On the multiple B-O bonding using the topological analysis of electron localisation function (ELF).

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Streszczenie

Topological analysis of the Electron Localisation Function (ELF) within the framework of Quantum Chemical Topology (QCT) has been applied to study the nature of the boron–oxygen bonds. A series of 16 compounds has been chosen, with the experimental BO bond length in the range of 1.481 Å (BO)–1.179 Å (BO). Topological results obtained for the DFT(M062X), DFT(B3LYP), MP2 and CCSD(T) optimised geometrical structures show that all the boron–oxygen bonds in the investigated compounds are described by the disynaptic bonding basin, V(B,O). All these bonds have a covalent-polarised character. The mean electron population of V(B,O) varies from 1.6e ($B(OH)_4^-$) to about 3.5e (HNCHCHCHNHBO). The polarity index values, $p_{BO,}$ lie between 0.77 (ClBO) and 0.89 (H_2BOCH_3), thus all boron–oxygen bonds are essentially polarised by the oxygen atom. According to the Lewis formula, four types of the bonds have been recognised. These are: a single bond with a mixture of the ionic hybrid (BO, B^+O^-), a single bond (BO), a single bond with a small contribution of the dative O→B bond (BO) and a single bond with a large contribution of the dative O→B bond (depleted BO bonds). There is a clear distinction between a group of 11 molecules chosen for this study, with the basin population value of the boron–oxygen bond between 1.6e and 2.4e, and the HBO, FBO, ClBO, HNCHCHCHNHBO and trans-[(Me3P)2BrPt(BO)] molecules that exhibit the basin population in the range: 3.3e–3.5e. The second group was postulated to have a triple bond, BO, but this statement has not been confirmed by our research.

Słowa kluczowe

Triple bond, Quantum Chemical Topology, QCT, Lewis structure, B-O, B=O