

Abstract

The nature of the covalent bond has been the subject of considerable discussion in the modern chemistry.

Although the Lewis formula was introduced well before the quantum chemistry era, a representation of the multiple covalent bond (i.e. $X-X$, $X=X$, $X\equiv X$) with shared electron pairs has been widely accepted and used in modern chemistry.

The problem of the nature of chemical bonding involves connection between all atoms in the periodic table, if only in a purely hypothetical aspect.

Straub et al, studied multiple B-X bonds ($X=N$, O, F, P, S, Cl), and described a correlation between a predicted bond order and its length, assuming the presence of eight electrons around boron. So, it appeared interesting to investigate the nature of the bonds formed by the boron atom using the modern method of bonding analysis rooted in quantum chemistry and topology - the topological analysis of electron localisation function (ELF).

The boron atom has two empty 2p orbitals, therefore, the existence of double and triple covalent bonds $B=X$, $B\equiv X$ could also be considered.

The theoretical (computational) results presented in this thesis are concerned with the local electronic nature of the chemical bonds formed by a boron atom with atoms of boron (BB), carbon (BC), nitrogen (BN), oxygen (BO), fluorine (BF), and chlorine (BCl). 124 molecules containing B-X ($X = B, C, N, O, F, Cl$) bonds have been investigated at various electronic states ($2S+1 = 1, 2, 3, 4$) and with a range of formal charges ($q = -1, 0, +1$). 72 small molecules, known only from theoretical considerations, and 52 large molecules characterised experimentally with a described crystal structure have been studied.

For all investigated BX ($X = B, C, N, O, F, Cl$) bonds, which have been described as covalent, the topological analysis of ELF showed the bonding disynaptic attractor $V(B,X)$.

Generally, the obtained values of the basin populations are close to formal values of 1, 2, 4 and 6e, while there are many cases of the molecules for which the values for the BX bonds can not be easily interpreted.

The basin populations of the BB, BC, and BN bonds support the formal concept of the triple ($B\equiv B$, $B\equiv C$, $B\equiv N$), double ($B=B$, $B=C$, $B=N$), and single ($B-B$, $B-N$, $B-C$) bonds. The possibility of multiple, $B=O$, $B\equiv O$, $B=F$, $B\equiv F$, and $B=Cl$, $B\equiv Cl$ bonds has been thoroughly investigated and the suggestion has not been confirmed.