Non Patent Literature 4: Metalorganic Catalysts for Synthesis and Polymerization, Springer-Verlag: Berlin, 1999; p. 170.

Non Patent Literature 5: Polypropylene Handbook, Kogyo Chosakai Publishing Co., Ltd., 1998, p. 135

Non Patent Literature 6: Polymer, 4083 (1993)

Non Patent Literature 7: J. Macromol. Sci. Part B Phys. (2002), 1121

Non Patent Literature 8: Chem. Rev. (2000), 100, 1253

Non Patent Literature 9: Polypropylene Handbook, Kogyo Chosakai Publishing Co., Ltd., 1998, p. 72

Non Patent Literature 10: J. Appl. Poly. Sci., Vol. 109, 1338 (2008)

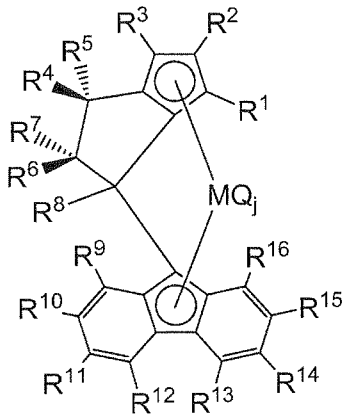
Non Patent Literature 11: Macromolecules (2007), 40, 6871

Non Patent Literature 12: Chem. Eur. J. (2012), 18, 4174-4178

SUMMARY ~~OF INVENTION~~

[0024a]

In one aspect of the present disclosure, there is provided a transition metal compound represented by General Formula [I] or an enantiomer thereof:

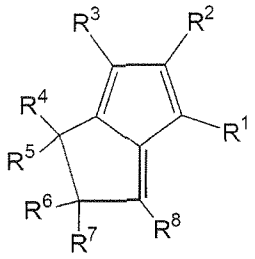


... [I]

[in Formula [I], R^1, R^3, R^6, R^7, R^8, R^9, R^{10}, R^{11}, R^{12}, R^{13}, R^{14}, R^{15} and R^{16} are each independently a hydrogen atom, a hydrocarbon group, a hetero atom-containing hydrocarbon group, or a silicon-containing group; R^2 is a hydrocarbon group, a hetero atom-containing hydrocarbon group, or a silicon-containing group; R^4 is a hydrogen atom; R^5 is a hydrocarbon group, or R^5 and R^7 are bonded to each other to form a ring; any two substituents of the substituents R^1 to R^{16} except R^4 may be bonded to each other to form a ring; M is a transition metal of Group IV; Q is a halogen atom, a hydrocarbon group, an anionic ligand, or a neutral ligand coordinatable with a lone electron pair; j is an integer of 1 to 4; and when j is an integer of 2 or greater, Qs may be the same or different from one another; in Formula [I], the MQ_j moiety is in front of the plane of the paper, and the hydrogen atom (R^4) is present on the same side as the M].

In another aspect of the present disclosure, there is provided an olefin polymerization catalyst comprising at least one transition metal compound selected from the transition metal compounds and the enantiomers thereof described herein.

In another aspect of the present disclosure, there is provided a process for producing the transition metal compound or the enantiomer thereof described herein, comprising a step of preparing a pentalene compound represented by General Formula (1a):



... (1a)

[in Formula (1a), R^1, R^3, R^6, R^7 and R^8 are each independently a hydrogen atom, a hydrocarbon group, a hetero atom-containing hydrocarbon group, or a silicon-containing group; R^2 is a hydrocarbon group, a hetero atom-containing hydrocarbon group, or a silicon-containing group; R^4 is a hydrogen atom; R^5 is a hydrocarbon group, or R^5 and R^7 are bonded to each other to form a ring; and any two substituents of the substituents R^1 to R^8 except R^4 may be bonded to each other to form a ring].

In a further aspect of the present disclosure, there is provided a process for producing an olefin polymer comprising a step of polymerizing propylene and optionally at least one olefin selected from ethylene and α-olefins having 4 to 30 carbon atoms in the presence of the olefin polymerization catalyst described herein,

the olefin polymer including propylene-derived structural units in the range of 50 to 100 mol% (wherein the total of the content of structural units derived from propylene and the content of structural units derived from the olefin(s) is 100 mol%).

In another aspect of the present disclosure, there is provided a process for producing a shaped article comprising an olefin polymer, which comprises a step of producing the olefin polymer by the production process described herein.

TECHNICAL PROBLEM

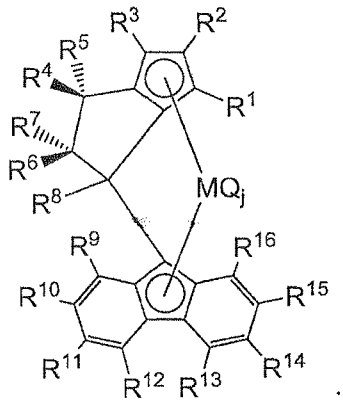
[0025]

An object of the invention is to provide transition metal compounds with excellent catalytic activity which can afford olefin polymers such as propylene polymers that have high stereoregularity and high molecular weight and may be easily formed into a β-phase. Another object of the invention is to

CLAIMS

[Claim 1]

A transition metal compound represented by General Formula [I] or an enantiomer thereof:



... [I]

[in Formula [I], R^1, R^3, R^5, R^6, R^7, R^8, R^9, R^{10}, R^{11}, R^{12}, R^{13}, R^{14}, R^{15} and R^{16} are each independently a hydrogen atom, a hydrocarbon group, a hetero atom-containing hydrocarbon group, or a silicon-containing group; R^2 is a hydrocarbon group, a hetero atom-containing hydrocarbon group, or a silicon-containing group; R^4 is a hydrogen atom; any two substituents of the substituents R^1 to R^{16} except R^4 may be bonded to each other to form a ring; M is a transition metal of Group IV; Q is a halogen atom, a hydrocarbon group, an anionic ligand, or a neutral ligand coordinatable with a lone electron pair; j is an integer of 1 to 4; and when j is an integer of 2 or greater, Qs may be the same or different from one another].

[Claim 2]

The transition metal compound or the enantiomer thereof

according to claim 1, wherein in General Formula [I], R^1 and R^3 are hydrogen atoms.

[Claim 3]

The transition metal compound or the enantiomer thereof according to claim 1 or 2, wherein in General Formula [I], R^2 is a hydrocarbon group having 1 to 20 carbon atoms.

[Claim 4]

The transition metal compound or the enantiomer thereof according to any one of claims 1 to 3, wherein in General Formula [I], R^2 is a substituent in which a carbon bonded to the cyclopentadienyl ring is a tertiary carbon.

[Claim 5]

The transition metal compound or the enantiomer thereof according to any one of claims 1 to 4, wherein in General Formula [I], R^5 and R^7 are bonded to each other to form a ring.

[Claim 6]

The transition metal compound or the enantiomer thereof according to any one of claims 1 to 5, wherein in General Formula [I], R^9, R^{12}, R^{13} and R^{16} are hydrogen atoms.

[Claim 7]

The transition metal compound or the enantiomer thereof according to any one of claims 1 to 6, wherein in General Formula [I], R^{10}, R^{11}, R^{14} and R^{15} are hydrocarbon groups, or R^{10} and R^{11} are bonded to each other to form a ring and R^{14} and R^{15} are bonded

to each other to form a ring.

[Claim 8]

An olefin polymerization catalyst comprising at least one transition metal compound selected from the transition metal compounds and the enantiomers thereof described in any one of claims 1 to 7.

[Claim 9]

The olefin polymerization catalyst according to claim 8, comprising:

at least one transition metal compound (A) selected from the transition metal compounds and the enantiomers thereof described in any one of claims 1 to 7; and

at least one compound (B) selected from

organometallic compounds (B-1),

organoaluminum-oxy compounds (B-2), and

compounds (B-3) capable of reacting with the transition metal compound (A) to form an ion pair.

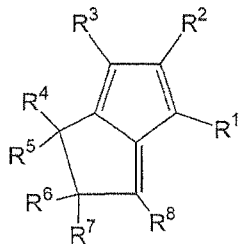
[Claim 10]

The olefin polymerization catalyst according to claim 9, wherein the olefin polymerization catalyst further comprises a carrier (C), and the transition metal compound (A) is supported on the carrier (C).

[Claim 11]

A process for producing the transition metal compound or

the enantiomer thereof described in claim 1, comprising a step of preparing a pentalene compound represented by General Formula (1a):



... (1a)

[in Formula (1a), R^1, R^3, R^5, R^6, R^7 and R^8 are each independently a hydrogen atom, a hydrocarbon group, a hetero atom-containing hydrocarbon group, or a silicon-containing group; R^2 is a hydrocarbon group, a hetero atom-containing hydrocarbon group, or a silicon-containing group; R^4 is a hydrogen atom; and any two substituents of the substituents R^1 to R^8 except R^4 may be bonded to each other to form a ring].

[Claim 12]

A process for producing an olefin polymer comprising a step of polymerizing propylene and optionally at least one olefin selected from ethylene and α-olefins having 4 to 30 carbon atoms in the presence of the olefin polymerization catalyst described in any one of claims 8 to 10,

the olefin polymer including propylene-derived structural units in the range of 50 to 100 mol% (wherein the total of the content of structural units derived from propylene

and the content of structural units derived from the olefin(s) is 100 mol%).

[Claim 13]

An olefin polymer obtained by the production process described in claim 12.

[Claim 14]

A propylene polymer having a meso pentad fraction of 97.0% to 99.5% and a total fraction of 2,1-insertions and 1,3-insertions of propylene monomers of 0.01 mol% to 0.06 mol% relative to all propylene-derived structural units as measured by ^{13}C-NMR.

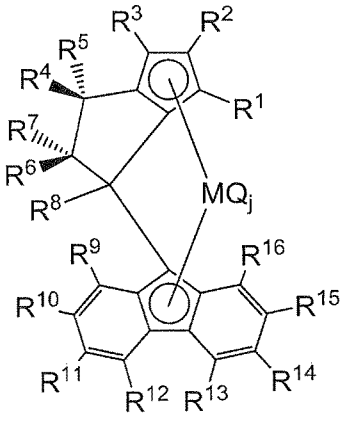
[Claim 15]

A shaped article comprising the propylene polymer described in claim 13 or 14.

CLAIMS

[Claim 1]

A transition metal compound represented by General Formula [I] or an enantiomer thereof:



... [I]

[in Formula [I], R^1, R^3, R^6, R^7, R^8, R^9, R^{10}, R^{11}, R^{12}, R^{13}, R^{14}, R^{15} and R^{16} are each independently a hydrogen atom, a hydrocarbon group, a hetero atom-containing hydrocarbon group, or a silicon-containing group; R^2 is a hydrocarbon group, a hetero atom-containing hydrocarbon group, or a silicon-containing group; R^4 is a hydrogen atom; R^5 is a hydrocarbon group, or R^5 and R^7 are bonded to each other to form a ring; any two substituents of the substituents R^1 to R^{16} except R^4 may be bonded to each other to form a ring; M is a transition metal of Group IV; Q is a halogen atom, a hydrocarbon group, an anionic ligand, or a neutral ligand coordinatable with a lone electron pair; j is an integer of 1 to 4; and when j is an integer of 2 or greater, Qs may be the same or different from one another; in Formula [I], the MQ_j moiety is in front

of the plane of the paper, and the hydrogen atom (R^4) is present on the same side as the M].

[Claim 2]

The transition metal compound or the enantiomer thereof according to claim 1, wherein in General Formula [I], R^1 and R^3 are hydrogen atoms.

[Claim 3]

The transition metal compound or the enantiomer thereof according to claim 1 or 2, wherein in General Formula [I], R^2 is a hydrocarbon group having 1 to 20 carbon atoms.

[Claim 4]

The transition metal compound or the enantiomer thereof according to any one of claims 1 to 3, wherein in General Formula [I], R^2 is a substituent in which a carbon bonded to the cyclopentadienyl ring is a tertiary carbon.

[Claim 5]

The transition metal compound or the enantiomer thereof according to any one of claims 1 to 4, wherein in General Formula [I], the hydrocarbon group in R^5 is an alkyl group having 2 or more carbon atoms, a cycloalkyl group or a cycloalkenyl group.

[Claim 6]

The transition metal compound or the enantiomer thereof according to any one of claims 1 to 5, wherein in General Formula [I], R^9, R^{12}, R^{13} and R^{16} are hydrogen atoms.

[Claim 7]

The transition metal compound or the enantiomer thereof according to any one of claims 1 to 6, wherein in General Formula [I], R^{10}, R^{11}, R^{14} and R^{15} are hydrocarbon groups, or R^{10} and R^{11} are bonded to each other to form a ring and R^{14} and R^{15} are bonded to each other to form a ring.

[Claim 8]

An olefin polymerization catalyst comprising at least one transition metal compound selected from the transition metal compounds and the enantiomers thereof described in any one of claims 1 to 7.

[Claim 9]

The olefin polymerization catalyst according to claim 8, comprising:

at least one transition metal compound (A) selected from the transition metal compounds and the enantiomers thereof described in any one of claims 1 to 7; and

at least one compound (B) selected from

organometallic compounds (B-1),

organoaluminum-oxy compounds (B-2), and

compounds (B-3) capable of reacting with the transition metal compound (A) to form an ion pair.

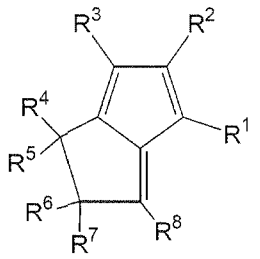
[Claim 10]

The olefin polymerization catalyst according to claim 9,

wherein the olefin polymerization catalyst further comprises a carrier (C), and the transition metal compound (A) is supported on the carrier (C).

[Claim 11]

A process for producing the transition metal compound or the enantiomer thereof described in claim 1, comprising a step of preparing a pentalene compound represented by General Formula (1a):



... (1a)

[in Formula (1a), R^1, R^3, R^6, R^7 and R^8 are each independently a hydrogen atom, a hydrocarbon group, a hetero atom-containing hydrocarbon group, or a silicon-containing group; R^2 is a hydrocarbon group, a hetero atom-containing hydrocarbon group, or a silicon-containing group; R^4 is a hydrogen atom; R^5 is a hydrocarbon group, or R^5 and R^7 are bonded to each other to form a ring; and any two substituents of the substituents R^1 to R^8 except R^4 may be bonded to each other to form a ring].

[Claim 12]

A process for producing an olefin polymer comprising a

step of polymerizing propylene and optionally at least one olefin selected from ethylene and α-olefins having 4 to 30 carbon atoms in the presence of the olefin polymerization catalyst described in any one of claims 8 to 10,

the olefin polymer including propylene-derived structural units in the range of 50 to 100 mol% (wherein the total of the content of structural units derived from propylene and the content of structural units derived from the olefin(s) is 100 mol%).

[Claim 13]

A process for producing a shaped article comprising an olefin polymer, which comprises a step of producing the olefin polymer by the production process described in claim 12.