Noble Gas Supported B_3^+ Cluster: Formation of Strong Covalent Boron-Noble Gas Bonds

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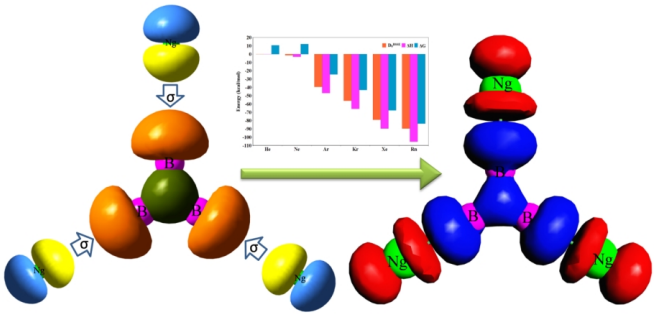
The stability of noble gas (Ng) bound B_3^+ clusters is assessed via an *in silico* study, highlighting their structure and nature of the Ng-B bonds.[1] Ar to Rn atoms are found to form exceptionally strong bonds with B_3^+ having each Ng-B bond dissociation energy in the range of 15.1-34.8 kcal/mol in $B_3Ng_3^+$ complexes with gradual increase in moving from Ar to Rn. The computed thermochemical parameters like enthalpy and free energy changes for the Ng dissociation processes from $B_3Ng_3^+$ also support the stability of Ar to Rn analogues for which the corresponding dissociation processes are endergonic in nature even at room temperature. The covalent nature of the Ng-B bonds is indicated by the localized natural Ng-B bond orbitals and high Wiberg bond indices (0.57-0.78) for Ng-B bonds. Electron density analysis also supports the covalency of these Ng-B bonds where the electron density gets accumulated in between Ng and B centres. The orbital interaction energy is the main contributor (*ca.* 63.0-64.4%) of the total attraction energy in Ng-B bonds..



Reference

1. Saha, R.; Pan, S.; Mandal, S.; Orozco, M.; Merino, G.; Chattaraj, P. K. Noble Gas Supported B3+ Cluster: Formation of Strong Covalent Boron-Noble Gas Bonds. *RSC Adv*. **2016**, *6*, 78611-78620.