

(19) World Intellectual Property
Organization
International Bureau



(43) International Publication Date
10 November 2005 (10.11.2005)

PCT

(10) International Publication Number
WO 2005/105864 A1

(51) International Patent Classification⁷: **C08F 10/00**,
4/64, C07F 17/00

(21) International Application Number:
PCT/US2005/008301

(22) International Filing Date: 11 March 2005 (11.03.2005)

(25) Filing Language: English

(26) Publication Language: English

(30) Priority Data:
60/562,861 16 April 2004 (16.04.2004) US

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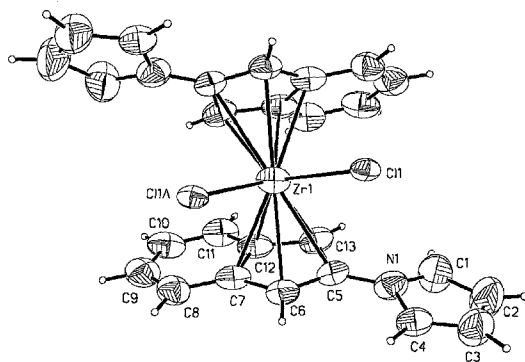
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(81) Designated States (unless otherwise indicated, for every kind of national protection available): AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW.

(84) Designated States (unless otherwise indicated, for every kind of regional protection available): ARIPO (BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW), Eurasian (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM),

[Continued on next page]

(54) Title: HETEROCYCLIC SUBSTITUTED METALLOCENE COMPOUNDS FOR OLEFIN POLYMERIZATION



Structural Representation of bis-(2-(pyrrol-1-yl)indenyl)zirconium dichloride (13) from X-ray crystallography.

(57) Abstract: This invention relates to metallocene compounds represented by formula (I): (I) Where in M is a group 3, 4, 5 or 6 transition metal atom, or a lanthanide metal atom, or actinide metal atom; E is an indenyl ligand that is substituted in any position of the indenyl ligand with at least one aromatic heterocyclic substituent or pseudoaromatic heterocyclic substituent that is bonded to the indenyl ring through a nitrogen or phosphorous ring heteroatom, and additionally, E may be substituted with 0, 1, 2, 3, 4, 5 or 6 R groups, where each R is, independently, a hydrocarbyl, substituted hydrocarbyl, halocarbyl, substituted halocarbyl, silylcarbyl, substituted silylcarbyl, germylcarbyl, or substituted germylcarbyl substituent, and optionally, two or more adjacent R substituents may join together to form a substituted or unsubstituted, saturated, partially unsaturated, or aromatic cyclic or polycyclic substituent; A is a substituted or unsubstituted cyclopentadienyl ligand, a substituted or unsubstituted heterocyclopentadienyl ligand, a substituted or unsubstituted indenyl ligand, a substituted or unsubstituted heteroindenyl ligand, a substituted or unsubstituted fluorenyl ligand, a substituted or unsubstituted heterofluorenyl ligand, or other mono-anionic ligand, or A may, independently, be defined as E; Y is an optional bridging group that is bonded to E and A, and is present when y is one and absent when y is zero; y is zero or one; X are, independently, univalent anionic ligands, or both X are joined and bound to the metal atom to form a metallocycle ring, or both X join to form a chelating ligand, a diene ligand, or an alkylidene ligand; and provided that when A is independently defined as E, and y is one, and Y is bonded to the one position of each indenyl ligand, and per indenyl ligand there is only one aromatic heterocyclic substituent or pseudoaromatic heterocyclic substituent that is bonded to the indenyl ligand, such substituent being bonded to the 4-position of the indenyl ligand, then such substituent is not an unsubstituted or hydrocarbyl substituted pyrrol-1-yl substituent including ring-fused hydrocarbyl substituted pyrrol-1-yl substituents such as indol-1-yl, isoindol-2-yl, carbazol-9-yl, 2,3,4,9-tetrahydrocarbazol-9-yl, and 1,2,3,4-tetrahydrocyclopenta[b]indol-4-yl. This invention further relates to a catalyst system comprised of the above metallocenes combined with an activator, and to a process to polymerize unsaturated monomers using such catalyst system.

orenyl ligand, a substituted or unsubstituted heterofluorenyl ligand, or other mono-anionic ligand, or A may, independently, be defined as E; Y is an optional bridging group that is bonded to E and A, and is present when y is one and absent when y is zero; y is zero or one; X are, independently, univalent anionic ligands, or both X are joined and bound to the metal atom to form a metallocycle ring, or both X join to form a chelating ligand, a diene ligand, or an alkylidene ligand; and provided that when A is independently defined as E, and y is one, and Y is bonded to the one position of each indenyl ligand, and per indenyl ligand there is only one aromatic heterocyclic substituent or pseudoaromatic heterocyclic substituent that is bonded to the indenyl ligand, such substituent being bonded to the 4-position of the indenyl ligand, then such substituent is not an unsubstituted or hydrocarbyl substituted pyrrol-1-yl substituent including ring-fused hydrocarbyl substituted pyrrol-1-yl substituents such as indol-1-yl, isoindol-2-yl, carbazol-9-yl, 2,3,4,9-tetrahydrocarbazol-9-yl, and 1,2,3,4-tetrahydrocyclopenta[b]indol-4-yl. This invention further relates to a catalyst system comprised of the above metallocenes combined with an activator, and to a process to polymerize unsaturated monomers using such catalyst system.



European (AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR), OAPI (BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG).

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- *as to the applicant's entitlement to claim the priority of the earlier application (Rule 4.17(iii)) for the following designations* AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW, ARIPO patent (BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW), Eurasian patent (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), European patent (AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR), OAPI patent (BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG)

Published:

- *with international search report*

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