Streszczenie pracy doktorskiej

Mariusz Michalczyk

„Oddziaływania niekowalencyjne w wybranych kompleksach donorów dziury typu σ lub π”

Interactions through σ- or π-holes are responsible for the formation of wide group of complexes. Genesis of both of these holes is connected with the effect of the anisotropic distribution of electron density in certain molecules which leads to decreasing this density around atoms bonded with electron-withdrawing substituents. As a consequence of this the regions of positive electrostatic potential rise. They act as potential binding sites for approaching nucleophiles. Taking into account the origin of element which produces particular hole, there are some categories of these bonds as: halogen, chalcogen, pnicogen, tetrel, triel and aerogen. All of them have gained constantly growing interest of scientific community. Complexes stabilized by these interactions are not only the subjects of theoretical studies but also find its purpose in crystal engineering, supramolecular and material chemistry or biochemistry as well. There is a rising number of structures deposited in crystal databases in which the patterns of discussed interactions are present.

In the frame of doctoral dissertation a guidebook to 7 articles belonging to the series describing various σ- and π-holes bonds is presented. The essential role of the isolated hole donor geometry distortion is described there. Deformation affects greatly the process of complexation which results in the complexes of higher than predicted interaction energies. The numerous examples of such structures have been thoroughly investigated by means of computational methods of quantum chemistry.

Beside the geometry deformation of monomers, the impact of other agents which cause the anomalies of obtained energy results has been studied. They are the negative hyperconjugation effect occurring in the some of Lewis bases and the presence of secondary interaction which hamper the calculations of interaction energy belonging to the σ-hole interaction solely. The results achieved in concerned publications may allow to understand better the self-organization processes of molecules embedded in many molecular systems.