom to the respective R^9, R^{10} or R^{11} radical, and preferably at least one Y is O,

[0195] R^9 is H, an optionally substituted straight-chain or branched C1- to C25-alkyl group, an optionally substituted straight-chain or branched C2- to C25-alkenyl group or an optionally substituted straight-chain or branched C2- to C18-alkynyl group, an optionally substituted C4- to C18-cycloalkyl group or an optionally substituted C4- to C18-aryl group, or a radical of the general structure (Vb),

[0196] R^{12} and R^{14} are each independently H or a radical from the group consisting of —R^{15}, —$COOR^{15}$ and —CN,

[0197] R^{13} is H or a radical from the group consisting of —CH_2—$COOR^{15}$, —$COOR^{15}$, —$CONHR^{15}$, —CON(R^{15}), —CN, —NO_2, —$PO(OR^{15})_2$, —SOR^{15} and —SO_2OR^{15},

[0198] R^{15} is a hydrocarbyl radical having 1 to 20 carbon atoms and optionally having at least one heteroatom,

[0199] R^9, R^{10} and R^{11} are independently H or C1- or C2-alkyl group, preferably at least R^9 is a C2-alkyl group, more preferably R^9 and R^{10} are a C2-alkyl group, and

[0200] m is 0 or 1 and, when m=0, the silicon atom is bonded directly to a carbon in the polymer backbone (P).

[0201] In a preferred embodiment, the composition of the invention comprises two catalysts A and B, where A is heptaisobutyl POSS-titanium(IV) ethoxide (TiPOSS) or heptaisobutyl POSS-tin(IV) ethoxide (SnPOSS) and B is dibutyltin laurate (DBTL) or heptaisobutyl POSS-tin(IV) ethoxide (SnPOSS) when A is not heptaisobutyl POSS-tin (IV) ethoxide (SnPOSS).

[0202] In a particularly preferred embodiment, the silylated polymer (SiP) is prepared by a synthesis of at least one isocyanate-reactive compound (component A) selected from the group of compounds having NH, OH or SH functions, and one or more compounds having at least one isocyanate group, selected from the group of isocyanates (Iso) and/or isocyanatosilanes (Iso-Si), catalysed by at least one mononuclear metal-siloxane-silanol(ate) compound.

[0203] In a further preferred embodiment, the silylated polymer (SiP) is prepared by a synthesis of at least one hydroxy-functionalized polymer (component A) selected from the group of polypropylene diols, polyester polyols, or mixtures thereof, and one or more compounds having at least one isocyanate group, selected from the group of 4,4'-methylene diphenyl isocyanate (4,4'-MDI), isophorone diisocyanate (IPDI) or mixtures thereof and/or 3-(triethoxysilyl)methyl isocyanate, 3-(triethoxysilyl)propyl isocyanate, or mixtures thereof, catalysed by at least one mononuclear single-cage metal-siloxane-silanol(ate) compound.

[0204] In a further preferred embodiment, the silylated polymer (SiP) is prepared by a synthesis of at least one hydroxy-functionalized polymer (component A) selected from the group of polypropylene diols, polyester polyols, or mixtures thereof, and one or more compounds having at least one isocyanate group, selected from the group of 4,4'-methylene diphenyl isocyanate (4,4'-MDI), isophorone diisocyanate (IPDI) or mixtures thereof and/or 3-(triethoxysilyl)methyl isocyanate, 3-(triethoxysilyl)propyl isocyanate, or mixtures thereof, catalysed by at least one mononuclear titanium-siloxane-silanol(ate) compound, especially by heptaisobutyl POSS-titanium(IV) ethoxide (TiPOSS).

[0205] In a further alternative embodiment of all the above combinations, the silylated polymer (SiP) is prepared by reaction with an aminosilane (AmSi) selected from the group of N-[3-(triethoxysilyl)methyl]butylamine, N-[3-(triethoxysilyl)propyl]butylamine, N-(3-triethoxysilylpropyl) aminosuccinic acid diethyl ester or a mixture thereof.

[0206] In a very particularly preferred embodiment, the silylated polymer (SiP) of the composition according to the invention is prepared by a heptaisobutyl POSS-titanium(IV) ethoxide (TiPOSS)-catalysed synthesis of a component A selected from the group of polypropylene diols, polyester polyols, or mixtures thereof, with a component B selected from the group of 3-(triethoxysilyl)methyl isocyanate, 3-(triethoxysilyl)propyl isocyanate or mixtures thereof.

[0207] In a further very particularly preferred embodiment, the silylated polymer (SiP) of the composition according to the invention is prepared by a heptaisobutyl POSS-titanium(IV) ethoxide (TiPOSS)-catalysed synthesis of a component A selected from the group of polypropylene diols, polyester polyols, or mixtures thereof, with a component B selected from the group of 4,4'-methylene diphenyl isocyanate (4,4'-MDI), isophorone diisocyanate (IPDI) or mixtures thereof, followed by silanization with an aminosilane selected from the group of N-[3-(triethoxysilyl)methyl] butylamine, N-[3-(triethoxysilyl)propyl]butylamine, N-(3-triethoxysilylpropyl)aminosuccinic acid diethyl ester or a mixture thereof.

[0208] In the most preferred embodiment, all the above combinations include heptaisobutyl POSS-titanium(IV) ethoxide (TiPOSS) as catalyst in the synthesis of the silylated polymer (SiP). In an alternative embodiment, all the above combinations in the embodiments, rather than heptaisobutyl POSS-titanium(IV) ethoxide (TiPOSS) in the synthesis of the silylated polymer (SiP), include heptaisobutyl POSS-tin(IV) ethoxide (SnPOSS) or a mixture of the two catalysts. In what is, however, the most preferred embodiment, heptaisobutyl POSS-titanium(IV) ethoxide (TiPOSS) only is present as catalyst in the synthesis of the silylated polymer (SiP).

[0209] The composition of the invention in all the above combinations, in a preferred embodiment, includes a further catalyst selected from metal-siloxane-silanol(ate) compounds, especially heptaisobutyl POSS-titanium(IV) ethoxide (TiPOSS) or heptaisobutyl POSS-tin(IV) ethoxide (SnPOSS), dibutyltin dilaurate (DBTL) or mixtures thereof.

[0210] In a particularly preferred embodiment, all the above combinations of the composition of the invention include dibutyltin dilaurate (DBTL) as second catalyst.

[0211] In a further-preferred embodiment, this comprises additives from the group comprising one or more fillers selected from the group of inorganic and organic fillers, especially natural, ground or precipitated calcium carbonates optionally coated with fatty acids, especially stearic acid, barite (heavy spar), talcs, quartz flours, quartz sand, dolomites, wollastonites, kaolins, calcined kaolins, mica (potassium aluminium silicate), molecular sieves, aluminium oxides, aluminium hydroxides, magnesium hydroxide, silicas including finely divided silicas from pyrolysis processes, industrially produced carbon blacks, graphite, metal powders such as aluminium, copper, iron, silver or steel, PVC powders or hollow beads, one or more adhesion promoters from the group of the silanes, especially aminosilanes such as 3-aminopropyltrimethoxysilane, 3-aminopropyldimethoxymethylsilane, N-(2-aminoethyl)-3-aminopropyltrimethoxysilane, N-(2-aminoethyl)-3-aminopropylmethyldimethoxysilane, N-(2-aminoethyl)-N'-[3-(trimethoxysilyl)propyl]ethylenediamine and analogues thereof having ethoxy or isopropoxy in place of the methoxy groups on the silicon, aminosilanes having secondary amino groups, such as, in particular, N-phenyl-, N-cyclohexyl- and N-alkylaminosilanes, and also mercaptosilanes, epoxysilanes, (meth)acryloylsilanes, anhydridosilanes, carbamatosilanes, alkylsilanes and iminosilanes, and oligomeric forms of these silanes, and adducts of primary aminosilanes with epoxysilanes or (meth)acryloylsilanes or anhydridosilanes. Especially suitable are 3-glycidoxypropyltrimethoxysilane, 3-aminopropyltrimethoxysilane, N-(2-aminoethyl)-3-aminopropyltrimethoxysilane, N-(2-aminoethyl)-N'-[3-(trimethoxysilyl)propyl]ethylenediamine, 3-mercaptopropyltrimethoxysilane, 3-ureidopropyltrimethoxysilane and the corresponding silanes having ethoxy groups in place of the methoxy groups, and oligomeric forms of these silanes, one or more moisture scavengers from the group of silanes, especially tetraethoxysilane, vinyltrimethoxy- or vinyltriethoxysilane or organoalkoxysilanes having a functional group in the a position to the silane group, especially N-(methyldimethoxysilylmethyl)-O-methyl carbamate, (methacryloyloxymethyl)silanes, methoxymethylsilanes, orthoformic esters, and calcium oxide or molecular sieves, one or more plasticizers from the group of carboxylic esters, such as phthalates, especially diisononyl cyclohexane-1,2-dicarboxylate, dioctyl phthalate, diisononyl phthalate or diisodecyl phthalate, adipates, especially dioctyl adipate, azelates, sebacates, polyols, especially polyoxyalkylene polyols or polyester polyols, glycol ethers, glycol esters, citrates, especially triethyl citrate, organic phosphoric and sulfonic esters, polybutenes, or fatty acid methyl or ethyl esters derived from natural fats or oils, one or more UV stabilizers from the group of organic (benzophenones, benzotriazoles, oxalanilides, phenyltriazines) and inorganic (titanium dioxide, iron oxide, zinc oxide) UV absorbers, and antioxidants from the group of sterically hindered phenols, amines, phosphites and phosphonites, one or more thixotropic agents from the group of sheet silicates such as bentonites, derivatives of castor oil, hydrogenated castor oil, polyamides, polyurethanes, urea compounds, fumed silicas, cellulose ethers or hydrophobically modified polyoxyethylenes, one or more wetting agents from the group of nonionic, anionic and cationic surfactants, or combinations of these.

[0212] In a further preferred embodiment, the composition of the invention additionally includes a water scavenger, preferably a vinylalkoxysilane, more preferably vinyltrimethoxysilane (VTMO). It is always possible here that the alkoxy substituents (e.g. methoxy or ethoxy) of the alkoxysilanes in the composition of at least one silylated polymer (SiP) can undergo mutual exchange with at least one water scavenger.

[0213] A preferred process for producing the composition comprises the following steps:

[0214] (i) synthesizing a polymer or silylated polymer (SiP) at a temperature of <80° C., preferably at <60° C., especially preferably at room temperature, by combining at least one hydroxy-functionalized polymer selected from the group consisting of polypropylene diols, polyester polyols, and mixtures thereof, preferably having number-average molar masses (Mn) of 500-35 000 g/mol, more preferably with about 2000 g/mol or about 19 000 g/mol or mixtures thereof with one or more isocyanates (Iso) selected from the group consisting of 4,4'-methylene diphenyl isocyanate (4,4'-MDI), isophorone diisocyanate (IPDI) or mixtures thereof and/or one or more isocyanatosilanes (Iso-Si) selected from the group consisting of 3-(triethoxysilyl) methyl isocyanate, 3-(triethoxysilyl)propyl isocyanate or mixtures thereof, using a metal-siloxane-silanol(ate) compound, especially heptaisobutyl POSS-titanium (IV) ethoxide (TiPOSS), heptaisobutyl POSS-tin(IV) ethoxide (SnPOSS) or mixtures thereof,

[0215] (ii) optionally reacting the polymer obtained from step (i) with an aminosilane (AmSi) selected from the group of N-[3-(triethoxysilyl)propyl]butylamine, N-[3-(triethoxysilyl)methyl]butylamine, N-(3-triethoxysilylpropyl)aminosuccinic acid diethyl ester or mixtures thereof to give the silylated polymer (SiP),

[0216] (iii) optionally admixing the silylated polymer (SiP) from step (i) or (ii) with a further catalyst selected from dibutyltin dilaurate (DBTL), heptaisobutyl POSS-titanium(IV) ethoxide (TiPOSS), heptaisobutyl POSS-tin(IV) ethoxide (SnPOSS) or mixtures thereof, preferably heptaisobutyl POSS-titanium(IV) ethoxide (TiPOSS).

[0217] In the inventive preparation of the silylated polymers (SiP), either the entirety of the isocyanate-containing compound (component B) or else the entirety of the isocyanate-reactive compound, especially the hydroxy-functionalized polymer (component A) is preferably first initially charged, then the respective other component A or B is added, followed by addition of at least one metal-siloxane-silanol(ate) compound, and the components are left to react with one another. The end product is optionally then prepared from the resulting intermediate by reaction with the aminosilane (AmSi). If one or more components are used in addition, these may in principle be added to the reaction mixture at any time.

[0218] The process according to the invention is preferably conducted at temperatures of at least 0° C., more preferably at least 20° C., and preferably at most 150° C., especially at most 80° C.

[0219] The process according to the invention is preferably conducted with exclusion of (air) humidity and at the pressure of the surrounding atmosphere, i.e. about 900 to 1100 hPa.

[0220] The process according to the invention can be effected continuously, for example in a tubular reactor or tube reactor having multiple metering sites in parallel or else in series, or batchwise, for example in a conventional reaction tank with stirrer system.

PARTICULARLY PREFERRED EMBODIMENTS OF THE INVENTION

[0221] 1. Composition comprising at least one silylated polymer (SiP) and at least two catalysts A and B, where catalyst A is selected from the group of the metal-siloxane-silanol(ate) compounds.

[0222] 2. Composition according to Embodiment 1, characterized in that catalyst A is selected from the group of the metal-siloxane-silanol(ate) compounds, preferably in that catalyst A is heptaisobutyl POSS-titanium(IV) ethoxide (TiPOSS), and catalyst B is likewise selected from the group of the metal-siloxane-silanol(ate) compounds.

[0223] 3. Composition according to Embodiment 1 or 2, characterized in that catalyst A is heptaisobutyl POSS-titanium(IV) ethoxide (TiPOSS) and catalyst B is heptaisobutyl POSS-tin(IV) ethoxide (SnPOSS).

[0224] 4. Composition according to Embodiment 1, characterized in that catalyst B is selected from a group of catalysts not including metal-siloxane-silanol(ate) compounds.

[0225] 5. Composition according to Embodiment 4, characterized in that catalyst B is selected from the group of organometallic compounds.

[0226] 6. Composition according to Embodiment 5, characterized in that catalyst B is selected from the group of organotin or organotitanium compounds.

[0227] 7. Composition according to any of Embodiments 4 to 6, characterized in that catalyst B is selected from the group consisting of tetraalkyl titanates, such as tetramethyl titanate, tetraethyl titanate, tetra-n-propyl titanate, tetraisopropyl titanate, tetra-n-butyl titanate, tetraisobutyl titanate, tetra-sec-butyl titanate, tetraoctyl titanate, tetra(2-ethylhexyl) titanate, dialkyl titanates ($(RO)_2TiO_2$ in which R is, for example, isopropyl, n-butyl, isobutyl), such as isopropyl n-butyl titanate; titanium acetylacetonate chelates, such as diisopropoxybis(acetylacetonate) titanate, diisopropoxybis(ethylacetylacetonate) titanate, di-n-butylbis(acetylacetonate) titanate, di-n-butylbis(ethylacetoacetate) titanate, triisopropoxidebis (acetylacetonate) titanate, zirconium tetraalkoxides, such as zirconium tetraethoxide, zirconium tetrabutoxide, zirconium tetrabutyrate, zirconium tetrapropoxide, zirconium carboxylates, such as zirconium diacetate; zirconium acetylacetonate chelates, such as zirconium tetra(acetylacetonate), tributoxyzirconium acetylacetonate, dibutoxyzirconium bisacetylacetonate, aluminium trisalkoxides, such as aluminium triisopropoxide, aluminium trisbutoxide; aluminium acetylacetonate chelates, such as aluminium tris(acetylacetonate) and aluminium tris(ethylacetylacetonate), organotin compounds such as dibutyltin dilaurate (DBTL), dibutyltin maleate, dibutyltin diacetate, tin(II) 2-ethylhexanoate (tin octoate), tin naphthenate, dimethyltin dineodecanoate, dioctyltin dineodecanoate, dimethyltin dioleate, dioctyltin dilaurate, dimethyl mercaptides, dibutyl mercaptides, dioctyl mercaptides, dibutyltin dithioglycolate, dioctyltin glycolate, dimethyltin glycolates, a solution of dibutyltin oxide, reaction products of zinc salts and organic carboxylic acids (carboxylates) such as zinc(II) 2-ethylhexanoate or zinc(II) neodecanoate, mixtures of bismuth carboxylates and zinc carboxylates, reaction products of bismuth salts and organic carboxylic acids, such as bismuth(III) tris(2-ethylhexanoate) and bismuth(III) tris (neodecanoate) and bismuth complexes, organolead compounds such as lead octoxide, organovanadium compounds, amine compounds such as butylamine, octylamine, dibutylamine, monoethanolamine, diethanolamine, triethanolamine, diethylenetriamine, oleylamine, cyclohexylamine, benzylamine, diethylaminopropylamine, xylylenediamine, triethylenediamine, guanidine, diphenylguanidine, 2,4,6-tris(dimethylaminomethyl)phenol, morpholine, N-methylmorpholine, 2-ethyl-4-methylimidazole and 1,8-diazabicyclo(5.4.0) undecene-7 (DBU), salts of these amines with carboxylic acids or other acids or mixtures thereof.

[0228] 8. Composition according to Embodiment 7, characterized in that catalyst B is selected from the group consisting of dibutyltin dilaurate (DBTL), tin(II)

2-ethylhexanoate (tin octoate), zinc(II) 2-ethylhexanoate, zinc(II) neodecanoate, bismuth(III) tris(2-ethylhexanoate), bismuth(III) tris(neodecanoate) or mixtures thereof.

[0229] 9. Composition according to Embodiment 7 or 8, characterized in that catalyst B is dibutyltin dilaurate (DBTL).

[0230] 10. Composition according to any of Embodiments 4 to 8, characterized in that catalyst A is selected from the group consisting of heptaisobutyl POSS-titanium(IV) ethoxide (TiPOSS) and heptaisobutyl POSS-tin(IV) ethoxide (SnPOSS), preferably in that the catalyst is heptaisobutyl POSS-titanium(IV) ethoxide (TiPOSS).

[0231] 11. Composition according to Embodiment 10, characterized in that it includes more than one catalyst A from the group of metal-siloxane-silanol(ate) compounds.

[0232] 12. Composition according to any of the preceding embodiments, characterized in that catalyst A is in the form of a monomer, oligomer and/or polymer, where the metal(s) are present terminally and/or within the chain.

[0233] 13. Composition according to Embodiment 12, characterized in that the metal-siloxane-silanol(ate) compound has the general formula $R^*_qSi_rO_sM_t$ where each R* is independently selected from the group consisting of optionally substituted C1- to C20-alkyl, optionally substituted C3- to C6-cycloalkyl, optionally substituted C2- to C20-alkenyl, optionally substituted C6- to C10-aryl, —OH and —O—(C1- to C10-alkyl), each M is independently selected from the group consisting of s- and p-block metals, d- and f-block transition metals, lanthanide and actinide metals and semimetals, especially from the group consisting of metals of transition groups 1, 2, 3, 4, 5, 8, 10 and 11 and metals of main groups 1, 2, 3, 4 and 5, preferably from the group consisting of Na, Zn, Sc, Nd, Ti, Zr, Hf, V, Fe, Pt, Cu, Ga, Sn and Bi; especially preferably from the group consisting of Zn, Ti, Zr, Hf, V, Fe, Sn and Bi,

[0234] q is an integer from 4 to 19,

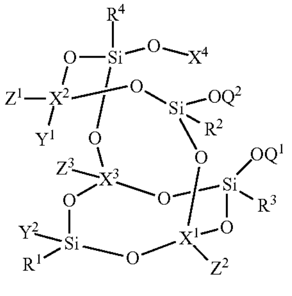
[0235] r is an integer from 4 to 10,

[0236] s is an integer from 8 to 30, and

[0237] t is an integer from 1 to 8.

[0238] 14. Composition according to any of the preceding embodiments, characterized in that the metal-siloxane-silanol(ate) compound has a general structure (I)

(I)



where

[0239] X^1, X^2 and X^3 are independently selected from Si and M^1, where M^1 is selected from the group consisting of s- and p-block metals, d- and f-block transition metals, lanthanide and actinide metals and semimetals,

[0240] especially from the group consisting of metals of transition groups 1, 2, 3, 4, 5, 8, 10 and 11 and metals of main groups 1, 2, 3, 4 and 5, preferably from the group consisting of Na, Zn, Sc, Nd, Ti, Zr, Hf, V, Fe, Pt, Cu, Ga, Sn and Bi; especially preferably from the group consisting of Zn, Ti, Zr, Hf, V, Fe, Sn and Bi,

[0241] Z^1, Z^2 and Z^3 are independently selected from the group consisting of L^2, R^5, R^6 and R^7, where L^2 is selected from the group consisting of —OH and —O—(C1-to C10-alkyl), especially —O—(C1- to C8-alkyl) or —O—(C1- to C6-alkyl), or where L^2 is selected from the group consisting of —OH, —O-methyl, —O-ethyl, —O-propyl, —O-butyl, —O-octyl, —O-isopropyl, and —O-isobutyl;

[0242] R^1, R^2, R^3, R^4, R^5, R^6 and R^7 are independently selected from the group consisting of optionally substituted C1- to C20-alkyl, optionally substituted C3- to C8-cycloalkyl, optionally substituted C2- to C20-alkenyl and optionally substituted C5- to C10-aryl;

[0243] Y^1 and Y^2 are independently —O-M^2-L^3_{Δ}, or Y^1 and Y^2 are associated and together are —O-M^2(L^3_{Δ})-O— or —O—, where L^3 is selected from the group consisting of —OH and —O—(C1- to C10-alkyl), especially —O—(C1- to C8-alkyl) or —O—(C1- to C6-alkyl), or where L^3 is selected from the group consisting of —OH, —O-methyl, —O-ethyl, —O-propyl, —O-butyl, —O-octyl, —O-isopropyl, and —O-isobutyl, and where M^2 is selected from the group consisting of s- and p-block metals, d- and f-block transition metals, lanthanide and actinide metals and semimetals,

[0244] especially from the group consisting of metals of transition groups 1, 2, 3, 4, 5, 8, 10 and 11 and metals of main groups 1, 2, 3, 4 and 5, preferably from the group consisting of Na, Zn, Sc, Nd, Ti, Zr, Hf, V, Fe, Pt, Cu, Ga, Sn and Bi; especially preferably from the group consisting of Zn, Ti, Zr, Hf, V, Fe, Sn and Bi, and

[0245] X^4 is -$M^3L^1_{\Delta}$ or M^3 and Q^1 and Q^2 are H or each is a single bond joined to M^3, where L^1 is selected from the group consisting of —OH and —O—(C1- to C10-alkyl), especially —O—(C1- to C8-alkyl) or —O—(C1- to C6-alkyl), or where L^1 is selected from the group consisting of —OH, —O-methyl, —O-ethyl, —O-propyl, —O-butyl, —O-octyl, —O-isopropyl, and —O-isobutyl, and where M^3 is selected from the group consisting of s- and p-block metals, d- and f-block transition metals, lanthanide and actinide metals and semimetals,

[0246] especially from the group consisting of metals of transition groups 1, 2, 3, 4, 5, 8, 10 and 11 and metals of main groups 1, 2, 3, 4 and 5, preferably from the group consisting of Na, Zn, Sc, Nd, Ti, Zr, Hf, V, Fe, Pt, Cu, Ga, Sn and Bi; especially preferably from the group consisting of Zn, Ti, Zr, Hf, V, Fe, Sn and Bi, or

[0247] X^4 is $-M^3L^1_\Delta$ and Q^2 is H or a single bond joined to M^3 and Q^1 is H, $M^4L^4_\Delta$ or —SiR^8, where M^4 is selected from the group consisting of s- and p-block metals, d- and f-block transition metals, lanthanide and actinide metals and semimetals,

[0248] especially from the group consisting of metals of transition groups 1, 2, 3, 4, 5, 8, 10 and 11 and metals of main groups 1, 2, 3, 4 and 5, preferably from the group consisting of Na, Zn, Sc, Nd, Ti, Zr, Hf, V, Fe, Pt, Cu, Ga, Sn and Bi; especially preferably from the group consisting of Zn, Ti, Zr, Hf, V, Fe, Sn and Bi,

[0249] and where L^4 is selected from the group consisting of —OH and —O—(C1- to C10-alkyl), especially —O—(C1- to C8-alkyl) or —O—(C1- to C6-alkyl), or where L^4 is selected from the group consisting of —OH, —O-methyl, —O-ethyl, —O-propyl, —O-butyl, —O-octyl, —O-isopropyl, and —O-isobutyl, and where R^8 is selected from the group consisting of optionally substituted C1- to C20-alkyl, optionally substituted C3- to C8-cycloalkyl, optionally substituted C2- to C20-alkenyl and optionally substituted C5- to C10-aryl, or

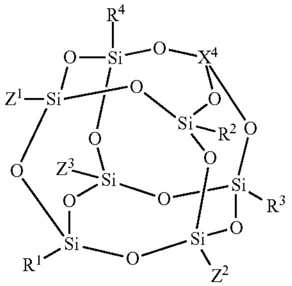
[0250] X^4, Q^1 and Q^2 are independently $-M^3L^1_\Delta$, or

[0251] X^4 is —$Si(R^8)$—$O-M^3L^1_A$, Q^2 is a single bond joined to the silicon atom of X^4 and Q^1 is $-M^4L^4_\Delta$, or

[0252] X^4 is —$Si(R^8)$—$O-M^3L^1_\Delta$, Q^2 is a single bond joined to the silicon atom of X^4 and Q^1 is a single bond joined to the M^3 atom of X^4.

[0253] 15. Composition according to any of the preceding embodiments, characterized in that the metal-siloxane-silanol(ate) compound has the structural formula (II)

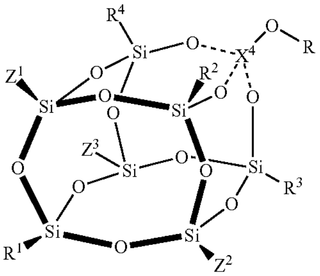
(II)



where X^4, R^1, R^2, R^3, R^4, Z^1, Z^2 and Z^3 are defined according to Embodiment 4.

[0254] 16. Composition according to Embodiment 15, characterized in that the metal-siloxane-silanol(ate) compound of the structure (IV) is a metal silsesquioxane

(IV)



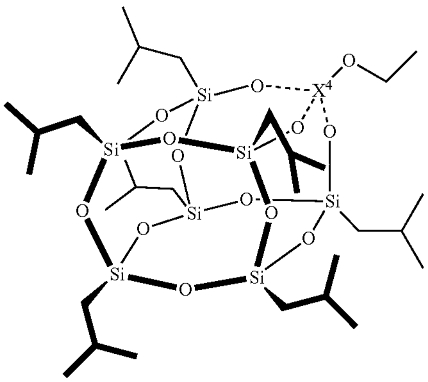
where

[0255] X^4 is selected from the group consisting of metals of transition groups 1, 2, 3, 4, 5, 8, 10 and 11 and metals of main groups 1, 2, 3, 4 and 5, preferably from the group consisting of Na, Zn, Sc, Nd, Ti, Zr, Hf, V, Fe, Pt, Cu, Ga, Sn and Bi; especially preferably from the group consisting of Zn, Ti, Zr, Hf, V, Fe, Sn and Bi, most preferably from the group consisting of Ti and Sn, and is most preferably Ti, and

[0256] X^4 is joined to OR where R is selected from the group consisting of —H, -methyl, -ethyl, -propyl, -butyl, -octyl, -isopropyl, and -isobutyl, Z^1, Z^2 and Z^3 are each independently C1- to C20-alkyl, C3- to C8-cycloalkyl, C2- to C20-alkenyl and C5- to C10-aryl, especially selected from the group consisting of methyl, ethyl, propyl, isopropyl, butyl, isobutyl, hexyl, heptyl, octyl, vinyl, allyl, butenyl and phenyl, and benzyl, and R^1, R^2, R^3 and R^4 are each independently C1- to C20-alkyl, C3- to C8-cycloalkyl, C2- to C20-alkenyl, and C5- to C10-aryl, especially selected from the group consisting of methyl, ethyl, propyl, isopropyl, butyl, isobutyl, hexyl, heptyl, octyl, vinyl, allyl, butenyl and phenyl, and benzyl.

[0257] 17. Composition according to Embodiment 16, characterized in that the metal-siloxane-silanol(ate) compound is a metal silsesquioxane of the structure (IVb)

(IVb)



[0258] where X^4 is selected from the group consisting of metals of transition groups 1, 2, 3, 4, 5, 8, 10 and 11 and metals of main groups 1, 2, 3, 4 and 5, preferably from the group consisting of Na, Zn, Sc, Nd, Ti, Zr, Hf, V, Fe, Pt, Cu, Ga, Sn and Bi; especially preferably from the group consisting of Zn, Ti, Zr, Hf, V, Fe, Sn and Bi, most preferably from the group consisting of Ti (and therefore is heptaisobutyl POSS-titanium(IV) ethoxide (TiPOSS)) and Sn (and therefore is heptaisobutyl POSS-tin(IV) ethoxide (SnPOSS)), and is most preferably Ti (and therefore is heptaisobutyl POSS-titanium(IV) ethoxide (TiPOSS)).

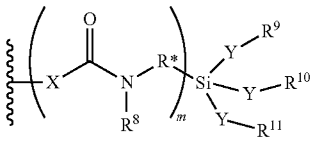
[0259] 18. Composition according to any of the preceding embodiments, characterized in that the silylated polymer (SiP) is obtainable by a synthesis, catalysed by a metal-siloxane-silanol(ate) compound, of at least one isocyanate-reactive compound, especially at least one hydroxy-functionalized polymer (component A), and one or more compounds having at least one isocyanate group (component B).

[0260] 19. Composition according to Embodiment 18, characterized in that the metal-siloxane-silanol(ate) compound for catalysed synthesis of component A and component B is defined according to any of Embodiments 11 to 16, especially in that the compound is heptaisobutyl POSS-titanium(IV) ethoxide (TiPOSS) and/or heptaisobutyl POSS-tin(IV) ethoxide (SnPOSS), preferably heptaisobutyl POSS-titanium(IV) ethoxide (TiPOSS).

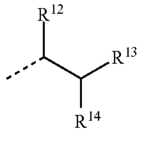
[0261] 20. Composition according to any of the preceding embodiments, characterized in that the polymer backbone (P) of the silylated polymer (SiP) has constituents selected from the group consisting of polyurethanes, polyureas, polyethers, polyesters, phenolic resins, polyalkylenes, poly(meth)acrylates, polyamides, polycaprolactones, polybutadienes or polyisoprenes, and polycarbonates or mixtures thereof, preferably from the group consisting of polyurethanes, polyureas, poly(meth)acrylates or polyethers or mixtures thereof, most preferably polyethers.

[0262] 21. Composition according to any of the preceding embodiments, characterized in that the silylated polymer (SiP) has at least two end groups of the general formula (V)

(V)



(Vb)



[0263] where

[0264] X is C, Si or a heteroatom and these, according to their valency, optionally have one or more R^8 radicals, preferably C, N, O, P, S, more preferably C, N or O, most preferably N or O, and each is bonded to a carbon in the polymer backbone,

[0265] R* is 0 or an optionally substituted straight-chain or branched C1- to C25-alkyl group or an optionally substituted C4- to C18-cycloalkyl group or an optionally substituted C4- to C18-aryl group and, when R*=0, the silicon atom is bonded directly to the nitrogen atom,

[0266] each Y is independently either O or a direct bond of the silicon atom to the respective R^9, R^{10} or R^{11} radical, and preferably at least one Y is O,

[0267] R^8 is H, an optionally substituted straight-chain or branched C1- to C16-alkyl group, an optionally substituted straight-chain or branched C2- to C16-alkenyl group or an optionally substituted straight-chain or branched C2- to C16-alkynyl group, an optionally substituted C4- to C14-cycloalkyl group or an optionally substituted C4- to C14-aryl group, or a radical of the general structure (Vb),

[0268] R^{12} and R^{14} are each independently H or a radical from the group consisting of —R^{15}, —$COOR^{15}$ and —CN,

[0269] R^{13} is H or a radical from the group consisting of —CH_2—$COOR^{15}$, —$COOR^{15}$, —$CONHR^{15}$, —$CON(R^{15})$, —CN, —NO_2, —$PO(OR^{15})_2$, —SOR^{15} and —SO_2OR^{15},

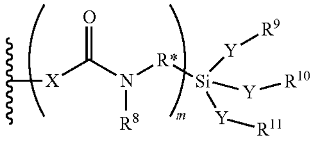
[0270] R^{15} is a hydrocarbyl radical having 1 to 20 carbon atoms and optionally having at least one heteroatom,

[0271] R^9, R^{10} and R^{11} are independently H, an optionally substituted straight-chain or branched C1- to C5-alkyl group, an optionally substituted straight-chain or branched C2- to C10-alkenyl group or an optionally substituted C4- to C14-cycloalkyl group or an optionally substituted C4- to C14-aryl group,

[0272] m is 0 or 1 and, when m=0, the silicon atom is bonded directly to a carbon in the polymer backbone (P).

[0273] 22. Composition according to Embodiment 21, characterized in that the silylated polymer (SiP) has a polyether polymer backbone having at least two end groups of the general formula (V)

(V)



where

[0274] X is N or O and N optionally has an R^9 radical,

[0275] R* is 0 or an optionally substituted straight-chain or branched C1- to C20-alkyl group or an optionally substituted C4- to C12-cycloalkyl group or an optionally substituted C4- to C12-aryl group, preferably an optionally substituted straight-chain or branched C1- to C15-alkyl group, and, when R*=0, the silicon atom is bonded directly to the nitrogen atom,

[0276] Y in Y—R^9 and Y—R^{10} are O and the Y in Y—R^{11} is either O or a direct bond of the silicon atom to the respective R^{11} radical, preferably at least one Y is O,

[0277] R^9 is H, an optionally substituted straight-chain or branched C1- to C10-alkyl group, an optionally substituted straight-chain or branched C2- to

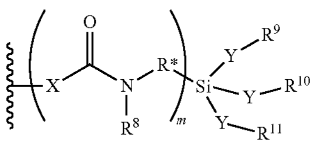
C10-alkenyl group or an optionally substituted straight-chain or branched C2- to C10-alkynyl group, an optionally substituted C4- to C10-cycloalkyl group or an optionally substituted C4- to C10-aryl group or a succinic acid derivative of the general structure (Vb) according to Embodiment 9,

[0278] R^9, R^{10} and R^{11} are independently H, an optionally substituted straight-chain or branched C1- to C4-alkyl group, an optionally substituted straight-chain or branched C2- to C5-alkenyl group or an optionally substituted C4- to C10-cycloalkyl group or an optionally substituted C4- to C10-aryl group, preferably independently H or a C1- to C2-alkyl group, and

[0279] m is 0 or 1 and, when m=0, the silicon atom is bonded directly to a carbon in the polymer backbone (P), preferably m=1.

[0280] 23. Composition according to Embodiment 22, characterized in that the silylated polymer (SiP) has a polyether polymer backbone having at least two end groups of the general formula (V)

(V)



where

[0281] R* is 0 or an optionally substituted straight-chain or branched C1- to C15-alkyl group or an optionally substituted C4- to C6-cycloalkyl group or an optionally substituted C4- to C6-aryl group, preferably an optionally substituted straight-chain or branched C1- to C10-alkyl group, more preferably a C1-alkyl group (=alpha-silane) or a C3-alkyl group (=gamma-silane), and, when R*=0, the silicon atom is bonded directly to the nitrogen atom,

[0282] R^9 is H, an optionally substituted straight-chain or branched C1- to C8-alkyl group, an optionally substituted straight-chain or branched C2- to C8-alkenyl group or an optionally substituted straight-chain or branched C2- to C8-alkynyl group, an optionally substituted C4- to C6-cycloalkyl group or an optionally substituted C4- to C6-aryl group,

[0283] R^9, R^{10} and R^{11} are independently H, an optionally substituted, straight-chain or branched C1- to C4-alkyl group, an optionally substituted, straight-chain or branched C2- to C5-alkenyl group or an optionally substituted C4- to C6-cycloalkyl group or an optionally substituted C4- to C6-aryl group, preferably independently H or a C1- to C2-alkyl group, and

[0284] m is 0 or 1 and, when m=0, the silicon atom is bonded directly to a carbon in the polymer backbone (P), preferably m=1.

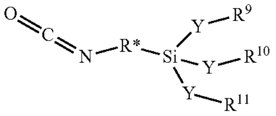
[0285] 24. Composition according to any of Embodiments 18 to 23, characterized in that the hydroxy-functionalized polymer is selected from the group consisting of polyoxyalkylene diols or polyoxyalkylene triols, especially polyoxyethylene di- and triols and polyoxypropylene di- and triols, higher-functionality polyols such as sorbitol, pentaerythritol-started polyols, ethylene oxide-terminated polyoxypropylene polyols, polyester polyols, styrene-acrylonitrile, acryloyl-methacrylate, (poly)urea-grafted or -containing polyether polyols, polycarbonate polyols, CO_2 polyols, polyhydroxy-functional fats and oils, especially castor oil, polyhydrocarbon polyols such as dihydroxypolybutadiene, polytetrahydrofuran-based polyethers (PTMEG), OH-terminated prepolymers based on the reaction of a polyetherol or polyesterol with a diisocyanate, polypropylene diols, polyester polyols or mixtures thereof, preferably polypropylene diols, polyester polyols, or mixtures thereof.

[0286] 25. Composition according to Embodiment 24, characterized in that the hydroxy-functionalized polymer is selected from the group consisting of polyoxyalkylene diols, polyoxyalkylene triols, especially polyoxyethylene di- and/or triols and/or polyoxypropylene di- and/or triols, KOH-catalysed hydroxy-functionalized polyethers or double metal cyanide complex-catalysed (DMC-catalysed) hydroxy-functionalized polyethers or mixtures thereof.

[0287] 26. Composition according to any of the preceding Embodiments 18 to 24, characterized in that component B is selected from the group consisting of aromatic and/or aliphatic isocyanates (Iso) of the general structure (VI) or mixtures thereof or isocyanatosilanes (Iso-Si) of the general structure (VII) or mixtures thereof

$$R^x\!\!+\!\!\left(N{=}C{=}O\right)_z \qquad \text{(VI)}$$

(VII)



where

[0288] R^x is a carbon-containing group, preferably at least one aromatic or aliphatic group or mixtures thereof, more preferably an optionally substituted straight-chain or branched C1- to C16-alkyl group, an optionally substituted straight-chain or branched C2- to C16-alkenyl group or an optionally substituted straight-chain or branched C2- to C16-alkynyl group, an optionally substituted C4- to C14-cycloalkyl group or an optionally substituted C4- to C14-aryl group, most preferably diphenylmethane, toluene, dicyclohexylmethane, hexane or methyl-3,5,5-trimethylcyclohexyl,

[0289] each Y is independently either O or a direct bond of the silicon atom to the respective R^9, R^{10} or R^{11} radical, and preferably at least one Y is O,

[0290] z is at least 1, preferably at least 2,

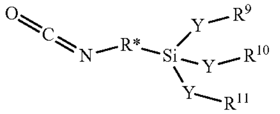
[0291] R^9, R^{10} and R^{11} are independently H, an optionally substituted straight-chain or branched C1- to C5-alkyl group, an optionally substituted straight-chain or branched C2- to C10-alkenyl group or an optionally substituted C4- to C8-cycloalkyl group or an optionally substituted C4- to C8-aryl group and

[0292] R* is 0 or an optionally substituted straight-chain or branched C1- to C25-alkyl group or an optionally substituted C4- to C18-cycloalkyl group or an optionally substituted C4- to C18-aryl group and, when R*=0, the silicon atom is bonded directly to the nitrogen atom.

[0293] 27. Composition according to any of Embodiments 18 to 26, characterized in that component B is selected from the group consisting of aromatic and/or aliphatic isocyanates (Iso) of the general structure (VI) or mixtures thereof or isocyanatosilanes (Iso-Si) of the general structure (VII) or mixtures thereof

$$R^x \text{—}(N{=}C{=}O)_z \qquad \text{(VI)}$$

(VII)



where

[0294] R^x is diphenylmethane, toluene, dicyclohexylmethane, hexane or methyl-3,5,5-trimethylcyclohexyl, preferably diphenylmethane or hexane or methyl-3,5,5-trimethylcyclohexyl, most preferably diphenylmethane or methyl-3,5,5-trimethylcyclohexyl, and

[0295] z is at least 2, preferably 2,

[0296] Y in Y—R^9 and Y—R^{10} are O and the Y in Y—R^{11} is either O or a direct bond of the silicon atom to the respective R^{11} radical, preferably at least one Y is O,

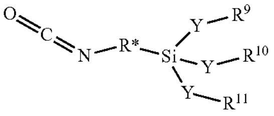
[0297] R^9, R^{10} and R^{11} are independently H, an optionally substituted straight-chain or branched C1- to C3-alkyl group and

[0298] R* is 0 or an optionally substituted straight-chain or branched C1- to C15-alkyl group or an optionally substituted C4- to C6-cycloalkyl group or an optionally substituted C4- to C6-aryl group, preferably an optionally substituted straight-chain or branched C1- to C10-alkyl group, more preferably a C1-alkyl group (=alpha-silane) or a C3-alkyl group (=gamma-silane), and, when R*=0, the silicon atom is bonded directly to the nitrogen atom.

[0299] 28. Composition according to Embodiment 27, characterized in that at least one isocyanate (Iso) of the general structure (VI) is selected from the group consisting of polymeric, oligomeric and monomeric methylene diphenyl isocyanate (MDI), especially from 4,4'-methylene diphenyl isocyanate (4,4'-MDI), 2,4'-methylene diphenyl isocyanate (2,4'-MDI), 2,2'-methylene diphenyl isocyanate (2,2'-MDI), 4,4'-diisocyanatodicyclohexylmethane (H12MDI), 2-methylpentamethylene 1,5-diisocyanate, dodecamethylene 1,12-diisocyanate, lysine and lysine ester diisocyanate, cyclohexane 1,3-diisocyanate, cyclohexane 1,4-diisocyanate, perhydro(diphenylmethane 2,4'-diisocyanate), perhydro(diphenylmethane 4,4'-diisocyanate), 1,4-diisocyanato-2,2,6-trimethylcyclohexane (TMCDI), 3-isocyanatomethyl-3,5,5-trimethylcyclohexyl isocyanate (=isophorone diisocyanate or IPDI), hexamethylene 1,6-diisocyanate (HDI) or the trimer thereof (HDI trimer), 2,2,4- and/or 2,4,4-trimethylhexamethylene 1,6-diisocyanate, 1,4-bis(isocyanato)cyclohexane, 1,4-bis(isocyanato)benzene (PPDI), 1,3- and/or 1,4-bis(isocyanatomethyl)cyclohexane, m- and/or p-xylylene diisocyanate (m- and/or p-XDI), m- and/or p-tetramethylxylylene 1,3-diisocyanate, m- and/or p-tetramethylxylylene 1,4-diisocyanate, bis(1-isocyanato-1-methylethyl)naphthalene, 1,3-bis(isocyanato-4-methylphenyl)-2,4-dioxo-1,3-diazetidine, naphthalene 1,5-diisocyanate (NDI), 3,3'-dimethyl-4,4'-diisocyanatodiphenyl (TODI), tolylene 2,4- and/or 2,6-diisocyanate (TDI), 1,3-bis(isocyanatomethyl)benzene or mixtures thereof, preferably 4,4'-methylene diphenyl isocyanate (4,4'-MDI) or isophorone diisocyanate (IPDI), hexamethylene 1,6-diisocyanate (HDI) or the trimer thereof (HDI trimer) or mixtures thereof, most preferably 4,4'-methylene diphenyl isocyanate (4,4'-MDI) or isophorone diisocyanate (IPDI) or mixtures thereof.

[0300] 29. Composition according to Embodiment 27, characterized in that at least one isocyanatosilane (Iso-Si) of the general structure (VII) is selected, or mixtures thereof,

(VII)

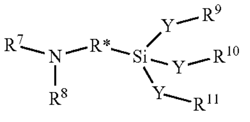


where R^9, R^{10}, R^{11} and R* are as defined in Embodiment 14 or 15, preferably R^9, R^{10}, R^{11} are a methyl or ethyl group or mixtures thereof, preferably selected from the group consisting of 3-(triethoxysilyl)methyl isocyanate, 3-(trimethoxysilyl)methyl isocyanate, 3-(triethoxysilyl)ethyl isocyanate, 3-(trimethoxysilyl)ethyl isocyanate, 3-(triethoxysilyl)propyl isocyanate, 3-(trimethoxysilyl)propyl isocyanate, 3-(triethoxysilyl)butyl isocyanate, 3-(trimethoxysilyl)butyl isocyanate, 3-(triethoxysilyl)pentyl isocyanate, 3-(trimethoxysilyl)pentyl isocyanate, 3-(triethoxysilyl)hexyl isocyanate, 3-(trimethoxysilyl)hexyl isocyanate or mixtures thereof, preferably 3-(trimethoxysilyl)methyl isocyanate, 3-(triethoxysilyl)methyl isocyanate, 3-(trimethoxysilyl)propyl isocyanate, 3-(triethoxysilyl)propyl isocyanate or mixtures thereof, more preferably 3-(trimethoxysilyl)propyl isocyanate, 3-(triethoxysilyl)propyl isocyanate, or mixtures thereof.

[0301] 30. Composition according to any of the preceding embodiments, characterized in that the silylated polymer (SiP) has been prepared by reaction with an aminosilane (AmSi).

[0302] 31. Composition according to Embodiment 30, characterized in that at least one aminosilane (AmSi) of the general structure (VIII) is selected, or is a mixture thereof,

(VIII)



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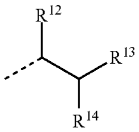
(Vb)



where

[0303] R^7 is H,

[0304] R^8 is H, an optionally substituted straight-chain or branched C1- to C25-alkyl group, an optionally substituted straight-chain or branched C2- to C25-alkenyl group or an optionally substituted C4- to C18-cycloalkyl group or an optionally substituted C4- to C18-aryl group, or a radical of the general structure (Vb),

[0305] R* is 0 or an optionally substituted straight-chain or branched C1- to C25-alkyl group or an optionally substituted C4- to C18-cycloalkyl group or an optionally substituted C4- to C18-aryl group and, when R*=0, the silicon atom is bonded directly to the nitrogen atom,

[0306] R^{12} and R^{14} are each independently H or a radical from the group consisting of $—R^{15}$, $—COOR^{15}$ and —CN,

[0307] R^{13} is H or a radical from the group consisting of $—CH_2—COOR^{15}$, $—COOR^{15}$, $—CONHR^{15}$, $—CON(R^{15})$, —CN, $—NO_2$, $—PO(OR^{15})_2$, $—SOR^{15}$ and $—SO_2OR^{15}$,

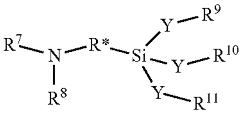
[0308] R^{15} is a hydrocarbyl radical having 1 to 20 carbon atoms and optionally having at least one heteroatom,

[0309] R^9, R^{10}, R^{11} and R* are defined according to Embodiment 22 or 23 and

[0310] each Y is independently either O or a direct bond of the silicon atom to the respective R^9, R^{10} or R^{11} radical, and preferably at least one Y is O.

[0311] 32. Composition according to Embodiment 31, characterized in that at least one aminosilane (AmSi) of the general structure (VIII) is selected, or is a mixture thereof,

(VIII)



where

[0312] R^8 is H, an optionally substituted straight-chain or branched C1- to C10-alkyl group, an optionally substituted straight-chain or branched C2- to C10-alkenyl group or an optionally substituted straight-chain or branched C2- to C10-alkynyl group, an optionally substituted C4- to C10-cycloalkyl group or an optionally substituted C4- to C10-aryl group or a succinic acid derivative of the general structure (Vb) according to Embodiment 19,

[0313] R* is 0 or an optionally substituted straight-chain or branched C1- to C20-alkyl group or an optionally substituted C4- to C12-cycloalkyl group or an optionally substituted C4- to C12-aryl group, preferably an optionally substituted straight-chain or branched C1- to C15-alkyl group, more preferably a C1-alkyl group (=alpha-silane) or a C3-alkyl group (=gamma-silane), and, when R*=0, the silicon atom is bonded directly to the nitrogen atom,

[0314] R^9, R^{10}, R^{11} are defined according to Embodiment 22 or 23, preferably R^9, R^{10}, R^{11} are a methyl or ethyl group or mixtures thereof, and

[0315] Y in $Y—R^9$ and $Y—R^{10}$ are O and the Y in $Y—R^{11}$ is either O or a direct bond of the silicon atom to the respective R^{11} radical.

[0316] 33. Composition according to any of the preceding Embodiments 30 to 32, characterized in that the aminosilane (AmSi) of the general structure (VIII) is selected from the group of N-[3-(trimethoxysilyl)methyl]butylamine, N-[3-(triethoxysilyl)methyl]butylamine, N-[3-(trimethoxysilyl)ethyl]butylamine, N-[3-(triethoxysilyl)ethyl]butylamine, N-[3-(trimethoxysilyl)propyl]butylamine, N-[3-(triethoxysilyl)propyl]butylamine, N-[3-(trimethoxysilyl)butyl]butylamine, N-[3-(triethoxysilyl)butyl]butylamine, N-[3-(trimethoxysilyl)pentyl]butylamine, N-[3-(triethoxysilyl)pentyl]butylamine, N-[3-(trimethoxysilyl)hexyl]butylamine, N-[3-(triethoxysilyl)hexyl]butylamine, 3-aminopropyltrimethoxysilane, 3-aminopropyltriethoxysilane, N-cyclohexyl-3-aminopropyltrimethoxysilane, N-cyclohexyl-3-aminopropyltriethoxysilane, N-(3-trimethoxysilylpropyl)aminosuccinic acid diethyl ester, N-(3-triethoxysilylpropyl)aminosuccinic acid diethyl ester or a mixture thereof, preferably N-[3-(trimethoxysilyl)methyl]butylamine, N-[3-(triethoxysilyl)methyl]butylamine, N-[3-(trimethoxysilyl)propyl]butylamine, N-[3-(triethoxysilyl)propyl]butylamine, N-(3-trimethoxysilylpropyl)aminosuccinic acid diethyl ester, N-(3-triethoxysilylpropyl)aminosuccinic acid diethyl ester, more preferably N-[3-(trimethoxysilyl)propyl]butylamine, N-[3-(triethoxysilyl)propyl]butylamine, N-[3-(trimethoxysilyl)methyl]butylamine, N-[3-(triethoxysilyl)methyl]butylamine, N-(3-trimethoxysilylpropyl)aminosuccinic acid diethyl ester, N-(3-triethoxysilylpropyl)aminosuccinic acid diethyl ester or a mixture thereof, most preferably N-(3-triethoxysilylpropyl)aminosuccinic acid diethyl ester, N-[3-(triethoxysilyl)propyl]butylamine, N-[3-(triethoxysilyl)methyl]butylamine or a mixture thereof.

[0317] 34. Composition according to any of the preceding Embodiments 18 to 33, characterized in that the metal-siloxane-silanol(ate) compound for catalysed synthesis is present in a molar concentration in the range from 0.000001 to 0.0001 mol/kg or 0.0001 to 0.1 mol/kg, especially from 0.00001 to 0.00005 mol/kg or 0.001 to 0.01 mol/kg, based in each case on the total weight of the composition.

[0318] 35. Composition according to any of the preceding Embodiments 18 to 34, characterized in that the metal-siloxane-silanol(ate) compound for catalysed synthesis is present with a proportion by weight of 0.001% to 1.5%, preferably of 0.002% to 0.5%, based in each case on the total weight of the composition.

[0319] 36. Composition according to any of the preceding embodiments, characterized in that the silylated polymer (SiP) has a viscosity in the range from 500 to 100 000 mPa·s, preferably in the range from 2000 to 25 000 mPa·s.

[0320] 37. Composition according to any of the preceding embodiments, characterized in that the silylated polymer (SiP) according to any of the preceding embodiments has a viscosity lower by >5% compared to a silylated polymer (SiP) prepared under dibutyltin dilaurate (DBTL) catalysis.

[0321] 38. Composition according to any of the preceding embodiments, characterized in that the silylated polymer (SiP) has a number-average molar mass (Mn) between 500 and 100 000 g/mol.

[0322] 39. Composition according to any of the preceding embodiments, characterized in that the silylated polymer (SiP) has a molar mass distribution (Mw/Mn) of about 1.6 or less.

[0323] 40. Composition according to any of the preceding embodiments, characterized in that the composition is moisture-curing, preferably with additional use of a catalyst.

[0324] 41. Composition according to any of the preceding embodiments, characterized in that it can cure through the influence of moisture and at room temperature, in the range of 10-30° C., preferably in the range of 18-25° C., more preferably at 20 to 23° C.

[0325] 42. Composition according to any of the preceding embodiments, wherein the composition further comprises one or more additives selected from the group consisting of filler, adhesion promoter, moisture scavenger, plasticizer, UV stabilizers, thixotropic agents, wetting agents or combinations thereof, where one or more additives is/are preferably a silane.

[0326] 43. Composition comprising the following components or obtainable by combining the following components:

[0327] 2 to 50 g of silylated polymer (SiP) defined according to any of the preceding embodiments,

[0328] 0 to 35 g of plasticizer

[0329] 5 to 65 g of chalk

[0330] 0 to 15 g of titanium dioxide

[0331] 0 to 5 g of water scavenger

[0332] 0 to 5 g of adhesion promoter, and

[0333] 0 to 2 g of a catalyst according to any of the preceding embodiments,

based in each case on the total weight of the composition.

[0334] 44. Composition according to Embodiment 43, comprising the following components or obtainable by combining the following components:

[0335] 10 to 40 g of silylated polymer (SiP) defined according to any of the preceding embodiments,

[0336] 5 to 30 g of plasticizer

[0337] 15 to 55 g of chalk

[0338] 1 to 10 g of titanium dioxide

[0339] 0.25 to 3 g of water scavenger

[0340] 0.25 to 3 g of adhesion promoter, and

[0341] 0 to 1 g of a catalyst according to any of the preceding embodiments,

based in each case on the total weight of the composition.

[0342] 45. Composition according to either of Embodiments 43 and 44, comprising the following components or obtainable by combining the following components:

[0343] 15 to 35 g of silylated polymer (SiP) defined according to any of the preceding embodiments,

[0344] 10 to 25 g of plasticizer

[0345] 25 to 50 g of chalk

[0346] 1.5 to 5 g of titanium dioxide

[0347] 0.5 to 2 g of water scavenger

[0348] 1 to 2.5 g of adhesion promoter, and

[0349] 0 to 0.8 g of a catalyst according to any of the preceding embodiments,

based in each case on the total weight of the composition.

[0350] 46. Process for producing the composition according to any of the preceding embodiments, comprising the following steps:

[0351] (i) synthesizing a polymer by combining at least one isocyanate-reactive compound, especially a hydroxy-functionalized polymer according to Embodiment 24 or 25, and with one or more isocyanates (Iso) according to Embodiment 26, 27 or 28, or one or more isocyanatosilanes (Iso-Si) according to Embodiment 26, 27 or 29 using a metal-siloxane-silanol(ate) compound according to any of the preceding embodiments, especially heptaisobutyl POSS-titanium(IV) ethoxide (TiPOSS) according to Embodiment 16 or 17, heptaisobutyl POSS-tin(IV) ethoxide (SnPOSS) according to Embodiment 16 or 17 or mixtures thereof,

[0352] (ii) optionally admixing the polymer from step (i) with a catalyst selected from dibutyltin dilaurate (DBTL) or a metal-siloxane-silanol(ate) compound according to any of the preceding embodiments, especially heptaisobutyl POSS-titanium(IV) ethoxide (TiPOSS) according to Embodiment 16 or 17, heptaisobutyl POSS-tin(IV) ethoxide (SnPOSS) according to Embodiment 16 or 17 or mixtures thereof.

[0353] 47. Process for producing the composition according to any of the preceding embodiments, comprising the following steps:

[0354] (i) synthesizing a polymer by combining at least one hydroxy-functionalized polymer selected from the group consisting of hydroxy-functionalized polymers according to Embodiment 24 or 25 having number-average molar masses (Mn) of 500-35 000 g/mol, preferably of about 2000 g/mol or about 19 000 g/mol, or mixtures thereof with one or more isocyanates (Iso) according to Embodiment 26, 27 or 28, or one or more isocyanatosilanes (Iso-Si) according to Embodiment 26, 27 or 29, preferably 3-(triethoxysilyl)methyl isocyanate or 3-(triethoxysilyl)propyl isocyanate or mixtures thereof, using a metal-siloxane-silanol(ate) compound according to any of the preceding embodiments, especially heptaisobutyl POSS-titanium(IV) ethoxide (TiPOSS) according to Embodiment 16 or 17, heptaisobutyl POSS-tin(IV) ethoxide (SnPOSS) according to Embodiment 16 or 17 or mixtures thereof,

[0355] (ii) optionally admixing the polymer from step (i) with a catalyst selected from dibutyltin dilaurate (DBTL) or a metal-siloxane-silanol(ate) compound according to any of the preceding embodiments, especially heptaisobutyl POSS-titanium(IV) ethoxide (TiPOSS) according to Embodiment 16 or 17, heptaisobutyl POSS-tin(IV) ethoxide (SnPOSS) according to Embodiment 16 or 17 or mixtures thereof.

[0356] 48. Process for producing the composition according to Embodiment 47, comprising the steps of:

[0357] (i) synthesizing a polymer at a temperature of <80° C. by combining at least one hydroxy-functionalized polymer selected from the group consisting of hydroxy-functionalized polymers according to Embodiment 24 or 25 having number-average molar masses (Mn) of 500-35 000 g/mol, preferably of about 2000 g/mol or about 19 000 g/mol, or mixtures thereof with one or more isocyanates (Iso) according to Embodiment 26, 27 or 28, or one or more isocyanatosilanes (Iso-Si) according to Embodiment 26, 27 or 29, preferably 3-(triethoxysilyl)methyl isocyanate or 3-(triethoxysilyl)propyl isocyanate or mixtures thereof, using a metal-siloxane-silanol(ate) compound according to any of the preceding embodiments, especially heptaisobutyl POSS-titanium(IV) ethoxide (TiPOSS) according to Embodiment 16 or 17, heptaisobutyl POSS-tin(IV) ethoxide (SnPOSS) according to Embodiment 16 or 17 or mixtures thereof,

[0358] (ii) optionally admixing the polymer from step (i) with a catalyst selected from dibutyltin dilaurate (DBTL) or a metal-siloxane-silanol(ate) compound according to any of the preceding embodiments, especially heptaisobutyl POSS-titanium(IV) ethoxide (TiPOSS) according to Embodiment 16 or 17, heptaisobutyl POSS-tin(IV) ethoxide (SnPOSS) according to Embodiment 16 or 17 or mixtures thereof.

[0359] 49. Process for producing the composition according to Embodiment 46, 47 or 48, characterized in that the polymer obtained in each case from step (i) is reacted with an aminosilane (AmSi) according to Embodiment 31, 32 or 33, preferably with N-[3-(triethoxysilyl)propyl]butylamine, N-[3-(trimethoxysilyl)propyl]butylamine, N-[3-(triethoxysilyl)methyl]butylamine, N-[3-(trimethoxysilyl)methyl]butylamine, N-(3-trimethoxysilylpropyl)aminosuccinic acid diethyl ester, N-(3-triethoxysilylpropyl)aminosuccinic acid diethyl ester or mixtures thereof.

[0360] 50. Use of the composition according to any of the preceding embodiments in CASE sectors (coatings, adhesives, sealants and elastomers).

[0361] 51. Use of the composition according to any of the preceding embodiments in adhesives and sealants.

EXAMPLES

Examples I)

[0362] Preparation of the Polymers Required for the Study:

[0363] The following materials were used for the preparation of the prepolymers and silane-terminated polymers:

[0364] 4,4'-methylene diphenyl isocyanate, Alfa Aesar

[0365] IPDI Wanate IPDI, DKSH

[0366] PolyU L 4000 (low monool polyoxypropylene diol, OH number 27 mg KOH/g, viscosity 1000 mPa·s), PolyU GmbH

[0367] PolyU L 12000 (low monool polyoxypropylene diol, OH number 10 mg KOH/g, viscosity 6000 mPa·s), PolyU GmbH

[0368] diethyl maleate, Acros Organics

[0369] 3-aminopropyltrimethoxysilane, Alfa Aesar

[0370] 3-aminopropyltriethoxysilane, Alfa Aesar

[0371] 3-(triethoxysilyl)propyl isocyanate, Acros Organics

[0372] 3-(trimethoxysilyl)propyl isocyanate, TCI

[0373] DBTL Kosmos 19, Evonik, 20% strength, dissolved in Hexamoll DINCH, BASF

[0374] TiPOSS, 20% strength, dissolved in Hexamoll DINCH, BASF

[0375] vinyltrimethoxysilane, VTMO, Acros Organics

[0376] vinyltriethoxysilane, VTEO, Alfa Aesar

[0377] Preparation of Triethoxysilane-Terminated Polymers (ESTP) and Trimethoxysilane-Terminated Polymers (MSTP)

[0378] A) Preparation of Triethoxysilane-Terminated Polymers (ESTP) and Trimethoxysilane-Terminated Polymers (MSTP) From the reaction of MDI Prepolymer With N-(3-triethoxysilylpropyl)aminosuccinic acid diethyl ester or N-(3-trimethoxysilylpropyl)aminosuccinic acid diethyl ester:

[0379] A1) Synthesis of Triethoxysilane-Terminated Polymer (ESTP)

[0380] Step 1; MDI Prepolymer Synthesis: Reaction of 4,4'-MDI With PolyU L 4000 and TiPOSS as Catalyst

[0381] In a reaction vessel under a nitrogen atmosphere, 31.3 g of 4,4'-methylene diphenyl isocyanate was melted at 55° C., and 250 g of PolyU L 4000 heated to 50° C. was added while stirring within 30 min. The mixture was cooled down to room temperature, and 0.625 g of a 1% TiPOSS solution (corresponding to 22 ppm of TiPOSS) in DINCH was added. After a reaction time of 3 h at room temperature, by means of titration, a content of free isocyanate groups of 1.9% by weight (calculated value: 1.9% by weight) was obtained. The viscosity of the resulting prepolymer was 5000 mPa·s.

[0382] Step 2, Aminosilane Synthesis: Reaction of Diethyl Maleate With 3-aminopropyltriethoxysilane

[0383] A reaction vessel was initially charged with 50 g of 3-aminopropyltriethoxysilane, and 38.9 g of diethyl maleate was added at room temperature within 30 min. The mixture was stirred at 80° C. for a further 12 h. 87 g of N-(3-triethoxysilylpropyl)aminosuccinic acid diethyl ester was obtained as a water-clear liquid.

[0384] Step 3, Synthesis of Triethoxysilane-Terminated Polymer ESTP 1:

[0385] To 171.2 g of MDI prepolymer with 0.0038 g of TiPOSS under a nitrogen atmosphere at room temperature was added 30 g of N-(3-triethoxysilylpropyl)aminosuccinic acid diethyl ester while stirring. The reaction was ended after 2 h at 80° C.; it was no longer possible to detect any free isocyanate. The viscosity of the resultant triethoxysilane-terminated polymer ESTP 1 was 18 000 mPa·s.

[0386] A2) Comparative Experiment for A1; Synthesis of Triethoxysilane-Terminated Polymer ESTP 2

[0387] For a comparison, the MDI prepolymer synthesis of step 1 of reaction sequence A1 was repeated using 0.625 g of a 1% DBTL solution in DINCH as catalyst. The subsequent steps were conducted analogously to the manner described above. A triethoxysilane-terminated polymer ESTP 2 with viscosity of 28 000 mPa·s was obtained.

[0388] A3) Trimethoxysilane-Terminated Polymers (MSTP)

[0389] Step 1; MDI Prepolymer Synthesis: Reaction of 4,4'-MDI With PolyU L 4000 and TiPOSS as Catalyst

[0390] As described under A1.

[0391] Step 2, Aminosilane Synthesis: Reaction of Diethyl Maleate With 3-aminopropyltrimethoxysilane

[0392] A reaction vessel was initially charged with 51 g of 3-aminopropyltrimethoxysilane, and 49 g of diethyl maleate was added at room temperature within 30 min. The mixture was stirred at room temperature for a further 2 h. 97.8 g of N-(3-trimethoxysilylpropyl)aminosuccinic acid diethyl ester was obtained as a water-clear liquid.

[0393] Step 3, Synthesis of Trimethoxysilane-Terminated Polymer MSTP 1:

[0394] To 240 g of MDI prepolymer with 0.006 g of TiPOSS under a nitrogen atmosphere at room temperature was added 37.5 g of N-(3-trimethoxysilylpropyl)aminosuccinic acid diethyl ester while stirring. The reaction was ended after 2 h; it was no longer possible to detect any free isocyanate. The viscosity of the resultant trimethoxysilane-terminated polymer MSTP 1 was 17 000 mPa·s.

[0395] A4) Comparative Experiment for A3; Synthesis of Trimethoxysilane-Terminated Polymer MSTP 2

[0396] For a comparison, the MDI prepolymer synthesis of step 1 of reaction sequence A1 was repeated using 0.625 g of a 1% DBTL solution in DINCH as catalyst. The subsequent steps were conducted analogously to the manner described above.

[0397] To 240 g of MDI prepolymer with 0.006 g of DBTL under a nitrogen atmosphere at room temperature was added 37.5 g of N-(3-trimethoxysilylpropyl)aminosuccinic acid diethyl ester while stirring. The reaction was ended after 2 h; it was no longer possible to detect any free isocyanate. A trimethoxysilane-terminated polymer MSTP 2 with viscosity of 25 000 mPa·s was obtained.

[0398] B) Preparation of Triethoxysilane-Terminated Polymers (ETSP) and Trimethoxysilane-Terminated Polymers (MSTP) From the Reaction of 3-(triethoxysilyl)propyl isocyanate or 3-(trimethoxysilyl)propyl isocyanate With PolyU L 12000

[0399] B1) Synthesis of Triethoxysilane-Terminated Polymer ESTP 3: Reaction of 3-(triethoxysilyl)propyl isocyanate and PolyU L 12000 With TiPOSS as Catalyst

[0400] A reaction vessel under a nitrogen atmosphere was initially charged with 250 g of PolyU L 12000, and 6.25 g of a 20% TiPOSS solution in DINCH was added while stirring. Subsequently, 10.98 g of 3-(triethoxysilyl)propyl isocyanate was added dropwise within 30 min. The reaction was ended after 2 h; it was no longer possible to detect any free isocyanate. The viscosity of the resultant triethoxysilane-terminated polymer was 7300 mPa·s. Finally, 2% VTEO was added.

[0401] B2) Comparative Experiment for B1; Synthesis of Triethoxysilane-Terminated Polymer ESTP 4: Reaction of 3-(triethoxysilyl)propyl isocyanate and PolyU L 12000 With DBTL as Catalyst

[0402] A reaction vessel under a nitrogen atmosphere was initially charged with 250 g of PolyU L 12000, and 6.25 g of a 20% DBTL solution in DINCH was added while stirring. Subsequently, 10.98 g of 3-(triethoxysilyl)propyl isocyanate was added dropwise within 30 min. The reaction was ended after 2 h; it was no longer possible to detect any free isocyanate. The viscosity of the resultant triethoxysilane-terminated polymer was 7700 mPa·s. Finally, 2% VTEO was added.

[0403] B3) Synthesis of Trimethoxysilane-Terminated Polymer MSTP 3: Reaction of 3-(trimethoxysilyl)propyl isocyanate and PolyU L 12000 With TiPOSS as Catalyst

[0404] A reaction vessel under a nitrogen atmosphere was initially charged with 200 g of PolyU L 12000, and 5 g of a 20% DBTL solution in DINCH was added while stirring. Subsequently, 7.31 g of 3-(trimethoxysilyl)propyl isocyanate was added dropwise within 30 min. The reaction was ended after 2 h; it was no longer possible to detect any free isocyanate. The viscosity of the resultant trimethoxysilane-terminated polymer was 8900 mPa·s. Finally, 2% VTMO was added.

[0405] B4) Synthesis of Trimethoxysilane-Terminated Hybrid Polymer MSTP 4: Reaction of 3-(trimethoxysilyl) propyl isocyanate and PolyU L 12000 With DBTL as Catalyst

[0406] A reaction vessel under a nitrogen atmosphere was initially charged with 200 g of PolyU L 12000, and 5 g of a 20% DBTL solution in DINCH was added while stirring. Subsequently, 7.31 g of 3-(trimethoxysilyl)propyl isocyanate was added dropwise within 30 min. The reaction was ended after 2 h; it was no longer possible to detect any free isocyanate. The viscosity of the resultant trimethoxysilane-terminated polymer was 9100 mPa·s. Finally, 2% VTMO was added.

[0407] C) Testing of the Curing Characteristics of Triethoxysilane-Terminated Polymers ESTP 1 to 4 and Trimethoxysilane-Terminated Polymers MSTP 1 to 4

[0408] The curing characteristics of the silane-terminated polymers were tested by determining the fibre time TT and tack-free time TFT on samples of thickness 2 mm at 23° C./50% RH. For this purpose, the samples were made up without catalyst and with TiPOSS, DBTL or with a combination of TiPOSS and DBTL and cured.

TABLE A

Curing characteristics of triethoxysilane-terminated polymers (ESTP 1 to 4) and trimethoxysilane-terminated polymers (MSTP 1 to 4) using TiPOSS and DBTL

		ESTP 1 TT/TFT 1	ESTP 2 TT/TFT 2	ESTP 3 TT/TFT 3	ESTP 4 TT/TFT 4	MSTP 1 TT/TFT 5	MSTP 2 TT/TFT 6	MSTP 3 TT/TFT 7	MSTP 4 TT/TFT 8
TS 1	No further addition of cat.	No reaction for 7 days	No reaction for 7 days	>48 h/ <72 h	>30 h/ 48 h	No reaction for 7 days	No reaction for 7 days	6 h/ 12 h	1 h/ 3.5 h

TABLE A-continued

Curing characteristics of triethoxysilane-terminated polymers (ESTP 1 to 4) and trimethoxysilane-terminated polymers (MSTP 1 to 4) using TiPOSS and DBTL

		ESTP 1 TT/TFT 1	ESTP 2 TT/TFT 2	ESTP 3 TT/TFT 3	ESTP 4 TT/TFT 4	MSTP 1 TT/TFT 5	MSTP 2 TT/TFT 6	MSTP 3 TT/TFT 7	MSTP 4 TT/TFT 8
TS 2	+0.5% by wt. TiPOSS	No reaction for 7 days	8 h/No through-curing	22 h/ <48 h	6 h/ 20 h	16 h/ 44 h	5 h/ No through-curing	40 min/ 1.5 h	15 min/ 45 min
TS 3	+0.5% by wt. DBTL	6.5 h/ <40 h	42 h/ 65 h	5 h/ 16 h	>24 h/ 48 h	1.5 h/ 5 h	2.5 h/ 8 h	15 min/ 45 min	40 min/ 2 h
TS 4	+0.5% by wt. TiPOSS; +0.5% by wt. DBTL	5.5 h/ <30 h	7 h/ <30 h	3 h/ 8 h	6 h/ 18 h	1 h/ 4 h	1.5 h/ 5.5 h	10 min/ 40 min	15 min/ 45 min

TS = test series

[0409] Columns 1, 2, 3 and 4 describe curing characteristics under air humidity (23° C./50% RH) of the triethoxysilane-terminated polymers to which additional catalyst (TiPOSS, by way of example DBTL, a 1:1 mixture of DBTL/TiPOSS) has or has not been added (ESTP 1 to 4). The triethoxysilane-terminated polymers have been obtained via the reaction of MDI prepolymer with N-(3-triethoxysilylpropyl)aminosuccinic acid diethyl ester (ESTP 1, TiPOSS-catalysed and ESTP 2, DBTL-catalysed) and via the reaction of triethoxysilylpropyl isocyanate with polyol (ESTP 3, TiPOSS-catalysed and ESTP 4, DBTL-catalysed).

[0410] Columns 5, 6, 7 and 8 describe, by way of comparison, the reactions of the corresponding trimethoxysilane-terminated polymers prepared in the same way (MSTP 1 to 4).

[0411] D) Conclusion:

[0412] It can be inferred overall from the examples of columns 1-8 that the combination of equal parts of TiPOSS and DBTL used by way of example (but also bismuth, zinc, tin, zirconium, aluminium catalysts etc.) has a particularly advantageous effect on the curing of silane-terminated polymers. All silane-terminated polymers of test series 4 lead to fully cured hybrid polymers. It is particularly surprising here that the triethoxysilane-terminated polymers that are normally of limited reactivity (ESTP 1 to 4, test series 4) cure fully within customary curing times (up to 40 h). The curing outcome from column 3, test series 3, and column 4, test series 2, corroborates this result since there is likewise a catalyst mixture in this case of TiPOSS and DBTL. In the table, the corresponding triethoxysilane-terminated polymers that cure in a particularly accelerated manner by virtue of the catalyst mixture of TiPOSS and DBTL are marked. Furthermore, it is clear from test series 1, in the case of the trimethoxysilane-terminated polymers (columns 5 to 8), that the polymers that have been prepared from the silylation using TiPOSS are much more stable with respect to curing with air humidity (test series 1, columns 5 and 7). All triethoxysilane-terminated polymers ESTP 1-4 (test series 1, columns 1 to 4) and polymers MSTP 1 and MSTP 2 (test series 1, columns 5 and 6) are of limited reactivity without additional catalysis and do not have an adequate curing tendency (skin formation) even after a number of days.

[0413] The main results of the curing tests can be summarized as follows:

[0414] 1) The moisture-induced curing of triethoxysilane-terminated polymers is greatly accelerated by the use of a catalyst combination of TiPOSS and DBTL (bismuth, zinc, tin, zirconium, aluminium etc.) and hence satisfies practical requirements.

[0415] 2) By contrast, the use of a single catalyst (TiPOSS or DBTL) does not lead to a practically appropriate curing rate of the triethoxysilanized hybrid polymers.

[0416] 3) The use of TiPOSS as sole catalyst for the synthesis of the silane-terminated polymers has the advantage that they are particularly stable with respect to ingress of water (humidity, residual moisture, formulation raw materials, etc.).

[0417] In order to demonstrate the practical suitability of an abovementioned triethoxysilane-terminated polymer (ESTP 3), it was processed as a polymer in an illustrative standard sealant and adhesive formulation. The resultant sealant and adhesive was examined with regard to curing characteristics (skin time, ST), hardness and density.

TABLE B

Composition in parts by weight and results of the evaluation of an illustrative standard sealant and adhesive using the ethoxysilane-terminated polymer ESTP 3

	Example 1
ESTP 3	25*
Chalk	45
Plasticizer	20
Titanium dioxide	3.35
Water scavenger	1.5
Adhesion promoter	1.95
DBTL	0.2
Skin time [min]	22
Shore A hardness	35
Density [g/cm^3]	1.43

*contains 0.13 part by weight of TiPOSS

[0418] The results for skin time and hardness obtained with this material are within the range of values achieved with comparable industrial adhesives and sealants.

Example II)

[0419] The present invention relates to the composition and to the process for preparing polyurethane prepolymers and polyurethane systems based on polyols, di- or polyisocyanates and a TiPOSS-based catalyst.

[0420] TiPOSS-based catalysts that are preferred in accordance with the invention are those disclosed in EP 2 989 155 B1 and EP 2 796 493 A1. The disclosure of these documents is fully incorporated with regard to the catalysts. Particular preference is given to the catalysts (metallosilsesquioxane) according to embodiment 5 of EP 2 989 155 B1.

[0421] The study of the activity of heptaisobutyl POSS-titanium(IV) ethoxide (TiPOSS) for the formation of polyurethane compounds was conducted by way of example in comparison with dibutyltin dilaurate (DBTDL) and tin(II) 2-ethylhexanoate (tin octoate) in various unfoamed and foamed polyurethane systems. Particular attention was paid to the effect on the preparation of the silylated polyurethanes (SPUR) by the IPDI route. The model formulations from the CASE application sectors, soft foam and flexible foam (slabstock foam), were examined here with regard to their curing characteristics at room temperature (23° C./50% RH) using various polyols and isocyanates with the same catalyst content of TiPOSS and DBTDL or tin octoate. For simplification, the studies have been conducted under the assumption that a complete stoichiometric reaction (index 100) can take place between isocyanate and polyol. In principle, the studies are also applicable to the preparation of prepolymers. The catalytic activity of the catalysts examined was determined by the determination and comparison of cream time, fibre time and tack-free time.

[0422] 1.) Study of TiPOSS/DBTDL in Unfoamed Polyurethane Formulations

[0423] a) Propylene glycol polyols

[0424] The polyol A component consisted of a polypropylene diol and the TiPOSS catalyst in the form of a 20% solution in diisononyl phthalate (DINP). For comparison of catalytic activity, a corresponding identical polyol A component was prepared using DBTDL. The amount of catalyst was 0.2 percent by weight in each case (neglecting the amount of solvent). In order to study the influence of molecular weight, the molecular weight was additionally varied from low (MW ~2000) to high (MW ~18 000), since it can be assumed that the reactivity of polypropylene polyols that are of limited reactivity in any case will decrease further with rising molecular weight, and hence differences in reactivity will be particularly readily observable.

[0425] The polypropylene polyols tested were accordingly those with MW ~2000 (Rokopol D2002, PCC Rokita), MW ~8000 (Rokopol LDB 8000), MW ~12 000 (Rokopol LDB 12000) and MW ~18 000 (Rokopol LDB 18000).

[0426] The crosslinker components used were the isocyanates P-MDI (Voranate M230, Dow), IPDI (Wanate IPDI, DKSH) and HDI trimer isocyanurates (Vestanat HT2500/100). The reaction between polyol A and isocyanate B component was effected by stirring the two components at 1000 rpm with a conventional propeller stirrer for 10 s. After the stirring process had ended, the resultant reaction mixture was cast into slabs of thickness ~6 mm (10 g). The curing characteristics were determined from the cream time, fibre time and tack-free time.

[0427] It was found that the TiPOSS-catalysed curing of polyurethane at room temperature is significantly accelerated using the polypropylene polyols described compared to the corresponding DBTDL-catalysed crosslinking. The acceleration of the reaction, according to the combination of polyol and isocyanate examined, is between a factor of 2 and a factor of 100. Viewed overall, the factor of reaction acceleration when TiPOSS is used particularly surprisingly increases for the HDI trimer of isocyanurate used, and to a lesser degree for IPDI.

[0428] Conclusion for SPUR Methodology:

[0429] Since the reaction between the DMC polyols and IPDI isocyanate is the crucial reaction for the commercial preparation of SPUR (hybrid polymers), this finding is of great significance. Since we are already able to establish a considerable increase in reaction at room temperature and with 1:1 stoichiometry, it can be expected that, under the customary conditions of SPUR prepolymer preparation, it is possible to work with considerably smaller amounts of catalyst (⅕ to ⅒) and/or a lower temperature (<80° C.) and/or shortening of the reaction time. Since the formation of by-products in this preparation leads to an unwanted increase in viscosity, a distinct improvement in the reaction regime and product quality is thus to be expected.

[0430] With regard to the ever-increasing economic significance of the SPUR products, the use of the TiPOSS catalyst is expected to lead both to a cost benefit over tin catalysts and to a product benefit.

[0431] a) Propylene glycol polyols, ethylene glycol-Tipped

[0432] In order to assess whether these observations are also applicable to more reactive polyether polyols, by way of example, polyether polyols with MW ~4000 and f=2 and MW ~4850 and f=3 tipped with ethoxy groups at the termini were examined. It has been found that the differences in reactivity of the polyol systems catalysed with TiPOSS and DBTDL are smaller in the case of use of reactive polyether triol. Here too, it is again observed that the acceleration in reactivity of the crosslinking by TiPOSS is particularly effective for the HDI trimer.

[0433] 2.) Study of the Activity of TiPOSS/DBTL in Silane-Terminated Polyurethanes

[0434] The speed of fibre formation and curing in silane-terminated polyurethanes was determined on 6 mm SPUR slabs that had been produced by mixing the silane-terminated polyurethanes with 0.2 percent by weight each of TiPOSS and DBTL (each in solution, 20% in DINP). The mixing was effected with exclusion of air in an argon inert gas atmosphere with a conventional propeller stirrer. The mixed material was cured at 23° C./50% RH.

[0435] 3.) Study of the Activity of TiPOSS/DBTDL in Flexible Polyurethane Foam Formulations

[0436] The polyol A component consisted of a reactive, ethoxy group-tipped polyether triol (Rokopol M 5020, f=3), water and the TiPOSS catalyst, in the form of a 20% solution in diisononyl phthalate (DINP). For comparison of catalytic activity, a corresponding identical polyol A component was prepared using DBTDL. The amount of catalyst was 0.2 percent by weight in each case (neglecting the DINP solvent). By way of comparison, the reaction was conducted using a less reactive polypropylene polyol (Rokopol D 2002, f=2).

[0437] The crosslinking component used was the isocyanate P-MDI (Voranate M230). The reaction between polyol A and isocyanate B component was effected by stirring the two components at 2500 rpm with a conventional propeller stirrer for 10 s. The reaction was stoichiometric. After the stirring process had ended, the reaction mixture obtained (20 g) was poured into cups. The curing characteristics were determined from the cream time and tack-free time.

[0438] It was found that the activity of TiPOSS when using ethoxylated polyols is comparable to that of DBTDL. By contrast, the curing process in the case of the formulation made from a pure polypropylene polyol is more significantly accelerated by TiPOSS.

[0439] 4.) Study of the Activity of TiPOSS/Tin Octoate in a Slabstock Polyurethane Foam Formulation

[0440] The polyol A component consisted of a standard polyester polyol based on Desmophen 2200 B, an amine catalyst (N,N-dimethylpiperazine and N,N-dimethylhexadecylamine), cell stabilizers, water and the TiPOSS catalyst, in the form of a 20% solution in DINP. For comparison of catalytic activity, a corresponding identical polyol A component was prepared using tin octoate. The amount of TiPOSS and tin octoate catalyst was 0.03 percent by weight in each case.

[0441] The crosslinking components used were the isocyanate Desmodur T65 and a prepolymer having an NCO content of about 12%. The reaction was effected in a stoichiometric ratio (index 100). The reaction between polyol A and isocyanate B components was effected by stirring the two components at 1000 rpm with a Visco Jet stirrer unit for 10 s. After the stirring process had ended, the resultant reaction mixture (~400 g) was poured into a 2 L wooden box, and the curing characteristics were determined from the cream time and tack-free time.

[0442] It was found that the activity of TiPOSS is comparable to that of tin octoate. The resultant foams from the reaction with TiPOSS have lower density; strength properties and indentation hardness are correspondingly lower.

[0443] 5.) Overall Conclusion/Applications

[0444] a) Use of TiPOSS in the Preparation of SPUR Prepolymers

[0445] The significant increase in reaction described in the reaction between the DMC polyols and IPDI can be used for the commercial production of SPUR (hybrid polymers). It can be expected here that it will be possible to use considerably smaller amounts of catalyst (⅕ to ⅒) and/or a lower temperature (<80° C.) and/or a shortened reaction time. Since, in general, the formation of by-products in this preparation leads to an unwanted increase in viscosity, a distinct improvement in the reaction regime and product quality, including lower product viscosity (very important for the formulator), is thus possible.

[0446] b) Preparation of KOH-Based PU Prepolymers With TiPOSS

[0447] The formation of prepolymers obtained from the reaction of KOH-based polyols and aliphatic and aromatic isocyanates can be brought about with considerably smaller amounts of TiPOSS catalyst (⅕ to ⅒) and/or a lower temperature (<80° C.) and/or a shortened reaction time. Since the formation of by-products in this preparation leads to an unwanted increase in viscosity, a distinct improvement in the reaction regime and product quality can thus be assumed.

[0448] c) Use of TiPOSS in 2-Component Clear Encapsulating Systems and PU Varnishes Based on HDI and Other Aliphatic Isocyanates

[0449] Use of TiPOSS as catalyst increases the curing rate in 2-component polyurethane clear encapsulating systems and PU varnishes. The increase in molecular weight distinctly improves the mechanical properties of the varnishes and encapsulating compounds.

[0450] d) TDI Foams/Use of TiPOSS in the Production of Slabstock Foams

[0451] In the production of TDI-based slabstock foams, through use of TiPOSS as catalyst, it is possible to dispense with the use of tin compounds that are harmful to health—as in all other applications mentioned in 5.). There is no loss here in product quality.

[0452] e) FIPFG (Foamed in Place Foam Gaskets)—Sealant Foams

[0453] The production of 2-component polyurethane systems for the FIPFG process based on TiPOSS-catalysed curing is particularly advantageous since the curing process is accelerated by the higher reactivity of TiPOSS compared to DBTL. Polyurethane products can additionally be produced without tin compounds that are harmful to health, which is particularly important for the production of sealant materials in the medical sector, kitchen applications, etc.

[0454] f) Use of TiPOSS in Moisture-Curing 1-Component Isocyanate-Terminated Prepolymers

[0455] The curing of 1-component isocyanate-terminated prepolymers can be accelerated by the use of TiPOSS. It is possible to dispense with the use of tin compounds that are harmful to health. This is of particular relevance when these prepolymers are used as adhesives for customary floor coverings, since it is thus possible to avoid possible contamination, even if only by small amounts of tin, via the skin of the foot.

[0456] 6.) Specific Embodiments

[0457] Studies on the activity of heptaisobutyl-POSS-titanium(IV) ethoxide TiPOSS in comparison to DBTL

TABLE 1

Isocyanate	Catalyst	Polyols from the KOH-catalyzed reaction f = 2, MW = 2000, PO f = 2, MW = 4000, PO, EO tipped f = 3, MW = 4800, PO, EO tipped
P-MDI*	TiPOSS 0.2% vs. DTBL 0.2%	+
P-MDI	TiPOSS 0.2% vs. DTBL 0.2%	++

TABLE 2

SPUR	Catalyst	activity
Silylated Polyurethane (nonaromatic)	TiPOSS 0.2% vs. DTBL 0.2%	+

[0458] List of Abbreviations

[0459] Coatings, Adhesives, Sealants, Elastomers (CASE)

[0460] Diisononyl phthalate (DINP)

[0461] Dibutyltin dilaurate (DBTDL or DBTL)

[0462] Tin(II) 2-ethylhexanoate (tin octoate)

[0463] Silylated polyurethanes/silylated polyurethane resins (SPUR)

[0464] Heptaisobutyl POSS-titanium(IV) ethoxide (TiPOSS)

[0465] Dimethylcyclosiloxane (DMC)

[0466] Polyurethane (PU)

[0467] Potassium hydroxide (KOH)

[0468] FIPFG (foamed in place foam gaskets—sealant foams)

[0469] Titanium (Ti)

[0470] Polyhedral oligomeric silsesquioxane (POSS)

[0471] Embodiments, especially for Examples II

[0472] 1. Process for preparing prepolymers by reacting a component A with a component B in the presence of a catalyst in a liquid medium, where component A is a polyol and component B a crosslinking component (crosslinker), characterized in that component A is in deficiency relative to component B, and component A and component B are especially used in a ratio of at least 1:1.05, preferably of 1:2.2, and the catalyst is selected from the group of the tin-free polyhedral oligomeric metallosilsesquioxanes, preferably from the group of the titanium(IV) polyoctahedral silsesquioxanes.

[0473] 2. Process for preparing polyurethanes by combining a two-component system having a component A and a component B in the presence of a catalyst in a liquid medium, where component A is a polyol and component B a crosslinking component (crosslinker), characterized in that components A and B are present separately, and the catalyst has preferably been formulated with component A, and components A and B are present in a ratio of 1.2:1.0 up to 1.0:1.2.

[0474] 3. Process for producing polyurethane systems, characterized in that the prepolymers are prepared or preparable according to either of Embodiments 1 and 2 using a catalyst selected from the group of the tin-free polyhedral oligomeric metallosilsesquioxanes, preferably from the group of the titanium(IV) polyoctahedral silsesquioxanes.

[0475] 4. Process according to Embodiment 3, characterized in that the prepolymers are functionalized before the reaction with aminosilanes.

[0476] 5. Process according to any of the preceding embodiments, characterized in that auxiliaries are added.

[0477] 6. Process according to Embodiment 5, characterized in that the auxiliaries are selected from the group consisting of water, cell stabilizers, amine catalysts, fillers, adhesion promoters, moisture scavengers, plasticizers, UV stabilizers, thixotropic agents, or combinations thereof, preferably with one or more additives being one or more silanes.

[0478] 7. Process according to Embodiment 6, characterized in that the amine catalyst may be N,N-dimethylpiperazine and/or N,N-dimethylhexadecylamine or a mixture thereof.

[0479] 8. Process according to any of the preceding embodiments, characterized in that the catalyst is R^1-POSS-titanium(IV) ethoxide (TiPOSS) where R^1 is an alkyl, allyl or aryl radical or mixtures thereof, and R^1 is preferably a heptaisobutyl radical.

[0480] 9. Process according to any of the preceding embodiments, characterized in that the catalyst content is between 0.0001% and 5% by weight, preferably between 0.001% and 2% by weight, further preferably between 0.01% and 0.3% by weight, especially preferably 0.2, more especially preferably 0.03.

[0481] 10. Process according to any of the preceding embodiments, characterized in that the crosslinker is an isocyanate.

[0482] 11. Process according to Embodiment 10, characterized in that the isocyanate is aromatic and/or aliphatic, preferably methylene diphenyl isocyanates (MDI) and/or isophorone diisocyanate (IPDI) and/or a hexamethylene diisocyanate trimer (HDI trimer) or a mixture thereof.

[0483] 12. Process according to any of the preceding embodiments, characterized in that the polyol is a polyoxypropylene diol, preferably having a molar mass between 2000 g/mol and 18 000 g/mol, more preferably having a molar mass between 12 000 g/mol and 18 000 g/mol.

[0484] 13. Process according to any of the preceding Embodiments 1 to 11, characterized in that the polyol is an ethoxylated polyol, preferably a polyether triol tipped with ethoxy groups, and more preferably has a molar mass between 2000 g/mol and 4850 g/mol.

[0485] 14. Process according to any of Embodiments 1 to 11, characterized in that the polyol is a polyester polyol, preferably Desmophen 2200 B.

[0486] 15. Process according to any of the preceding embodiments, characterized in that the polyol comes from a KOH- and/or DMC-catalysed reaction.

[0487] 16. Process according to any of the preceding embodiments, characterized in that the liquid medium is an organic solvent, preferably diisononyl phthalate (DINP).

[0488] 17. Process according to any of the preceding embodiments, characterized in that it is tin-free.

1. A composition comprising at least one silylated polymer (SiP) and at least two catalysts A and B, wherein catalyst A is a metal-siloxane-silanol(ate) compound.

2. The composition according to claim **1**, wherein catalyst A is heptaisobutyl POSS-titanium(IV) ethoxide (TiPOSS), and catalyst B is a metal-siloxane-silanol(ate) compound.

3. The composition according to claim **2**, wherein catalyst A is heptaisobutyl POSS-titanium(IV) ethoxide (TiPOSS), and catalyst B is heptaisobutyl POSS-tin(IV) ethoxide (SnPOSS).

4. The composition according to claim **1**, wherein catalyst B is not a metal-siloxane-silanol(ate) compound.

5. The composition according to claim **4**, wherein catalyst B is an organometallic compound.

6. The composition according to claim **4**, wherein catalyst B is selected from the group consisting of tetraalkyl titanates, such as tetramethyl titanate, tetraethyl titanate, tetra-n-propyl titanate, tetraisopropyl titanate, tetra-n-butyl titanate, tetraisobutyl titanate, tetra-sec-butyl titanate, tetraoctyl titanate, tetra(2-ethylhexyl) titanate, dialkyl titanates ($(RO)_2TiO_2$ in which R is, for example, isopropyl, n-butyl, isobutyl), such as isopropyl n-butyl titanate; titanium acetylacetonate chelates, such as diisopropoxybis(acetylacetonate) titanate, diisopropoxybis(ethylacetylacetonate) titanate, di-n-butylbis(acetylacetonate) titanate, di-n-butylbis(ethylacetoacetate) titanate, triisopropoxidebis(acetylacetonate) titanate, zirconium tetraalkoxides, such as zirconium tetraethoxide, zirconium tetrabutoxide, zirconium tetrabutyrate, zirconium tetrapropoxide, zirconium carboxylates, such as zirconium diacetate; zirconium acetylacetonate chelates, such as zirconium tetra(acetylacetonate), tributoxyzirconium acetylacetonate, dibutoxyzirconium bisacetylacetonate, aluminium trisalkoxides, such as aluminium triisopropoxide, aluminium trisbutoxide; aluminium acetylacetonate chelates, such as aluminium tris(acetylacetonate) and aluminium tris(ethylacetylacetonate), organotin compounds such as dibutyltin dilaurate (DBTL), dibutyltin maleate, dibutyltin diacetate, tin(II) 2-ethylhexanoate (tin octoate), tin naphthenate, dimethyltin dineodecanoate, dioctyltin dineodecanoate, dimethyltin dioleate, dioctyltin dilaurate, dimethyl mercaptides, dibutyl mercaptides, dioctyl mercaptides, dibutyltin dithioglycolate, dioctyltin glycolate, dimethyltin glycolates, a solution of dibutyltin oxide, reaction products of zinc salts and organic carboxylic acids (carboxylates) such as zinc(II) 2-ethylhexanoate or zinc(II) neodecanoate, mixtures of bismuth carboxylates and zinc carboxylates, reaction products of bismuth salts and organic carboxylic acids, such as bismuth(III) tris(2-ethylhexanoate) and bismuth(III) tris(neodecanoate) and bismuth complexes, organolead compounds such as lead octoxide, organovanadium compounds, amine compounds such as butylamine, octylamine, dibutylamine, monoethanolamine, diethanolamine, triethanolamine, diethylenetriamine, oleylamine, cyclohexylamine, benzylamine, diethylaminopropylamine, xylylenediamine, triethylenediamine, guanidine, diphenylguanidine, 2,4,6-tris(dimethylaminomethyl)phenol, morpholine, N-methylmorpholine, 2-ethyl-4-methylimidazole and 1,8-diazabicyclo(5.4.0)undecene-7 (DBU), salts of these amines with carboxylic acids or other acids or mixtures thereof.

7. The composition according to claim **6**, wherein catalyst B is selected from the group consisting of dibutyltin dilaurate (DBTL), tin(II) 2-ethylhexanoate (tin octoate), zinc(II) 2-ethylhexanoate, zinc(II) neodecanoate, bismuth(III) tris(2-ethylhexanoate), bismuth(III) tris(neodecanoate) or mixtures thereof.

8. The composition according to claim **6**, wherein catalyst B is dibutyltin dilaurate (DBTL).

9. The composition according to claim **3**, wherein catalyst A is selected from the group consisting of heptaisobutyl POSS-titanium(IV) ethoxide (TiPOSS) and heptaisobutyl POSS-tin(IV) ethoxide (SnPOSS), preferably in that the catalyst is heptaisobutyl POSS-titanium(IV) ethoxide (TiPOSS).

10. The composition according to claim **9**, wherein said composition includes more than one catalyst A metal-siloxane-silanol(ate) compound.

11. The composition according to claim **1**, wherein the metal-siloxane-silanol(ate) compound has the general formula R*qSirOsMt where each R* is independently selected from the group consisting of optionally substituted C1- to C20-alkyl, optionally substituted C3- to C6-cycloalkyl, optionally substituted C2- to C20-alkenyl, optionally substituted C6- to C10-aryl, —OH and —O—(C1- to C10-alkyl), each M is independently selected from the group consisting of s- and p-block metals, d- and f-block transition metals, lanthanide and actinide metals and semimetals, especially from the group consisting of metals of transition groups 1, 2, 3, 4, 5, 8, 10 and 11 and metals of main groups 1, 2, 3, 4 and 5, preferably from the group consisting of Na, Zn, Sc, Nd, Ti, Zr, Hf, V, Fe, Pt, Cu, Ga, Sn and Bi; especially preferably from the group consisting of Zn, Ti, Zr, Hf, V, Fe, Sn and Bi,

q is an integer from 4 to 19,

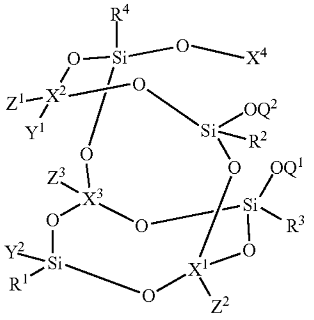
r is an integer from 4 to 10,

s is an integer from 8 to 30, and

t is an integer from 1 to 8.

12. The composition according to claim **1**, wherein the metal-siloxane-silanol(ate) compound has a general structure (I)

(I)



where

X^1, X^2 and X^3 are independently selected from Si and M^1, where M^1 is selected from the group consisting of s- and p-block metals, d- and f-block transition metals, lanthanide and actinide metals and semimetals,

especially from the group consisting of metals of transition groups 1, 2, 3, 4, 5, 8, 10 and 11 and metals of main groups 1, 2, 3, 4 and 5, preferably from the group consisting of Na, Zn, Sc, Nd, Ti, Zr, Hf, V, Fe, Pt, Cu, Ga, Sn and Bi; especially preferably from the group consisting of Zn, Ti, Zr, Hf, V, Fe, Sn and Bi,

Z^1, Z^2 and Z^3 are independently selected from the group consisting of L^2, R^5, R^6 and R^7, where L^2 is selected from the group consisting of —OH and —O—(C1- to C10-alkyl), especially —O—(C1- to C8-alkyl) or —O—(C1- to C6-alkyl), or where L^2 is selected from the group consisting of —OH, —O-methyl, —O-ethyl, —O-propyl, —O-butyl, —O-octyl, —O-isopropyl, and —O-isobutyl;

R^1, R^2, R^3, R^4, R^5, R^6 and R^7 are independently selected from the group consisting of optionally substituted C1- to C20-alkyl, optionally substituted C3- to C8-cycloalkyl, optionally substituted C2- to C20-alkenyl and optionally substituted C5- to C10-aryl;

Y^1 and Y^2 are independently —O-M^2-L^3_Δ, or Y^1 and Y^2 are associated and together are —O-$M^2(L^3_\Delta)$-O— or —O—, where L^3 is selected from the group consisting of —OH and —O—(C1- to C10-alkyl), especially —O—(C1- to C8-alkyl) or —O—(C1- to C6-alkyl), or where L^3 is selected from the group consisting of —OH, —O-methyl, —O-ethyl, —O-propyl, —O-butyl, —O-octyl, —O-isopropyl, and —O-isobutyl, and where M^2 is selected from the group consisting of s- and p-block metals, d- and f-block transition metals, lanthanide and actinide metals and semimetals,

especially from the group consisting of metals of transition groups 1, 2, 3, 4, 5, 8, 10 and 11 and metals of main groups 1, 2, 3, 4 and 5, preferably from the group consisting of Na, Zn, Sc, Nd, Ti, Zr, Hf, V, Fe, Pt, Cu, Ga, Sn and Bi; especially preferably from the group consisting of Zn, Ti, Zr, Hf, V, Fe, Sn and Bi,

and

X^4 is $-M^3L^1_\Delta$ or M^3 and Q^1 and Q^2 are H or each is a single bond joined to M^3, where L^1 is selected from the group consisting of —OH and —O—(C1- to C10-alkyl), especially —O—(C1- to C8-alkyl) or —O—(C1- to C6-alkyl), or where L^1 is selected from the group consisting of —OH, —O-methyl, —O-ethyl, —O-propyl, —O-butyl, —O-octyl, —O-isopropyl, and —O-isobutyl, and where M^3 is selected from the group consisting of s- and p-block metals, d- and f-block transition metals, lanthanide and actinide metals and semimetals,

especially from the group consisting of metals of transition groups 1, 2, 3, 4, 5, 8, 10 and 11 and metals of main groups 1, 2, 3, 4 and 5, preferably from the group consisting of Na, Zn, Sc, Nd, Ti, Zr, Hf, V, Fe, Pt, Cu, Ga, Sn and Bi; especially preferably from the group consisting of Zn, Ti, Zr, Hf, V, Fe, Sn and Bi,

or

X^4 is $-M^3L^1_\Delta$ and Q^2 is H or a single bond joined to M^3 and Q^1 is H, $M^4L^4_\Delta$ or where M^4 is selected from the group consisting of s- and p-block metals, d- and f-block transition metals, lanthanide and actinide metals and semimetals,

especially from the group consisting of metals of transition groups 1, 2, 3, 4, 5, 8, 10 and 11 and metals of main groups 1, 2, 3, 4 and 5, preferably from the group consisting of Na, Zn, Sc, Nd, Ti, Zr, Hf, V, Fe, Pt, Cu, Ga, Sn and Bi; especially preferably from the group consisting of Zn, Ti, Zr, Hf, V, Fe, Sn and Bi,

and where L^4 is selected from the group consisting of —OH and —O—(C1- to C10-alkyl), especially —O—(C1- to C8-alkyl) or —O—(C1- to C6-alkyl), or where L^4 is selected from the group consisting of —OH, —O-methyl, —O-ethyl, —O-propyl, —O-butyl, —O-octyl, —O-isopropyl, and —O-isobutyl, and where R^8 is selected from the group consisting of optionally substituted C1- to C20-alkyl, optionally substituted C3- to C8-cycloalkyl, optionally substituted C2- to C20-alkenyl and optionally substituted C5- to C10-aryl,

or

X^4, Q^1 and Q^2 are independently $-M^3L^1_\Delta$,

or

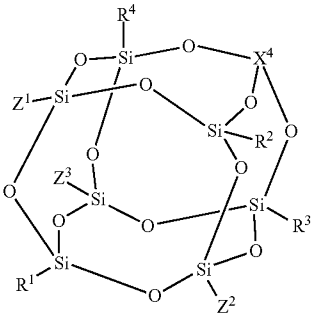
X^4 is $—Si(R^8)—O-M^3L^1_\Delta$, Q^2 is a single bond joined to the silicon atom of X^4 and Q^1 is $-M^4L^4_\Delta$,

or

X^4 is $—Si(R^8)—O-M^3L^1_\Delta$, Q^2 is a single bond joined to the silicon atom of X^4 and Q^1 is a single bond joined to the M^3 atom of X^4.

13. The composition according to claim **1**, wherein the metal-siloxane-silanol(ate) compound has the structural formula (II)

(II)



where

Z^1, Z^2 and Z^3 are independently selected from the group consisting of L^2, R^5, R^6 and R^7, where L^2 is selected from the group consisting of —OH and —O—(C1- to C10-alkyl), especially —O—(C1- to C8-alkyl) or —O—(C1- to C6-alkyl), or where L^2 is selected from the group consisting of —OH, —O-methyl, —O-ethyl, —O-propyl, —O-butyl, —O-octyl, —O-isopropyl, and —O-isobutyl

R^1, R^2, R^3 and R^4 are independently selected from the group consisting of optionally substituted C1- to C20-alkyl, optionally substituted C3- to C8-cycloalkyl, optionally substituted C2- to C20-alkenyl and optionally substituted C5- to C10-aryl;

and

X^4 is $-M^3L^1_\Delta$ or M^3 and Q^1 and Q^2 are H or each is a single bond joined to M^3, where L^1 is selected from the group consisting of —OH and —O—(C1- to C10-alkyl), especially —O—(C1- to C8-alkyl) or —O—(C1- to C6-alkyl), or where L^1 is selected from the group consisting of —OH, —O-methyl, —O-ethyl, —O-propyl, —O-butyl, —O-octyl, —O-isopropyl, and —O-isobutyl, and where M^3 is selected from the group consisting of s- and p-block metals, d- and f-block transition metals, lanthanide and actinide metals and semimetals,

especially from the group consisting of metals of transition groups 1, 2, 3, 4, 5, 8, 10 and 11 and metals of main groups 1, 2, 3, 4 and 5, preferably from the group consisting of Na, Zn, Sc, Nd, Ti, Zr, Hf, V, Fe, Pt, Cu, Ga, Sn and Bi; especially preferably from the group consisting of Zn, Ti, Zr, Hf, V, Fe, Sn and Bi,

or

X^4 is $-M^3L^1_\Delta$ and Q^2 is H or a single bond joined to M^3 and Q^1 is H, $M^4L^4_\Delta$ or where M^4 is selected from the group consisting of s- and p-block metals, d- and f-block transition metals, lanthanide and actinide metals and semimetals,

especially from the group consisting of metals of transition groups 1, 2, 3, 4, 5, 8, 10 and 11 and metals of main groups 1, 2, 3, 4 and 5, preferably from the group consisting of Na, Zn, Sc, Nd, Ti, Zr, Hf, V, Fe, Pt, Cu, Ga, Sn and Bi; especially preferably from the group consisting of Zn, Ti, Zr, Hf, V, Fe, Sn and Bi,

and where L^4 is selected from the group consisting of —OH and —O—(C1- to C10-alkyl), especially —O—(C1- to C8-alkyl) or —O—(C1- to C6-alkyl), or where L^4 is selected from the group consisting of —OH, —O-methyl, —O-ethyl, —O-propyl, —O-butyl, —O-octyl, —O-isopropyl, and —O-isobutyl, and where R^8 is selected from the group consisting of optionally substituted C1- to C20-alkyl, optionally substituted C3- to C8-cycloalkyl, optionally substituted C2- to C20-alkenyl and optionally substituted C5- to C10-aryl,

or

X^4, Q^1 and Q^2 are independently $-M^3L^1_{\Delta}$,

or

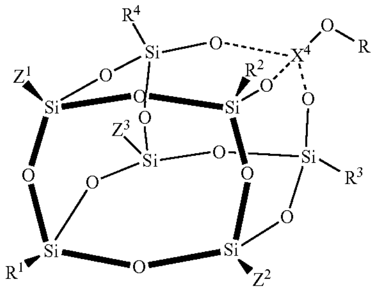
X^4 is —Si(R^8)—O-$M^3L^1_{\Delta}$, Q^2 is a single bond joined to the silicon atom of X^4 and Q^1 is $-M^4L^4_{\Delta}$,

or

X^4 is —Si(R^8)—O-$M^3L^1_{\Delta}$, Q^2 is a single bond joined to the silicon atom of X^4 and Q^1 is a single bond joined to the M^3 atom of X^4.

14. The composition according to claim **13**, wherein the metal-siloxane-silanol(ate) compound is a metal silsesquioxane of the structure (IV)

(IV)



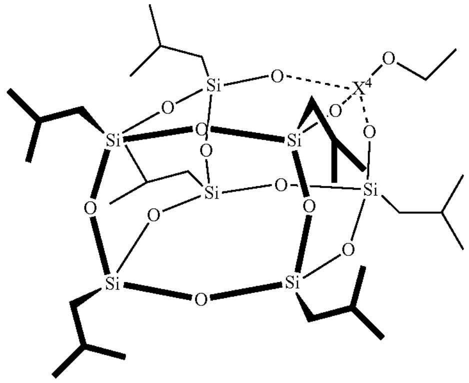
where

X4 is selected from the group consisting of metals of transition groups 1, 2, 3, 4, 5, 8, 10 and 11 and metals of main groups 1, 2, 3, 4 and 5, preferably from the group consisting of Na, Zn, Sc, Nd, Ti, Zr, Hf, V, Fe, Pt, Cu, Ga, Sn and Bi; especially preferably from the group consisting of Zn, Ti, Zr, Hf, V, Fe, Sn and Bi, most preferably from the group consisting of Ti and Sn, and is most preferably Ti, and

X4 is joined to OR where R is selected from the group consisting of —H, -methyl, -ethyl, -propyl, -butyl, -octyl, -isopropyl, and -isobutyl, Z^1, Z^2 and Z^3 are each independently C1- to C20-alkyl, C3- to C8-cycloalkyl, C2- to C20-alkenyl and C5- to C10-aryl, especially selected from the group consisting of methyl, ethyl, propyl, isopropyl, butyl, isobutyl, hexyl, heptyl, octyl, vinyl, allyl, butenyl and phenyl, and benzyl, and R^1, R^2, R^3 and R^4 are each independently C1- to C20-alkyl, C3- to C8-cycloalkyl, C2- to C20-alkenyl, and C5- to C10-aryl, especially selected from the group consisting of methyl, ethyl, propyl, isopropyl, butyl, isobutyl, hexyl, heptyl, octyl, vinyl, allyl, butenyl and phenyl, and benzyl.

15. The composition according to claim **14**, wherein the metal-siloxane-silanol(ate) compound is a metal silsesquioxane of the structure (IVb)

(IVb)



where X4 is selected from the group consisting of metals of transition groups 1, 2, 3, 4, 5, 8, 10 and 11 and metals of main groups 1, 2, 3, 4 and 5, preferably from the group consisting of Na, Zn, Sc, Nd, Ti, Zr, Hf, V, Fe, Pt, Cu, Ga, Sn and Bi; especially preferably from the group consisting of Zn, Ti, Zr, Hf, V, Fe, Sn and Bi, most preferably from the group consisting of Ti (and therefore is heptaisobutyl POSS-titanium(IV) ethoxide (TiPOSS)) and Sn (and therefore is heptaisobutyl POSS-tin(IV) ethoxide (SnPOSS)), and is most preferably Ti (and therefore is heptaisobutyl POSS-titanium(IV) ethoxide (TiPOSS)).

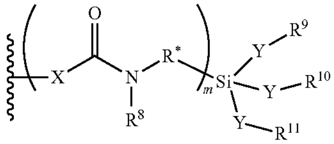
16. The composition according to claim **1**, wherein the silylated polymer (SiP) is obtainable by a synthesis, catalysed by a metal-siloxane-silanol(ate) compound, of at least one isocyanate-reactive compound, especially at least one hydroxy-functionalized polymer (component A), and one or more compounds having at least one isocyanate group (component B).

17. The composition according to claim **16**, wherein the metal-siloxane-silanol(ate) compound for catalysed synthesis of component A and component B is heptaisobutyl POSS-titanium(IV) ethoxide (TiPOSS) and/or heptaisobutyl POSS-tin(IV) ethoxide (SnPOSS), preferably heptaisobutyl POSS-titanium(IV) ethoxide (TiPOSS).

18. The composition according to claim **1**, wherein the polymer backbone (P) of the silylated polymer (SiP) has constituents selected from the group consisting of polyurethanes, polyureas, polyethers, polyesters, phenolic resins, polyalkylenes, poly(meth)acrylates, polyamides, polycaprolactones, polybutadienes or polyisoprenes, and polycarbonates or mixtures thereof, preferably from the group consisting of polyurethanes, polyureas, poly(meth)acrylates or polyethers or mixtures thereof, most preferably polyethers.

19. The composition according to claim **1**, wherein the silylated polymer (SiP) has at least two end groups of the general formula (V)

(V)



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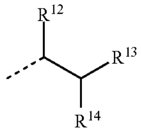
(Vb)



where

X is C, Si or a heteroatom and these, according to their valency, optionally have one or more R^8 radicals, preferably C, N, O, P, S, more preferably C, N or O, most preferably N or O, and each is bonded to a carbon in the polymer backbone,

R* is 0 or an optionally substituted straight-chain or branched C1- to C25-alkyl group or an optionally substituted C4- to C18-cycloalkyl group or an optionally substituted C4- to C18-aryl group and, when R*=0, the silicon atom is bonded directly to the nitrogen atom,

each Y is independently either O or a direct bond of the silicon atom to the respective R^9, R^{10} or R^{11} radical, and preferably at least one Y is O,

R^8 is H, an optionally substituted straight-chain or branched C1- to C16-alkyl group, an optionally substituted straight-chain or branched C2- to C16-alkenyl group or an optionally substituted straight-chain or branched C2- to C16-alkynyl group, an optionally substituted C4- to C14-cycloalkyl group or an optionally substituted C4- to C14-aryl group, or a radical of the general structure (Vb),

R^{12} and R^{14} are each independently H or a radical from the group consisting of $—R^{15}$, $—COOR^{15}$ and —CN,

R^{13} is H or a radical from the group consisting of $—CH_2—COOR^{15}$, $—COOR^{15}$, $—CONHR^{15}$, $—CON(R^{15})$, —CN, $—NO_2$, $—PO(OR^{15})_2$, $—SOR^{15}$ and $—SO_2OR^{15}$,

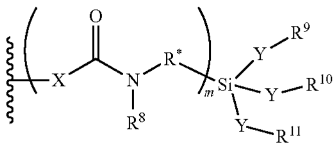
R^{15} is a hydrocarbyl radical having 1 to 20 carbon atoms and optionally having at least one heteroatom,

R^9, R^{10} and R^{11} are independently H, an optionally substituted straight-chain or branched C1- to C5-alkyl group, an optionally substituted straight-chain or branched C2- to C10-alkenyl group or an optionally substituted C4- to C14-cycloalkyl group or an optionally substituted C4- to C14-aryl group,

m is 0 or 1 and, when m=0, the silicon atom is bonded directly to a carbon in the polymer backbone (P).

20. The composition according to claim **19**, wherein the silylated polymer (SiP) has a polyether polymer backbone having at least two end groups of the general formula (V)

(V)



where

X is N or O and N optionally has an R^8 radical,

R* is 0 or an optionally substituted straight-chain or branched C1- to C20-alkyl group or an optionally substituted C4- to C12-cycloalkyl group or an optionally substituted C4- to C12-aryl group, preferably an optionally substituted straight-chain or branched C1- to C15-alkyl group, and, when R*=0, the silicon atom is bonded directly to the nitrogen atom,

Y in $Y—R^9$ and $Y—R^{10}$ are O and the Y in $Y—R^{11}$ is either O or a direct bond of the silicon atom to the respective R^{11} radical,

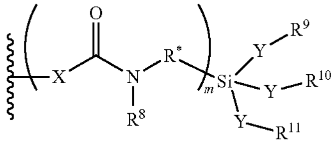
R^8 is H, an optionally substituted straight-chain or branched C1- to C10-alkyl group, an optionally substituted straight-chain or branched C2- to C10-alkenyl group or an optionally substituted straight-chain or branched C2- to C10-alkynyl group, an optionally substituted C4- to C10-cycloalkyl group or an optionally substituted C4- to C10-aryl group or a succinic acid derivative of the general structure (Vb),

R^9, R^{10} and R^{11} are independently H, an optionally substituted straight-chain or branched C1- to C4-alkyl group, an optionally substituted straight-chain or branched C2- to C5-alkenyl group or an optionally substituted C4- to C10-cycloalkyl group or an optionally substituted C4- to C10-aryl group, preferably independently H or a C1- to C2-alkyl group, and

m is 0 or 1 and, when m=0, the silicon atom is bonded directly to a carbon in the polymer backbone (P), preferably m=1.

21. The composition according to claim **20**, wherein the silylated polymer (SiP) has a polyether polymer backbone having at least two end groups of the general formula (V)

(V)



where

R* is 0 or an optionally substituted straight-chain or branched C1- to C15-alkyl group or an optionally substituted C4- to C6-cycloalkyl group or an optionally substituted C4- to C6-aryl group, preferably an optionally substituted straight-chain or branched C1- to C10-alkyl group, more preferably a C1-alkyl group (=alpha-silane) or a C3-alkyl group (=gamma-silane), and, when R*=0, the silicon atom is bonded directly to the nitrogen atom,

R^8 is H, an optionally substituted straight-chain or branched C1- to C8-alkyl group, an optionally substituted straight-chain or branched C2- to C8-alkenyl group or an optionally substituted straight-chain or branched C2- to C8-alkynyl group, an optionally substituted C4- to C6-cycloalkyl group or an optionally substituted C4- to C6-aryl group,

R^9, R^{10} and R^{11} are independently H, an optionally substituted straight-chain or branched C1- to C4-alkyl group, an optionally substituted straight-chain or branched C2- to C5-alkenyl group or an optionally substituted C4- to C6-cycloalkyl group or an optionally substituted C4- to C6-aryl group, preferably independently H or a C1- to C2-alkyl group, and

m is 0 or 1 and, when m=0, the silicon atom is bonded directly to a carbon in the polymer backbone (P), preferably m=1.

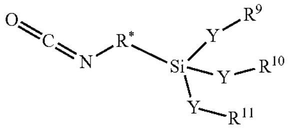
22. The composition according to claim **16**, wherein the hydroxy-functionalized polymer is selected from the group consisting of polyoxyalkylene diols or polyoxyalkylene triols, especially polyoxyethylene di- and triols and polyoxypropylene di- and triols, higher-functionality polyols such as sorbitol, pentaerythritol-started polyols, ethylene oxide-terminated polyoxypropylene polyols, polyester polyols, styrene-acrylonitrile, acryloyl-methacrylate, (poly)urea-grafted or -containing polyether polyols, polycarbonate polyols, CO_2 polyols, polyhydroxy-functional fats and oils, especially castor oil, polyhydrocarbon polyols such as dihydroxypolybutadiene, polytetrahydrofuran-based polyethers (PTMEG), OH-terminated prepolymers based on the reaction of a polyetherol or polyesterol with a diisocyanate, polypropylene diols, polyester polyols or mixtures thereof, preferably polypropylene diols, polyester polyols, or mixtures thereof.

23. The composition according to claim **22**, wherein the hydroxy-functionalized polymer is selected from the group consisting of polyoxyalkylene diols, polyoxyalkylene triols, especially polyoxyethylene di- and/or triols and/or polyoxypropylene di- and/or triols, KOH-catalysed hydroxy-functionalized polyethers or double metal cyanide complex-catalysed (DMC-catalysed) hydroxy-functionalized polyethers or mixtures thereof.

24. The composition according to claim **16**, wherein component B is selected from the group consisting of aromatic and/or aliphatic isocyanates (Iso) of the general structure (VI) or mixtures thereof or isocyanatosilanes (Iso-Si) of the general structure (VII) or mixtures

$$R^x\text{—}(N{=}C{=}O)_z \quad \text{(VI)}$$

(VII)



R^x is a carbon-containing group, preferably at least one aromatic or aliphatic group or mixtures thereof, more preferably an optionally substituted straight-chain or branched C1- to C16-alkyl group, an optionally substituted straight-chain or branched C2- to C16-alkenyl group or an optionally substituted straight-chain or branched C2- to C16-alkynyl group, an optionally substituted C4- to C14-cycloalkyl group or an optionally substituted C4- to C14-aryl group, most preferably diphenylmethane, toluene, dicyclohexylmethane, hexane or methyl-3,5,5-trimethylcyclohexyl,

each Y is independently either O or a direct bond of the silicon atom to the respective R^9, R^{10} or R^{11} radical, and preferably at least one Y is O,

z is at least 1, preferably at least 2,

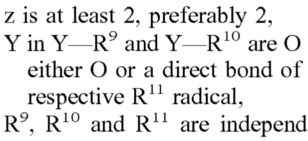
R^9, R^{10} and R^{11} are independently H, an optionally substituted straight-chain or branched C1- to C5-alkyl group, an optionally substituted straight-chain or branched C2- to C10-alkenyl group or an optionally substituted C4- to C8-cycloalkyl group or an optionally substituted C4- to C8-aryl group and

R* is 0 or an optionally substituted straight-chain or branched C1- to C25-alkyl group or an optionally substituted C4- to C18-cycloalkyl group or an optionally substituted C4- to C18-aryl group and, when R*=0, the silicon atom is bonded directly to the nitrogen atom.

25. The composition according to claim **16**, wherein component B is selected from the group consisting of aromatic and/or aliphatic isocyanates (Iso) of the general structure (VI) or mixtures thereof or isocyanatosilanes (Iso-Si) of the general structure (VII) or mixtures thereof

$$R^x\text{—}(N{=}C{=}O)_z \quad \text{(VI)}$$

(VII)



where

R^x is diphenylmethane, toluene, dicyclohexylmethane, hexane or methyl-3,5,5-trimethylcyclohexyl, preferably diphenylmethane or hexane or methyl-3,5,5-trimethylcyclohexyl, most preferably diphenylmethane or methyl-3,5,5-trimethylcyclohexyl, and

z is at least 2, preferably 2,

Y in Y—R^9 and Y—R^{10} are O and the Y in Y—R^{11} is either O or a direct bond of the silicon atom to the respective R^{11} radical,

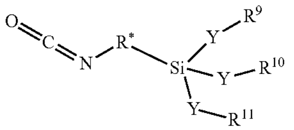
R^9, R^{10} and R^{11} are independently H, an optionally substituted straight-chain or branched C1- to C3-alkyl group and

R* is 0 or an optionally substituted straight-chain or branched C1- to C15-alkyl group or an optionally substituted C4- to C6-cycloalkyl group or an optionally substituted C4- to C6-aryl group, preferably an optionally substituted straight-chain or branched C1- to C10-alkyl group, more preferably a C1-alkyl group (=alpha-silane) or a C3-alkyl group (=gamma-silane), and, when R*=0, the silicon atom is bonded directly to the nitrogen atom.

26. The composition according to claim **25**, wherein Component B is at least one isocyanate (Iso) of the general structure (VI) selected from the group consisting of polymeric, oligomeric and monomeric methylene diphenyl isocyanate (MDI), especially from 4,4'-methylene diphenyl isocyanate (4,4'-MDI), 2,4'-methylene diphenyl isocyanate (2,4'-MDI), 2,2'-methylene diphenyl isocyanate (2,2'-MDI), 4,4'-diisocyanatodicyclohexylmethane (H12MDI), 2-methylpentamethylene 1,5-diisocyanate, dodecamethylene 1,12-diisocyanate, lysine and lysine ester diisocyanate, cyclohexane 1,3-diisocyanate, cyclohexane 1,4-diisocyanate, perhydro(diphenylmethane 2,4'-diisocyanate), perhydro(diphenylmethane 4,4'-diisocyanate), 1,4-diisocyanato-2,2,6-trimethylcyclohexane (TMCDI), 3-isocyanatomethyl-3,5,5-trimethylcyclohexyl isocyanate (=isophorone diisocyanate or IPDI), hexamethylene 1,6-diisocyanate (HDI) or the trimer thereof (HDI trimer), 2,2,4- and/or 2,4,4-trimethylhexamethylene 1,6-diisocyanate, 1,4-bis(isocyanato)cyclohexane, 1,4-bis(isocyanato)benzene (PPDI), 1,3- and/or 1,4-bis(isocyanatomethyl)cyclohexane, m- and/or p-xylylene diisocyanate (m- and/or p-XDI), m- and/or p-tetramethylxylylene 1,3-diisocyanate, m- and/or p-tetramethylxylylene 1,4-diisocyanate, bis(1-isocyanato-1-methylethyl)naphthalene, 1,3-bis(isocyanato-4-methylphenyl)-2,4-dioxo-1,3-diazetidine, naphthalene 1,5-diisocyanate (NDI), 3,3'-dimethyl-4,4'-diisocyanatodiphenyl (TODI), tolylene 2,4- and/or 2,6-diisocyanate (TDI), 1,3-bis(isocyanatomethyl) benzene or mixtures thereof, preferably 4,4'-methylene diphenyl isocyanate (4,4'-MDI) or isophorone diisocyanate (IPDI), hexamethylene 1,6-diisocyanate (HDI) or the trimer thereof (HDI trimer) or mixtures thereof, most preferably 4,4'-methylene diphenyl isocyanate (4,4'-MDI) or isophorone diisocyanate (IPDI) or mixtures thereof.

27. The composition according to claim **26**, wherein Component B is at least one isocyanatosilane (Iso-Si) of the general structure (VII) is selected, or mixtures thereof,

(VII)

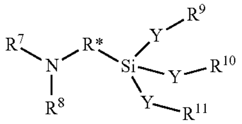


where R^9, R^{10} , and R^{11} and are preferably a methyl or ethyl group or mixtures thereof, preferably selected from the group consisting of 3-(triethoxysilyl)methyl isocyanate, 3-(trimethoxysilyl)methyl isocyanate, 3-(triethoxysilyl)ethyl isocyanate, 3-(trimethoxysilyl) ethyl isocyanate, 3-(triethoxysilyl)propyl isocyanate, 3-(trimethoxysilyl)propyl isocyanate, 3-(triethoxysilyl) butyl isocyanate, 3-(trimethoxysilyl)butyl isocyanate, 3-(triethoxysilyl)pentyl isocyanate, 3-(trimethoxysilyl) pentyl isocyanate, 3-(triethoxysilyl)hexyl isocyanate, 3-(trimethoxysilyl)hexyl isocyanate or mixtures thereof, preferably 3-(trimethoxysilyl)methyl isocyanate, 3-(triethoxysilyl)methyl isocyanate, 3-(trimethoxysilyl)propyl isocyanate, 3-(triethoxysilyl)propyl isocyanate or mixtures thereof, more preferably 3-(trimethoxysilyl)propyl isocyanate, 3-(triethoxysilyl) propyl isocyanate, or mixtures thereof.

28. The composition according to claim **1**, wherein the silylated polymer (SiP) has been prepared by reaction with an aminosilane (AmSi).

29. The composition according to claim **28**, wherein the aminosilane (AmSi) is at least one aminosilane (AmSi) of the general structure (VIII) is selected, or is a mixture thereof,

(VIII)



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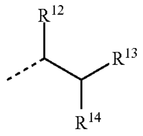
(Vb)



where

R^7 is H,

R^8 is H, an optionally substituted straight-chain or branched C1- to C25-alkyl group, an optionally substituted straight-chain or branched C2- to C25-alkenyl group or an optionally substituted C4- to C18-cycloalkyl group or an optionally substituted C4- to C18-aryl group, or a radical of the general structure (Vb),

R* is 0 or an optionally substituted straight-chain or branched C1- to C25-alkyl group or an optionally substituted C4- to C18-cycloalkyl group or an optionally substituted C4- to C18-aryl group and, when R*=0, the silicon atom is bonded directly to the nitrogen atom,

R^{12} and R^{14} are each independently H or a radical from the group consisting of —R^{15}, —$COOR^{15}$ and —CN,

R^{13} is H or a radical from the group consisting of —CH_2—$COOR^{15}$, —$COOR^{15}$, —$CONHR^{15}$, —$CON(R^{15})$, —CN, —NO_2, —$PO(OR^{15})_2$, —SOR^{15} and —SO_2OR^{15},

R^{15} is a hydrocarbyl radical having 1 to 20 carbon atoms and optionally having at least one heteroatom,

R^9, R^{10} and R^{11} are independently H, an optionally substituted straight-chain or branched C1- to C4-alkyl group, an optionally substituted straight-chain or branched C2- to C5-alkenyl group or an optionally substituted C4- to C10-cycloalkyl group or an optionally substituted C4- to C10-aryl group, preferably independently H or a C1- to C2-alkyl group, and

each Y is independently either O or a direct bond of the silicon atom to the respective R^9, R^{10} or R^{11} radical, and preferably at least one Y is O.

30. The composition according to claim **29**, wherein the aminosilane (AmSi) of the general structure (VIII) is selected from the group of N-[3-(trimethoxysilyl)methyl] butylamine, N-[3-(triethoxysilyl)methyl]butylamine, N-[3-(trimethoxysilyl)ethyl]butylamine, N-[3-(triethoxysilyl) ethyl]butylamine, N-[3-(trimethoxysilyl)propyl]butylamine, N-[3-(triethoxysilyl)propyl]butylamine, N-[3-(trimethoxysilyl)butyl]butylamine, N-[3-(triethoxysilyl)butyl] butylamine, N-[3-(trimethoxysilyl)pentyl]butylamine, N-[3-(triethoxysilyl)pentyl]butylamine, N-[3-(trimethoxysilyl) hexyl]butylamine, N-[3-(triethoxysilyl)hexyl]butylamine, 3-aminopropyltrimethoxysilane, 3-aminopropyltriethoxysilane, N-cyclohexyl-3-aminopropyltrimethoxysilane, N-cyclohexyl-3-aminopropyltriethoxysilane, N-(3-trimethoxysilylpropyl)aminosuccinic acid diethyl ester, N-(3-triethoxysilylpropyl)aminosuccinic acid diethyl ester or a mixture thereof, preferably N-[3-(trimethoxysilyl)methyl] butylamine, N-[3-(triethoxysilyl)methyl]butylamine, N-[3-(trimethoxysilyl)propyl]butylamine, N-[3-(triethoxysilyl) propyl]butylamine, N-(3-trimethoxysilylpropyl) aminosuccinic acid diethyl ester, N-(3-triethoxysilylpropyl) aminosuccinic acid diethyl ester, more preferably N-[3-(trimethoxysilyl)propyl]butylamine, N-[3-(triethoxysilyl)propyl]butylamine, N-[3-(trimethoxysilyl)methyl]butylamine, N-[3-(triethoxysilyl)methyl]butylamine, N-(3-triethoxysilylpropyl)aminosuccinic acid diethyl ester, N-(3-trimethoxysilylpropyl)aminosuccinic acid diethyl ester or a mixture thereof, most preferably N-(3-triethoxysilylpropyl)aminosuccinic acid diethyl ester, N-[3-(triethoxysilyl)propyl]butylamine, N-[3-(triethoxysilyl)methyl]butylamine or a mixture thereof.

31. (canceled)

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