Synthesis and Molecular Structure of \(\text{(BuOO)(BuO)Al(\mu-O\text{Bu})_2}\text{Al(mesal)}_2\). The First Structurally Characterized (Alkylperoxo)aluminum Compound

Janusz Lewiński,* Janusz Zachara, and Elżbieta Grabaska

Department of Chemistry
Warsaw University of Technology
Noakowskiego 3, 00-664 Warsaw, Poland

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Organoauminum compounds are usually very sensitive toward dioxygen and very often inflame spontaneously in the air. Mild oxidation of these compounds by controlled introduction of oxygen leads to alkoxide compounds via unstable alkyl peroxide intermediates.\(^1\) Although the reactions of a variety of aluminum trialkyls with dioxygen and organic peroxides have been under investigation for many years,\(^2\) no structural data are available for aluminum alkyl peroxide. Only recently the first available for aluminum alkyl peroxide. Only recently the first

The interaction of \(\text{(Bu)_2 Al(mesal)}\) with dioxygen results in the formation of the corresponding monoalkoxide compound \(\text{[(Bu)_2 Al(\mu-O\text{Bu})_2]}\).\(^3\) We report here the isolation and structural characterization of the first (alkylperoxo)aluminum compound derived from the oxidation of di-tert-butylnuclear magnetic resonance (1H, Ar) ppm, C\(_6\)D\(_6\)): 1.38 (s, 9H, tBuO), 1.49 (s, 9H, tBuO), 1.60 (s, 9H, tBuO), 1.98 (s, 9H, tBuO), 3.05 (s, 3H, OCH\(_3\)), 6.34 (td, 1H, Ar H), 7.47 (dd, 1H, Ar H).

(\text{Bu}_3\text{Al(AlOEt}_2 + \text{mesalH} \rightarrow \text{(Bu)_2 Al(mesal)} + \text{BuH}) \quad (1)

The solid state structure of \(\text{(Bu}_3\text{Al(AlOEt}_2 + \text{mesalH})}\) has been confirmed by X-ray crystallography\(^8\) and is essentially consistent with spectroscopic data.\(^7\) The molecular structure of \(\text{2}\) is shown in Figure 1. The molecule has an unsymmetric dinuclear structure with two aluminum atoms of different coordination. The Al(1) atom is bonded to a tert-butyl peroxide group and one terminal tert-butoxide group and Al(2) to two chelating mesal ligands. Both aluminum sites are joined by bridging \(\text{µ-O\text{Bu}}\) atoms with refined occupancy factors 0.75(1) and 0.25(1). \(\text{Molecular structure of (BuOO)(BuO)Al(µ-OBu)Al(mesal)}_2\).

The tert-butyl substituted dialkylaluminum chelate compound was obtained from the equimolar reaction of \(\text{(Bu)_2 Al(OEt}_2 + \text{methyl salicylate (mesalH)}\) in a near quantitative yield (eq 1).\(^5\)

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Communications to the Editor


Studies on the interaction of dialkylaluminum chelate complexes with dioxygen and the stability and reactivity of alkyl peroxide aluminum compounds are underway in our laboratory.

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Supporting Information Available: A listing of crystallographic data, atomic parameters, anisotropic thermal parameters, and complete bond distances and angles for 2 (8 pages). See any current masthead page for ordering and Internet access instructions.