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Influence of alkoxy ligands on the Cp-Al bonding mode in $[Cp_2Al\text{-}\mu\text{-}OR]_2$ from X-ray crystallographic and ^{27}Al-NMR spectroscopic solution studies.

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The dicyclopentadienylaluminium alkoxides of general formula $[Cp_2Al\text{-}\mu\text{-}OR]_2$ where R=Me, Et, *n*-Bu, *i*-Bu, CH_2*t*-Bu, *s*-Bu, CH_2Ph, C_6H_4-4-*t*-Bu (**1**–**8**) were prepared by reacting CpNa with $ROAlCl_2$ at the molar ratio 2:1, respectively (**2**–**8**) or from the reaction of Cp_3Al with alcohol (**1**). The compounds were characterised by multinuclear NMR (^{1}H, ^{13}C, ^{27}Al) method. The molecular structures of compounds **2**, **5** and **6** were determined by X-ray crystallography. The Cp–Al bonding mode in dicyclopentadienylaluminium alkoxides regarding the steric demands of alkoxy groups is discussed based on ^{27}Al-NMR chemical shifts and structural data obtained. The meaningful correlation between Cp ring-slippage and ^{27}Al-NMR chemical shifts was observed.The dicyclopentadienylaluminium alkoxides of general formula $[Cp_2Al\text{-}\mu\text{-}OR]_2$ where R=Me, Et, *n*Bu, *i*Bu, CH_2*t*Bu, *s*Bu, CH_2Ph, C_6H_4-4-*t*Bu (**1**–**8**) were synthesised and structurally characterised by multinuclear NMR and compounds **2**, **5**, **6** by X-ray crystallography as well. The analysis of Cp–Al bond mode in dicyclopentadienylaluminium alkoxides regarding the steric demands of alkoxy groups was presented and the meaningful correlation between Cp ring-slippage and ^{27}Al-NMR chemical shifts was observed.

Słowa kluczowe

Alkoxy ligands, X-ray crystallography, Cp–Al bond mode

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