Noncovalent Interactions of Boron Clusters

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Polychedral 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-hole interactions [2]. The counterintuitive ability of heteroboranes to form strong σ-hole interactions 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-Cl₂-closo-1,2-P₂B₁₀H₈. The ESP range in kcal mol⁻¹. Adopted from reference [6].

References