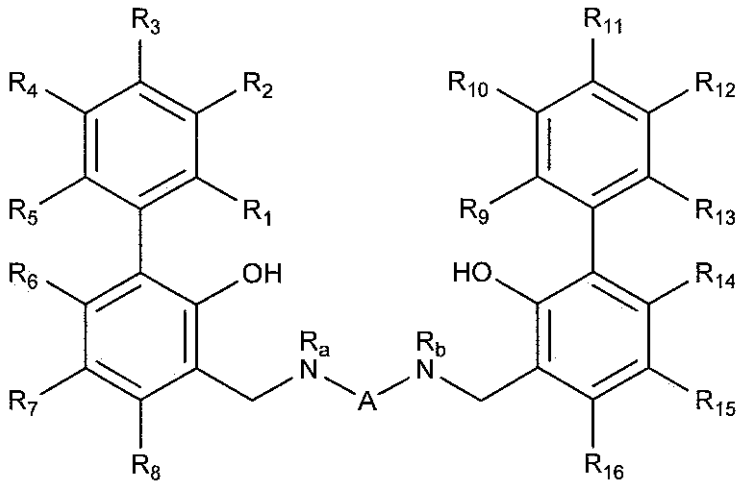
wherein each of R_1, R_2, R_3, R_4, R_5, R_6, R_7, R_8, R_9, R_{10}, R_{11}, R_{12}, R_{13}, R_{14}, R_{15} and R_{16} is independently selected from the group consisting of hydride, halide, optionally substituted hydrocarbyl, heteroatom-containing optionally substituted hydrocarbyl, alkoxy, aryloxy, silyl, boryl, dialkyl amino, alkylthio, arylthio and seleno, with the proviso that none of R_1, R_2, R_3, R_4, R_5, R_9, R_{10}, R_{11}, R_{12} and R_{13} comprise fluorine; optionally two or more R groups can combine together into ring structures with such ring structures having from 3 to 100 non-hydrogen atoms in the ring; A is a bridging group having from one to 50 non-hydrogen atoms; R_a and R_b are independently selected from hydride or optionally substituted hydrocarbyl, or, optionally, R_a and R_b may be joined to form a bridging group, E, having from one to 50 non-hydrogen atoms; and when R_a and R_b are not joined to form a bridging group, A is not $-(CH_2-CH_2)-$.

[0005a] In one aspect, there is provided a bis(aminophenylphenol) ligand of formula (I):



(I)

wherein each of R_1, R_2, R_3, R_4, R_5, R_6, R_7, R_8, R_9, R_{10}, R_{11}, R_{12}, R_{13}, R_{14}, R_{15} and R_{16} is independently selected from the group consisting of hydride, halide, optionally substituted hydrocarbyl, heteroatom-containing optionally substituted hydrocarbyl, alkoxy, aryloxy, silyl, boryl, dialkyl amino, alkylthio, arylthio and seleno, with the proviso that none of R_1, R_2, R_3, R_4, R_5, R_9, R_{10}, R_{11}, R_{12} and R_{13} comprise fluorine; optionally two or more R groups can combine together into ring structures with such ring structures having from 3 to 100 non-hydrogen atoms in the ring; A is a bridging group having from one to 50 non-hydrogen atoms; R_a and R_b are joined to form a bridging group, E, having from one to 50 non-hydrogen atoms; and

wherein R_a and R_b are joined to form a bridging group, E, wherein said bridging group is selected from the group consisting of optionally substituted divalent hydrocarbyl and divalent heteroatom containing hydrocarbyl; or

wherein, R_a and R_b are joined to form a bridging group, E, wherein said bridging group is selected from the group consisting of optionally substituted divalent alkyl, optionally substituted divalent cycloalkyl, alkenyl, alkynyl, heteroalkyl, heterocycloalkyl, heteroalkenyl, heteroalkynyl, carbocycle, heterocarbocycle, aryl, heteroaryl and silyl; or

wherein R_a and R_b are joined to form a bridging group represented by the general formula—$(QR^{18}_{2-z''})_{z'}$—wherein each Q is either carbon or silicon and each R^{18} may be the same or different from the others such that each R^{18} is selected from the group consisting of hydride and optionally substituted hydrocarbyl and heteroatom containing hydrocarbyl, and optionally two or more R^{18} groups may be joined into a ring structure having from 3 to 50 atoms in the ring structure not counting hydrogen atoms; z′ is an integer from 1 to 10; and z″ is 0, 1 or 2.

[0006] Each of R_1, R_2, R_3, R_4, R_5, R_6, R_7, R_8, R_9, R_{10}, R_{11}, R_{12}, R_{13}, R_{14}, R_{15} and R_{16} may be independently selected from the group consisting of hydride, halide, optionally substituted alkyl, heteroalkyl, aryl, heteroaryl, alkoxyl, aryloxyl, silyl, dialkylamino, alkylthio, and arylthio, with the proviso that none of R_1, R_2, R_3, R_4, R_5, R_9, R_{10}, R_{11}, R_{12} and R_{13} comprise fluorine.

[0007] Each of R_1, R_2, R_3, R_4, R_5, R_6, R_7, R_8, R_9, R_{10}, R_{11}, R_{12}, R_{13}, R_{14}, R_{15} and R_{16} may be independently selected from the group consisting of hydride, halide, optionally substituted alkyl, heteroalkyl, aryl, heteroaryl, alkoxyl, and aryloxyl, with the proviso that none of R_1, R_2, R_3, R_4, R_5, R_9, R_{10}, R_{11}, R_{12} and R_{13} comprise fluorine.

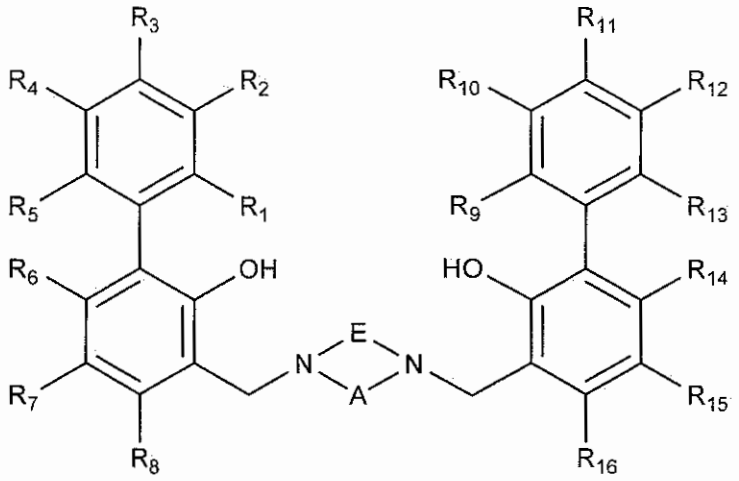
[0008] The bridging group A may be selected from the group consisting of optionally substituted divalent hydrocarbyl and divalent heteroatom containing hydrocarbyl.

[0009] The bridging group A may be selected from the group consisting of optionally substituted divalent alkyl, alkenyl, alkynyl, heteroalkyl, heteroalkenyl, heteroalkynyl, carbocycle, heterocarbocycle, aryl, heteroaryl and silyl.

[0010] The bridging group A may be represented by the general formula—$(QR^{17}_{2-z''})_{z'}$—wherein each Q is either carbon or silicon and each R^{17} may be the same or different from the others such that each R^{17} is selected from the group consisting of hydride and optionally substituted hydrocarbyl and heteroatom containing hydrocarbyl, and optionally two or more R^{17} groups may be joined into a ring structure having from 3 to 50 atoms in the ring structure not counting hydrogen atoms; z′ is an integer from 1 to 10; and z″ is 0, 1 or 2.

[0011] R_a and R_b may be independently selected from hydride or optionally substituted alkyl.

[0012] R_a and R_b may be joined to form a bridging group, E, wherein said bridging group may be selected from the group consisting of optionally substituted divalent hydrocarbyl and divalent heteroatom containing hydrocarbyl.



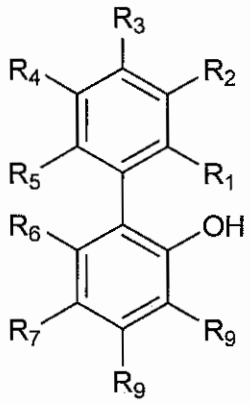
(III)

wherein each of R_1, R_2, R_3, R_4, R_5, R_6, R_7, R_8, R_9, R_{10}, R_{11}, R_{12}, R_{13}, R_{14}, R_{15} and R_{16} is as hereinbefore defined and A and E are independently optionally substituted divalent alkyl.

[0017] The bridging groups A and E may be the same or different divalent alkyl containing from 1 to 10, or from 2 to 6 carbon atoms.

[0018] There is also provided a method for preparing a bis(aminophenylphenol) ligand of formula (I), (II) or (III) wherein the method comprises at least one step of reductive amination or Mannich aminoalkylation.

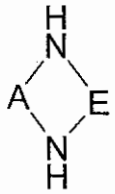
[0018a] In another aspect, there is provided a method of preparing a ligand as defined herein, wherein the method comprises at least one step of reductive amination or Mannich aminoalkylation and the step of treating an arylphenol of formula (VI):



(VI)

wherein R_1 to R_7 and R_9, are as defined above,

with a heterocycle of formula (VII):



(VII)

wherein A and E are as defined above,

in the presence of formaldehyde, or a source of formaldehyde, to yield the bis(aminophenylphenol) ligand of formula (I) or formula (III) as defined above.

[0019] The method may also comprise at least one step of aryl coupling, such as Suzuki coupling.

[0020] The method may comprise the steps of:

(a) treating an arylphenol carboxaldehyde of formula (IV) with a diamine of formula (V); and

(b) treating the product formed in (a) with a reducing agent;

so as to yield the bis(aminophenylphenol) ligand of formula (I) or formula (II).

[0030] In any one of the hereinbefore disclosed methods R_a and R_b may be joined to form a bridging group, E, wherein said bridging group may be selected from the group consisting of optionally substituted divalent hydrocarbyl and divalent heteroatom containing hydrocarbyl.

[0031] In any one of the hereinbefore disclosed methods R_a and R_b may be joined to form a bridging group, E, wherein said bridging group may be selected from the group consisting of optionally substituted divalent alkyl, alkenyl, alkynyl, heteroalkyl, heteroalkenyl, heteroalkynyl, carbocycle, heterocarbocycle, aryl, heteroaryl and silyl.

[0032] In any one of the hereinbefore disclosed methods R_a and R_b may be joined to form a bridging group represented by the general formula—$(QR^{18}_{2-z''})_{z'}$—wherein each Q is either carbon or silicon and each R^{18} may be the same or different from the others such that each R^{18} is selected from the group consisting of hydride and optionally substituted hydrocarbyl and heteroatom containing hydrocarbyl, and optionally two or more R^{18} groups may be joined into a ring structure having from 3 to 50 atoms in the ring structure not counting hydrogen atoms; z′ is an integer from 1 to 10; and z″ is 0, 1 or 2.

[0033] In any one of the hereinbefore disclosed embodiments the catalyst may comprise a nickel or palladium catalyst.

[0034] In any one of the hereinbefore disclosed embodiments the palladium catalyst may comprise a palladium phosphine catalyst. The palladium catalyst may also comprise, for example, bis(tri-tert-butylphosphine)palladium, tetrakis(triphenylphosphine)palladium(0) ($Pd(PPh_3)_4$), bis[1,2-bis(diphenylphosphino)ethane]palladium(0) ($Pd(dppe)_2$), 1,1'-bis(diphenylphosphino)ferrocene palladium (Pd(dppf)), (2,2'-bis(diphenylphosphino)-1,1'-binaphthyl palladium (Pd(BINAP).

[0035] In any one of the hereinbefore disclosed embodiments the reducing agent may be a metal hydride. A non-limiting example includes sodium borohydride.

[0036] The herein disclosed methods may comprise any combination of the hereinbefore disclosed embodiments.

[0037] The present disclosure provides a ligand of formula (I), (II) or (III) prepared by any one of the hereinbefore disclosed methods.

[0038] The present disclosure further provides a transition metal compound formed from any one of the ligands of formula (I), (II) or (III). The transition metal compounds may comprise a titanium, a zirconium or a hafnium atom.

[0038a] In another aspect, there is provided a transition metal compound comprising a ligand as defined herein, wherein the transition metal compound comprises one or more titanium, zirconium or hafnium atoms.

[0039] In another aspect there is provided a catalyst composition comprising one or more transition metal compounds as hereinbefore disclosed, and one or more activators. The activator may comprise one or more alumoxanes. The activator may comprise methylalumoxane.

[0040] In another aspect there is provided a supported catalyst composition comprising one or more transition metal compounds as hereinbefore disclosed, one or more activators and one or more support materials. The activator may comprise one or more alumoxanes. The activator may comprise methylalumoxane. The support may be silica.

[0041] The catalyst composition or supported catalyst composition may comprise two or more transition metal compounds. The transition metal compounds may be selected from any one of those hereinbefore described or at least one of the transition metal compounds may be different from those hereinbefore described. For example, at least one of the transition metal compounds may be a metallocene.

[0042] The present disclosure further provides a process for polymerizing olefins, the process comprising:

contacting olefins with one or more catalyst compositions or supported catalyst compositions comprising at least one transition metal compound as hereinbefore disclosed in a reactor under polymerization conditions to produce an olefin polymer or copolymer.

[0042a] In another aspect, there is provided a process for polymerizing olefins, the process comprising:

contacting olefins with one or more catalyst compositions or supported catalyst compositions as defined herein in a reactor under polymerization conditions to produce an olefin polymer or copolymer.

BRIEF DESCRIPTION OF THE DRAWINGS

[0043] Figure 1 depicts the chemical structures of exemplary compounds in accordance with this disclosure.

[0044] Figures 2 to 6 depict exemplary reaction schemes in accordance with this disclosure.

DETAILED DESCRIPTION

[0045] Before the present compounds, components, compositions, and/or methods are disclosed and described, it is to be understood that unless otherwise indicated this invention is not limited to specific compounds, components, compositions, reactants, reaction conditions, ligands, transition metal compounds, or the like, as such may vary, unless otherwise specified. It is also to be understood that the terminology used herein is for the purpose of describing particular embodiments only and is not intended to be limiting.

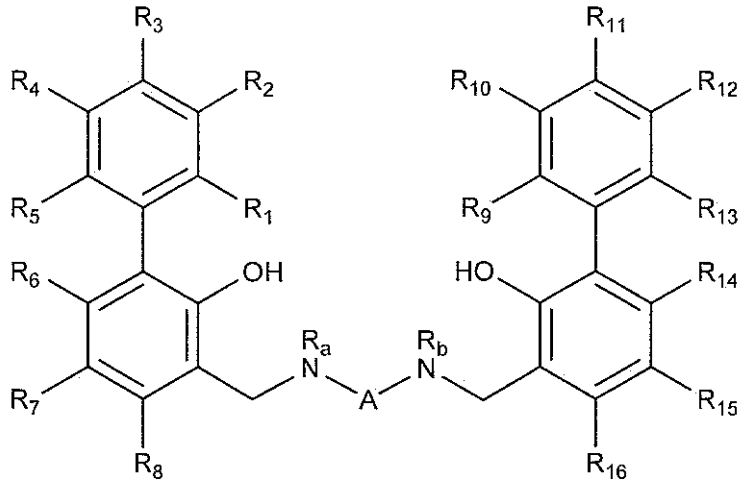
[0046] It must also be noted that, as used in the specification and the appended claims, the singular forms "a," "an" and "the" include plural referents unless otherwise specified. Thus, for example, reference to "a halogen atom" as in a moiety "substituted with a halogen atom" includes more than one halogen atom, such that the moiety may be substituted with two or more halogen atoms, reference to "a substituent" includes one or more substituents, reference to "a ligand" includes one or more ligands, and the like.

[0047] As used herein, all reference to the Periodic Table of the Elements and groups thereof is to the NEW NOTATION published in HAWLEY'S CONDENSED CHEMICAL DICTIONARY, Thirteenth Edition, John Wiley & Sons, Inc., (1997) (reproduced there with

CLAIMS

What is claimed is:

1. A bis(aminophenylphenol) ligand of formula (I):



(I)

wherein each of R_1, R_2, R_3, R_4, R_5, R_6, R_7, R_8, R_9, R_{10}, R_{11}, R_{12}, R_{13}, R_{14}, R_{15} and R_{16} is independently selected from the group consisting of hydride, halide, optionally substituted hydrocarbyl, heteroatom-containing optionally substituted hydrocarbyl, alkoxy, aryloxy, silyl, boryl, dialkyl amino, alkylthio, arylthio and seleno, with the proviso that none of R_1, R_2, R_3, R_4, R_5, R_9, R_{10}, R_{11}, R_{12} and R_{13} comprise fluorine; optionally two or more R groups can combine together into ring structures with such ring structures having from 3 to 100 non-hydrogen atoms in the ring; A is a bridging group having from one to 50 non-hydrogen atoms; R_a and R_b are joined to form a bridging group, E, having from one to 50 non-hydrogen atoms; and

wherein R_a and R_b are joined to form a bridging group, E, wherein said bridging group is selected from the group consisting of optionally substituted divalent hydrocarbyl and divalent heteroatom containing hydrocarbyl; or

wherein, R_a and R_b are joined to form a bridging group, E, wherein said bridging group is selected from the group consisting of optionally substituted divalent alkyl, optionally substituted divalent cycloalkyl, alkenyl, alkynyl, heteroalkyl, heterocycloalkyl, heteroalkenyl, heteroalkynyl, carbocycle, heterocarbocycle, aryl, heteroaryl and silyl; or

wherein R_a and R_b are joined to form a bridging group represented by the general formula—$(QR^{18}_{2-z''})_{z'}$—wherein each Q is either carbon or silicon and each R^{18} may be the same or different from the others such that each R^{18} is selected from the group consisting of hydride and optionally substituted hydrocarbyl and heteroatom containing hydrocarbyl, and optionally two or more R^{18} groups may be joined into a ring structure having from 3 to 50 atoms in the ring structure not counting hydrogen atoms; z′ is an integer from 1 to 10; and z″ is 0, 1 or 2.

2. A ligand according to claim 1, wherein each of R_1, R_2, R_3, R_4, R_5, R_6, R_7, R_8, R_9, R_{10}, R_{11}, R_{12}, R_{13}, R_{14}, R_{15} and R_{16} is independently selected from the group consisting of hydride, halide, optionally substituted alkyl, optionally substituted cycloalkyl, heteroalkyl, heterocycloalkyl, aryl, heteroaryl, alkoxyl, aryloxyl, silyl, dialkylamino, alkylthio, and arylthio; or

wherein each of R_1, R_2, R_3, R_4, R_5, R_6, R_7, R_8, R_9, R_{10}, R_{11}, R_{12}, R_{13}, R_{14}, R_{15} and R_{16} is independently selected from the group consisting of hydride, halide, optionally substituted alkyl, optionally substituted cycloalkyl, heteroalkyl, heterocycloalkyl, aryl, heteroaryl, alkoxyl, and aryloxyl; or

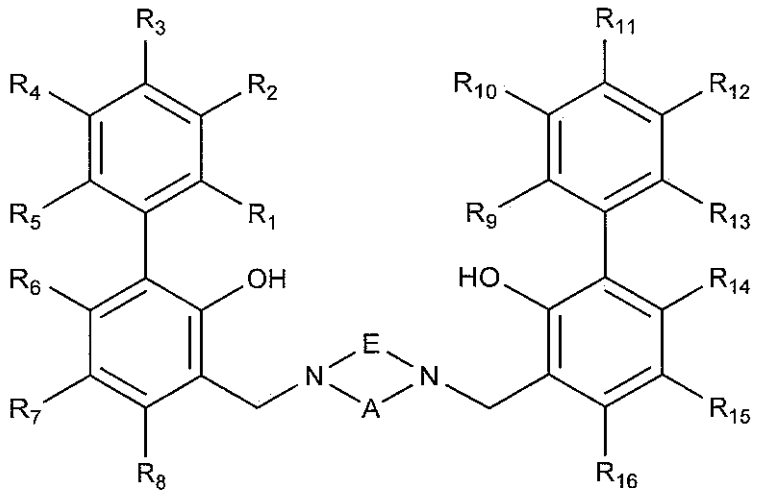
wherein the bridging group A is selected from the group consisting of optionally substituted divalent hydrocarbyl and divalent heteroatom containing hydrocarbyl; or

wherein the bridging group A is selected from the group consisting of optionally substituted divalent alkyl, optionally substituted cycloalkyl alkenyl, alkynyl, heteroalkyl, heterocycloalkyl,heteroalkenyl, heteroalkynyl, carbocycle, heterocarbocycle, aryl, heteroaryl and silyl; or

wherein the bridging group A is represented by the general formula—$(QR^{17}_{2-z''})_{z'}$—wherein each Q is either carbon or silicon and each R^{17} may be the same or different from the others such that each R^{17} is selected from the group consisting of hydride and optionally substituted hydrocarbyl and heteroatom containing hydrocarbyl, and optionally two or more R^{17} groups may be joined into a ring structure having from 3 to 50 atoms in the ring structure not counting hydrogen atoms; z′ is an integer from 1 to 10; and z″ is 0, 1 or 2; or

wherein R_a and R_b are independently selected from hydride or optionally substituted alkyl or cycloalkyl.

3. A ligand according to claim 1 having formula (III):

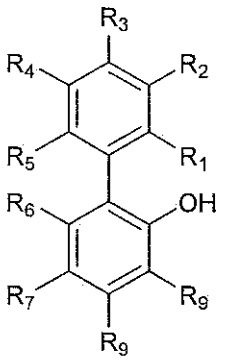


(III)

wherein each of R_1, R_2, R_3, R_4, R_5, R_6, R_7, R_8, R_9, R_{10}, R_{11}, R_{12}, R_{13}, R_{14}, R_{15} and R_{16} is as defined in claim 1 and A and E are independently optionally substituted divalent alkyl or cycloalkyl; or

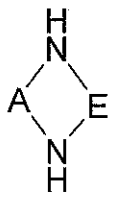
wherein the bridging groups A and E are the same or different divalent alkyl groups or cycloalkyl groups, containing from 1 to 10 carbon atoms.

4. A method of preparing a ligand according to any one of claims 1 to 3, wherein the method comprises at least one step of reductive amination or Mannich aminoalkylation and the step of treating an arylphenol of formula (VI):



(VI)

wherein R_1 to R_7 and R_9, are as defined in claim 1, with a heterocycle of formula (VII):



(VII)

wherein A and E are as defined in claim 1,

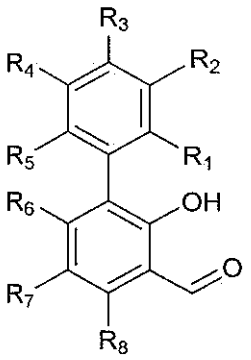
in the presence of formaldehyde, or a source of formaldehyde, to yield the bis(aminophenylphenol) ligand of formula (I) as defined in claim 1 or formula (III) as defined in claim 3.

5. A method according to claim 4, wherein the method further comprises at least one step of aryl coupling; or

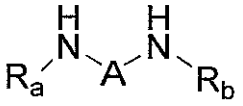
wherein the method comprises the steps of:

(a) treating an arylphenol carboxaldehyde of formula (IV) with a diamine of formula (V); and

(b) treating the product formed in (a) with a reducing agent, to yield the bis(aminophenylphenol) ligand of formula (I) as defined in claim 1;



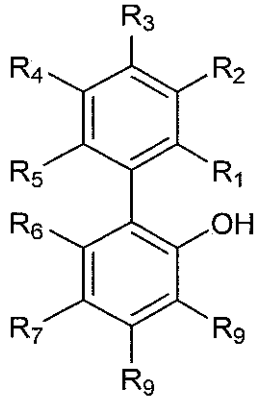
(IV)



(V)

wherein R_1 to R_8, A, R_a and R_b are as defined in claim 1; or

wherein the method comprises the step of treating an arylphenol of formula (VI), with a diamine of formula (V) in the presence of formaldehyde, or a source of formaldehyde, to yield the bis(aminophenylphenol) ligand of formula (I)

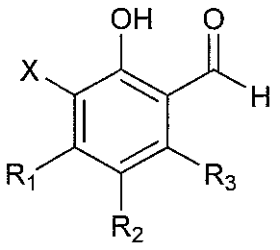


(VI)

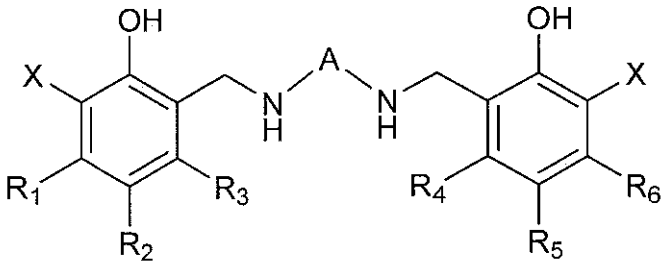
wherein R_1 to R_7 and R_9 are as defined in claim 1; or

wherein the method comprises the steps of:

a) treating a halophenol of formula (VIII) with a diamine of formula (V), to yield the dihalo compound of formula (IX);

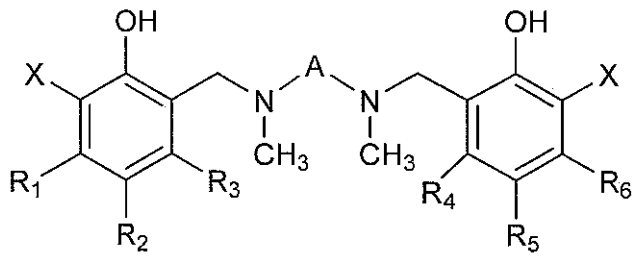


(VIII)



(IX)

b) treating the compound of formula (IX) with formaldehyde, or a source of formaldehyde, in the presence of a reducing agent, to yield a compound of formula (X);



(X)

c) treating the compound of formula (X) with an aryl-boron compound ($ArBR^c_2$ or $ArBF_3^-M^+$) in the presence of a catalyst, so as yield a compound of formula (I) as defined in claim 1, wherein Ar is optionally substituted aryl or optionally substituted heteroaryl; R^c is independently selected from hydride, alkyl, cycloalkyl, hydroxy and alkoxy, wherein when both of R^c are alkoxy, optionally they may combine to form a ring structure of formula $BO_2R^c_2$, M^+ is an alkali metal cation, R_1 to R_6 and A are as defined in claim 1.

6. A method according to claim 4 or 5 wherein each of R_1, R_2, R_3, R_4, R_5, R_6, R_7, R_8, R_9, R_{10}, R_{11}, R_{12}, R_{13}, R_{14}, R_{15} and R_{16} is independently selected from the group consisting of hydride, halide, optionally substituted alkyl, optionally substituted cycloalkyl, heteroalkyl, heterocycloalkyl,aryl, heteroaryl, alkoxyl, aryloxyl, silyl, dialkylamino, alkylthio, and arylthio; or

wherein each of R_1, R_2, R_3, R_4, R_5, R_6, R_7, R_8, R_9, R_{10}, R_{11}, R_{12}, R_{13}, R_{14}, R_{15} and R_{16} is independently selected from the group consisting of hydride, halide, optionally substituted alkyl, optionally substituted cycloalkyl, heteroalkyl, heterocycloalkyl, aryl, heteroaryl, alkoxyl, and aryloxyl; or

wherein the bridging group A is selected from the group consisting of optionally substituted divalent hydrocarbyl and divalent heteroatom containing hydrocarbyl; or
wherein the bridging group A is selected from the group consisting of optionally substituted divalent alkyl, optionally substituted divalent cycloalkyl, alkenyl, alkynyl, heteroalkyl, heterocycloalkyl, heteroalkenyl, heteroalkynyl, carbocycle, heterocarbocycle, aryl, heteroaryl and silyl; or

wherein the bridging group A is represented by the general formula—$(QR^{17}_{2-z''})_{z'}$—wherein each Q is either carbon or silicon and each R^{17} may be the same or different from the others such that each R^{17} is selected from the group consisting of hydride and optionally substituted hydrocarbyl and heteroatom containing hydrocarbyl, and optionally two or more R^{17} groups may be joined into a ring structure having

from 3 to 50 atoms in the ring structure not counting hydrogen atoms; z′ is an integer from 1 to 10; and z″ is 0, 1 or 2; or

wherein R_a and R_b is independently selected from hydride or optionally substituted alkyl or cycloalkyl; or

wherein R_a and R_b are joined to form a bridging group, wherein said bridging group is selected from the group consisting of optionally substituted divalent hydrocarbyl and divalent heteroatom containing hydrocarbyl; or

wherein R_a and R_b are joined to form a bridging group, wherein said bridging group is selected from the group consisting of optionally substituted divalent alkyl, optionally substituted divalent cycloalkyl, alkenyl, alkynyl, heteroalkyl, heterocycloalkyl, heteroalkenyl, heteroalkynyl, carbocycle, heterocarbocycle, aryl, heteroaryl and silyl; or

wherein R_a and R_b are joined to form a bridging group represented by the general formula—$(QR^{18}{}_{2-z''})_{z'}$—wherein each Q is either carbon or silicon and each R^{18} may be the same or different from the others such that each R^{18} is selected from the group consisting of hydride and optionally substituted hydrocarbyl and heteroatom containing hydrocarbyl, and optionally two or more R^{18} groups may be joined into a ring structure having from 3 to 50 atoms in the ring structure not counting hydrogen atoms; z′ is an integer from 1 to 10; and z″ is 0, 1 or 2.

7. A transition metal compound comprising a ligand according to any one of claims 1 to 3, wherein the transition metal compound comprises one or more titanium, zirconium or hafnium atoms.

8. A catalyst composition comprising one or more transition metal compounds according to claim 7 and one or more activators; or

a supported catalyst composition comprising one or more transition metal compounds according to claim 7, one or more activators and one or more support materials;

wherein the activator comprises methyalumoxane; or

wherein the supported catalyst composition comprises one or more other transition metal compounds.

9. A process for polymerizing olefins, the process comprising:

contacting olefins with one or more catalyst compositions or supported catalyst compositions according to claim 8 in a reactor under polymerization conditions to produce an olefin polymer or copolymer.