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On the existence of MH_n species with M=Al., Ga and *n*= 4,5,6. Computational study of structures, stabilities and bonding.

Autorzy

Jerzy Moc

Karolina Bober

Jarosław Panek

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Streszczenie

Based on second-order perturbation theory (MP2) predictions with large 6-311 + + G(3df, 3pd) basis set we have reviewed the possible structures and stabilities of a series of neutral MH_n(M = Al, Ga; n = 4, 5, 6) species. For AlH_4 and AlH_5, our results confirm the previous theoretical findings, which indicate the dihydrogen C_s complexes ($^2A'$) AlH_2 (H_2) and ($^1A'$) AlH_3 (H_2), respectively, as the lowest energy isomers. We found, similarly, C_s ($^2A'$) GaH_2 (H_2) and (^{1} A′) GaH_3 (H_2) van der Waals complexes as the most stable species of the gallium analogues GaH_4 and GaH_5. The calculated H_2 dissociation energies (D_e) for AlH_2 (H_2) and AlH_3(H_2) are of the order 1.8-2.5 kcalmol^1, whereas this range of values for GaH_2(H_2) and GaH_3(H_2) is 1.4-1.8 kcalmol^1. Symmetry-adapted perturbation theory (SAPT) was used to analyze the interaction energies of these dihydrogen complexes (for n = 5) to determine why the Ga species show a smaller binding energy than the Al species. The SAPT partitioning of the interaction energy showed significant differences between AlH_3 (H_2) and GaH_3(H_2), resulting from the much stronger "hydride" character of the aluminum species. The experimental observation of AlH_2(H_2) and AlH_3(H_2), and likely GaH_3 (H_2), via low-temperature matrix isolation has been reported recently by Pullumbi et al. and Andrews et al., supporting the theoretical predictions. For n = 6, we found the degenerate C_2 (^2A) and C_s($^2A'$) MH_2 $(H_2)_2$ "double H_2" type van der Waals complexes as the lowest energy species for both M = Al and Ga.

Słowa kluczowe

Ab initio calculations, Aluminum and gallium van der Waals complexes, SAPT

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