On the multiple B-N bonding in boron compounds using the topological analysis of electron localization function (ELF).

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Streszczenie

Topological analysis of the Electron Localization Function (ELF) within the framework of Quantum Chemical Topology (QCT) has been applied to study the nature of the boron–nitrogen bonds. A series of 10 compounds have been chosen, with the B–N bond length ranging between 1.698 Å (B–N) and 1.258 Å (BN). According to the Lewis formula three types of bonds have been recognized. These are: the single B–N bond with a basin population of 1.91 ÷ 2.09e, the double BN bond with a population of 3.78 ÷ 4.28e, and the triple BN bond with a basin population of 5.72 ÷ 5.74e. In the case of partial double bonds (BN), where formally two or more resonance hybrids have to be considered, our calculations strongly support the concept of double boron–nitrogen bonding (BN).

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