The formation of a σ-bond complex vs. an oxidation addition product in reaction of [M(CO)$_4$(η^4-nbd)] (M = W, Mo) and H–EEt$_3$ (E= Si, Ge, Sn): DFT optimized structures and predicted chemical shifts of hydride ligands.

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Streszczenie

Density functional theory calculations have been employed to understand the bonding and structural features of the key intermediate complexes formed during the catalytic cycle for the hydrogermylation, hydrosilylation and hydrostannation of norbornadiene (nbd) in the photochemical reaction of the tungsten(0) and molybdenum(0) carbonyl complex [M(CO)$_4$(η^4-nbd)] (M = Mo, W) and H–EEt$_3$ (E = Si, Ge, Sn). The structure of the *σ*-bond complexes [M(CO)$_3$(η^2-H–EEt$_3$)(η^4-nbd)] (**1**) and the seven-coordinate hydride complexes [MH(EEt$_3$)(CO)$_3$(η^4-nbd)] (**2**) have been optimized. The calculated values of the chemical shift for the *σ*-bond proton in complex **1** and the terminal hydride ligand in the oxidative addition product complex **2** have been compared with recently published experimental data for complexes of this type.

Słowa kluczowe

σ-Bond activation, Metal hydrides, DFT calculation, Hydrosilylation, Hydrogermylation, Hydrostannation

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