

Zirconium and hafnium complexes of the thio(bisphenolato) ligand: synthesis structural characterization and testing as 1-hexene polymerization catalysts.

Autorzy

Zofia Janas

Dorota Godbole

Tomasz A. Nerkowski

Krzysztof Szczegot

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Streszczenie

Thio(bisphenolato) complexes of the type $[M_2(\mu\text{-tbop-}\kappa^3\text{O,S,O})_2\text{Cl}_4]$ [$M = \text{Zr } \mathbf{1}$, $\text{Hf } \mathbf{2}$ and $\text{tbop} = 2,2'$ -thiobis{4-(1,1,3,3-tetramethyl-butyl)phenolate}] were prepared by HCl elimination from tbopH_2 and MCl_4 . Substitution of the chlorides in $\mathbf{1}$ and $\mathbf{2}$ by 2,6-diisopropylphenolato groups (dipp) generates new compounds $[M_2(\mu\text{-tbop-}\kappa^3\text{O,S,O})_2(\text{dipp})_4]$ ($M = \text{Zr } \mathbf{3}$, $\text{Hf } \mathbf{4}$). The structures of $\mathbf{1-4}$ were confirmed by NMR spectroscopy; complexes $\mathbf{3}$ and $\mathbf{4}$ were further investigated by X-ray crystallography. These studies showed $\mathbf{1-4}$ to be dimers either in the solid state or in solution and to have metal centers adopting distorted octahedral geometry. However treatment of MCl_4 with $[\text{Al}_2(\mu\text{-OEt})_2(\text{tbop-}\kappa^3\text{O,S,O})_2]$ or $[\text{Al}_2(\mu\text{-tbop-}\kappa^3\text{O,S,O})_2\text{Me}_2]$ gave heterotrimeric complexes $[M(\text{tbop-}\kappa^3\text{O,S,O})_2\text{Cl}_2(\mu\text{-AlX}_2)_2]$ ($M = \text{Zr}$, $\text{X} = \text{Cl } \mathbf{5}$, $\text{X} = \text{Me } \mathbf{7}$ and $M = \text{Hf}$, $\text{X} = \text{Cl } \mathbf{6}$, $\text{X} = \text{Me } \mathbf{8}$) for which the single-crystal X-ray diffraction analysis showed zirconium and hafnium centers to have eight-coordinate dodecahedral geometry. Complexes $\mathbf{1-6}$ after activation with aluminium alkyls and supporting on MgCl_2 showed a lack of activity in the ethene polymerization process and moderate activity towards 1-hexene producing high molecular weight atactic poly(1-hexenes).

Adres publiczny

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