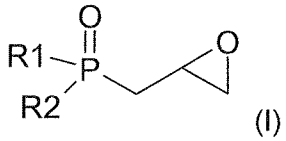
WO 2007/066383 describes hyperbranched polyesters which were reacted with phosphorus compounds, such as 9,10-dihydro-9-oxa-10-phosphaphenanthrene 10-oxide, and also the use of these as flame retardants for resins. The low thermal and hydrolytic stability of the ester groups is disadvantageous.

It was therefore an object of the embodiments disclosed herein to provide a halogen-free flame retardant which can also be used in the production of polyurethanes.

Another object of the embodiments disclosed herein was to provide flame retardants whose use does not lead to emissions in polymers, in particular in polyurethanes, and specifically in polyurethane foams, and whose use in polymers, in particular in polyurethanes and specifically in polyurethane foams, does not lead to impairment of properties, in particular of mechanical properties.

These objects of the disclosureare achieved by a phosphorus containing alcohol, obtainable or obtained by a process comprising the reaction of at least one alcohol with a phosphorus containing compound of the general formula (I):

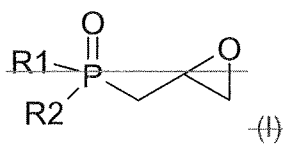


(I)

wherein

R1, R2 are equal or different linear or branched C_1-C_{18}-alkyl, linear or branched C_2-C_{18}-alkenyl, linear or branched C_2-C_{18}-alkinyl, C_3-C_{10}-cycloalkyl, C_6-C_{10}-aryl, heteroaryl, C_6-C_{10}-aryl-C_1-C_{10}-alkyl, benzyl, OR^3, SR^3, or R^1 and R^2 in combination with the P atom which they are bound to form a 4 to 8-membered ring system;
R^3 is linear or branched C_1-C_{16}-alkyl, linear or branched C_2-C_{16}-alkenyl, linear or branched C_2-C_{16}-alkinyl, C_3-C_{10}-cycloalkyl, C_6-C_{10}-aryl, heteroaryl or C_6-C_{10}-aryl-C_1-C_{10}-alkyl, benzyl.

In an aspect, there is provided a process for preparing a phosphorus containing alcohol comprising at least one phosphorus-containing group~~, obtainable or obtained by a process comprising the reaction of at least one alcohol with a phosphorus containing compound of the general formula (I):~~



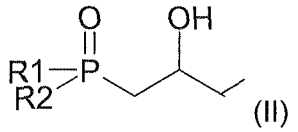
~~(I)~~

~~wherein~~

~~R1, R2 are equal or different linear or branched C_1-C_{18}-alkyl, linear or branched C_2-C_{18}-alkenyl, linear or branched C_2-C_{18}-alkinyl, C_3-C_{10}-cycloalkyl, C_6-C_{10}-aryl, heteroaryl, C_6-C_{10}-aryl-C_1-C_{10}-alkyl, benzyl, OR^3, SR^3, or R^1 and R^2 in combination with the P atom which they are bound to form a 4 to 8-membered ring system;~~

~~R^3 is hydrogen, linear or branched C_1-C_{16}-alkyl, linear or branched C_2-C_{16}-alkenyl, linear or branched C_2-C_{16}-alkinyl, C_3-C_{10}-cycloalkyl, C_6-C_{10}-aryl, heteroaryl or C_6-C_{10}-aryl-C_1-C_{10}-alkyl, benzyl, and~~

wherein the at least one phosphorus-containing group is a group of the general formula (II):



(II)

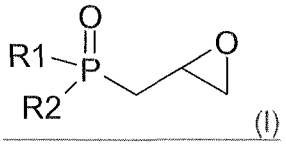
wherein

R1, R2 are equal or different linear or branched C_1-C_{18}-alkyl, linear or branched C_2-C_{18}-alkenyl, linear or branched C_2-C_{18}-alkinyl, C_3-C_{10}-cycloalkyl, C_6-C_{10}-aryl, heteroaryl, C_6-C_{10}-aryl-C_1-C_{10}-alkyl, benzyl, OR^3, SR^3, or R^1 and R^2 in combination with the P atom which they are bound to form a 4 to 8-membered ring system;

R^3 is hydrogen, linear or branched C_1-C_{16}-alkyl, linear or branched C_2-C_{16}-alkenyl, linear or branched C_2-C_{16}-alkinyl, C_3-C_{10}-cycloalkyl, C_6-C_{10}-aryl, heteroaryl or C_6-C_{10}-aryl-C_1-C_{10}-alkyl, benzyl,

and wherein the phosphorus is present in the form of phosphate, phosphonate or phosphinate groups or metal salts thereof

the process comprising the reaction of at least one polyol with a phosphorus containing compound of the general formula (I) in the presence of a catalyst:



(I)

wherein

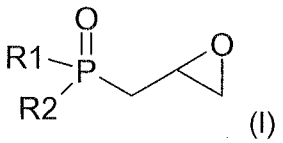
R1, R2 are equal or different linear or branched C_1-C_{18}-alkyl, linear or branched C_2-C_{18}-alkenyl, linear or branched C_2-C_{18}-alkinyl, C_3-C_{10}-cycloalkyl, C_6-C_{10}-aryl, heteroaryl, C_6-C_{10}-aryl-C_1-C_{10}-alkyl, benzyl, OR^3, SR^3, or R^1 and R^2 in combination with the P atom which they are bound to form a 4 to 8-membered ring system;

R^3 is hydrogen, linear or branched C_1-C_{16}-alkyl, linear or branched C_2-C_{16}-alkenyl, linear or branched C_2-C_{16}-alkinyl, C_3-C_{10}-cycloalkyl, C_6-C_{10}-aryl, heteroaryl or C_6-C_{10}-aryl-C_1-C_{10}-alkyl, benzyl, and

~~wherein the at least one alcohol is a polyol and~~

wherein the phosphorus containing alcohol has a phosphorus content of from 3 to 30 % by weight based on the total weight of the phosphorus containing alcohol, has an OH-functionality of from 1 to 8, and a molecular weight of from 100 to 6000 g/mol.

The phosphorus containing alcohols according to the present disclosure can be prepared by a process for preparing a phosphorus containing alcohol, comprising the reaction of at least one alcohol with a phosphorus containing compound of the general formula (I):

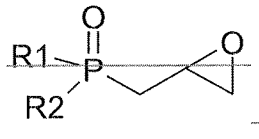


(I)

wherein

R1, R2 are equal or different linear or branched C_1-C_{18}-alkyl, linear or branched C_2-C_{18}-alkenyl, linear or branched C_2-C_{18}-alkinyl, C_3-C_{10}-cycloalkyl, C_6-C_{10}-aryl, heteroaryl, C_6-C_{10}-aryl-C_1-C_{10}-alkyl, benzyl, OR^3, SR^3, or R^1 and R^2 in combination with the P atom which they are bound to form a 4 to 8-membered ring system;
R^3 is linear or branched C_1-C_{16}-alkyl, linear or branched C_2-C_{16}-alkenyl, linear or branched C_2-C_{16}-alkinyl, C_3-C_{10}-cycloalkyl, C_6-C_{10}-aryl, heteroaryl or C_6-C_{10}-aryl-C_1-C_{10}-alkyl, benzyl,
which is also subject of the present disclosure.

~~In another aspect, there is provided a process for preparing a phosphorus containing alcohol comprising at least one phosphorus-containing group, comprising the reaction of at least one alcohol with a phosphorus containing compound of the general formula (I):~~

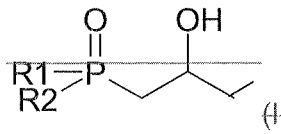


~~(I)~~

~~wherein~~

~~R1, R2 are equal or different linear or branched C_1-C_{18}-alkyl, linear or branched C_2-C_{18}-alkenyl, linear or branched C_2-C_{18}-alkinyl, C_3-C_{10}-cycloalkyl, C_6-C_{10}-aryl, heteroaryl, C_6-C_{10}-aryl-C_1-C_{10}-alkyl, benzyl, OR^3, SR^3, or R^1 and R^2 in combination with the P atom which they are bound to form a 4 to 8-membered ring system;~~
~~R^3 is hydrogen, linear or branched C_1-C_{16}-alkyl, linear or branched C_2-C_{16}-alkenyl, linear or branched C_2-C_{16}-alkinyl, C_3-C_{10}-cycloalkyl, C_6-C_{10}-aryl, heteroaryl or C_6-C_{10}-aryl-C_1-C_{10}-alkyl, benzyl, and~~

~~wherein the at least one phosphorus-containing group is a group of the general formula (II):~~



~~(II)~~

~~wherein~~
~~R1, R2 are equal or different linear or branched C_1-C_{18}-alkyl, linear or branched C_2-C_{18}-alkenyl, linear or branched C_2-C_{18}-alkinyl, C_3-C_{10}-cycloalkyl, C_6-C_{10}-aryl, heteroaryl, C_6-C_{10}-aryl-C_1-C_{10}-alkyl, benzyl, OR^3, SR^3, or R^1 and R^2 in combination with the P atom which they are bound to form a 4 to 8-membered ring system;~~
~~R^3 is hydrogen, linear or branched C_1-C_{16}-alkyl, linear or branched C_2-C_{16}-alkenyl, linear or branched C_2-C_{16}-alkinyl, C_3-C_{10}-cycloalkyl, C_6-C_{10}-aryl, heteroaryl or C_6-C_{10}-aryl-C_1-C_{10}-alkyl, benzyl,~~

~~wherein the at least one alcohol is a polyol and~~

~~wherein the phosphorus containing alcohol has a phosphorus content of from 3 to 30 % by weight based on the total weight of the phosphorus containing alcohol.~~

In another aspect, there is provided a phosphorus containing alcohol obtainable or obtained by the process as defined above.

~~In another aspect, there is provided the use of a phosphorus containing alcohol as defined above or a phosphorus containing alcohol obtainable or obtained according to the process as defined above as a flame retardant.~~

~~In another aspect, there is provided the use of a phosphorus containing alcohol as defined above or a phosphorus containing alcohol obtainable or obtained according to the process as defined above for the preparation of a polyurethane with improved flammability properties.~~

In another aspect, there is provided a process for the preparation of a polyurethane comprising the reaction of at least one isocyanate (a), at least one polyol (b) and at least one phosphorus containing alcohol obtainable or obtained according to the process as defined above or a phosphorus containing alcohol ~~obtainable or obtained according to the process~~ as defined above

wherein the at least one phosphorus containing alcohol is used in an amount of 1 to 30 % of the total of all polyols and alcohols used.

In another aspect, there is provided a polyurethane obtainable or obtained by a process as defined above.

As a solution the phosphorus containing alcohols according to the disclosure were found. The synthesis is an easy one-step reaction based on cheap raw materials. Due to the diversity of alcohols which can be used as starting materials, a wide range of phosphorus containing alcohols can be easily obtained to adjust performance and processing as desired.

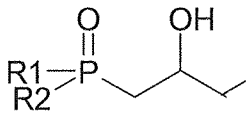
The alcohol used for the preparation of the phosphorus containing alcohols according to the invention can be any suitable alcohol including monoalcohols, and polyols. In the context of the present invention, a polyol is defined as having at least two OH groups, for example two, three, four, five, six or more OH-groups. Therefore, the resulting phosphorus containing alcohol according to the invention might also be a phosphorus containing alcohol.

The phosphorus containing alcohols according to the present invention work as flame retardants and at the same time can improve mechanical properties (or prevent deterioration of properties as observed with non-reactive flame retardants). The flame retardancy is not only influenced by the phosphorus content but also by the OH-functionality as well as the type of alcohol.

By varying the degree of partial functionalization, the hydroxyl-number of the resulting product can be adjusted to OH-values common either for flexible or for rigid foam. Thus the phosphorus containing alcohol can be easily blended with common polyols and show minimum interference

on foaming. Thus tailor-made flame retardants for flexible and rigid polyurethane foams are provided.

The phosphorus containing alcohol according to the present invention comprises at least one phosphorus-containing group. This at least one phosphorus-containing group is preferably a group of the general formula (II):



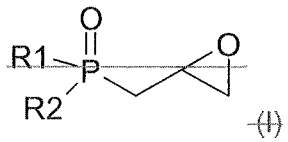
(II)

wherein

R1, R2 are equal or different linear or branched C_1-C_{18}-alkyl, linear or branched C_2-C_{18}-alkenyl, linear or branched C_2-C_{18}-alkinyl, C_3-C_{10}-cycloalkyl, C_6-C_{10}-aryl, heteroaryl, C_6-C_{10}-aryl-C_1-C_{10}-

Claims

1. A process for preparing a Pphosphorus containing alcohol comprising at least one phosphorus-containing group, ~~obtainable or obtained by a process comprising the reaction of at least one alcohol with a phosphorus containing compound of the general formula (I):~~



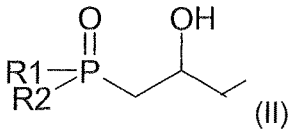
~~(I)~~

~~wherein~~

~~R1, R2 are equal or different linear or branched C_1-C_{18}-alkyl, linear or branched C_2-C_{18}-alkenyl, linear or branched C_2-C_{18}-alkinyl, C_3-C_{10}-cycloalkyl, C_6-C_{10}-aryl, heteroaryl, C_6-C_{10}-aryl-C_1-C_{10}-alkyl, benzyl, OR^3, SR^3, or R^1 and R^2 in combination with the P atom which they are bound to form a 4 to 8-membered ring system;~~

~~R^3 is hydrogen, linear or branched C_1-C_{16}-alkyl, linear or branched C_2-C_{16}-alkenyl, linear or branched C_2-C_{16}-alkinyl, C_3-C_{10}-cycloalkyl, C_6-C_{10}-aryl, heteroaryl or C_6-C_{10}-aryl-C_1-C_{10}-alkyl, benzyl, and~~

wherein the at least one phosphorus-containing group is a group of the general formula (II):



(II)

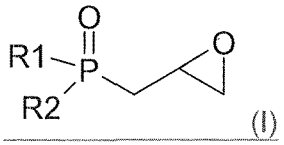
wherein

R1, R2 are equal or different linear or branched C_1-C_{18}-alkyl, linear or branched C_2-C_{18}-alkenyl, linear or branched C_2-C_{18}-alkinyl, C_3-C_{10}-cycloalkyl, C_6-C_{10}-aryl, heteroaryl, C_6-C_{10}-aryl-C_1-C_{10}-alkyl, benzyl, OR^3, SR^3, or R^1 and R^2 in combination with the P atom which they are bound to form a 4 to 8-membered ring system;

R^3 is hydrogen, linear or branched C_1-C_{16}-alkyl, linear or branched C_2-C_{16}-alkenyl, linear or branched C_2-C_{16}-alkinyl, C_3-C_{10}-cycloalkyl, C_6-C_{10}-aryl, heteroaryl or C_6-C_{10}-aryl-C_1-C_{10}-alkyl, benzyl,

and wherein the phosphorus is present in the form of phosphate, phosphonate or phosphinate groups or metal salts thereof

the process comprising the reaction of at least one polyol with a phosphorus containing compound of the general formula (I) in the presence of a catalyst:



(I)

wherein

R1, R2 are equal or different linear or branched C_1-C_{18}-alkyl, linear or branched C_2-C_{18}-alkenyl, linear or branched C_2-C_{18}-alkinyl, C_3-C_{10}-cycloalkyl, C_6-C_{10}-aryl, heteroaryl, C_6-C_{10}-aryl-C_1-C_{10}-alkyl, benzyl, OR^3, SR^3, or R^1 and R^2 in combination with the P atom which they are bound to form a 4 to 8-membered ring system;

R^3 is hydrogen, linear or branched C_1-C_{16}-alkyl, linear or branched C_2-C_{16}-alkenyl, linear or branched C_2-C_{16}-alkinyl, C_3-C_{10}-cycloalkyl, C_6-C_{10}-aryl, heteroaryl or C_6-C_{10}-aryl-C_1-C_{10}-alkyl, benzyl, and

~~wherein the at least one alcohol is a polyol and~~

wherein the phosphorus containing alcohol has a phosphorus content of from 3 to 30 % by weight based on the total weight of the phosphorus containing alcohol, has an OH-functionality of from 1 to 8, and a molecular weight of from 100 to 6000 g/mol.

~~2. The phosphorus containing alcohol according to claim 1, wherein the phosphorus is present in the form of phosphate, phosphonate or phosphinate groups or metal salts thereof.~~

~~3. The phosphorus containing alcohol according to claim 1 or 2, wherein the phosphorus containing alcohol has an OH-functionality of from 1 to 8.~~

4. The ~~phosphorus containing alcohol~~process according to ~~any of~~ claims ~~1 to 3~~, wherein the polyol is selected from the group of the polyether polyols, polyester polyols, and mixtures thereof.

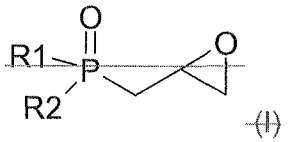
~~5. The phosphorus containing alcohol according to any of claims 1 to 4, wherein the phosphorus containing alcohol has a molecular weight of from 100 to 6000 g/mol.~~

6. The ~~phosphorus containing alcohol~~process according to any of claims 1 ~~to 5~~or 2, wherein the phosphorus containing alcohol has an OH number in the range of 2 to 800.

~~7. The phosphorus containing alcohol according to any of claims 1 to 6, wherein the reaction of the at least one alcohol with the phosphorus containing compound of the general formula (I) takes place in the presence of a catalyst.~~

8. The ~~phosphorus containing alcohol~~process according to any of claims 1 orto ~~7~~3, wherein in the process, ethylene oxide or propylene oxide or a mixture of ethylene oxide and propylene oxide is used as further reactant.

~~9. A process for preparing a phosphorus containing alcohol comprising at least one phosphorus-containing group, comprising the reaction of at least one alcohol with a phosphorus containing compound of the general formula (I):~~

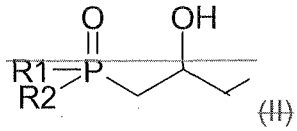


~~(I)~~

~~wherein~~

~~R1, R2 are equal or different linear or branched C_1-C_{18}-alkyl, linear or branched C_2-C_{18}-alkenyl, linear or branched C_2-C_{18}-alkinyl, C_3-C_{10}-cycloalkyl, C_6-C_{10}-aryl, heteroaryl, C_6-C_{10}-aryl-C_1-C_{10}-alkyl, benzyl, OR^3, SR^3, or R^1 and R^2 in combination with the P atom which they are bound to form a 4 to 8-membered ring system;~~
~~R^3 is hydrogen, linear or branched C_1-C_{16}-alkyl, linear or branched C_2-C_{16}-alkenyl, linear or branched C_2-C_{16}-alkinyl, C_3-C_{10}-cycloalkyl, C_6-C_{10}-aryl, heteroaryl or C_6-C_{10}-aryl-C_1-C_{10}-alkyl, benzyl, and~~

~~wherein the at least one phosphorus-containing group is a group of the general formula (II):~~



~~(II)~~

~~wherein~~

~~R1, R2 are equal or different linear or branched C_1-C_{18}-alkyl, linear or branched C_2-C_{18}-alkenyl, linear or branched C_2-C_{18}-alkinyl, C_3-C_{10}-cycloalkyl, C_6-C_{10}-aryl, heteroaryl, C_6-C_{10}-aryl-C_1-C_{10}-alkyl, benzyl, OR^3, SR^3, or R^1 and R^2 in combination with the P atom which they are bound to form a 4 to 8-membered ring system;~~

~~R^3 is hydrogen, linear or branched C_1-C_{16}-alkyl, linear or branched C_2-C_{16}-alkenyl, linear or branched C_2-C_{16}-alkinyl, C_3-C_{10}-cycloalkyl, C_6-C_{10}-aryl, heteroaryl or C_6-C_{10}-aryl-C_1-C_{10}-alkyl, benzyl,~~

~~wherein the at least one alcohol is a polyol and~~

~~wherein the phosphorus containing alcohol has a phosphorus content of from 3 to 30 % by weight based on the total weight of the phosphorus containing alcohol.~~

5. Phosphorus containing alcohol obtainable or obtained by a process according to any of claims 1 to 4.

~~10. Use of a phosphorus containing alcohol according to any of claims 1 to 8 or a phosphorus containing alcohol obtainable or obtained according to the process of claim 9 as a flame retardant.~~

~~11. Use of a phosphorus containing alcohol according to any of claims 1 to 8 or a phosphorus containing alcohol obtainable or obtained according to the process of claim 9 for the preparation of a polyurethane with improved flammability properties.~~

~~12~~6. A process for the preparation of a polyurethane comprising the reaction of at least one isocyanate (a), at least one polyol (b) and at least one phosphorus containing alcohol obtainable or obtained according to the process of any of claims 1 to ~~4~~8 or a phosphorus containing alcohol ~~obtainable or obtained according to the process of claim 9~~according to claim 5

wherein the at least one phosphorus containing alcohol is used in an amount of 1 to 30 % of the total of all polyols and alcohols used.

~~13. The process according to claim 12, wherein the at least one phosphorus containing alcohol is used in an amount of 1 to 30 % of the total of all polyols and alcohols used.~~

~~14~~7. Polyurethane obtainable or obtained by a process according to ~~any of~~ claims ~~12 or 13~~6.

~~15~~8. The polyurethane according to claim ~~7~~14, wherein the polyurethane is a polyurethane foam, a thermoplastic polyurethane, a coating, an adhesive, a sealant, or an elastomer.