

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

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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 ( $^1A'$ )  $GaH_3(H_2)$  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<sup>-1</sup>, whereas this range of values for  $GaH_2(H_2)$  and  $GaH_3(H_2)$  is 1.4-1.8 kcalmol<sup>-1</sup>. 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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Strona internetowa wydawcy

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