Noncovalent Interactions of Boron Clusters

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Polyhedral boron clusters (boranes, boron hydrides) are large group of compounds with unique properties and unusual noncovalent interactions, which include dihydrogen bonds [1] and σ-hole interactions [2]. The counterintuitive ability of heteroboranes to form strong σ-hole interactions might be attributed to the multicenter bonding [3]. It breaks the classical electronegativity concept and results in areas of highly positive electrostatic potential (called σ-holes) on heteroatoms that are incorporated into the skeleton via multicenter type of bonding [3]. Group V, VI and VII elements in neutral heteroboranes can have highly positive σ-holes that are responsible for strong σ-hole interactions [2]. We have observed the S···π [4], Br···π [5], P···π [6] and Sb···H-B [7] types of σ-hole interactions of heteroboranes experimentally in the corresponding crystal packings.

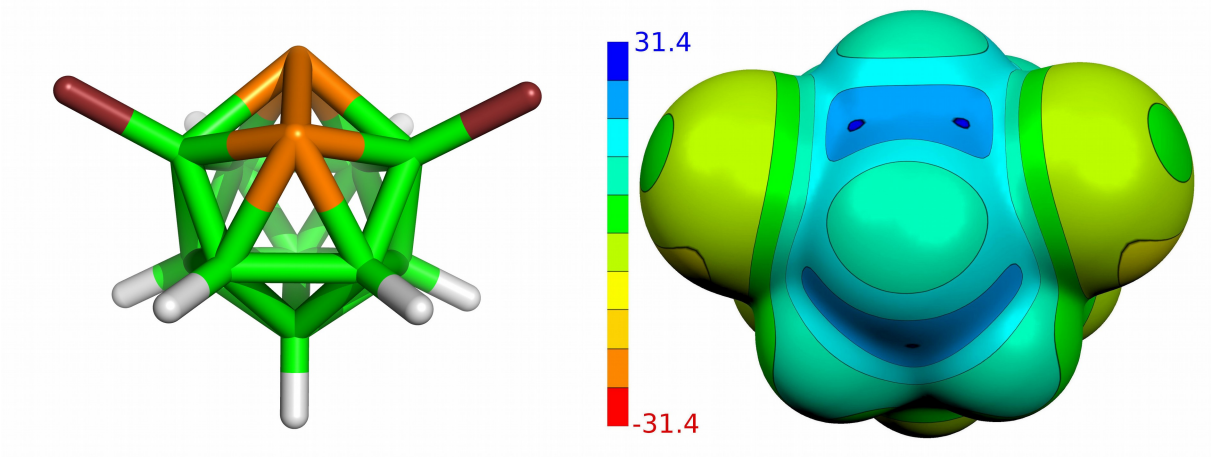

Figure 1: Molecular diagram (left) and electrostatic potential (right) on the 0.001 a.u. molecular surface of 3,6-Cl_2-closo-1,2-$P_2B_{10}H_8$. The ESP range in kcal mol^{-1}. Adopted from reference [6].

References

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