CHEMICAL BOND AND INTERMOLECULAR INTERACTIONS: WILL BE THE PARADIGM CHANGED?

Tsirelson V.G.

D.I. Mendeleev University of Chemical Technology, Moscow, Miusskaya Sq. 9

In the XX-th century the basic concepts of chemistry was firmly inscribed in the system of scientific knowledge. A significant part of chemistry is based on the representation of a spatial arrangement of atoms in molecules, molecular systems and crystals, the chemical bond between them, and the dependence of physical and chemical properties of crystals from their composition and structure. The most significant elements of classical chemical paradigm are the theory of symmetry, the concept of the atom as a structural unit and the theory of the chemical bond and intermolecular interactions. We will focus on existing chemical ideas about the nature and relationship between quantum and electrostatic component of atomic and molecular interactions in molecules and crystals and compare them with new data about the structure of these entities at the level of continuous electronic continuum (plus nuclei). These data are available thanks to the development of precision X-ray structural analysis, quantum-chemical calculation methods and methods of interpretation of the obtained results. The main conclusion that is not based on model representations is that the atom as a structural unit of the chemical picture of the world gradually ”splits” at the subatomic elements associated with the peculiarities of the electron density in the bounded systems. This allows one to more exhaustively and accurately describe chemical bonding and intermolecular interactions in complex systems.

This work is supported by the Russian Foundation for Basic Research; project 16-03-00057a.