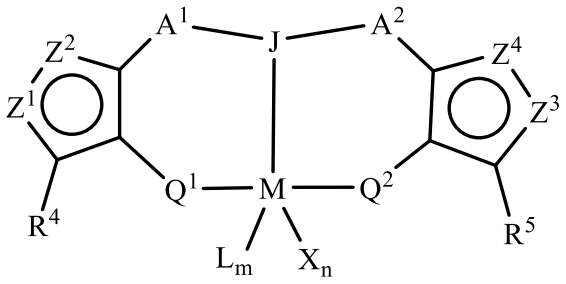
CLAIMS

What is claimed is:

1. A catalyst compound represented by Formula (**I**):



(**I**)

wherein:

M is a group 3, 4, or 5 metal;

each A^1 and A^2 is independently an aromatic, a substituted aromatic, or alkenediyl group;

heterocyclic ring fragments -(Z^1Z^2)- and –(Z^3Z^4)- are independently selected from –(Z^5Z^6)- or –(Z^6Z^5)-, with Z^5 being selected from oxygen, sulfur, S(O), $S(O)_2$, and N(R^{50}), and Z^6 being selected from nitrogen and C(R^{51}), wherein each R^{50} and R^{51} is independently hydrogen, C_1-C_{40} hydrocarbyl, C_1-C_{40} substituted hydrocarbyl, a monovalent heteroatom, or a heteroatom-bonded monovalent group;

each of R^4 and R^5 is independently hydrogen, C_1-C_{40} hydrocarbyl, C_1-C_{40} substituted hydrocarbyl, a monovalent heteroatom, or a heteroatom-bonded monovalent group;

J is a heterocyclic Lewis base;

each Q^1 and Q^2 are independently selected from oxygen, sulfur, N(R^{30}), or P(R^{30}), wherein R^{30} is C_1-C_{40} hydrocarbyl, substituted C_1-C_{40} hydrocarbyl, a monovalent heteroatom, or a heteroatom-bonded monovalent group;

L is a Lewis base, optionally any two L groups join together to form a bidentate Lewis base;

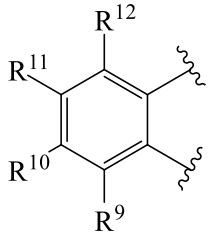
X is an anionic ligand, optionally an X group is joined to an L group to form a monoanionic bidentate group, or optionally, any two X groups are joined together to form a dianionic ligand;

n is 1, 2 or 3;

m is 0, 1, or 2; and

n+m is not greater than 4.

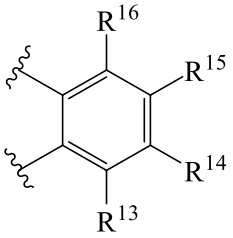
2. The catalyst compound of claim 1, wherein A^1 is represented by the formula:



wherein ~ indicates a connection to the catalyst compound, and

each of R^9, R^{10}, R^{11}, and R^{12} is independently hydrogen, C_1-C_{40} hydrocarbyl, C_1-C_{40} substituted hydrocarbyl, a monovalent heteroatom, or a heteroatom-bonded monovalent group, or one or more of R^9 and R^{10}, R^{10} and R^{11}, or R^{11} and R^{12} may be joined to form one or more substituted hydrocarbyl rings, unsubstituted hydrocarbyl rings, substituted heterocyclic rings, or unsubstituted heterocyclic rings each having 5, 6, 7, or 8 ring atoms.

3. The catalyst compound of claim 1, wherein A^2 is represented by the formula:



wherein ~ indicates a connection to the catalyst compound, and

each of R^{13}, R^{14}, R^{15}, and R^{16} is independently hydrogen, C_1-C_{40} hydrocarbyl, C_1-C_{40} substituted hydrocarbyl, a monovalent heteroatom, or a heteroatom-bonded monovalent group, or one or more of R^{13} and R^{14}, R^{14} and R^{15}, or R^{15} and R^{16} may be joined to form one or more substituted hydrocarbyl rings, unsubstituted hydrocarbyl rings, substituted heterocyclic rings, or unsubstituted heterocyclic rings each having 5, 6, 7, or 8 ring atoms.

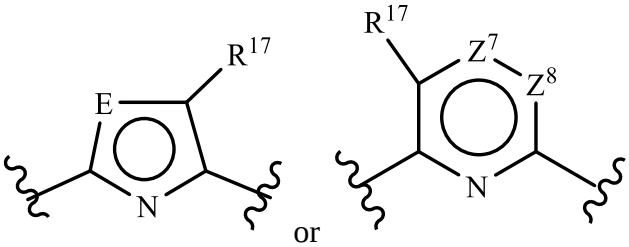
4. The catalyst compound of claim 1, wherein the compound features a tridentate dianionic ligand that is coordinated to the metal to form a pair of 8-membered metallocycle rings.

5. The catalyst compound of claim 1, wherein J is a group 15-containing heterocycle, or a group 16-containing heterocycle.

6. The catalyst compound of claim 1, wherein J is a nitrogen-containing heterocycle, an oxygen-containing heterocycle, a phosphorus-containing heterocycle, or a sulfur-containing heterocycle.

7. The catalyst compound of any of claims 1 to 6, wherein J is selected from a pyridine, a pyrimidine, a pyrazine, a thiazole, an oxazole, an oxazoline, an imidazole, a furan, or a thiofuran.

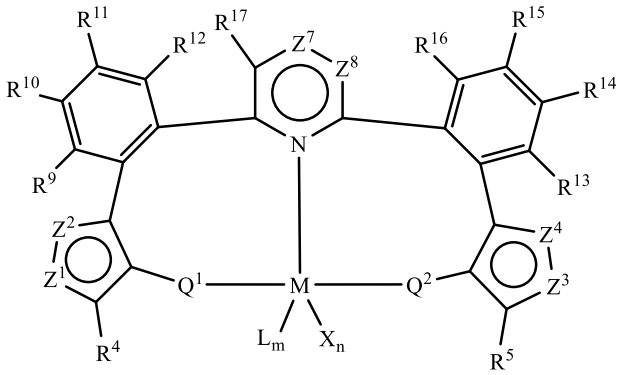
8. The catalyst compound of any of claims 1 to 6, wherein J is represented by the formula:



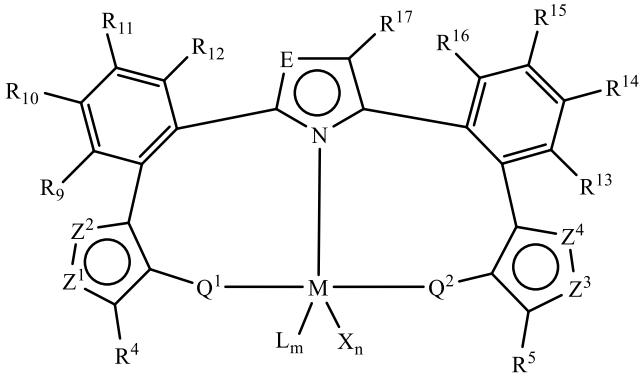
or

wherein ~ indicates a connection to the catalyst compound; E is oxygen, sulfur, or NR^{17}; Z^7 is selected from nitrogen and $C(R^{18})$; Z^8 is selected from nitrogen and $C(R^{19})$; and each of R^{17} and R^{18} and R^{19} are selected from hydrogen, C_1-C_{40} hydrocarbyl, C_1-C_{40} substituted hydrocarbyl, a monovalent heteroatom, or a heteroatom-bonded monovalent group..

9. The catalyst compound of claim 1, wherein the catalyst compound represented by Formula (**I**) is represented by Formula (**II**) or Formula (**III**):



(**II**)



(**III**)

wherein:

each Q^1 and Q^2 are independently selected from oxygen, sulfur, $N(R^{30})$, or $P(R^{30})$, wherein R^{30} is C_1-C_{40} hydrocarbyl, substituted C_1-C_{40} hydrocarbyl, a monovalent heteroatom, or a heteroatom-bonded monovalent group;

heterocyclic ring fragments -(Z^1Z^2)- and –(Z^3Z^4)- are selected from –(Z^5Z^6)- or –(Z^6Z^5)-, with Z^5 being selected from oxygen, sulfur, S(O), $S(O)_2$, and $N(R^{50})$, and Z^6 being selected from nitrogen and $C(R^{51})$, wherein each R^{50} and R^{51} is independently hydrogen, C_1-C_{40} hydrocarbyl, C_1-C_{40} substituted hydrocarbyl, a monovalent heteroatom, or a heteroatom-bonded monovalent group;

Z^7 is selected from nitrogen and $C(R^{18})$;

Z^8 is selected from nitrogen and $C(R^{19})$;

E is oxygen, sulfur, or $N(R^{20})$;

each of R^4 and R^5 is independently hydrogen, C_1-C_{40} hydrocarbyl, C_1-C_{40} substituted hydrocarbyl, a monovalent heteroatom, or a heteroatom-bonded monovalent group;

each of R^9, R^{10}, R^{11}, and R^{12} is independently hydrogen, C_1-C_{40} hydrocarbyl, C_1-C_{40} substituted hydrocarbyl, a monovalent heteroatom, or a heteroatom-bonded monovalent group, or one or more of R^9 and R^{10}, R^{10} and R^{11}, or R^{11} and R^{12} may be joined to form one or more substituted hydrocarbyl rings, unsubstituted hydrocarbyl rings, substituted heterocyclic rings, or unsubstituted heterocyclic rings each having 5, 6, 7, or 8 ring atoms;

each of R^{13}, R^{14}, R^{15}, and R^{16} is independently hydrogen, C_1-C_{40} hydrocarbyl, C_1-C_{40} substituted hydrocarbyl, a monovalent heteroatom, or a heteroatom-bonded monovalent group, or one or more of R^{13} and R^{14}, R^{14} and R^{15}, or R^{15} and R^{16} may be joined to form one or more substituted hydrocarbyl rings, unsubstituted hydrocarbyl rings, substituted heterocyclic rings, or unsubstituted heterocyclic rings each having 5, 6, 7, or 8 ring atoms;

each of R^{17}, R^{18}, R^{19} and R^{20} is hydrogen, C_1-C_{40} hydrocarbyl, C_1-C_{40} substituted hydrocarbyl, a monovalent heteroatom, or a heteroatom-bonded monovalent group, or one or

more of R^{17} and R^{18}, R^{18} and R_{19} may be joined together to form one or more substituted hydrocarbyl rings, unsubstituted hydrocarbyl rings, substituted heterocyclic rings, or unsubstituted heterocyclic rings each having 5, 6, 7, or 8 ring atoms;

M is a group 3, 4, or 5 metal;

L is a Lewis base;

X is an anionic ligand;

n is 1, 2 or 3;

m is 0, 1, or 2;

n+m is not greater than 4;

any two L groups may be joined together to form a bidentate Lewis base;

an X group may be joined to an L group to form a monoanionic bidentate group; and any two X groups may be joined together to form a dianionic ligand.

10. The catalyst compound of claim 9, wherein M is zirconium or hafnium.

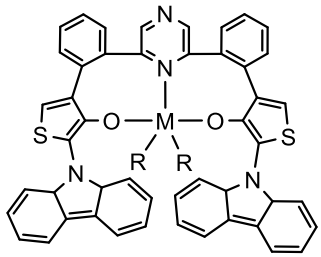
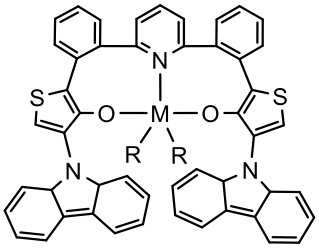
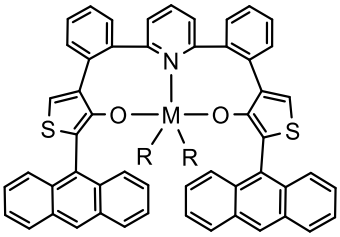
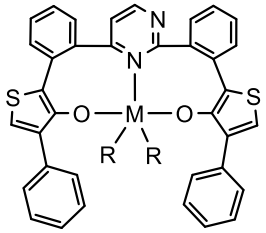
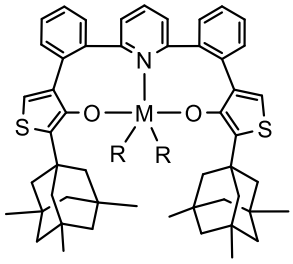
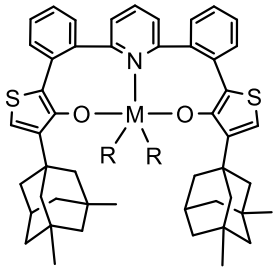
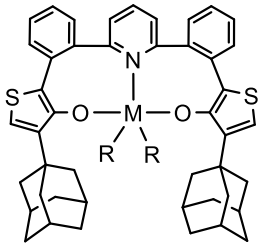
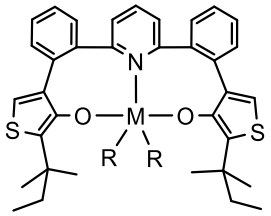
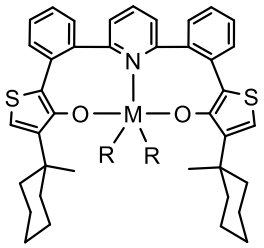
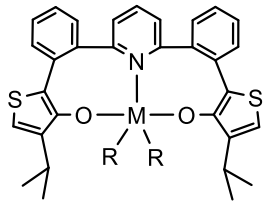
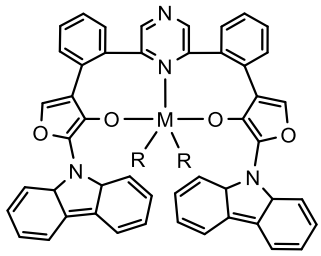
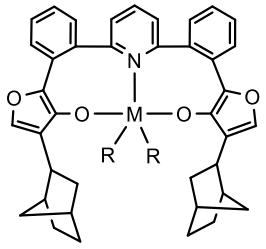
11. The catalyst compound of claim 10, wherein R^9 through R^{17} are hydrogen.

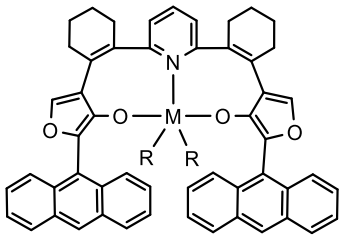
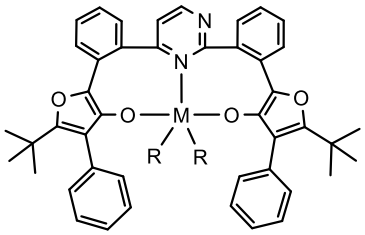
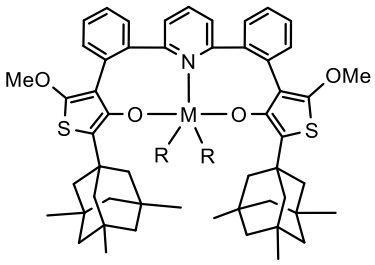
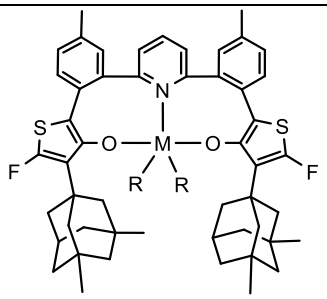
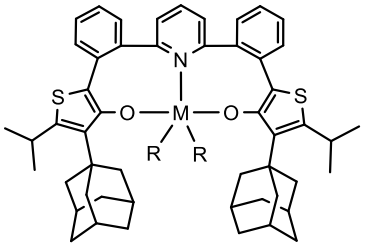
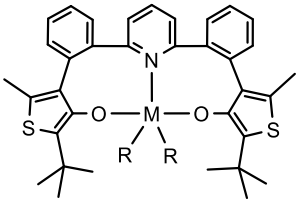
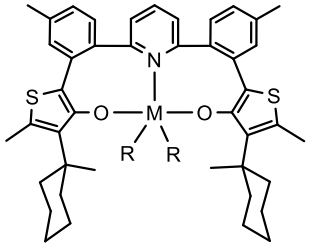
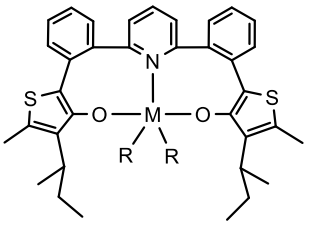
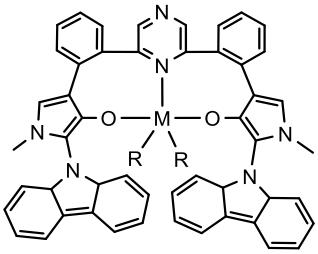
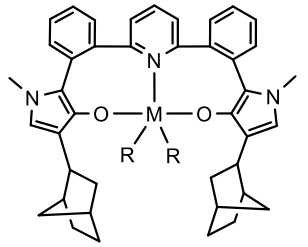
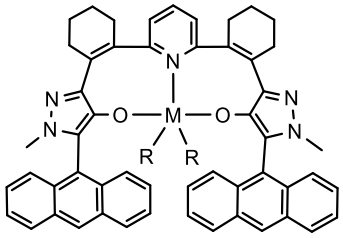
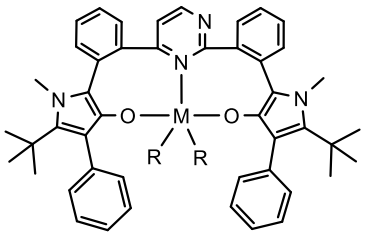
12. The catalyst compound of claim 11, wherein R^4 and R^5 are each selected from C_1-C_{40} hydrocarbyl, C_1-C_{40} substituted hydrocarbyl, or a heteroatom-bonded monovalent group containing up to 40 atoms, wherein -(Z^1Z^2)- and –(Z^3Z^4)- are selected from –(Z^5Z^6)- or –(Z^6Z^5)-, with Z^5 being oxygen or sulfur, and wherein R^4 and R^5 are each selected from C_4-C_{40} cyclic tertiary hydrocarbyl groups.

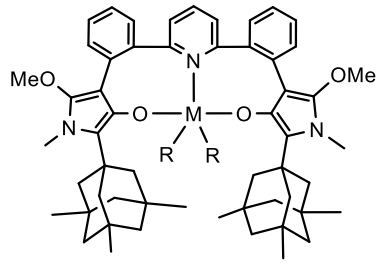
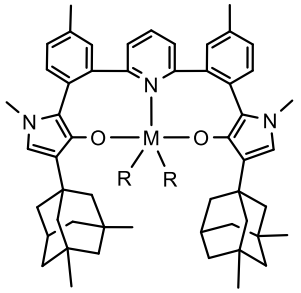
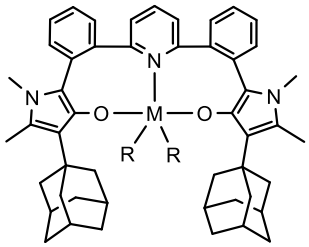
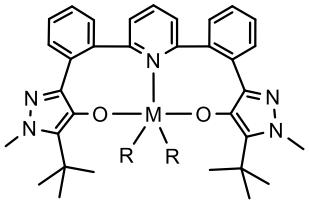
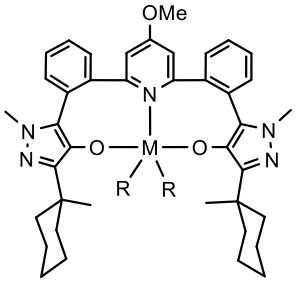
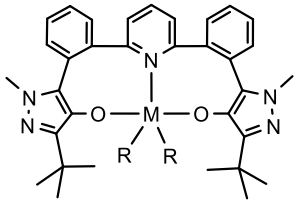
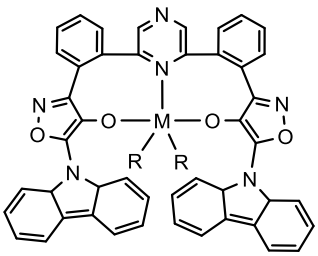
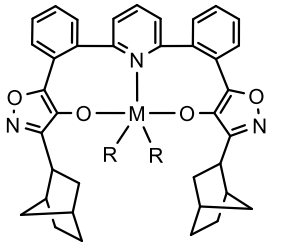
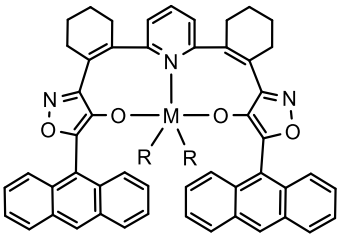
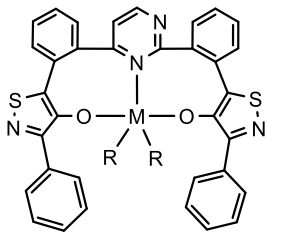
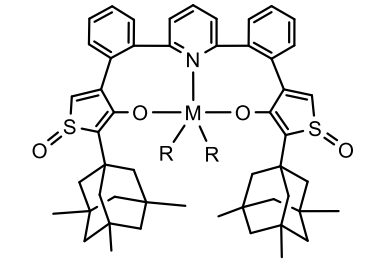
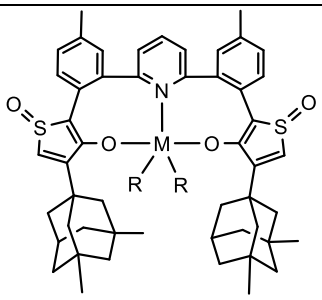
13. The catalyst compound (**II**) of claim 9, wherein Z^7 is C(R^{18}), wherein R^{18} is selected from hydrogen, trifluoromethyl, methoxy, Me_2N, or halogen atom, wherein Z^8 is C(R^{19}), wherein R^{18} is hydrogen, wherein R^4 and R^5 are each selected from C_4-C_{20} hydrocarbyls, tertiary hydrocarbyl, or cyclic tertiary hydrocarbyl, and wherein each of R^9, R^{10}, R^{11}, R^{12}, R^{13}, R^{14}, R^{15}, R^{16}, and R^{17} is independently hydrogen or C_1-C_{10} alkyl.

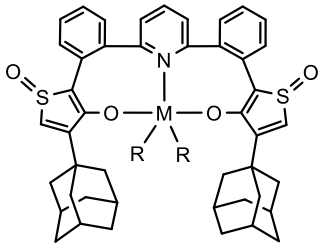
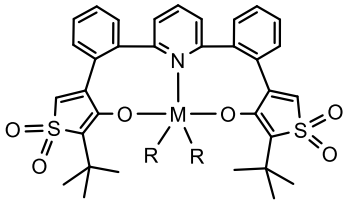
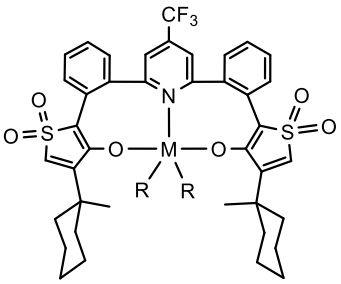
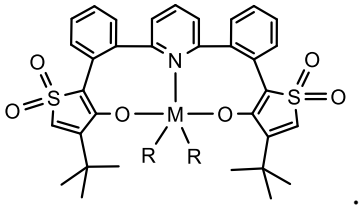
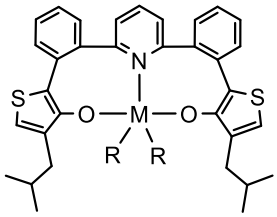
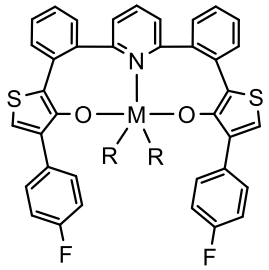
14. The catalyst compound of claim 1, wherein R^4 and R^5 are each selected from C_6-C_{20} aryls, tertiary hydrocarbyl, or cyclic tertiary hydrocarbyl, preferably adamantan-1-yl, 3,5-dimethyladamantan-1-yl, and 3,5,7-trimethyladamantan-1-yl.

15. The catalyst compound of claim 1, wherein the catalyst compound is selected from the following, with M = Zr or Hf; and R = C_1-C_{20} hydrocarbyl, a monovalent heteroatom, or a heteroatom-bonded monovalent group:

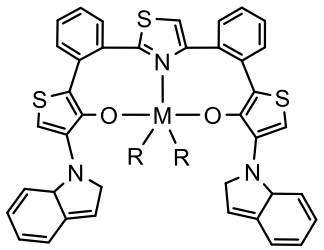
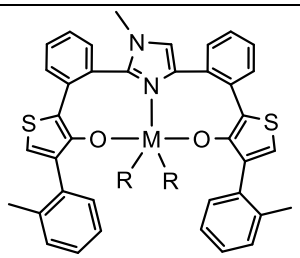
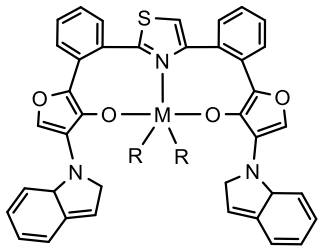
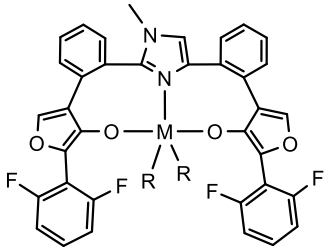
	
	
	
	
	
	

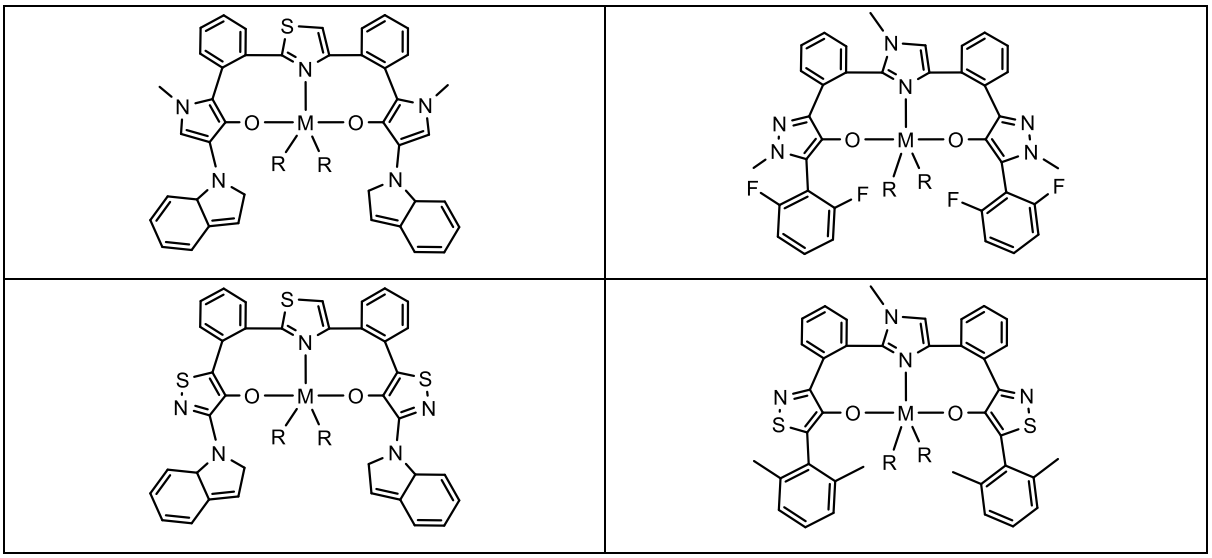
	
	
	
	
	
	

16. The catalyst compound of claim 1, wherein the catalyst compound is selected from the following, with M = Zr or Hf; and R = C_1-C_{20} hydrocarbyl, a monovalent heteroatom, or a heteroatom-bonded monovalent group:



17. A catalyst system comprising an activator and the catalyst compound of claim 1.

18. A process for the production of an ethylene based polymer comprising: polymerizing ethylene by contacting the ethylene with a catalyst system of claim 17, in one or more continuous stirred tank reactors or loop reactors, in series or in parallel, at a reactor pressure of from 0.05 MPa to 1,500 MPa and a reactor temperature of from 30°C to 230°C.

19. The process of claim 18, wherein the ethylene based polymer has an Mw value of from 2,000 to 3,000,000 g/mol, Mn value of from 1,000 to 2,000,000 g/mol, Mz value of from 10,000 to 10,000,000 g/mol, and an Mw/Mn of from 1 to 5.

20. The process of claim 18, wherein the ethylene based polymer has a melting point of from 110°C to 150°C.

21. A process for the production of a propylene based polymer comprising: polymerizing propylene by contacting the propylene with a catalyst system of claim 17, in one or more continuous stirred tank reactors or loop reactors, in series or in parallel, at a reactor pressure of from 0.05 MPa to 1,500 MPa and a reactor temperature of from 30°C to 230°C.

22. The process of claim 21, wherein the propylene based polymer has an Mw value of from 500 to 15,000 g/mol, Mn value of from 500 to 15,000 g/mol, Mz value of from 500 to 20,000 g/mol, and an Mw/Mn of from 1 to 5.

23. The process of claim 21, wherein the propylene based polymer has a melting point of from 50°C to 150°C.

24. A process for the production of an ethylene alpha-olefin copolymer comprising: polymerizing ethylene and at least one C_3-C_{20} alpha-olefin by contacting the ethylene and the at least one C_3-C_{20} alpha-olefin with a catalyst system of claim 17, in one or more continuous stirred tank reactors or loop reactors, in series or in parallel, at a reactor pressure of from 0.05 MPa to 1,500 MPa and a reactor temperature of from 30°C to 230°C.

25. The process of claim 24, wherein the ethylene alpha-olefin copolymer has a comonomer content of 0.1 to 50 wt%, an Mw value of from 1,000 to 3,000,000 g/mol, and Mz value of from 1,000 to 10,000,000 g/mol, an Mn value of from 1,000 to 1,000,000 g/mol, and an Mw/Mn of from 1 to 5.

26. The process of claim 24, wherein the ethylene alpha-olefin copolymer has a melting point of from 100°C to 140°C.

27. A process for the production of a propylene alpha-olefin copolymer comprising: polymerizing propylene and at least one ethylene or at least one C_4-C_{20} alpha-olefin by contacting the propylene and the at least one ethylene or at least one C_3-C_{20} alpha-olefin with a catalyst system of claim 17, in one or more continuous stirred tank reactors or loop reactors, in series or in parallel, at a reactor pressure of from 0.05 MPa to 1,500 MPa and a reactor temperature of from 30°C to 230°C.

28. The process of claim 27, wherein the propylene alpha-olefin copolymer has a comonomer content of 0.1 to 35 wt%, an Mw value of from 1,000 to 3,000,000 g/mol, and Mz value of from 1,000 to 10,000,000 g/mol, an Mn value of from 1,000 to 1,000,000 g/mol, and an Mw/Mn of from 1 to 5.

29. The process of claim 27, wherein the propylene alpha-olefin copolymer has a melting point of from 100°C to 140°C.