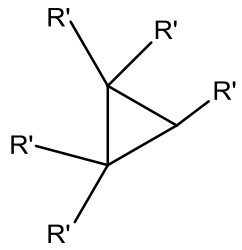
CLAIMS:

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 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 each A is the same,

wherein 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:



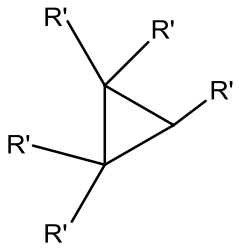
where each R' is, independently, hydrogen, a substituted or unsubstituted hydrocarbyl group, or a halogen; M is a transition metal atom having a coordination number of n and selected from group 3, 4, or 5 of the Periodic Table of Elements, or a lanthanide metal atom, or actinide metal atom; n is 3, 4, 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. 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;

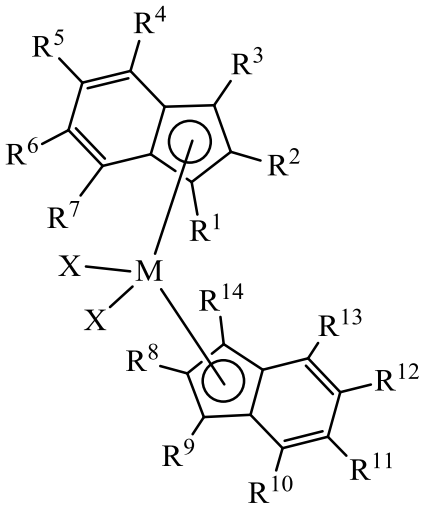
e is 2; each A is a substituted monocyclic or polycyclic ligand that is pi-bonded to M and optionally includes one or more ring heteroatoms selected from boron, a group 14 atom that is not carbon, a group 15 atom, or a group 16 atom, each A is the same,

wherein 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:

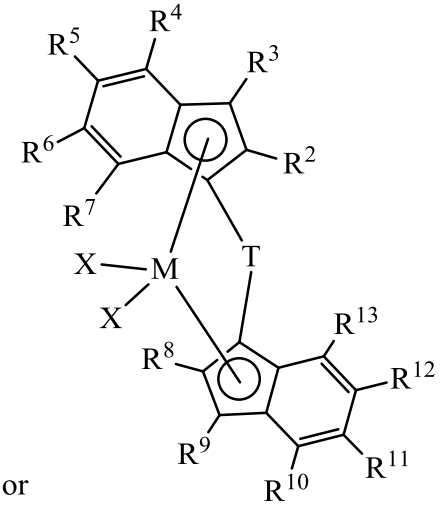


where each R' is, independently, hydrogen, a substituted or unsubstituted hydrocarbyl group, or a halogen; M is a transition metal atom having a coordination number of n and selected from group 3, 4, or 5 of the Periodic Table of Elements, or a lanthanide metal atom, or actinide metal atom; n is 3, 4, 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. A metallocene compound represented by one of the following formulae:



or



formula (1a) formula (1b)

where

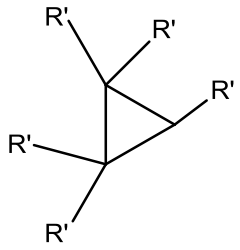
M is a transition metal atom having a coordination number of n* and selected from group 3, 4, or 5 of the Periodic Table of Elements, or a lanthanide metal atom, or actinide metal atom; n* is 3, 4, or 5;

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;

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 la and lb, 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 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 A is a monocyclic ligand selected from the group consisting of substituted or unsubstituted cyclopentadienyl, heterocyclopentadienyl, and heterophenyl ligands.

5. The metallocene compound of claim 1 or 2, wherein 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.

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 A is a substituted indenyl ligand substitutedwith at least one cyclopropyl substituent, preferably in the 2 and/or 4 and/or 6 positions.

9. The metallocene compound of any of claims 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 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. 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;

bis(2-cyclopropylindenyl)zirconium 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;

dimethylsilylene-bis(2-cyclopropyl-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, the dichloride in any of the compounds listed above is optionally 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 halide.

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.