

Experimental and computational insights into carbon dioxide fixation by RZnOH species.

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Streszczenie

Organozinc hydroxides, RZnOH, possessing the proton-reactive alkylzinc group and the CO₂-reactive Zn OH group, represent an intriguing group of organometallic precursors for the synthesis of novel zinc carbonates. Comprehensive experimental and computational investigations on 1) solution and solid-state behavior of tBuZnOH (1) species in the presence of Lewis bases, namely, THE and 4-methylpyridine; 2) step-by-step sequence of the reaction between 1 and CO₂; and 3) the effect of a donor ligand and/or an excess of tBu(2)Zn as an external proton acceptor on the reaction course are reported. DFT calculations for the insertion of carbon dioxide into the dinuclear alkylzinc hydroxide 12 are fully consistent with H-1 NMR spectroscopy studies and indicate that this process is a multistep reaction, in which the insertion of CO₂ seems to be the rate-determining step. Moreover, DFT studies show that the mechanism of the rearrangement between key intermediates, that is, the primary alkylzinc bicarbonate with a proximal position of hydrogen and the secondary alkylzinc bicarbonate with a distal position of hydrogen, most likely proceeds through internal rotation of the dinuclear bicarbonate.

Słowa kluczowe

carbon dioxide fixation, computational chemistry, density functional calculations, reaction mechanisms, zinc, zinc hydroxide

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