PROCATALYST COMPOSITION WITH SUBSTITUTED AMIDE ESTER INTERNAL ELECTRON DONOR

BACKGROUND

[0001] The present disclosure relates to procatalyst compositions containing a substituted amide ester, the incorporation of the same in catalyst compositions and the process of making olefin-based polymer using said catalyst compositions and the resultant olefin-based polymers produced therefrom.

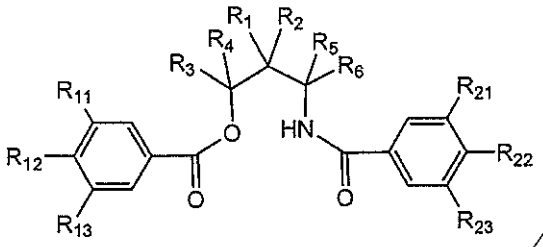
[0002] Worldwide demand for olefin-based polymers continues to grow as applications for these polymers become more diverse and more sophisticated. Olefin-based polymers with broad molecular weight distribution (MWD), for example, find increasing applications in thermoforming; pipe-, foam-, blow-molding; and films. Known are Ziegler-Natta catalyst compositions for the production of olefin-based polymers, particularly propylene-based polymers, with broad MWD. Ziegler-Natta catalyst compositions typically include a procatalyst composed of a transition metal halide (*i.e.*, titanium, chromium, vanadium) supported on a metal or metalloid compound, such as magnesium chloride or silica, the procatalyst complexed with a cocatalyst such as an organoaluminum compound. Production of olefin-based polymers with broad MWD produced by way of Ziegler-Natta catalysts, however, is typically limited to a single reactor process requiring rigorous process control and/or a series reactor process requiring multiple reactors.

[0003] Given the perennial emergence of new applications for olefin-based polymers, the art recognizes the need for olefin-based polymers with improved and varied properties. Desirable would be a Ziegler-Natta catalyst composition that produces olefin-based polymer, and propylene-based polymer in particular, with broad molecular weight distribution (MWD) with less process constraints and less equipment.

SUMMARY

[0004] The present disclosure is directed to procatalyst compositions containing substituted amide ester as an internal electron donor and the application of the same in catalyst compositions and polymerization processes. Catalyst compositions containing the substituted amide ester find application in olefin polymerization processes. The present substituted amide ester-containing catalyst compositions have high catalyst activity and/or high selectivity and produce propylene-based olefins with high isotacticity and broad molecular weight distribution.

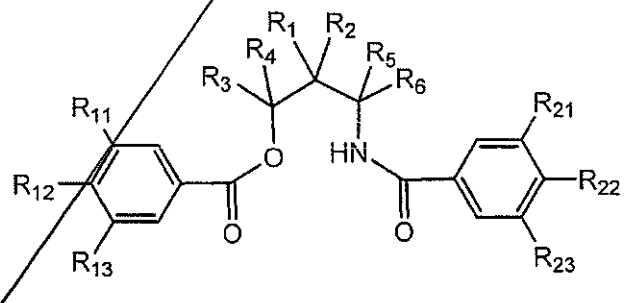
[0005] In an embodiment, a procatalyst composition is provided. The procatalyst composition includes a combination of a magnesium moiety, a titanium moiety and an internal electron donor. The internal electron donor includes a substituted amide ester. The substituted amide ester has the structure (II) below.



(II)

[0006] R_1-R_6 are the same or different. Each of R_1-R_6 is selected from hydrogen and a hydrocarbyl group having 1-20 carbon atoms. At least one of R_1-R_6 is a hydrocarbyl group having at least two carbon atoms. Alternatively, each of R_3 and R_5 is a hydrocarbyl group having 1-20 carbon atoms. R_{11}-R_{13} and R_{21}-R_{23} are the same or different. Each of R_{11}-R_{13} and R_{21}-R_{23} is selected from hydrogen and a hydrocarbyl group having 1-20 carbon atoms.

[0007] In an embodiment, another procatalyst composition is provided. The procatalyst composition includes a combination of a magnesium moiety, a titanium moiety and an internal electron donor. The internal electron donor includes a substituted amide ester. The substituted amide ester has the structure (II) below.



(II)

[0008] R_1-R_6, R_{11}-R_{13}, and R_{21}-R_{23} are the same or different. Each of R_1-R_6, R_{11}-R_{13}, and R_{21}-R_{23} is selected from hydrogen and a hydrocarbyl group having 1-20 carbon atoms. At least one of R_1-R_6 is a hydrocarbyl group having 1-20 carbon atoms. At least one of R_{11}-R_{13}, R_{21}-R_{23} is a hydrocarbyl group having 1-20 carbon atoms.

[0009] In an embodiment, a catalyst composition is provided. The catalyst composition includes a procatalyst composition. The procatalyst composition includes a substituted amide ester of structure (II). The procatalyst composition also includes a cocatalyst.

[0010] In an embodiment, a process for producing an olefin-based polymer is provided. The process includes contacting, under polymerization conditions, an olefin with a catalyst composition comprising a substituted amide ester, and forming an olefin-based polymer.

[0011] An advantage of the present disclosure is the provision of an improved procatalyst composition.

[0012] An advantage of the present disclosure is the provision of an improved catalyst composition for the polymerization of olefin-based polymers.

[0013] An advantage of the present disclosure is the provision of a phthalate-free catalyst composition and a phthalate-free olefin-based polymer produced therefrom.

[0014] An advantage of the present disclosure is a catalyst composition that produces a propylene-based polymer with broad molecular weight distribution and/or high isotacticity.

[0015] An advantage of the present disclosure is a catalyst composition that produces a propylene-based polymer with broad molecular weight distribution in a single reactor.

DETAILED DESCRIPTION

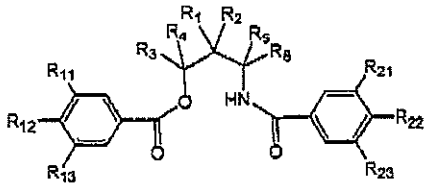
[0016] The present disclosure provides a procatalyst composition. In an embodiment, a procatalyst composition is provided and includes a combination of a magnesium moiety, a titanium moiety and an internal electron donor. The internal electron donor includes a substituted amide ester. In other words the procatalyst composition is a reaction product of a procatalyst precursor, a substituted amide ester, an optional halogenating agent, and an optional titanating agent.

[0017] The procatalyst composition is produced by halogenating/titanating a procatalyst precursor in the presence of the internal electron donor. As used herein, an "internal electron donor" is a compound added or otherwise formed during formation of the procatalyst composition that donates at least one pair of electrons to one or more metals present in the resultant procatalyst composition. The internal electron donor includes the substituted amide ester. Not wishing to be bound by any particular theory, it is believed that during halogenation and titanation the internal electron donor (1) regulates the formation of active sites, (2) regulates the position of titanium on the magnesium-based support and thereby enhances catalyst

REPLACEMENT SHEET

1. A procatalyst composition comprising:

a combination of a magnesium moiety, a titanium moiety and an internal electron donor comprising a substituted amide ester having the structure (II):



(II)

R_1-R_6 are the same or different, each of R_1-R_6 is selected from the group consisting of hydrogen and a hydrocarbyl group having 1-20 carbon atoms,

wherein at least one of R_1-R_6 is a hydrocarbyl group having at least 2 carbon atoms, or

each of R_3 and R_5 is a hydrocarbyl group having 1-20 carbon atoms; and

R_{11}-R_{13} and R_{21}-R_{23} are the same or different, each of R_{11}-R_{13} and R_{21}-R_{23} is selected from the group consisting of hydrogen and a hydrocarbyl group having 1-20 carbon atoms.

2. The procatalyst composition of claim 1 wherein at least two of R_1-R_6 are a hydrocarbyl group having at least 2 carbon atoms.

3. The procatalyst composition of any of claims 1-2 wherein each of R_1 and R_2 is a hydrocarbyl group with at least two carbon atoms.

4. The procatalyst composition of any of claims 1-3 wherein at least one of R_{11}-R_{13} and at least one of R_{21}-R_{23} is a hydrocarbyl group having 1-20 carbon atoms.

5. The procatalyst composition of any of claims 1-4 wherein each of R_1 and R_2 is are selected from the group consisting of an isopropyl group, an isobutyl group, a sec-butyl group, a cyclopentyl group, and a cyclohexyl group.

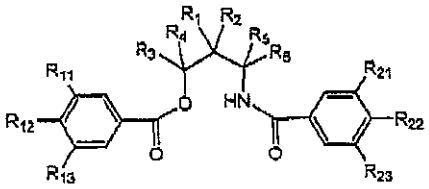
6. The procatalyst composition of claim 1 wherein each of R_1, R_2, R_4, and R_6 is hydrogen and each of R_3 and R_5 is a methyl group.

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REPLACEMENT SHEET

7. A procatalyst composition comprising:

a combination of a magnesium moiety, a titanium moiety and an internal electron donor comprising a substituted amide ester having the structure (II):



(II)

wherein R_1-R_6, R_{11}-R_{13}, and R_{21}-R_{23} are the same or different, each of R_1-R_6, R_{11}-R_{13}, and R_{21}-R_{23} is selected from the group consisting of hydrogen and a hydrocarbyl group having 1-20 carbon atoms,

wherein at least one of R_1-R_6 is a hydrocarbyl group having 1-20 carbon atoms, and at least one of R_{11}-R_{13}, R_{21}-R_{23} is a hydrocarbyl group having 1-20 carbon atoms.

8. The procatalyst composition of claim 7 wherein each of R_1 and R_2 is a methyl group and each of R_{12} and R_{22} is selected from the group consisting of ethyl, butyl, and phenyl.

9. The procatalyst composition of any of claims 1-8 comprising a mixed external electron donor comprising the substituted amide ester of structure (II) and an electron donor component.

10. A catalyst composition comprising:

a procatalyst composition of claim 1or claim 7; and

a cocatalyst.

11. The catalyst composition of claim 10 comprising an external electron donor selected from the group consisting of a silicon compound, a bidentate compound, a diether, a diol ester, a carboxylate, an amine, a phosphite, and combinations thereof.

12. The catalyst composition of any of claims 10-11 comprising two or more alkoxysilane external electron donors.

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REPLACEMENT SHEET

13. The catalyst composition of any of claims 10-12 comprising an activity limiting agent selected from the group consisting of a carboxylic acid ester, a diether, a diol ester, and combinations thereof.

14. A process for producing an olefin-based polymer comprising:

contacting, under polymerization conditions, an olefin with a catalyst composition comprising a procatalyst composition of claim 1 or claim 7; and

forming an olefin-based polymer comprising a substituted amide ester.

15. The process of claim 14 wherein the olefin is propylene, the process comprising forming a propylene-based polymer having a polydispersity index from about 5.0 to about 20.0.

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BACKGROUND

[0001] The present disclosure relates to procatalyst compositions containing a substituted amide ester, the incorporation of the same in catalyst compositions and the process of making olefin-based polymer using said catalyst compositions and the resultant olefin-based polymers produced therefrom.

[0002] Worldwide demand for olefin-based polymers continues to grow as applications for these polymers become more diverse and more sophisticated. Olefin-based polymers with broad molecular weight distribution (MWD), for example, find increasing applications in thermoforming; pipe-, foam-, blow-molding; and films. Known are Ziegler-Natta catalyst compositions for the production of olefin-based polymers, particularly propylene-based polymers, with broad MWD. Ziegler-Natta catalyst compositions typically include a procatalyst composed of a transition metal halide (i.e. , titanium, chromium, vanadium) supported on a metal or metalloid compound, such as magnesium chloride or silica, the procatalyst complexed with a cocatalyst such as an organoaluminum compound. Production of olefin-based polymers with broad MWD produced by way of Ziegler-Natta catalysts, however, is typically limited to a single reactor process requiring rigorous process control and/or a series reactor process requiring multiple reactors.

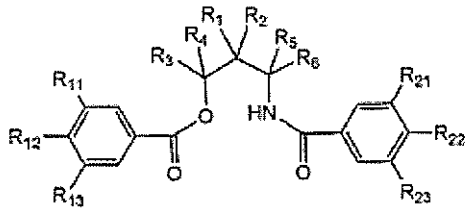
[0003] Given the perennial emergence of new applications for olefin-based polymers, the art recognizes the need for olefin-based polymers with improved and varied properties. Desirable would be a Ziegler-Natta catalyst composition that produces olefin-based polymer, and propylene-based polymer in particular, with broad molecular weight distribution (MWD) with less process constraints and less equipment.

SUMMARY

[0004] The present disclosure is directed to procatalyst compositions containing substituted amide ester as an internal electron donor and the application of the same in catalyst compositions and polymerization processes. Catalyst compositions containing the substituted amide ester find application in olefin polymerization processes. The present substituted amide ester-containing

catalyst compositions have high catalyst activity and/or high selectivity and produce propylene-based olefins with high isotacticity and broad molecular weight distribution.

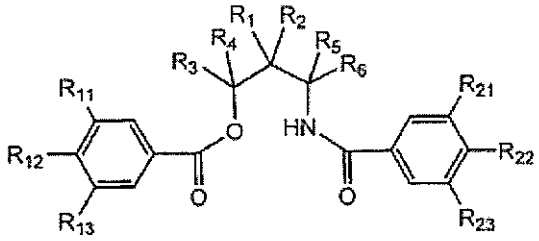
[0005] With the foregoing in view, the invention, in its broadest aspect resides in a procatalyst composition comprising a combination of a magnesium moiety, a titanium moiety and an internal electron donor comprising a substituted amide ester having the structure (II)



(II)

[0006] R_1-R_6 are the same or different, each of R_1-R_6 is selected from the group consisting of hydrogen and a hydrocarbyl group having 1-20 carbon atoms, or each of R_3 and R_5 is a hydrocarbyl group having 1-20 carbon atoms and each of R_{11}-R_{13} and R_{21}-R_{23} is selected from the group consisting of hydrogen and a hydrocarbyl group having 1-20 carbon atoms.

[0007] In another aspect the invention resides in a procatalyst composition comprising a combination of a magnesium moiety, a titanium moiety and an internal electron donor-comprising a substituted amide ester having the structure (II)



(II)

[0008] wherein R_1-R_6, R_{11}-R_{13}, and R_{21}-R_{23} are the same or different, each of R_1-R_6, R_{11}-R_{13}, and R_{21}-R_{23} is selected from the group consisting of hydrogen and a hydrocarbyl group having 1-20 carbon atoms wherein at least one of R_1-R_6 is a hydrocarbyl group having 1-20 carbon atoms. At least one of R_{11}-R_{13}, and R_{21}-R_{23} is a hydrocarbyl group having 1-20 carbon atoms.

[0009] In another aspect the invention resides in a catalyst composition which includes a procatalyst. The procatalyst composition includes a substituted amide ester of structure (II). The procatalyst composition also includes a cocatalyst.

[0010] In another aspect the invention resides in a process for producing an olefin-based polymer comprising contacting, under polymerization conditions, an olefin with a catalyst composition comprising a procatalyst composition as specified herein, and forming an olefin-based polymer comprising a substituted amide ester.

[0011] An advantage of the present disclosure is the provision of an improved procatalyst composition.

[0012] An advantage of the present disclosure is the provision of an improved catalyst composition for the polymerization of olefin-based polymers.

[0013] An advantage of the present disclosure is the provision of a phthalate-free catalyst composition and a phthalate-free olefin-based polymer produced therefrom.

[0014] An advantage of the present disclosure is a catalyst composition that produces a propylene-based polymer with broad molecular weight distribution and/or high isotacticity.

[0015] An advantage of the present disclosure is a catalyst composition that produces a propylene-based polymer with broad molecular weight distribution in a single reactor.

DETAILED DESCRIPTION

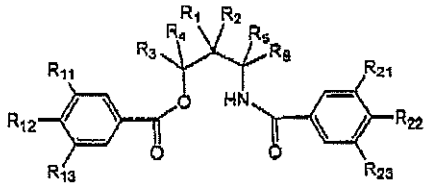
[0016] The present disclosure provides a procatalyst composition. In an embodiment, a procatalyst composition is provided and includes a combination of a magnesium moiety, a titanium moiety and an internal electron donor. The internal electron donor includes a substituted amide ester. In other words the procatalyst composition is a reaction product of a procatalyst precursor, a substituted amide ester, an optional halogenating agent, and an optional titanating agent.

[0017] The procatalyst composition is produced by halogenating/titanating a procatalyst precursor in the presence of the internal electron donor. As used herein, an "internal electron donor" is a compound added or otherwise formed during formation of the procatalyst composition that donates at least one pair of electrons to one or more metals present in the resultant procatalyst composition. The internal electron donor includes the substituted amide ester. Not wishing to be bound by any particular theory, it is believed that during halogenation and titanation the internal electron donor (1) regulates the formation of active sites, (2) regulates the position of titanium on the magnesium-based support and thereby enhances catalyst

CLAIMS

1. A procatalyst composition comprising:

a combination of a magnesium moiety, a titanium moiety and an internal electron donor comprising a substituted amide ester having the structure (II):



(II)

R_1-R_6 are the same or different, each of R_1-R_6 is selected from the group consisting of hydrogen and a hydrocarbyl group having 1-20 carbon atoms,

wherein at least one of R_1-R_6 is a hydrocarbyl group having at least 2 carbon atoms, or

each of R_3 and R_5 is a hydrocarbyl group having 1-20 carbon atoms; and

R_{11}-R_{13} and R_{21}-R_{23} are the same or different, each of R_{11}-R_{13} and R_{21}-R_{23} is selected from the group consisting of hydrogen and a hydrocarbyl group having 1-20 carbon atoms.

2. The procatalyst composition of claim 1 wherein at least two of R_1-R_6 are a hydrocarbyl group having at least 2 carbon atoms.

3. The procatalyst composition of any of claims 1-2 wherein each of R_1 and R_2 is a hydrocarbyl group with at least two carbon atoms.

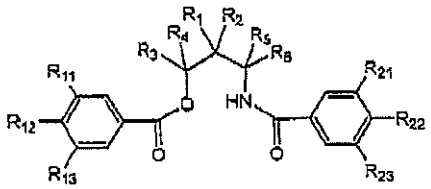
4. The procatalyst composition of any of claims 1-3 wherein at least one of R_{11}-R_{13} and at least one of R_{21}-R_{23} is a hydrocarbyl group having 1-20 carbon atoms.

5. The procatalyst composition of any of claims 1-4 wherein each of R_1 and R_2 is are selected from the group consisting of an isopropyl group, an isobutyl group, a sec-butyl group, a cyclopentyl group, and a cyclohexyl group.

6. The procatalyst composition of claim 1 wherein each of R_1, R_2, R_4, and R_6 is hydrogen and each of R_3 and R_5 is a methyl group.

7. A procatalyst composition comprising:

a combination of a magnesium moiety, a titanium moiety and an internal electron donor comprising a substituted amide ester having the structure (II):



(II)

wherein R_1-R_6, R_{11}-R_{13}, and R_{21}-R_{23} are the same or different, each of R_1-R_6, R_{11}-R_{13}, and R_{21}-R_{23} is selected from the group consisting of hydrogen and a hydrocarbyl group having 1-20 carbon atoms,

wherein at least one of R_1-R_6 is a hydrocarbyl group having 1-20 carbon atoms, and at least one of R_{11}-R_{13}, R_{21}-R_{23} is a hydrocarbyl group having 1-20 carbon atoms.

8. The procatalyst composition of claim 7 wherein each of R_1 and R_2 is a methyl group and each of R_{12} and R_{22} is selected from the group consisting of ethyl, butyl, and phenyl.

9. The procatalyst composition of any of claims 1-8 comprising a mixed external electron donor comprising the substituted amide ester of structure (II) and an electron donor component.

10. A catalyst composition comprising:

a procatalyst composition of claim 1or claim 7; and

a cocatalyst.

11. The catalyst composition of claim 10 comprising an external electron donor selected from the group consisting of a silicon compound, a bidentate compound, a diether, a diol ester, a carboxylate, an amine, a phosphite, and combinations thereof.

12. The catalyst composition of any of claims 10-11 comprising two or more alkoxysilane external electron donors.

13. The catalyst composition of any of claims 10-12 comprising an activity limiting agent selected from the group consisting of a carboxylic acid ester, a diether, a diol ester, and combinations thereof.

14. A process for producing an olefin-based polymer comprising:

contacting, under polymerization conditions, an olefin with a catalyst composition comprising a procatalyst composition of claim 1or claim 7; and

forming an olefin-based polymer comprising a substituted amide ester.

15. The process of claim 14 wherein the olefin is propylene, the process comprising forming a propylene-based polymer having a polydispersity index from about 5.0 to about 20.0.