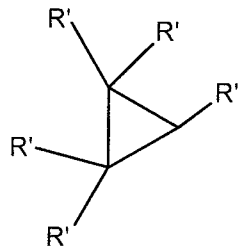
CLAIMS:

We claim:

1. A metallocene compound represented by the formula (1): A_eMX_{n-e}, or the formula (lc) TA_2MX_{n-2},

wherein: e is 1 or 2; T is a bridging group between two A groups; each A is a substituted monocyclic or polycyclic ligand that is pi-bonded to M and optionally includes one or more ring heteroatoms selected from boron, a group 14 atom that is not carbon, a group 15 atom, or a group 16 atom, and when e is 2 each A may be the same or different, provided that at least one A is substituted with at least one cyclopropyl substituent directly bonded to any sp^2 carbon atom at a bondable ring position of the ligand, wherein the cyclopropyl substituent is represented by the formula:



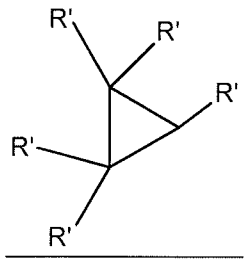
where each R' is, independently, hydrogen, a substituted or unsubstituted hydrocarbyl group, or a halogen; M is a transition metal atom having a coordination number of n and selected from group 3, 4, or 5 of the Periodic Table of Elements, or a lanthanide metal atom, or actinide metal atom; n is 3, 4, or 5; and each X is a univalent anionic ligand, or two Xs are joined and bound to the metal atom to form a metallocycle ring, or two Xs are joined to form a chelating ligand, a diene ligand, or an alkylidene ligand.

2. ~~The metallocene compound of claim 1, where the compound is~~ A metallocene compound represented by the formula: $T_y(A)_e(E)MX_{n-e-1}$

where E is $J\text{-}R''_{x-1-y}$, J is a heteroatom with a coordination number of three from group 15 or with a coordination number of two from group 16 of the Periodic Table of Elements; R" is a C_1-C_{100} substituted or unsubstituted hydrocarbyl radical; x is the coordination number of the heteroatom J where "x-l-y" indicates the number of R" substituents bonded to J; T is a bridging group between A and E, A and E are bound to M, y is 0 or 1; ~~and A, e, M, X and n are as defined in paragraph 1~~

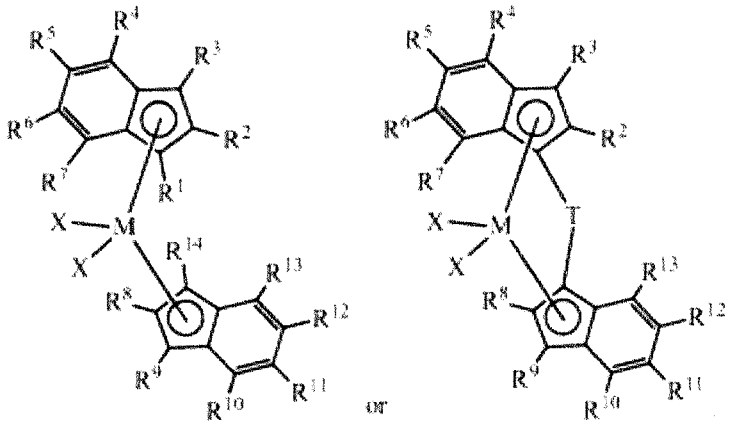
e is 1 or 2; each A is a substituted monocyclic or polycyclic ligand that is pi-bonded to M and optionally includes one or more ring heteroatoms selected from boron, a group 14 atom that is not carbon, a group 15 atom, or a group 16 atom, and when e is 2 each A may be the same or different, provided that at least one A is substituted with at least one cyclopropyl

substituent directly bonded to any sp^2 carbon atom at a bondable ring position of the ligand, wherein the cyclopropyl substituent is represented by the formula:

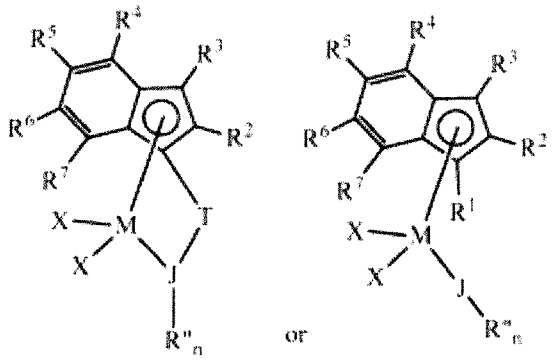


where each R' is, independently, hydrogen, a substituted or unsubstituted hydrocarbyl group, or a halogen; M is a transition metal atom having a coordination number of n and selected from group 3, 4, or 5 of the Periodic Table of Elements, or a lanthanide metal atom, or actinide metal atom; n is 3, 4, or 5; and each X is a univalent anionic ligand, or two Xs are joined and bound to the metal atom to form a metallocycle ring, or two Xs are joined to form a chelating ligand, a diene ligand, or an alkylidene ligand.

3. ~~The metallocene compound of claim 1 or 2, wherein the~~ A metallocene compound ~~is~~ represented by one of the following formulae:



formula (1a) formula (1b)



formula (2a) formula (2b);

where ~~M, T, X, are as defined in claim 1; J, R", and n are as defined in paragraph 2,~~

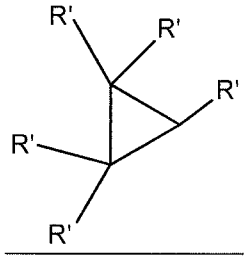
M is a transition metal atom having a coordination number of n* and selected from group 3, 4, or 5 of the Periodic Table of Elements, or a lanthanide metal atom, or actinide metal atom; n* is 3, 4, or 5;

T is a bridging group;

each X is a univalent anionic ligand, or two Xs are joined and bound to the metal atom to form a metallocycle ring, or two Xs are joined to form a chelating ligand, a diene ligand, or an alkylidene ligand;

J is a heteroatom with a coordination number of three from group 15 or with a coordination number of two from group 16 of the Periodic Table of Elements; R" is a C_1-C_{100} substituted or unsubstituted hydrocarbyl radical; n is the coordination number of the heteroatom J where "n" indicates the number of R" substituents bonded to J; and

each 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}, or R^{14} is, independently, hydrogen, a substituted hydrocarbyl group, an unsubstituted hydrocarbyl group, or a halide, provided that in formula Ia and Ib, at least one 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}, or R^{14} is a cyclopropyl substituent and in formula 2a and 2b at least one of R^1, R^2, R^3, R^4, R^5, R^6, or R^7, is a cyclopropyl substituent; and provided that any adjacent R^1 to R^{14} groups that are not a cyclopropyl substituent may form a fused ring or multicenter fused ring system where the rings may be aromatic, partially saturated or saturated, wherein the cyclopropyl substituent is represented by the formula:



where each R' is, independently, hydrogen, a substituted or unsubstituted hydrocarbyl group, or a halogen.

4. The metallocene compound of claim 1 or 2, wherein at least one A is monocyclic ligand selected from the group consisting of substituted or unsubstituted cyclopentadienyl, heterocyclopentadienyl, and heterophenyl ligands provided that when e is one, the monocyclic ligand is substituted with at least one cyclopropyl substituent.

5. The metallocene compound of claim 1 or 2, wherein at least one A is a polycyclic ligand selected from the group consisting of substituted or unsubstituted indenyl, fluorenyl, cyclopenta[*a*]naphthyl, cyclopenta[*b*]naphthyl, heteropentalenyl, heterocyclopentapentalenyl, heteroindenyl, heterofluorenyl, heterocyclopentanaphthyl, heterocyclopentaindenyl, and heterobenzocyclopentaindenyl ligands, provided that when e is one, the polycyclic ligand is substituted with at least one cyclopropyl substituent.

6. The metallocene compound of claim 1, 2, 3, 4, or 5, wherein M is a group 4 metal, preferably Hf, Ti or Zr.

7. The metallocene compound of any of claims 1 to 6, wherein each R' is hydrogen.

8. The metallocene compound of any of claims 1 to 7, wherein at least one A is a substituted or unsubstituted indenyl ligand, provided that when e is one, the indenyl ligand is substituted with at least one cyclopropyl substituent, preferably in the 2 and/or 4 and/or 6 positions.

9. The metallocene compound of any of claims ~~2~~1 to 8, wherein T is represented by the formula, $(R'''_2G)_g$, where each G is C, Si, or Ge, g is 1 or 2, and each R''' is, independently, hydrogen, halogen, C_1 to C_{20} hydrocarbyl or a C_1 to C_{20} substituted hydrocarbyl, and two or more R''' can form a cyclic structure including aromatic, partially saturated, or saturated cyclic or fused ring system.

10. The metallocene compound of any of claims 3 to 9 wherein R^2 and/or R^8 are cyclopropyl substituents and/ or R^4 and/or R^{10} are cyclopropyl substituents.

11. The metallocene compound of any of claims 3 to 10 wherein when one of R^1, R^2, R^3, R^4, R^5, R^6, and R^7 is a cyclopropyl substituent, at least one of the other R^1 to R^7 ~~substitutents~~ substituents is not hydrogen, and when one of R^8, R^9, R^{10}, R^{11}, R^{12}, R^{13}, and R^{14} is a cyclopropyl substituent, at least one of the other R^8 to R^{14} groups is not hydrogen.

12. The metallocene of compound of any of claims 3 to 11 wherein R^2 and R^8 are cyclopropyl and / or R^4 and/or R^{10} are hydrocarbyl or halogen.

13. The metallocene compound of any of claims 3 to 12, wherein J is nitrogen, phosphorus, oxygen or sulfur.

14. ~~The metallocene catalyst compound of claim 1, wherein the metallocene compound is one or more of~~ A metallocene catalyst selected from:

dimethylsilylene-bis(2-cyclopropyl-4-carbazol-9-ylindenyl)zirconium dichloride;

dimethylsilylene-bis(2-cyclopropyl-4-naphth-l-ylindenyl)zirconium dichloride;

dimethylsilyl(2-cyclopropyl-4-carbazol-9-ylindenyl)(2-cyclopropyl-4-phenylindenyl)zirconium dichloride;

dimethylsilylene-(2-cyclopropyl-4-carbazol-9-ylindenyl)(2-methyl-4-phenylindenyl) zirconium dichloride;
bis(2-cyclopropylindenyl)zirconium dichloride;
dimethylsilylene-(2-cyclopropylindenyl)(tert-butylamido)zirconium dichloride;
dimethylsilylene-(2-cyclopropylindenyl)(tert-butylamido)titanium dichloride;
dimethylsilylene-bis(2-cyclopropyl-4-para-tert-butylphenylindenyl)zirconium dichloride;
dimethylsilylene-bis(2-cyclopropyl-4-naphth-1 -ylindenyl)hafnium dichloride;
dimethylsilylene-bis(2-cyclopropyl-4-chloroindenyl)zirconium dichloride;
dimethylsilylene-bis(2-cyclopropyl-4,7-dimethylindenyl)zirconium dichloride;
dimethylsilylene-bis(2-cyclopropyl-4,7-dimethylindenyl)hafnium dichloride;
dimethylsilylene-bis(2-cyclopropyl-4-carbazol-9-ylindenyl)hafnium dichloride;
dimethylsilylene-bis(2-methyl-4-cyclopropylindenyl)zirconium dichloride;
cyclotetramethylenesilylene-(2-cyclopropyl-4-phenylindenyl)(2-cyclopropyl-4-carbazol-9-ylindenyl) zirconium dichloride;
dimethylsilylene-bis(2-cyclopropyl-4-phenylindenyl)zirconium dichloride;
dimethylsilylene-(2-cyclopropyl-4-para-tert-butylphenylindenyl)(2-methyl-4-phenylindenyl)zirconium dichloride;
dimethylsilylene-bis(2-cyclopropyl-4-para-tert-butylphenylindenyl)hafnium dichloride;
cyclotetramethylenesilylene-(bis(2-methyl-4-cyclopropylindenyl)zirconium dichloride;
dimethylsilylene-bis(2,4-dicyclopropylindenyl)zirconium dichloride;
dimethylsilylene-bis(2-methyl-4-cyclopropylindenyl)hafnium dichloride; where, in alternate embodiments, the dichloride in any of the compounds listed above may be replaced with dialkyl, dialkaryl, diflouride, diiodide, or dibromide, or a combination thereof.

15. A catalyst system comprising activator and the metallocene catalyst compound of any of claims 1 to 14.

16. The catalyst system of claim 15, wherein the activator comprises alumoxane or a non-coordinating anion activator.

17. The catalyst system of claim 15, wherein the activator is one or more of: N,N-dimethylanilinium tetrakis(perfluoronaphthyl)borate, N,N-dimethylanilinium tetrakis(perfluorobiphenyl)borate, N,N-dimethylanilinium tetrakis(3,5-bis(trifluoromethyl)phenyl)borate, triphenylcarbenium tetrakis(perfluoronaphthyl)borate, triphenylcarbenium tetrakis(perfluorobiphenyl)borate, triphenylcarbenium tetrakis(3,5-bis(trifluoromethyl)phenyl)borate, triphenylcarbenium tetrakis(perfluorophenyl)borate, $[Ph_3C^+]$ $[B(C_6F_5)_4^-]$, $[Me_3NH^+][B(C_6F_5)_4^-]$; l-(4-(tris(pentafluorophenyl)borate)-2,3,5,6-

tetrafluorophenyl)pyrrolidinium; tetrakis(pentafluorophenyl)borate, and 4-(tris(pentafluorophenyl)borate)-2,3,5,6-tetrafluoropyridine.

18. The catalyst system of claim 15, wherein the catalyst system is supported, preferably on silica.

19. A process to polymerize olefins comprising contacting one or more olefins with the catalyst system of any of claims 15 to 18.

20. The process of claim 19, wherein the process occurs in solution, preferably at a temperature of from about 0°C to about 300°C, at a pressure in the range of from about 0.35 MPa to about 10 MPa, and at a time up to 300 minutes.

21. The process of claim 20 further comprising obtaining polymer, preferably polymer comprising ethylene and or propylene.

22. The process of claim 20 or 21, wherein an ethylene polymer (preferably a homopolymer of ethylene or a copolymer of ethylene and one or more of propylene, butene, hexene or octene) is obtained.

23. The process of claim 20 or 21, wherein a propylene polymer (preferably a homopolymer of propylene or a copolymer of propylene and one or more of ethylene, butene, hexene or octene) is obtained.

24. The process of claim 20 or 21, wherein an isotactic polymer is obtained, preferably an isotactic propylene polymer.

25. The metallocene catalyst compound of claim 1 wherein when A is a substituted indenyl, the 2 position of the substituted indenyl is hydrogen, an unsubstituted hydrocarbyl group, or a halid.

26. The metallocene catalyst compound of claim 3, wherein the compound is of formula (1a) or (1b), each R^2 and R^8, is independently, hydrogen, an unsubstituted hydrocarbyl group, or a halide.

27. The metallocene catalyst compound of claim 3, wherein the compound is of formula (1a) or (1b), each R^2 and R^8 is cyclopropyl.