Molecular Crystal Structures from Low-Resolution Powder Diffraction Data: Reliability and Validation of the Results Obtained

Vladimir V. Chernyshev, *Department of Chemistry, Moscow State University, 199992 Moscow, Russia.* E-mail: vladimir@struct.chem.msu.ru

In recent years, an obvious progress has occurred in the determination of molecular crystal structures *ab initio* from powder diffraction data. There are no doubts now, the molecular crystal structures with the known connectivity set in the molecule(s) can be routinely solved even from the data measured at the laboratory powder diffractometer. However, there are the questions still waiting for an exhaustive answering. One of them is a question on how to estimate the reliability of the solution obtained. An another one concerns the accuracy of structural parameters extracted. These questions are exceptionally important for the results obtained at laboratory commonly used devices. There are problems, which can not be clarified with the use of laboratory data only. So the problem of positioning of the selected hydrogens is beyond the facilities of many laboratory X-ray powder diffractometers, which are virtually "insensitive" to the position of H atoms. In this particular case, the neutron diffraction often helps to find a correct position, especially when some, or even all, of the hydrogens are replaced by the deuteriums.

For the new crystal structure solved from laboratory powder data we have a good chance to validate its correctness by the comparison of the results with those, obtained either from high-resolution synchrotron data or, in some cases, from neutron powder diffraction data. The aforementioned comparison allows us to estimate the real accuracy of the results derived from the laboratory powder pattern. This will be demonstrated on a number of molecular structures solved from laboratory data and validated later with the use of synchrotron and/or neutron data.

Keywords: crystal structure determination x-ray powder data, synchrotron powder diffraction, neutron powder diffraction