The hydrogenated aluminium trimer: a theoretical examination of the formation and interconversion pathways.

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Streszczenie

Five doublet isomers of the Al_3H_2 cluster lying within a narrow range of 5 kcal/mol, along with the isomerization transition states connecting them, have been located with the coupled-cluster CCSD(T) and DFT methods. The two most stable doublet structures, the C_{2v} planar including the two Hs bound terminally and C_1 non-planar showing one H in terminal site and the other in threefold site are found to be essentially degenerate. Although the reaction of Al_3 with H_2 to yield Al_3H_2 is found to be significantly exothermic, by 23.5 kcal/mol, this hydrogenation is impeded by a considerable kinetic barrier of 16 kcal/mol. Our result is consistent with the observed lack of reactivity of Al_n towards $H_2(D_2)$ for n=3 under thermal conditions [3]. The quartet Al_3H_2 isomers are predicted to lie 16–21 kcal/mol higher in energy than the doublet analogues. Further dimerization of Al_3H_2 to form Al_6H_4 has also been examined.

Adres publiczny

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http://link.springer.com