# A family of group 4 metal alkoxo complexes with an $M_3(\mu_3\text{-}O)$ core relevant to Ziegler-Natta catalyst intermediates.

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Streszczenie

Highly optimized syntheses of interesting model intermediates in Ziegler–Natta catalysis are described. These zirconium and hafnium alkoxo complexes have a stable $(\mu_3\text{-}O)M_3$ core and incorporate an alkaline earth metal containing moiety, as illustrated. Their formation pathway gives an insight into the mechanism of Z–N procatalyst formation. Solvent polarity plays a pivotal role in formation of the final product. Reactions of $[Mg(thffo)_2]$ (**1**) or $[Ca(thffo)_2]$ (**2**) with $ZrCl_4$ or $HfCl_4$ in a $CH_2Cl_2$/THF/$CH_3CN$ mixture give thermall stable neutral heterobimetallic tetranuclear complexes $[M_3M'(\mu_x\text{-}O)(\mu,\eta^2\text{-}thffo)_6(Cl)_6]$ (thffo=tetrahydrofurfuroxide; M/M′/*x*: **3**, Zr/Mg/3; **4**, Hf/Mg/3; **5**, Zr/Ca/4; **6**, Hf/Ca/4) as colorless crystals in 75–82 % yield. X-ray diffraction studies show complexes **3**–**5** to contain oxo-bridged $M_3$ triangles that are capped by an alkaline earth metal-containing moiety to form species of $C_3$ symmetry. Reactions of $ZrCl_4$ and $HfCl_4$ with pure tetrahydrofurfuryl alcohol in EtOH and MeOH provide ionic complexes $[M_3(\mu_3\text{-}O)(\mu,\eta^2\text{-}thffo)_3(L)_3(Cl)_6]Cl$ (M/L: **8**, Zr/EtOH; **9**, Hf/EtOH; **10**, Zr/MeOH) in 66–79 % yield. Complexes **8**–**10** consist of $M_3$ triangles that are analogous to those in **3**–**6** and possess similar overall symmetry, as shown by X-ray crystallography. Changes in the reaction conditions afforded the asymmetric neutral dimer $[Zr_2(\mu\text{-}thffo)_2(thffoH)(Cl)_6]$ (**7**) and the homometallic $[Zr_3(\mu_3\text{-}O)(\mu,\eta^2\text{-}thp)_3(thf)_2(Cl)_7]$ (**11**).

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