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Crystal chemistry at the present stage

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The available information about the disposition in space of atoms in molecules and crystals and of molecules in different condensed phases is nowadays used so vigorously that it would not be a great exaggeration to apply the term structural chemistry to modern chemistry. Indeed, very many branches of chemistry are based on structural ideas. The source of the most complete, reliable, and exact information about the structure of substances has become crystal chemistry, which is based mainly on X-ray diffraction analysis. In the 1950s–1960s, the accumulation of systematic data on the structures of a wide variety of chemical compounds began on the basis of this method. These data have found extensive applications in the consideration of properties of not only crystals but also of liquids, solutions, amorphous substances, and mesophases.

By virtue of the wide-scale employment of automatic diffractometers, the development of computer technique and computer programs, and the appreciable increase in the number of research workers using X-ray diffraction data, crystal chemistry is living through a qualitatively new stage of its development. A fairly complete idea of this is provided by the articles in the present issue of "Uspekhi Khimii". The principal features of the present stage are as follows.

Firstly, it has now become possible to accumulate rapidly a large amount of structural information about a wide range of representatives of the class of chemical compounds investigated (including fairly complex compounds). This has led to the rapid development of systematic crystal chemistry, which reveals the regularities and specific features in the structure of substances belonging to the given chemical class. An example of such studies is provided by the review by L M Skhol'nikova and M A Porai-Koshits on aminoalkylcarboxylic and aminoalkylphosphonic complexones. It is significant that, within the framework of systematic crystal chemistry, it is frequently possible to interpret and predict successfully properties of substances which are of practical importance, for example, the photochemical properties of spiropyrans (the review by S M Aldoshin), the electrical conductivity of dithiolate complexes (the review by V E Shklover, S S Nagapetyan, and Yu T Struchkov), and phase formation in oxide systems (the review by V A Efremov).

Secondly, by virtue of the development of precision low-temperature studies, it has become possible to investigate substances which are liquid at room temperature and to obtain previously unavailable information, for example, information about the mean square displacement of atoms in thermal vibrations (the review by M Yu Antipin).

Thirdly, precision X-ray diffraction analysis has led to the possibility of thorough investigation of the details of the distribution of electron density in chemical compounds, which has given rise to new prospects for the development of the theory of the chemical bond (the review by P M Zorkii and A E Marsunov).

As a result of the development of the last two aspects of X-ray diffraction studies, the concept of the model of the crystal structure has been significantly transformed. It can now be regarded both as a dynamic structure (with atoms in the form of thermal ellipsoids and in certain cases also with allowance for anharmonicity) and as a continuous distribution of electron density in which atomic nuclei are incorporated. These advances constitute an important achievement not only in crystal chemistry but in chemistry as a whole.