DUAL-HEADED ORGANOALUMINUM COMPOSITIONS

CROSS-REFERENCE TO RELATED APPLICATIONS

This application claims priority to, and the benefit of, U.S. provisional application no. 62/611,680, filed on December 29, 2017, and incorporated herein in its entirety.

FIELD

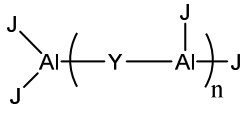
[0001] Embodiments relate to dual-headed organoaluminum compositions and processes to prepare the same. Such compositions may be capable of chain shuttling and/or chain transfer. In at least one aspect, the dual-headed organoaluminum compositions can be used in olefin polymerization.

BACKGROUND

[0002] In recent years, advances in polymer design have been seen with the use of compositions capable of chain shuttling, i.e., chain shuttling agents (CSAs). For example, chain shuttling agents having reversible chain transfer ability with transition metal catalysts have enabled the production of novel olefin block copolymers (OBCs). Currently, the best known compositions capable of chain shuttling are simple metal alkyls that typically contain only a single point of attachment to the metal for each polymer chain, such as diethyl zinc which produces polymer chains terminated with zinc metal at one end. More sophisticated compositions capable of chain shuttling, such as dual-headed chain shuttling agents, with the alkane moiety attached to two metals, are also known. Indeed, dual-headed compositions capable of chain shuttling are of great interest since they can enable the production of new polyolefins, such as telechelic functional polymers, triblock copolymers, etc.

SUMMARY

[0003] In certain examples, this disclosure relates to a dual-headed organoaluminum composition of formula (I):



(I), wherein:

n is a number from 1 to 100;

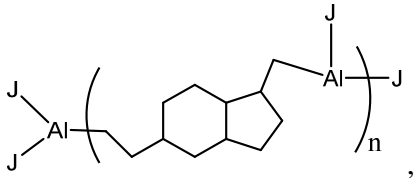
Y is a linking group composed of a linear, branched, or cyclic C_4 to C_{100} hydrocarbylene group that optionally includes at least one heteroatom and that is

aliphatic or aromatic, wherein Y comprises two points of attachments to Al atoms and at least one of the two points of attachments is $–CH_2–$;

each J group is independently hydrogen or a substituted or unsubstituted acyclic alkyl group; and

two J groups attached to the same Al atom can be optionally covalently linked together.

[0003a] In one aspect, the present disclosure refers to a compound of formula :



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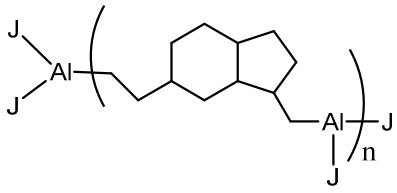

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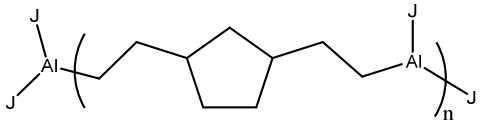


wherein:

n is a number from 1 to 100;

each J group is independently hydrogen or a substituted or unsubstituted acyclic alkyl group; and

two J groups attached to the same Al atom can be optionally covalently linked together.

[0004] In further examples, this disclosure relates to a process for preparing a dual-headed organoaluminum composition of formula (I), the process comprising: (a) combining an aluminum compound, a linking agent, and an optional solvent at a temperature of from 25 °C to 200 °C, and (b) obtaining the composition of formula (I), wherein the aluminum compound has the formula $Al(J)_3$, wherein each J is independently hydrogen or a substituted or unsubstituted acyclic alkyl group, and, optionally, two J groups can be covalently linked together; and the linking agent is a C_4

to C_{100} hydrocarbon comprising either at least two vinyl groups or a vinyl group and a cyclic olefin group and, optionally, includes at least one heteroatom.

[0004a] In another aspect, the present disclosure refers to a process for preparing an organoaluminum composition, the process comprising:

(a) combining an aluminum compound, a linking agent, and an optional solvent at a temperature of from 25 °C to 200 °C, and

(b) obtaining the organoaluminum composition, wherein:

the aluminum compound has the formula $Al(J)_3$, wherein each J group is independently hydrogen or a substituted or unsubstituted acyclic alkyl group, and, optionally, two J groups can be covalently linked together; and the linking agent is 1,2,4-trivinylcyclohexane or 1,3-divinylcyclopentane and, optionally, includes at least one heteroatom.

[0005] In further examples, this disclosure relates to a dual-headed organoaluminum composition of formula (I) comprising the reaction product of: an aluminum compound, a linking agent, and an optional solvent, wherein the aluminum compound has the formula $Al(J)_3$, wherein each J group is independently hydrogen or a substituted or unsubstituted acyclic alkyl group, and, optionally, two J groups can be covalently linked together; and the linking agent is a C_4 to C_{100} hydrocarbon comprising either at least two vinyl groups or a vinyl group and a cyclic olefin group and, optionally, includes at least one heteroatom.

BRIEF DESCRIPTION OF DRAWINGS

[0006] FIG. 1 is the ^1H NMR spectra for Example 1.

[0007] FIGS. 2A and 2B are the GC/MS spectra for Example 1.

[0008] FIG. 3 is the reaction scheme for Example 1.

[0009] FIG. 4 is the GC/MS spectrum for Example 2.

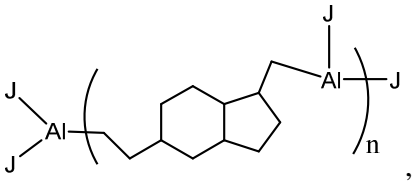
[0010] FIG. 5 is the NMR spectrum for Example 4.

DEFINITIONS

[0011] All references to the Periodic Table of the Elements refer to the Periodic Table of the Elements published and copyrighted by CRC Press, Inc., 2003. Also, any

What is claimed is:

1. A compound of formula :



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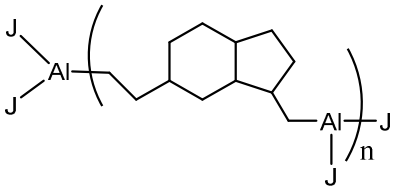

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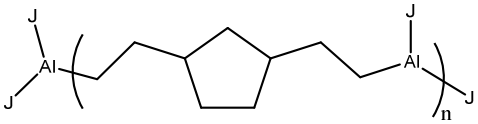


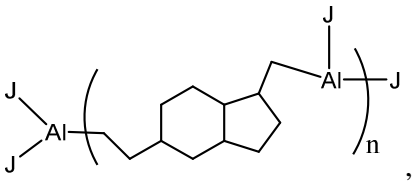
wherein:

n is a number from 1 to 100;

each J group is independently hydrogen or a substituted or unsubstituted acyclic alkyl group; and

two J groups attached to the same Al atom can be optionally covalently linked together.

2. The compound of Claim 1 having the following formulae:



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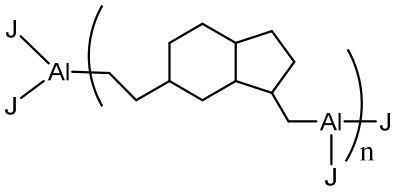

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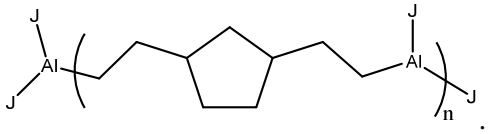
3. The compound of Claim 1 having the following formula:



4. The compound of any of the preceding claims, wherein each J is hydrogen or a C_1 to C_{20} acyclic alkyl group.

5. The compound of any of the preceding claims, wherein n is a number from 1 to 10.

6. The compound of any of the preceding claims, wherein n is a number from 1 to 3.

7. A process for preparing an organoaluminum composition, the process comprising:

(a) combining an aluminum compound, a linking agent, and an optional solvent at a temperature of from 25 °C to 200 °C, and

(b) obtaining the organoaluminum composition, wherein:

the aluminum compound has the formula $Al(J)_3$, wherein each J group is independently hydrogen or a substituted or unsubstituted acyclic alkyl group, and, optionally, two J groups can be covalently linked together; and the linking agent is 1,2,4-trivinylcyclohexane or 1,3-divinylcyclopentane and, optionally, includes at least one heteroatom.

8. The process of Claim 7, wherein the linking agent is 1,2,4-trivinylcyclohexane.

9. The process of Claim 7, wherein the linking agent is 1,3-divinylcyclopentane.