Boron Nanowheels with Axles Containing Noble Gas Atoms: Viable Noble Gas Bound M©B10 ? Clusters (M=Nb, Ta)

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The viability of noble gas axled boron nanowheels NgnM©B10 ? (Ng=Ar?Rn; M=Nb, Ta; n=1, 2) is explored by ab initio computations. In the resulting Ng2?M complexes, the Ng-M-Ng nanorod passes through the center of the B10 ? ring, providing them with an inverse sandwich-like structure. While in the singly Ng bound analogue, the Ng binding enthalpy Hb at 298 K ranges from 2.5 to 10.6 kcal mol?1, in doubly Ng bound cases it becomes very low for the Ng2M©B10 ??Ng+NgM©B10 ? dissociation channel, except for the case of Rn, for which the corresponding Hb values are 3.4 (Nb) and 4.0 kcal mol?1 (Ta). For a given Ng, Ta has slightly higher Ng-binding ability than Nb. The corresponding free-energy changes indicate that these systems, particularly the Xe and Rn complexes, are good candidates for experimental realization in a low-temperature matrix. The Ng?M bonds were found to be covalent in nature, as reflected in their large Wiberg bond indices, formation of a 2c?2e ? orbital between Ng and M centers in natural bond orbital and adaptive natural density partitioning (AdNDP) analyses, and the short Ng?M distances. Energy decomposition analysis and a study on the natural orbitals for chemical valence show that the Ng?M contact is supported mainly by the orbital and electrostatic interactions, with almost equal contributions. Although both the Ng?M ? donation and Ng?M ? backdonation play roles in the origin of orbital interaction, the former is significantly dominant over the latter. Further, AdNDP analysis indicates that the doubly aromatic

character (both ? and ?) in MB10 ? clusters is not perturbed by the interaction with Ng atoms. © 2018 Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim

ab initio calculations

boron

cluster compounds

noble gases

transition metals

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Boron

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