AMIDE ESTER INTERNAL ELECTRON DONOR AND PROCESS

BACKGROUND

[0001] The present disclosure relates to procatalyst compositions with amide ester internal electron donor, catalyst compositions containing the same, and polymer 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 amide ester internal electron donors and the use of same in procatalyst and catalyst compositions. Catalyst compositions containing the amide ester internal electron donor find application in olefin polymerization processes. The present amide ester-containing catalyst compositions have high catalyst activity, high catalyst selectivity, and produce propylene-based olefins with high isotacticity and broad molecular weight distribution.

[0005] In an embodiment, a process is provided and includes pre-halogenating a procatalyst precursor with a halogenating agent, and adding an amide ester to the halogenated procatalyst

precursor in a reaction mixture. The process further includes forming a procatalyst composition comprising a magnesium moiety, a titanium moiety, and an internal electron donor comprising the amide ester.

[0006] In an embodiment, a procatalyst composition is provided and includes a combination of a magnesium moiety, a titanium moiety, and a mixed internal electron donor. The mixed internal electron donor includes an amide ester and an electron donor component. The electron donor component may be a benzoate.

[0007] In an embodiment, a catalyst composition is provided and includes a procatalyst composition and a cocatalyst. The procatalyst composition includes a combination of a magnesium moiety, a titanium moiety, and a mixed internal electron donor. The mixed internal electron donor includes an amide ester and an electron donor component. The electron donor component may be a benzoate.

[0008] 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. The catalyst composition includes a mixed internal electron donor. The mixed internal electron donor includes an amide ester and an electron donor component. The process further includes forming an olefin-based polymer.

[0009] An advantage of the present disclosure is the provision of a process for producing improved procatalyst composition.

[0010] An advantage of the present disclosure is the provision of an improved procatalyst composition.

[0011] An advantage of the present disclosure is the provision of an improved catalyst composition for the polymerization of olefin-based polymers.

[0012] An advantage of the present disclosure is an amide-ester containing catalyst composition with improved catalyst activity and/or improved catalyst selectivity.

[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.

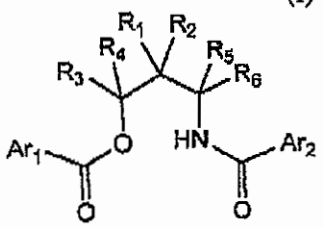
REPLACEMENT SHEET

1. A process comprising:

pre-halogenating a procatalyst precursor with a halogenating agent;

adding an amide ester to the halogenated procatalyst precursor in a reaction mixture, the amide ester having the structure (I);

(I)



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

forming a procatalyst composition comprising a magnesium moiety, a titanium moiety, and an internal electron donor comprising the amide ester.

2. The process of claim 1 comprising pre-halogenating a procatalyst precursor selected from a group consisting of a magnesium moiety compound, a magnesium mixed metal compound, a benzoate-containing magnesium chloride compound, and combinations thereof.

3. The process of any of claims 1-2 comprising reacting the amide ester with a benzoate-containing magnesium chloride compound procatalyst precursor in the presence of titanium tetrachloride.

4. The process of any of claims 1-4 comprising introducing, to the reaction mixture, an electron donor component; and

forming a procatalyst composition comprising a mixed internal electron donor comprising the amide ester and the internal electron donor component.

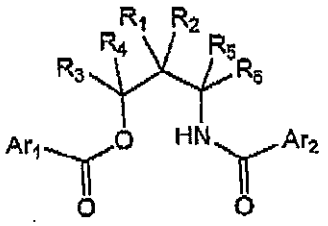
5. A procatalyst composition comprising:

a combination of a magnesium moiety, a titanium moiety, and a mixed internal electron donor comprising an amide ester and an electron donor component, the amide ester having the structure (I)

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REPLACEMENT SHEET

(I)



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

6. The procatalyst composition of claim 5 wherein the electron donor component is a benzoate.

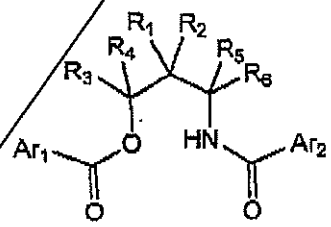
7. The procatalyst composition of claim 6 wherein the benzoate is selected from the group consisting of ethyl benzoate and 1-methoxypropan-2-yl benzoate.

8. The procatalyst composition of any of claims 5-7 comprising from about 0.5 wt % to about 10 wt % benzoate.

9. A catalyst composition comprising:

a procatalyst composition comprising a mixed internal electron donor comprising an amide ester and an electron donor component, the amide ester having the structure (I)

(I)



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

a cocatalyst.

10. The catalyst composition of claim 9 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.

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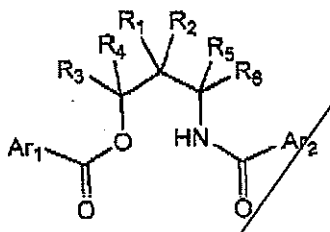
REPLACEMENT SHEET

11. The catalyst composition of any of claims 9-10 comprising an activity limiting agent selected from the group consisting of a carboxylic acid ester, a diether, a diol ester, a poly(alkene glycol), and combinations thereof.

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

contacting, under polymerization conditions, an olefin with a catalyst composition comprising a mixed internal electron donor comprising an amide ester and an electron donor component, the amide ester having the structure (I)

(I)



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

forming an olefin-based polymer.

13. The process of claim 12 comprising forming an olefin-based polymer comprising an amide ester.

14. The process of any of claims 12-13 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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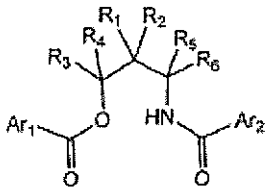
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SUMMARY

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

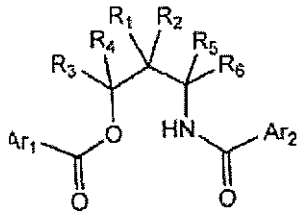
[0005] With the foregoing in view, there is broadly provided in one aspect a process comprising pre-halogenating a procatalyst precursor with a halogenating agent; adding an amide ester to the halogenated procatalyst precursor in a reaction mixture, the amide ester having the structure (I);



(I)

wherein R_1-R_6 are the same or different, each R_1-R_6 is selected from the group consisting of hydrogen, a halogen, and a hydrocarbyl group having 1-20 carbon atoms; and forming a procatalyst composition comprising a magnesium moiety, a titanium moiety, and an internal electron donor comprising the amide ester.

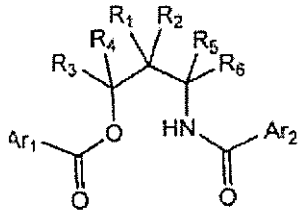
[0006] There is broadly provided in another aspect a procatalyst composition comprising: a combination of a magnesium moiety, a titanium moiety, and a mixed internal electron donor comprising an amide ester and an electron donor component, the amide ester having the structure (I)



(I)

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

[0007] There is broadly provided in another aspect a catalyst composition comprising: a procatalyst composition comprising a mixed internal electron donor comprising an amide ester and an electron donor component, the amide ester having the structure (I)



(I)

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

[0008] In an embodiment, a procatalyst composition is provided and includes a combination of a magnesium moiety, a titanium moiety, and a mixed internal electron donor. The mixed internal electron donor includes an amide ester and an electron donor component. The electron donor component may be a benzoate. In an embodiment, a catalyst composition is provided and includes a procatalyst composition and a cocatalyst. The procatalyst composition includes a combination of a magnesium moiety, a titanium moiety, and a mixed internal electron donor. The mixed internal electron donor includes an amide ester and an electron donor component. The electron donor component may be a benzoate. 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. The catalyst composition includes a mixed internal electron donor. The mixed internal electron donor includes an amide ester and an electron donor component. The process further includes forming an olefin based polymer.

[0009] An advantage of the present disclosure is the provision of a process for producing improved procatalyst composition.

[0010] An advantage of the present disclosure is the provision of an improved procatalyst composition.

[0011] An advantage of the present disclosure is the provision of an improved catalyst composition for the polymerization of olefin-based polymers.

[0012] An advantage of the present disclosure is an amide-ester containing catalyst composition with improved catalyst activity and/or improved catalyst selectivity.

[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.

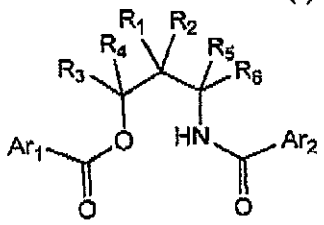
CLAIMS

1. A process comprising:

pre-halogenating a procatalyst precursor with a halogenating agent;

adding an amide ester to the halogenated procatalyst precursor in a reaction mixture, the amide ester having the structure (I);

(I)



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

forming a procatalyst composition comprising a magnesium moiety, a titanium moiety, and an internal electron donor comprising the amide ester.

2. The process of claim 1 comprising pre-halogenating a procatalyst precursor selected from a group consisting of a magnesium moiety compound, a magnesium mixed metal compound, a benzoate-containing magnesium chloride compound, and combinations thereof.

3. The process of any of claims 1-2 comprising reacting the amide ester with a benzoate-containing magnesium chloride compound procatalyst precursor in the presence of titanium tetrachloride.

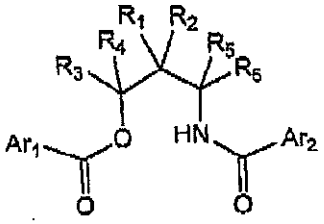
4. The process of any of claims 1-4 comprising introducing, to the reaction mixture, an electron donor component; and

forming a procatalyst composition comprising a mixed internal electron donor comprising the amide ester and the internal electron donor component.

5. A procatalyst composition comprising:

a combination of a magnesium moiety, a titanium moiety, and a mixed internal electron donor comprising an amide ester and an electron donor component, the amide ester having the structure (I)

(I)



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

6. The procatalyst composition of claim 5 wherein the electron donor component is a benzoate.

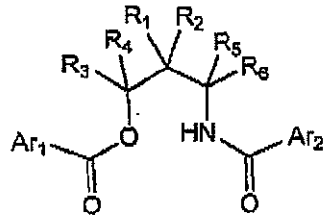
7. The procatalyst composition of claim 6 wherein the benzoate is selected from the group consisting of ethyl benzoate and 1-methoxypropan-2-yl benzoate.

8. The procatalyst composition of any of claims 5-7 comprising from about 0.5 wt % to about 10 wt % benzoate.

9. A catalyst composition comprising:

a procatalyst composition comprising a mixed internal electron donor comprising an amide ester and an electron donor component, the amide ester having the structure (I)

(I)



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

a cocatalyst.

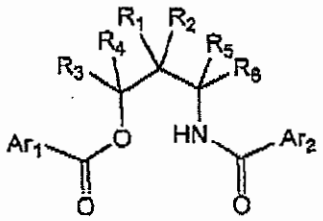
10. The catalyst composition of claim 9 comprising an external electron donor selected from the group consisting of a silicon compound, a bidentate compound, a diether, a diol ester, a carboxylate, an amine, a phosphite, and combinations thereof.

11. The catalyst composition of any of claims 9-10 comprising an activity limiting agent selected from the group consisting of a carboxylic acid ester, a diether, a diol ester, a poly(alkene glycol), and combinations thereof.

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

contacting, under polymerization conditions, an olefin with a catalyst composition comprising a mixed internal electron donor comprising an amide ester and an electron donor component, the amide ester having the structure (I)

(I)



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

forming an olefin-based polymer.

13. The process of claim 12 comprising forming an olefin-based polymer comprising an amide ester.

14. The process of any of claims 12-13 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.