s8.m27.p26 **Routine crystal structure determination from laboratory X-ray powder diffraction data.** Xuelian Xu,[a] Alastair Florence,[a] Norman Shankland,[b] Kenneth Shankland,[c] William I.F. David [c] and Alan R. Kennedy [d]. [a]*University of Strathclyde, Department of Pharmaceutical Sciences, 27 Taylor Street, Glasgow G4 0NR, UK,* [b]*CrystallografX Ltd., Queen Street, Glasgow., UK,* [c]*ISIS Facility, Rutherford Appleton Laboratory, Chilton, Didcot, Oxon., OX11 0QX, UK,* [d]*Department of Pure and Applied Chemistry, University of Strathclyde, Glasgow G1 1XL, UK. E-mail: x.xu@strath.ac.uk*

Keywords: X-ray powder diffraction; Crystal structure determination; Global optimisation

The crystal structures of 25 organic molecular compounds have been determined from laboratory X-ray powder diffraction (XRPD) data collected with transmission capillary geometry and CuKa1 radiation using the global optimisation approach embodied within the DASH structure solution package [1]. Compounds were selected to cover a wide range of structural complexity including multiple fragments (salts, solvates, Z' > 1) and conformational flexibility. Crystal structure determination using laboratory XRPD data and direct space global optimisation alone, is shown to be highly accurate and reproducible for problems comprising low degrees of freedom (<15). Such structures typically yield low R.M.S. differences (< 0.1Å) between the atomic positions obtained from the global optimisation approach and their single-crystal equivalents. The solutions are also highly reproducible as indicated by a high frequency of success reaching the global minimum. The challenges to the global optimisation procedure are somewhat greater with complex molecules (D.O.F. > 20) where accuracy is typically reduced (R.M.S. > 0.1Å) and the rate of success in reaching the global minimum may fall below 5%. In such cases it is shown that the application of torsional constraints to restrict the global-search space offers significant benefits in terms of the time taken to solve a structure and the frequency of success.

[1] W. I. F. David, K. Shankland, N. Shankland, *Chem. Commun*., 931-932, 1998

s8.m28.p1 **Quantitative Electron Diffraction Structure Analysis.** A. Avilov, *Institute of Crystallography RAS, E-mail: avilov@ns.crys.ras.ru*

Keywords: Electron diffraction; Structure analysis; Electrostatic potential

The development of the electron diffractometry methods jointly the analytical methods of electrostatic potential (ESP) reconstruction and its topological analysis allowed one to proceed to the quality new level of electron diffraction structure analysis (EDSA): investigation inner crystalline electrostatic field, which knowledge permitts to study the relation of the atomic structure with physical properties of crystals. The review of the last achivements in this direction, obtained particularly in the Institute of Crystallography of Russian Academy of Sciences, in which EDSA method was discovered, and elsewere will be done. The possibility of the EDSA method to solve precise problems of quantitative analysis of the electrostatic potential will be shown on the examples of investigations of the ESP distributions and chemical bonding in crystals with NaCl-type structure and covalent crystal Ge. The reliability of experimental results obtained was confirmed by the *ab initio* calculations by the Hartree-Fock method. Quantitative data on the potential distribution in addition to the topological analysis of the electron density considerably enlarge conceptions on the nature of interatomic and intermolecular interactions in crystals. The importance of this circumstance promotes the EDSA to the leading position in physics and chemistry of solids.

So the main contents of the lecture is:

[1] State of the methods of the precise EDSA:
- Electron diffractometry;
- Problem of kinematic - dynamic scattering in thin polycrystalline films;
- Using of the precession technics for EDSA.

[2] Reconstruction of the ESP by Fourier and analytical methods.

[3] Quantitative investigations of the chemical bonding and ESP by EDSA.

[4] Quantitative analysis of ESP in EDSA.

[5] The perspectives of development of the quantitative EDSA.