

4. ABSTRACT

Selected effects accompanying weak interactions in two- and three-body systems

A chemical bond is formed when forces acting between atoms or groups of atoms form a permanent connection. Recently, the issue of noncovalent interactions has attracted the attention of many researchers. Noncovalent interactions occur between the fragment of the electron acceptor (Lewis acid) and the fragment of the electron donor (Lewis base), playing an important role, among others, in living organisms. Intermolecular interactions are increasingly discussed in many scientific publications. Recently, the most-discussed among noncovalent interactions are hydrogen bonds, next to which the number of works describing halogen or chalcogen bond increases. These interactions are significant in the processes that occur in living organisms, which is why they have also become the main subject of this doctoral dissertation.

The main purpose of the work was the analysis of energy parameters, as well as the most important topological parameters at the bond critical points (BCP), which gave the opportunity to compare the strength of interactions and showed the effect of mutual interaction (cooperativity/anticooperativity effect). The many-body interaction approach was used in order to estimate the energy of individual bonds in the complex and the nonadditive contribution to total interaction energy.

In this work, the quantum-chemical calculations were performed for series of representative model systems. In the first step of the analysis the geometries of the investigated systems have been optimized using the Gaussian 09 program. The next step was the topological analysis of the electron density using the Quantum Theory of „Atoms in molecules" by Richard Bader (QTAIM). In addition, the supermolecular method was used to determine the energy of intermolecular interactions, in which the obtained energies are with the correction for basis set superposition error, BSSE.

The first section discusses the analysis of halogen bonds supported by double charge, in particular their impact on the parameters of the investigated systems, including charge transfer (CT) and two-center delocalization index $\delta(A, B)$. Quinuclidine is an organic compound from the group of bicyclic heterocyclic compounds. This compound consists of the bicyclo[2.2.2]octane moiety, wherein one of the carbon nodes is nitrogen.

For comparison, model systems consisting of bicyclo[2.2.2]octane moiety and its unsaturated analogue were analyzed.

The second section concerned model systems in which the dual role of a halogen atom, acting as an electron acceptor and donor, can be observed. The many-body interaction approach was used to analyze interactions between hydrogen and halogen bonds in complexes.

In the third section, the main goal of study was to confirm the dual role of the sulfur atom, acting as the electron donor and the electron acceptor, simultaneously. Model systems that are fragments of larger counterparts found in Crystallographic Database were selected for studies in such a way that the resulting complexes (dimers and trimers) were stabilized by various types of noncovalent interactions, that is, the hydrogen bonds, halogen bonds and chalcogen bonds.

Key words: halogen bond, hydrogen bond, chalcogen bond, noncovalent interaction, QTAIM, charge transfer