

Activation and adsorption of multiple H₂ molecules on a Pd₅ cluster: a density functional study.

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Rok wydania

2003

Czasopismo

Journal of Physical Chemistry
A

Numer woluminu

107

Strony

4929-4939

DOI

10.1021/jp0343436

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

The density functional study of the activation and adsorption of several H₂ molecules on Pd_{*n*} clusters is extended to *n* = 5. Detailed mechanisms of H–H activation by the trigonal bipyramidal (tbp) Pd₅ cluster are described. They encompass various reaction pathways initiated by binding the first and second H₂ to the axial/equatorial atoms of the Pd₅ core, leading to the formation of Pd₅(H)₂ and Pd₅(H)₄ activation products, respectively. The Pd₅ + H₂ → Pd₅(H)₂ reaction involves spin crossing, and the most stable product, which is a singlet, prefers both hydrogens at cap sites of the nonadjacent faces of Pd₅. By contrast to the cases for *n* = 3 and 4 studied previously, the activation of the second H₂ through the reaction Pd₅(H)₂ + H₂ → Pd₅(H)₄ is found to be exothermic with an associated barrier (ΔH (298.15 K)) lying below the Pd₅(H)₂ + H₂ asymptote. The subsequent steps of the hydrogenation of Pd₅ take place via molecular adsorption onto the Pd₅(H)₄ dissociative complex, ultimately giving the hydrogen-rich cluster Pd₅(H)₄(H₂)₅, consistent with experiment. A comprehensive set of the non-hydrogen-saturated species that contain the Pd₅(H)₄ core structure have also been predicted. The thermodynamic stabilities of the Pd₅(H)₄(H₂)_{*m*} (*m* = 1–5) hydrogenated clusters are discussed in terms of ΔH and ΔG values at *T* = 298.15 and 70 K.

Słowa kluczowe

Molecular structure, Palladium, Cluster chemistry, Chemical reactions, Chemical structure

Adres publiczny

<https://doi.org/10.1021/jp0343436>

Strona internetowa wydawcy

<https://www.acs.org/content/acs/en.html>

Plik został wygenerowany dnia 2026-10-10 19:59:05

Adres w repozytorium <https://old.chem.uni.wroc.pl/pl/repozytorium/z6cbYhp>.