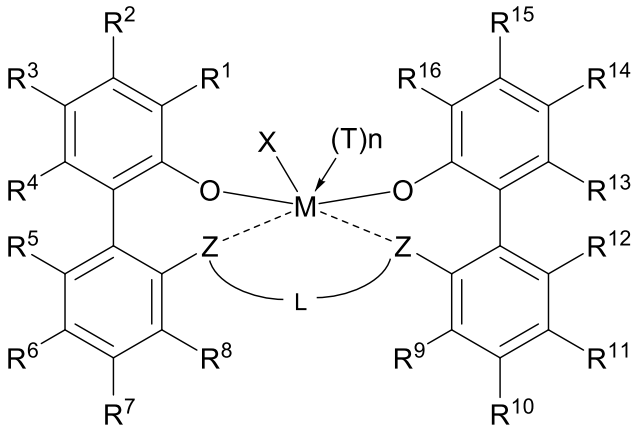
CLAIMS

1. A metal–ligand complex according to formula (I):



(I)

where:

M is scandium, yttrium, or a lanthanide metal having an oxidation state of +3;

X is a ligand chosen from (C_1−C_{40})hydrocarbyl, (C_1−C_{40})heterohydrocarbyl, -$CH_2Si(R^C)_{3-Q}(OR^C)_Q$, −$Si(R^C)_{3-Q}(OR^C)_Q$, -$OSi(R^C)_{3-Q}(OR^C)_Q$, −$CH_2Ge(R^C)_{3-Q}(OR^C)_Q$, −$Ge(R^C)_{3-Q}(OR^C)_Q$, −$P(R^C)_{2-W}(OR^C)_W$, −$P(O)(R^C)_{2-W}(OR^C)_W$, −$N(R^C)_2$, −$NH(R^C)$, −$N(Si(R^C)_3)_2$, −$NR^CSi(R^C)_3$, −$NHSi(R^C)_3$, −$OR^C$, −$SR^C$, −$NO_2$, −CN, −$CF_3$, −$OCF_3$, −$S(O)R^C$, −$S(O)_2R^C$, −$OS(O)_2R^C$, −$N{=}C(R^C)_2$, −$N{=}CH(R^C)$, −$N{=}CH_2$, −$N{=}P(R^C)_3$, −$OC(O)R^C$, −$C(O)OR^C$, −$N(R^C)C(O)R^C$, −$N(R^C)C(O)H$, −$NHC(O)R^C$, −$C(O)N(R^C)_2$, −$C(O)NHR^C$, −$C(O)NH_2$, a halogen, $B(R^Y)_4$, $Al(R^Y)_4$, or $Ga(R^Y)_4$, or a hydrogen, wherein each R^C is independently a substituted or unsubstituted (C_1−C_{30})hydrocarbyl, or a substituted or unsubstituted (C_1−C_{30})heterohydrocarbyl, and each Q is 0, 1, 2 or 3, and each W is 0, 1, or 2; each R^Y is –H, (C_1−C_{30})hydrocarbyl, or halogen atom;

each T is independently Lewis Base;

n is 0, 1, or 2, when n is 1, X and T are optionally linked, when n is 2, X and one of T are optionally linked;

the metal–ligand complex is overall charge-neutral;

each Z is independently chosen from −O−, −S−, −$N(R^N)$−, or –$P(R^P)$−, wherein the dotted line optionally defines a dative bond;

R^1 and R^{16} are independently selected from the group consisting of $(C_1–C_{40})$hydrocarbyl, $(C_1–C_{40})$heterohydrocarbyl, $–Si(R^C)_3$, $–Ge(R^C)_3$, $–P(R^P)_2$, $–N(R^N)_2$, $–OR^C$, $–SR^C$, $–NO_2$, –CN, $–CF_3$, $R^CS(O)–$, $R^CS(O)_2–$, $–N=C(R^C)_2$, $R^CC(O)O–$, $R^COC(O)–$, $R^CC(O)N(R)–$, $(R^C)_2NC(O)–$, or halogen;

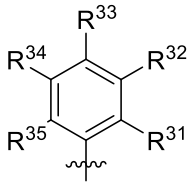
R^2, R^3, R^4, R^5, R^6, R^7, R^8, R^9, R^{10}, R^{11}, R^{12}, R^{13}, R^{14}, and R^{15} are independently selected from –H, $(C_1–C_{40})$hydrocarbyl, $(C_1–C_{40})$heterohydrocarbyl, $–Si(R^C)_3$, $–Ge(R^C)_3$, $–P(R^P)_2$, $–N(R^N)_2–OR^C$, $–SR^C$, $–NO_2$, –CN, $–CF_3$, $R^CS(O)–$, $R^CS(O)_2–$, $(R^C)_2C=N–$, $(R^C)_2P=N–$, $R^CC(O)O–$, $R^COC(O)–$, $R^CC(O)N(R)–$, $(R^C)_2NC(O)–$, and halogen;

provided that when M is yttrium or a lanthanide metal, R^1 is not –H, phenyl or *tert*-butyl; and R^{16} is not –H, phenyl or *tert*-butyl;

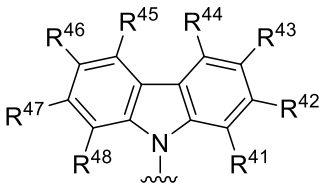
L is $(C_1–C_{40})$hydrocarbylene or $(C_1–C_{40})$heterohydrocarbylene; and

each R^C, R^P, and R^N in formula (I) is independently a $(C_1–C_{30})$hydrocarbyl, $(C_1–C_{30})$heterohydrocarbyl, or –H.

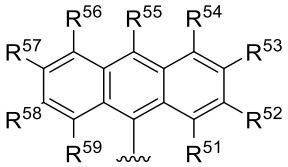
2. The metal–ligand complex according to claim 1, where R^1 and R^{16} are chosen from radicals having formula (II), radicals having formula (III), and radicals having formula (IV):



(II)



(III)



(IV)

where each of $R^{31–35}$, $R^{41–48}$, and $R^{51–59}$ is independently chosen from –H, $(C_1–C_{40})$hydrocarbyl, $(C_1–C_{40})$heterohydrocarbyl, $–Si(R^C)_3$, $–Ge(R^C)_3$, $–P(R^P)_2$, $–N(R^N)_2$, $–OR^C$, $–SR^C$, $–NO_2$, –CN, $–CF_3$, $R^CS(O)–$, $R^CS(O)_2–$, $(R^C)_2C=N–$, $R^CC(O)O–$, $R^COC(O)–$, $R^CC(O)N(R^N)–$, $(R^C)_2NC(O)–$, or halogen; provided that when R^1 and R^{16} are formula (II), at least one of R^{31} to R^{35} is not –H.

3. The metal–ligand complex of claim 1 or claim 2, wherein when M is yttrium or a lanthanide metal, at least one of $R^{5–8}$ is not –H and at least one of $R^{9–12}$ is not –H.

~~4. The metal–ligand complex according to claim 1 or claim 2, wherein R^1 and R^{16} are identical.~~

~~5~~4. The metal−ligand complex according to claim 2, wherein at least one of R^1 and R^{16} is a radical having formula (III) and R^{42} and R^{47} are (C_1-C_{20})hydrocarbyl, –Si[(C_1-C_{20})hydrocarbyl]$_3$, or –Ge[(C_1-C_{20})hydrocarbyl]$_3$; or R^{43} and R^{46} are (C_1-C_{20})hydrocarbyl, –Si[(C_1-C_{20})hydrocarbyl]$_3$, or –Ge[(C_1-C_{20})hydrocarbyl]$_3$.

~~6. The metal−ligand complex according to claim 5, wherein R^{42} and R^{47} are (C_1-C_{20})hydrocarbyl, Si[(C_1-C_{20})hydrocarbyl]$_3$, or Ge[(C_1-C_{20})hydrocarbyl]$_3$.~~

~~7. The metal−ligand complex according to claim 5, wherein R^{43} and R^{46} are (C_1-C_{20})hydrocarbyl, Si[(C_1-C_{20})hydrocarbyl]$_3$, or Ge[(C_1-C_{20})hydrocarbyl]$_3$.~~

~~8. The metal−ligand complex according to claims 5-7, wherein optionally R^{42} and R^{43} are bonded together, and optionally R^{46} and R^{47} are bonded together.~~

~~9~~5. The metal−ligand complex according to claim 2, wherein at least one of R^1 and R^{16} is a radical having formula (II), ~~wherein~~and at least one of R^{31} to R^{35} is not –H or R^{32} and R^{34} are (C_1-C_{20})hydrocarbyl, –Si[(C_1-C_{20})hydrocarbyl]$_3$, or –Ge[(C_1-C_{20})hydrocarbyl]$_3$.

~~10. The metal−ligand complex according to claim 9, wherein R^{32} and R^{34} are (C_1-C_{20})hydrocarbyl, Si[(C_1-C_{20})hydrocarbyl]$_3$, or Ge[(C_1-C_{20})hydrocarbyl]$_3$.~~

~~11~~6. The metal−ligand complex according to claim 2, wherein at least one of R^1 and R^{16} is a radical having formula (IV) and wherein at least two of R^{52}, R^{53}, R^{55}, R^{57}, and R^{58} are (C_1-C_{20})hydrocarbyl, –Si[(C_1-C_{20})hydrocarbyl]$_3$, or –Ge[(C_1-C_{20})hydrocarbyl]$_3$.

~~12. The metal−ligand complex according to claim 11, wherein at least two of R^{52}, R^{53}, R^{55}, R^{57}, and R^{58} are (C_1-C_{20})hydrocarbyl, Si[(C_1-C_{20})hydrocarbyl]$_3$, or Ge[(C_1-C_{20})hydrocarbyl]$_3$.~~

~~13. The metal−ligand complex according to claim 11 or claim 12, wherein optionally R^{52} and R^{53} are linked to form a cyclic structure, and optionally R^{57} and R^{58} are linked to form a cyclic structure.~~

~~14. The metal−ligand complex according to any of the preceding claims, wherein:~~
~~at least one of R^6, R^7, and R^8 is halogen; and~~
~~at least one of R^9, R^{10}, and R^{11} is halogen.~~

~~15~~7. The metal−ligand complex according to any one of claims 1 to ~~12~~6, wherein ~~at least one of~~ R^8 and R^9 ~~is not H~~are methyl.

~~16~~8. The metal−ligand complex according to any of the preceding claims, wherein R^3 and R^{14} are $(C_1–C_{10})$alkyl, methyl, *tert*-octyl, *n*-octyl, or *n*-octylalkoxy, $–OR^C$, wherein R^C is $(C_1–C_{30})$hydrocarbyl.

~~17. The metal−ligand complex according to any one of the preceding claims, wherein R^3 and R^{14} are methyl, R^6 and R^{11} are halogen.~~

~~18. The metal−ligand complex according to any one of claims 1-15, wherein R^3 and R^{14} are $–OR^C$, wherein R^C is $(C_1–C_{30})$hydrocarbyl.~~

~~19~~9. The metal−ligand complex according to any one of claims ~~1-15~~1 to 7, wherein R^6 and R^{11} are *tert*-butyl or halogen.

~~20. The metal−ligand complex according to any one of claims 1 to 15, wherein R^3 and R^{14} are *tert*-octyl, *n*-octyl, or *n*-octylalkoxy.~~

~~21~~10. The metal−ligand complex according to any one of the preceding claims, where L is chosen from $–CH_2–$, $–CH_2(CH_2)_mCH_2–$ where m is from 0 to 3, $–CH_2Si(R^C)_2CH_2–$, $–CH_2Ge(R^C)_2CH_2–$, $–CH(CH_3)CH_2CH^*(CH_3)$, and $–CH_2$(phen-1,2-di-yl)$CH_2–$, where each R^C in L is $(C_1–C_{20})$hydrocarbyl, and "C*" is a carbon atom from which a hydrogen atom is removed to form a secondary or tertiary alkyl radical.

~~22~~11. The metal−ligand complex according to any one of the preceding claims, wherein X is $–CH_2Si[(C_1–C_{20})alkyl]_3$, $(C_1–C_{12})$alkyl, or halogen atom.

~~23~~12. The metal−ligand complex according to any one of the preceding claims, wherein n is 1 or 2; and at least one T is $(C_1–C_{20})$heterohydrocarbon, wherein the hetero atom of the heterohydrocarbon is oxygen.

~~24~~13. The metal−ligand complex according to any one of the preceding claims, wherein n is 1 or 2; and at least one T is tetrahydrofuran, diethyl ether, or methyl *tert*-butyl ether (MTBE).

~~25. The metal−ligand complex according to any one of the preceding claims, wherein:~~

~~R^2, R^4, R^5, R^{12}, R^{13}, and R^{15} are hydrogen; and~~

~~each Z is oxygen.~~

14. The metal-ligand complex according to any one of the preceding claims, where M is scandium.

~~26~~15. A polymerization process comprising:

polymerizing ethylene and one or more olefins in the presence of a catalyst system comprising the metal−ligand complex of any one of claims 1-~~24~~14, under olefin polymerizing conditions to form an ethylene-based polymer.

~~27~~16. The polymerization process of claim ~~26~~15, wherein the catalyst system further comprises at least one co-catalyst.

~~28~~17. The polymerization process of claim ~~26~~15, wherein a co-catalyst is absent from the catalyst system.

~~29~~18. The polymerization process of any one of claims ~~26 to 28~~15 to 17, wherein the polymerization process is a solution polymerization process.

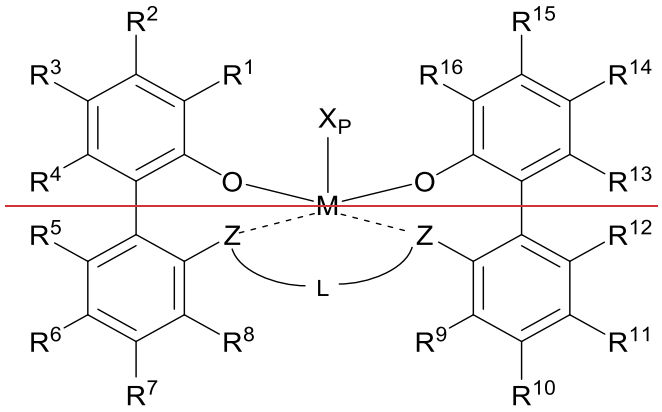
~~30~~19. The polymerization process of any one of claims ~~26 to 29~~15 to 18, wherein the catalyst system further comprises an additive.

~~31~~20. The polymerization process of claim ~~30~~19, wherein the additive is modified methylaluminoxane or alkylaluminum.

~~32. The polymerization process of claim 30, wherein the additive is alkylaluminum.~~

~~33. The polymerization process of claim 26, wherein the polymerizing ethylene occurs in the presence of a borate based additive.~~

34. An olefin propogating catalytic species according to formula (Ia):



(Ia)

where:

M is scandium, yttrium, or a lanthanide metal having an oxidation state of +3;

X_P is a ligand chosen from hydrocarbyl, wherein the hydrocarbyl is branched or unbranched having at least 30 carbon atoms;

each Z is independently chosen from –O–, –S–, –N(R^N)–, or –P(R^P)–, wherein the dotted line optionally defines a dative bond;

R^1 and R^{16} are independently selected from the group consisting of (C_1–C_{40})hydrocarbyl, (C_1–C_{40})heterohydrocarbyl, –Si(R^C)$_3$, –Ge(R^C)$_3$, –P(R^P)$_2$, –N(R^N)$_2$, –OR^C, –SR^C, –NO_2, –CN, –CF_3, R^CS(O)–, R^CS(O)$_2$–, –N=C(R^C)$_2$, R^CC(O)O–, R^COC(O)–, R^CC(O)N(R)–, (R^C)$_2$NC(O)–, or halogen;

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}, and R^{15} are independently selected from –H, (C_1–C_{40})hydrocarbyl, (C_1–C_{40})heterohydrocarbyl, –Si(R^C)$_3$, –Ge(R^C)$_3$, –P(R^P)$_2$, –N(R^N)$_2$, –OR^C, –SR^C, –NO_2, –CN, –CF_3, R^CS(O)–, R^CS(O)$_2$–, (R^C)$_2$C=N–, (R^C)$_2$P=N–, R^CC(O)O–, R^COC(O)–, R^CC(O)N(R)–, (R^C)$_2$NC(O)–, and halogen;

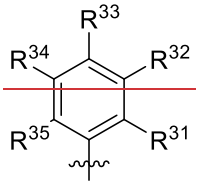
provided that when M is yttrium or a lanthanide metal, R^1 is not –H, phenyl or *tert*-butyl; and R^{16} is not –H, phenyl or *tert*-butyl;

L is (C_1–C_{40})hydrocarbylene or (C_1–C_{40})heterohydrocarbylene; and

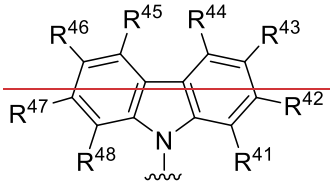
each R^C, R^P, and R^N in formula (I) is independently a (C_1–C_{30})hydrocarbyl, (C_1–C_{30})heterohydrocarbyl, or –H.

35. The olefin propogating catalytic species of claim 34, wherein M is yttrium or a lanthanide metal, at least one of $R^{5–8}$ is not –H and at least one of $R^{9–12}$ is not –H.

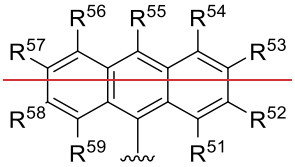
36. The olefin propogating catalytic species of claim 34 or claim 35, where R^1 and R^{16} are chosen from radicals having formula (II), radicals having formula (III), and radicals having formula (IV):



(II)



(III)



(IV)

where each of R^{31-35}, R^{41-48}, and R^{51-59} is independently chosen from –H, $(C_1–C_{40})$hydrocarbyl, $(C_1–C_{40})$heterohydrocarbyl, $–Si(R^C)_3$, $–Ge(R^C)_3$, $–P(R^P)_2$, $–N(R^N)_2$, $–OR^C$, $–SR^C$, $–NO_2$, –CN, $–CF_3$, $R^CS(O)–$, $R^CS(O)_2–$, $(R^C)_2C=N–$, $R^CC(O)O–$, $R^COC(O)–$, $R^CC(O)N(R^N)–$, $(R^C)_2NC(O)–$, or halogen; provided that when R^1 and R^{16} are formula (II), at least one of R^{31} to R^{35} is not –H.

37. The olefin propogating catalytic species of claim 34 or claim 35, wherein at least one of R^8 and R^9 is not –H.

38. The olefin propogating catalytic species of any one of claims 34 to 36, wherein R^3 and R^{14} are $(C_1–C_{10})$alkyl.

39. The olefin propogating catalytic species of any one of claims 34 to 37, wherein R^3 and R^{14} are $–OR^C$, wherein R^C is $(C_1–C_{30})$hydrocarbyl.

40. The olefin propogating catalytic species of any one of claims 34 to 37, wherein R^3 and R^{14} are *tert*-octyl, *n*-octyl, or *n*-octylalkoxy.

41. The olefin propogating catalytic species of any one of claims 34 to 40, wherein R^6 and R^{11} are *tert*-butyl.

42. The olefin propogating catalytic species of any one of claims 34 to 41, wherein R^1 and R^{16} are chosen from radicals having formula (III) and optionally R^{42} and R^{43} are linked to form a cyclic structure, and optionally R^{46} and R^{47} are linked to form a cyclic structure.

43. The olefin propogating catalytic species of any one of claims 34 to 42, where L is chosen from $–CH_2–$, $–CH_2(CH_2)_mCH_2–$ where m is from 0 to 3, $–CH_2Si(R^C)_2CH_2–$,

~~$=CH_2Ge(R^C)_2CH_2=$, $=CH(CH_3)CH_2CH^*(CH_3)$, and $=CH_2$(phen-1,2-di-yl)$CH_2=$, where each R^C in L is (C_1–C_{20})hydrocarbyl, and "C*" is a carbon atom from which a hydrogen atom is removed to form a secondary or tertiary alkyl radical.~~

~~44. A catalyst structure comprising a scandium, yttria, or a lanthanide metal having an oxidation state of +3 coordinated to a bis(phenylphenoxy) ligand.~~