H-Ge bond activation by tungsten carbonyls: an experimental and theoretical study.

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Rok wydania

2012

Czasopismo

Polyhedron

Numer woluminu

31

Strony

622-631

DOI

10.1016/j.poly.2011.10.040

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

The activation of the Ge–H bond and the formation of several hydride complexes, characterized by high-field resonances, have been detected during the ^{1}H NMR spectroscopy monitoring of the photochemical reaction of Et_3GeH and Et_2GeH_2 with $W(CO)_6$ and the norbornadiene complex $[W(CO)_4(\eta^4\text{-nbd})]$. The activation of the Ge–H bond of triethylgermane in the photochemical reactions of tungsten(0) complexes has been applied in the hydrogermylation of norbornadiene (nbd), which leads to the formation of *endo*-triethylgermylnorbornene as the major product. The complex $[\{W(\mu\text{-}\eta^2\text{-H–GeEt}_2)(CO)_4\}_2]$ has been fully characterized by NMR spectroscopy and by a single-crystal X-ray diffraction study. Evidence for the hydride ligand of the $W(\mu\text{-}\eta^2\text{-H–GeEt}_2)$ group has been provided by ^{1}H NMR spectroscopy (δ = −9.02, $^{1}J_{H–W}$ = 31 Hz) and by DFT calculations. A DFT study of the structural properties and ^{1}H NMR chemical shifts of several possible intermediate σ and hydride complexes formed during the photochemical reaction of $W(CO)_6$ and Et_2GeH_2 has been performed.

Słowa kluczowe

Tungsten, Germane, σ-Bond activation, Hydrogermylation, Photolysis, DFT calculation

Adres publiczny

https://doi.org/10.1016/j.poly.2011.10.040

Strona internetowa wydawcy

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