Valence bonds in elongated boron clusters

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Analyzing bonding patterns in complex systems remains a challenge. While chemists are used to the Lewis-type localized bonding, this approach works mainly for simple cases. As a result, resonance introduced as a concept to explain any further difficulties. A tool, the Adaptive Natural Density Partitioning (AdNDP)[1, 2], which reconciles both types of localized and delocalized bonding, will be presented. This method is an extension of the Natural Bond Analysis (NBO)[3] and performs search for up to *n*c-2e bonds, where *n* ranging up to the total number of atoms in a system. It provides a quantitative picture of bonding in many non–classical chemical structures such as boron clusters. Further, a well defined class of planar or quasi-planar elongated boron clusters, of type B_{7+3n}^{q-}, will serve as a basis to identify the valence bond picture of delocalized boron networks. Specific electron counting rules will be used for both π and σ-multi-center bonding. The analysis supports 4c-2e bonds as an alternative to the common 3c-2e bonds. The results are validated by symmetry induction and *ab initio* calculations[4].

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