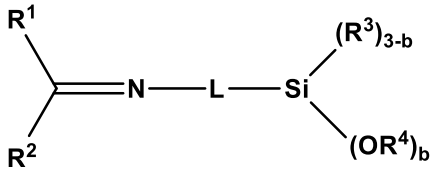
measure the change in viscosity of both natural and synthetic rubbers due to functionalization with silane terminal groups is the Mooney viscosity test.

[0005] It is generally accepted that the viscosity increase is due to the formation of Si-O-Si bonds resulting from the condensation over time of silanol or alkoxysilane groups on the silane terminal groups. The Si-O-Si bond formation results in links between polymer chains, resulting in longer chains, and thus increased viscosity.

[0006] The use of a protecting group on a silane compound has also shown technical challenges associated with the stability of the protecting group (U.S. 10,457,697). Therefore, there is a need for improved silane compounds and methods to prepare such silane compounds to overcome the technical challenges of conventional silane compounds and methods to prepare them.

BRIEF SUMMARY OF THE DISCLOSURE

[0007] In one aspect, the present disclosure provides a silane compound of Formula (I):



Formula (I)

wherein

[0008] each R^1 and R^2 independently is hydrogen; an optionally substituted alkyl group having from 1 to 20 carbon atoms, where the optional substituent is one or more heteroatom; an optionally substituted alkenyl group having from 2 to 20 carbon atoms, where the optional substituents is one or more heteroatom; an optionally substituted cycloalkyl group having from 3 to 10 carbon atoms, where the optional substituent is one or more heteroatom; an optionally substituted aryl group having from 6 to 12 carbon atoms, where the optional substituent is one or more heteroatom; or an optionally substituted aralkyl group having from 7 to 16 carbon atoms, where the optional substituent is one or more heteroatom;

[0009] L is an optionally substituted alkylene group having from 1 to 20 carbon atoms, where the optional substituent is one or more heteroatom; an optionally substituted alkenylene group having from 2 to 20 carbon atoms, where the optional substituent is one or more heteroatom; an optionally substituted cycloalkylene group having from 3 to 10

group, a branched or unbranched C_2-C_{30} alkenyl group, a C_6-C_{30} aryl group, or a C_7-C_{30} aralkyl group; and m is an integer of 1 to 30; and

[0014] b is 2 or 3.

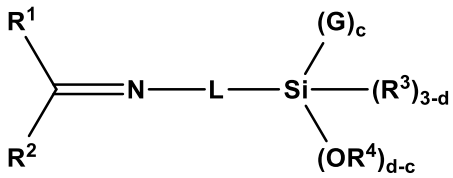
[0014a] In another aspect, the present disclosure provides a polymer comprising:

(i) a conjugated diene-based polymer having an active chain end; and

(ii) a silane compound as described herein;

wherein the polymer is a reaction product between the conjugated diene-based polymer and the silane compound.

[0015] In another aspect, the present disclosure provides a polymer represented by Formula (II)



Formula (II)

wherein

[0016] each R^1 and R^2 independently is hydrogen; an optionally substituted alkyl group having from 1 to 20 carbon atoms, where the optional substituent is one or more heteroatom; an optionally substituted alkenyl group having from 2 to 20 carbon atoms, where the optional substituents is one or more heteroatom; an optionally substituted cycloalkyl group having from 3 to 10 carbon atoms, where the optional substituent is one or more heteroatom; an optionally substituted aryl group having from 6 to 12 carbon atoms, where the optional substituent is one or more heteroatom; or an optionally substituted aralkyl group having from 7 to 16 carbon atoms, where the optional substituent is one or more heteroatom;

[0017] L is an optionally substituted alkylene group having from 1 to 20 carbon atoms, where the optional substituent is one or more heteroatom; an optionally substituted alkenylene group having from 2 to 20 carbon atoms, where the optional substituent is one or more heteroatom; an optionally substituted cycloalkylene group having from 3 to 10 carbon atoms, where the optional substituent is one or more heteroatom; an optionally substituted arylene group having from 6 to 12 carbon atoms, where the optional

substituent is one or more heteroatom; or an optionally substituted aralkylene group having from 7 to 16 carbon atoms, where the optional substituent is one or more heteroatom;

[0018] R^3 is an optionally substituted alkyl group having from 1 to 20 carbon atoms, where the optional substituent is one or more heteroatom; an optionally substituted alkenyl group having from 2 to 20 carbon atoms, where the optional substituent is one or more heteroatom; an optionally substituted cycloalkyl group having from 3 to 10 carbon atoms, where the optional substituent is one or more heteroatom; an optionally substituted

aryl group having from 6 to 12 carbon atoms, where the optional substituent is one or more heteroatom; or an optionally substituted aralkyl group having from 7 to 16 carbon atoms, where the optional substituent is one or more heteroatom;

[0019] each R^4 independently is an optionally substituted alkyl group having from 6 to 30 carbon atoms, where the optional substituent is one or more heteroatom; an optionally substituted alkenyl group having from 6 to 30 carbon atoms, where the optional substituent is one or more heteroatom; an optionally substituted alkynyl group having from 6 to 30 carbon atoms, where the optional substituent is one or more heteroatom; an optionally substituted cycloalkyl group having from 3 to 10 carbon atoms, where the optional substituent is one or more heteroatom; an optionally substituted aryl group having from 6 to 12 carbon atoms, where the optional substituent is one or more heteroatom; an optionally substituted aralkyl group having from 7 to 20 carbon atoms, where the optional substituent is one or more heteroatom; or an optionally substituted cyclic silane; or

[0020] R^4 is R^{23}, where each R^{23} independently is an optionally substituted straight chain or branched chain alkyl group, having from 1 to 10 carbon atoms, where two R^{23} combine with each other to form a ring together with the –O-Si-O- atoms to which they are bonded, and where the optional substituent is one or more heteroatom, and wherein the two R^{23} can be the same or different; or

[0021] each R^4 independently is a group represented by $-(R^5-O)_m-R^6$, where each R^5 is the same as or different from each other and each represents a branched or unbranched C_1-C_{30} divalent hydrocarbon group; R^6 represents a branched or unbranched C_1-C_{30} alkyl group, a branched or unbranched C_2-C_{30} alkenyl group, a C_6-C_{30} aryl group, or a C_7-C_{30} aralkyl group; and m is an integer of 1 to 30;

[0022] each G is independently a polymer fragment having a backbone of carbon atoms covalently bonded together by C—C single bond, C—C double bond, or a combination of C—C single bonds and C—C double bonds;

[0023] c is 1 or 2, with the proviso that c is equal to or less than d; and

[0024] d is 1, 2, or 3.

[0025] In another aspect, the present disclosure provides a polymer represented by Formula (IV)

[0029] R^4 is R^{23}, where each R^{23} independently is an optionally substituted straight chain or branched chain alkyl group, having from 1 to 10 carbon atoms, where two R^{23} combine with each other to form a ring together with the –O-Si-O- atoms to which they are bonded, and where the optional substituent is one or more heteroatom, and wherein the two R^{23} can be the same or different; or

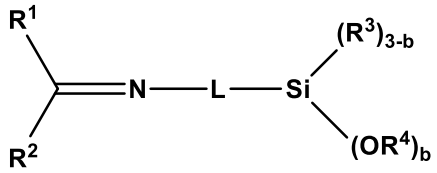
[0030] each R^4 independently is a group represented by $-(R^5-O)_m-R^6$, where each R^5 is the same as or different from each other and each represents a branched or unbranched C_1-C_{30} divalent hydrocarbon group; R^6 represents a branched or unbranched C_1-C_{30} alkyl group, a branched or unbranched C_2-C_{30} alkenyl group, a C_6-C_{30} aryl group, or a C_7-C_{30} aralkyl group; and m is an integer of 1 to 30;

[0031] c is 1 or 2, with the proviso that c is equal to or less than d;

[0032] d is 2 or 3; and

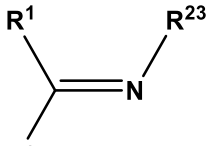
[0033] each G is independently a polymer fragment having a backbone of carbon atoms covalently bonded together by C—C single bond, C—C double bond, or a combination of C—C single bonds and C—C double bonds.

[0033a] In another aspect, the present disclosure provides a method of making the silane compound of Formula (I)

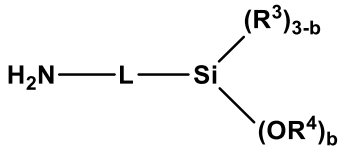


Formula (I)

as described herein, comprising:

reacting a compound of Formula (V) 

Formula (V) with a compound of Formula (VI)



Formula (VI);

wherein

each R^1 and R^2 independently is hydrogen; an optionally substituted alkyl group having from 1 to 20 carbon atoms, where the optional substituent is one or more heteroatom; an optionally substituted alkenyl group having from 2 to 20 carbon atoms, where the optional substituents is one or more heteroatom; an optionally substituted cycloalkyl group having from 3 to 10 carbon atoms, where the optional substituent is one or more heteroatom; an optionally substituted aryl group having from 6 to 12 carbon atoms, where the optional substituent is one or more heteroatom; or an optionally substituted aralkyl group having from 7 to 16 carbon atoms, where the optional substituent is one or more heteroatom;

L is an optionally substituted alkylene group having from 1 to 20 carbon atoms, where the optional substituent is one or more heteroatom; an optionally substituted alkenylene group having from 2 to 20 carbon atoms, where the optional substituent is one or more heteroatom; an optionally substituted cycloalkylene group having from 3 to 10 carbon atoms, where the optional substituent is one or more heteroatom; an optionally substituted arylene group having from 6 to 12 carbon atoms, where the optional substituent is one or more heteroatom; or an optionally substituted aralkylene group having from 7 to 16 carbon atoms, where the optional substituent is one or more heteroatom;

R^3 is an optionally substituted alkyl group having from 1 to 20 carbon atoms, where the optional substituent is one or more heteroatom; an optionally substituted alkenyl group having from 2 to 20 carbon atoms, where the optional substituent is one or more heteroatom; an optionally substituted cycloalkyl group having from 3 to 10 carbon atoms, where the optional substituent is one or more heteroatom; an optionally substituted aryl group having from 6 to 12 carbon atoms, where the optional substituent is one or more heteroatom; or an optionally substituted aralkyl group having from 7 to 16 carbon atoms, where the optional substituent is one or more heteroatom;

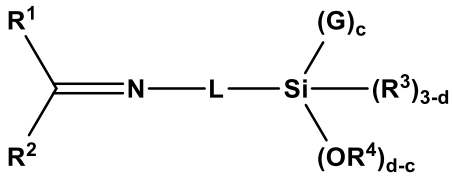
each R^4 independently is an optionally substituted alkyl group having from 6 to 30 carbon atoms, where the optional substituent is one or more heteroatom; an optionally substituted alkenyl group having from 6 to 30 carbon atoms, where the optional substituent is one or more heteroatom; an optionally substituted alkynyl group having from 6 to 30 carbon atoms, where the optional substituent is one or more heteroatom; an optionally substituted cycloalkyl group having from 3 to 10 carbon atoms, where the optional substituent is one or more heteroatom; an optionally substituted aryl group having from 6 to 12 carbon atoms, where the optional substituent is one or more heteroatom; an optionally substituted aralkyl group having from 7 to 20 carbon atoms, where the optional substituent is one or more heteroatom; or an optionally substituted cyclic silane; or

R^4 is R^{23}, where each R^{23} independently is an optionally substituted straight chain or branched chain alkyl group, having from 1 to 10 carbon atoms, where two R^{23} combine with each other to form a ring together with the –O-Si-O- atoms to which they are bonded, and where the optional substituent is one or more heteroatom, and wherein the two R^{23} can be the same or different; or

each R^4 independently is a group represented by $-(R^5-O)_m-R^6$, where each R^5 is the same as or different from each other and each represents a branched or unbranched C_1-C_{30} divalent hydrocarbon group; R^6 represents a branched or unbranched C_1-C_{30} alkyl group, a branched or unbranched C_2-C_{30} alkenyl group, a C_6-C_{30} aryl group, or a C_7-C_{30} aralkyl group; and m is an integer of 1 to 30; and

b is 2 or 3.

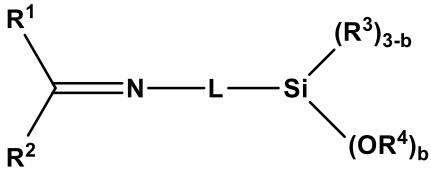
[0033b] In another aspect, the present disclosure provides a method of making the polymer as described herein, wherein the polymer is represented by Formula (II)



Formula (II), and is prepared by

(i) reacting a polymer fragment having a backbone of carbon atoms covalently bonded together by C—C single bond, C—C double bond, or a combination of C—C single bonds and C—C double bonds with an anionic initiator to form a polymer fragment G; and

(ii) reacting the polymer fragment G of (i) with a silane compound of Formula (I)



Formula (I)

wherein

each R^1 and R^2 independently is hydrogen; an optionally substituted alkyl group having from 1 to 20 carbon atoms, where the optional substituent is one or more heteroatom; an optionally substituted alkenyl group having from 2 to 20 carbon atoms, where the optional substituents is one or more heteroatom; an optionally substituted cycloalkyl group having from 3 to 10 carbon atoms, where the optional substituent is one or more heteroatom; an optionally substituted aryl group having from 6 to 12 carbon atoms, where the optional substituent is one or more heteroatom; or an optionally substituted aralkyl group having from 7 to 16 carbon atoms, where the optional substituent is one or more heteroatom;

L is an optionally substituted alkylene group having from 1 to 20 carbon atoms, where the optional substituent is one or more heteroatom; an optionally substituted alkenylene group having from 2 to 20 carbon atoms, where the optional substituent is one or more heteroatom; an optionally substituted cycloalkylene group having from 3 to 10 carbon atoms, where the optional substituent is one or more heteroatom; an optionally substituted arylene group having from 6 to 12 carbon atoms, where the optional substituent is one or more heteroatom; or an optionally substituted aralkylene group having from 7 to 16 carbon atoms, where the optional substituent is one or more heteroatom;

R^3 is an optionally substituted alkyl group having from 1 to 20 carbon atoms, where the optional substituent is one or more heteroatom; an optionally substituted alkenyl group having from 2 to 20 carbon atoms, where the optional substituent is one or more heteroatom; an optionally substituted cycloalkyl group having from 3 to 10 carbon atoms, where the optional substituent is one or more heteroatom; an optionally substituted aryl group having from 6 to 12 carbon atoms, where the optional substituent is one or more heteroatom; or an optionally substituted aralkyl group having from 7 to 16 carbon atoms, where the optional substituent is one or more heteroatom;

each R^4 independently is an optionally substituted alkyl group having from 6 to 30 carbon atoms, where the optional substituent is one or more heteroatom; an optionally substituted alkenyl group having from 6 to 30 carbon atoms, where the optional substituent is one or more heteroatom; an optionally substituted alkynyl group having from 6 to 30 carbon atoms, where the optional substituent is one or more heteroatom; an optionally substituted cycloalkyl group having from 3 to 10 carbon atoms, where the optional substituent is one or more heteroatom; an optionally substituted aryl group having from 6 to 12 carbon atoms, where the optional substituent is one or more heteroatom; an optionally substituted aralkyl group having from 7 to 20 carbon atoms, where the optional substituent is one or more heteroatom; or an optionally substituted cyclic silane; or

R^4 is R^{23}, where each R^{23} independently is an optionally substituted straight chain or branched chain alkyl group, having from 1 to 10 carbon atoms, where two R^{23} combine with each other to form a ring together with the –O-Si-O- atoms to which they are bonded, and where the optional substituent is one or more heteroatom, and wherein the two R^{23} can be the same or different; or

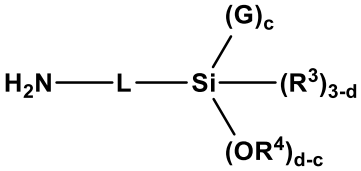
each R^4 independently is a group represented by $-(R^5-O)_m-R^6$, where where each R^5 is the same as or different from each other and each represents a branched or unbranched C_1-C_{30} divalent hydrocarbon group; R^6 represents a branched or unbranched C_1-C_{30} alkyl group, a branched or unbranched C_2-C_{30} alkenyl group, a C_6-C_{30} aryl group, or a C_7-C_{30} aralkyl group; and m is an integer of 1 to 30;

b is 2 or 3;

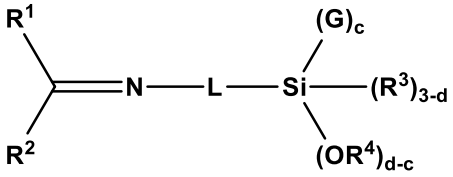
c is 1 or 2, with the proviso that c is less than or equal to d; and

d is 1, 2, or 3.

[0033c] In another aspect, the present disclosure provides a method of making the polymer as described herein, wherein the polymer is represented by Formula (VII)



Formula (VII), comprising reacting a polymer of Formula (II)



Formula (II) with water,

wherein

each R^1 and R^2 independently is hydrogen; an optionally substituted alkyl group having from 1 to 20 carbon atoms, where the optional substituent is one or more heteroatom; an optionally substituted alkenyl group having from 2 to 20 carbon atoms, where the optional substituents is one or more heteroatom; an optionally substituted cycloalkyl group having from 3 to 10 carbon atoms, where the optional substituent is one or more heteroatom; an optionally substituted aryl group having from 6 to 12 carbon atoms, where the optional substituent is one or more heteroatom; or an optionally substituted aralkyl group having from 7 to 16 carbon atoms, where the optional substituent is one or more heteroatom;

L is an optionally substituted alkylene group having from 1 to 20 carbon atoms, where the optional substituent is one or more heteroatom; an optionally substituted alkenylene group having from 2 to 20 carbon atoms, where the optional substituent is one or more heteroatom; an optionally substituted cycloalkylene group having from 3 to 10 carbon atoms, where the optional substituent is one or more heteroatom; an optionally substituted arylene group having from 6 to 12 carbon atoms, where the optional substituent is one or more heteroatom; or an optionally substituted aralkylene group having from 7 to 16 carbon atoms, where the optional substituent is one or more heteroatom;

R^3 is an optionally substituted alkyl group having from 1 to 20 carbon atoms, where the optional substituent is one or more heteroatom; an optionally substituted alkenyl group having from 2 to 20 carbon atoms, where the optional substituent is one or more heteroatom; an optionally substituted cycloalkyl group having from 3 to 10 carbon atoms, where the optional substituent is one or more heteroatom; an optionally substituted aryl group having from 6 to 12 carbon atoms, where the optional substituent is one or more heteroatom; or an optionally substituted aralkyl group having from 7 to 16 carbon atoms, where the optional substituent is one or more heteroatom;

each R^4 independently is an optionally substituted alkyl group having from 6 to 30 carbon atoms, where the optional substituent is one or more heteroatom; an optionally substituted alkenyl group having from 6 to 30 carbon atoms, where the optional substituent is one or more heteroatom; an optionally substituted alkynyl group having from 6 to 30 carbon atoms, where the optional substituent is one or more heteroatom; an optionally substituted cycloalkyl group having from 3 to 10 carbon atoms, where the optional substituent is one or more heteroatom; an optionally substituted aryl group having from 6 to 12 carbon atoms, where the optional substituent is one or more heteroatom; an optionally substituted aralkyl group having from 7 to 20 carbon atoms, where the optional substituent is one or more heteroatom; or an optionally substituted cyclic silane; or

R^4 is R^{23}, where each R^{23} independently is an optionally substituted straight chain or branched chain alkyl group, having from 1 to 10 carbon atoms, where two R^{23} combine with each other to form a ring together with the –O-Si-O- atoms to which they are bonded, and where the optional substituent is one or more heteroatom, and wherein the two R^{23} can be the same or different; or

each R^4 independently is a group represented by $-(R^5-O)_m-R^6$, where where each R^5 is the same as or different from each other and each represents a branched or unbranched C_1-C_{30} divalent hydrocarbon group; R^6 represents a branched or unbranched C_1-C_{30} alkyl group, a branched or unbranched C_2-C_{30} alkenyl group, a C_6-C_{30} aryl group, or a C_7-C_{30} aralkyl group; and m is an integer of 1 to 30;

G is is a polymer fragment having a backbone of carbon atoms covalently bonded together by C—C single bond, C—C double bond, or a combination of C—C single bonds and C—C double bonds;

c is 1 or 2, with the proviso that c is less than or equal to d; and

d is 1, 2, or 3.

[0033d] In another aspect, the present disclosure provides a rubber composition comprising one or more polymers as described herein.

[0033e] In another aspect, the present disclosure provides use of the rubber composition as described herein in the manufacture of a tire tread, a tire undertread, a tire carcass, a tire sidewall, or a tire bead.

[0033f] In another aspect, the present disclosure provides a tire comprising the rubber composition as described herein, wherein at least a tread of a tire or a sidewall of a tire is formed with the rubber composition.

BRIEF DESCRIPTION OF THE FIGURE

[0034] FIG. 1 is a pictorial representation of a method used to prepare the functionalized SSBRs of the present disclosure. The anionic polymerization initiated using n-butyl lithium is very sensitive to moisture and thus, precautions were necessary to prevent the initiator from being quenched.

DETAILED DESCRIPTION

I. Definitions

[0035] As used above, and throughout the description, the following terms, unless otherwise indicated, shall be understood to have the following meanings.

[0036] Unless stated otherwise, the terms "a" and "an" and "the" and similar references used in the context of describing a particular aspect of the application (especially in the context of claims) can be construed to cover both the singular and the plural. The recitation of ranges of values herein is merely intended to serve as a shorthand method of referring individually to each separate value falling within the range. Unless otherwise