

The nature of the triple $B\equiv B$, double, $B=B$, single, $B-B$, and one-electron, $B\cdot B$ boron-boron bonds from the topological analysis of electron localisation function (ELF) perspective.

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Streszczenie

Local nature of the boron-boron (BB) bond has been investigated in 23 molecules using the topological analysis of Electron Localisation Function (ELF) and the electron density (AIM) frameworks. The wave function has been approximated using the CCSD//CCSD(T), CASSCF and DFT(M062x) methods and triple-zeta basis sets. The calculations yielded a formally triple bond, BB, with population of 5.87–4.67e, a double bond BB with population of 4.39–3.58e, a single bond, $B-B$ with population of 2.49–2.04e and one electron bond, $B\cdot B$ with 0.38e. Topological analysis of $\rho(r)$ field has shown the non-nuclear attractor, NNA, for the BB bond in ten molecules (CCSD, DFT) with $r_{\text{opt}}(B,B)$ smaller than 1.6 Å. Population of the pseudo-atom basin ranges from 0.28e to 1.42e (CCSD) and from 0.32e to 1.27e (DFT). An overview of the results from topological analysis of ELF together with a detailed discussion of electronic structure for 14 small molecules has been presented.

Słowa kluczowe

chemical bond, one-electron bond, boron, $B-B$, Double bond, triple bond, Quantum chemical topology, QCT, electron localisation, ELF, topology

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