

Theoretical insights and quantitative prediction of the nature of boron–chalcogen (O, S, Se, Te) interactions using the electron density and the electron localisation function (ELF).

Autorzy

Michał Michalski

Agnieszka J. Gordon

Sławomir Berski

Rok wydania

2021

Czasopismo

Polyhedron

Numer woluminu

210

Strony

115495/1-115495/8

DOI

10.1016/j.poly.2021.115495

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

Local electronic structure of the boron–chalcogen bond B–Ch (Ch = O, S, Se, Te) has been investigated from the perspective of topological analysis of the electron localisation function (ELF) and the electron density. Calculations were carried out for H_3BO_3 and 27 experimentally known organoboron compounds with B–Ch bonds deposited in Cambridge Structural Database (CSD), and showed that the B–Ch bonds are covalent with similar values of basin populations (1.50–2.26e). They can be characterised as 2-center-2-electron bonds and the nature of the B–O bond differs from the B–Ch (Ch = S, Se, Te) bonds. The AIM analysis shows positive values of the Laplacian of $\rho(r)$ for BCP characterising the B–O bonding and negative values for the B–Ch (Ch = S, Se, Te) bonding. The covalency of the B–O bond may come from dative mechanism. The topological analysis of the ELF shows the B–O bond exhibits the highest median polarity of 0.82 among the studied B–Ch bonds, mainly formed by electrons from the O atom. Polarity is clearly smaller for B–Ch (Ch = S, Se, Te) bonds and its values are between 0.03 and 0.55. The covalency of the boron–chalcogen bond, predicted by calculating differences between electronegativity values is anticorrelated with the basin population for the $V(\text{B}, \text{Ch})$ basin.

Słowa kluczowe

boron, chalcogen, ELF, AIM, organoboron

Adres publiczny

<http://dx.doi.org/10.1016/j.poly.2021.115495>

Strona internetowa wydawcy

<http://www.elsevier.com>

