

Can gallium dimer react effectively with three H₂ molecules to form digallane?

Autorzy

Jerzy Moc

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Streszczenie

Distinct routes of formation of digallane (4) Ga₂H₄ and digallane (6) Ga₂H₆ starting with gallium atoms/H₂ and gallium dimers/H₂ are compared based on the high level ab initio single-reference CCSD(T) and CASSCF based SOCI and hybrid density functional theory calculations of the mechanisms involved. The predicted reaction paths are of relevance to the recent matrix IR studies on the gallium hydrides, notably the extensive one by Wang and Andrews [X. Wang, L. Andrews, J. Phys. Chem. A 107 (2003) 11371] who isolated and assigned the series of mono- and digallium hydrides including the two digallanes.

Słowa kluczowe

Gallium hydrides, Hydrogenation, Gallium clusters, Reaction paths, Ab initio and density functional calculations

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