The electronic structure of molecules with the B—F and B—Cl bond in light of the topological analysis of electron localization function: possibility of multiple bonds?

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Streszczenie

Topological analysis of electron localisation function (ELF) has been used to study the nature of the B-X (X = F, Cl) bonds in 26 molecules. Twelve small molecules with formal B-X, B=X, and B≡X bonds and 14 organoboron molecules with the B-Cl bond from the Cambridge Structural Database have been studied using CCSD, DFT(M062x) methods. As the *V*(B,F) basin population for the investigated molecules is smaller than 4 and 6e, the existence of B=X, B≡X bonds is not confirmed. The results show higher polarity of B-F bonds as compared to the B-Cl bonds. Electronic structure of selected molecules has been discussed from the ELF-topological perspective.

Słowa kluczowe

B-Cl, B-F, chemical bond, Double bond, electron localitasion function, Lewis structure, QCT, Quantum chemical topology, triple bond

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