

On the nature of the boron-copper interaction. Topological study of the electron localisation function (ELF).

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Streszczenie

Topological analysis of the Electron Localization Function (ELF) has been applied to study the nature of the boron–copper bonds in the BCu molecule and a series of 18 organoboron compounds with bond lengths between 1.994 and 2.671 Å. The three-center and two-center covalent bonds have been found through localisation of the $V(B,Cu,A)$, $A = Mn, Cu, B, H$ and C , and $V(B,Cu)$ attractors with the basin populations from 1.49 to 3.13e and from 2.49 to 2.99e, respectively. For $r_{opt}(B,Cu) > 2.5$ Å, $B \cdots Cu$ interactions, characterised by very small basin populations, between 0.12 and 0.49e have been observed. Topological analysis of ELF has not proven the existence of a triple BCu bond.

Adres publiczny

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