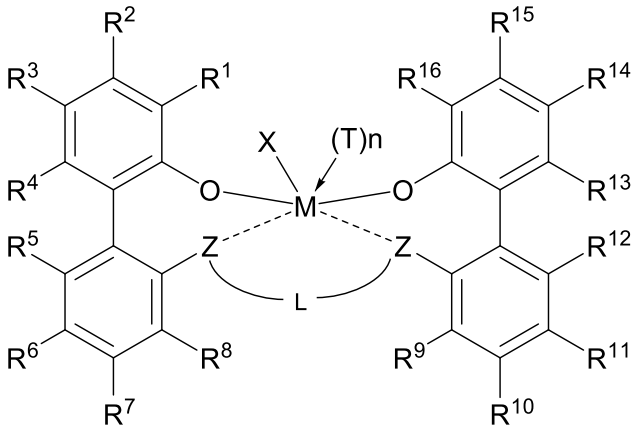
CLAIMS

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;

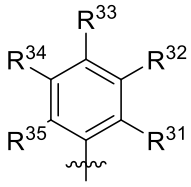
R^2, R^3, R^4, R^5, R^6, R^7, R^8, R^9, R^{10}, R^{11}, R^{12}, R^{13}, R^{14}, and R^{15} are independently selected from –H, $(C_1–C_{40})$hydrocarbyl, $(C_1–C_{40})$heterohydrocarbyl, $–Si(R^C)_3$, $–Ge(R^C)_3$, $–P(R^P)_2$, $–N(R^N)_2–OR^C$, $–SR^C$, $–NO_2$, –CN, $–CF_3$, $R^CS(O)–$, $R^CS(O)_2–$,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

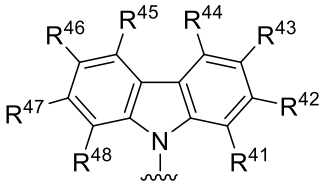
L is $(C_1–C_{40})$hydrocarbylene or $(C_1–C_{40})$heterohydrocarbylene; and

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.

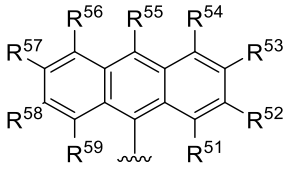
2. The metal−ligand complex according to claim 1, where R^1 and R^{16} are chosen from radicals having formula (II), radicals having formula (III), and radicals having formula (IV):



(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 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]$_3$.

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), 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]$_3$.

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]$_3$.

7. The metal−ligand complex according to any one of claims 1 to 6, wherein R^8 and R^9 are methyl.

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.

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

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.

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.

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.

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).

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

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 1-14, under olefin polymerizing conditions to form an ethylene-based polymer.

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

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

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

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

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