MS42-O1 **Small molecule Crystallography on Macromolecular Biology Beam Line at the ESRF.** David Flot[a]. [a]*ESRF, 6 rue Jules Horowitz, BP220 38043 Grenoble Cedex 9, France.*
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The third generation synchrotron beam lines can provide a high photon flux and small beam size. Modern goniometers such as those of the MD2 family [1], present on the macromolecular crystallography (MX) beam lines at the ESRF, combine excellent sample visualization, an accurate rotation axis and easy sample alignment. As a consequence, synchrotron single crystal data collection at synchrotrons are routinely made for biological macromolecules and it allows the collection of diffraction data from small samples (small molecules or proteins). X-ray beams can be focused down to less than 10 microns in diameter, allowing data collection from very small samples, from several positions, or to probe small volume from a larger but inhomogeneous sample and to define the best part. This technique or strategy are regularly used for macromolecular crystals and a similar approach can be used for small molecule single crystals; this will be presented, with hints on sample preparation and data reduction.

[1] Perrakis A, Cipriani F, Castagna JC, Claustre L, Burghammer M, Riekel C, Cusack S. *Acta Crystallogr D Biol Crystallogr* 1999, **55**: 1765-1770.

MS42-O2 **When small molecule data are lacking resolution.** Michal Dušek, Václav Petříček, Karla Fejfarová, *Institute of Physics ASCR, v.v.i., Na Slovance 2, Prague 8, Czech Republic*
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Low resolution is a typical problem of crystallography of large organic molecules. Special methods facing the lack of observed Bragg reflections needed for detailed solution of large structures have been developed especially for proteins. Small and medium structures usually provide sufficient number of reflections per refined parameters, provided that good quality samples are available. However, statistic disorder may occur in such structures, causing uniformly distributed diffuse scattering and corresponding decrease of Bragg intensities. With low resolution the structural information becomes less distinct even for small structures and some of the wide spectrum of parameters saving methods must be used. Here we shall focus to techniques available in the computing system Jana2006 [1]. The most natural is usage of rigid body, with a shape refined only for the model, which is placed to actual positions in the structure *via* refined translations and rotations. Collective atomic displacements of such rigid body can be refined in a form of TLS tensors. Another method is based on restrained refinement, where bond lengths, angles or torsion angles are kept on desired value with a user defined weight. Planes of atoms or shape of structure fragments can be also fixed using constraints, including possibility to derive atomic positions from positions of another atoms, as routinely used for decorating structure model with hydrogen atoms.

The methods for solution of medium-sized structures from low resolution data will be presented with two strongly disordered compounds: (**1**) β-Cyclodextrin duplex [2], (**2**) unpublished structure of valinomycine. **1** contains also electron density of an undetermined solvent, which was "filtered out" by using of anharmonic displacement tensors. While **1** was successfully solved and published, **2** represents an example on the borderline between normal-sized structures and macromolecules. Here the methods for small molecules become too laborious but the data still provide much more details comparing with e.g. proteins, opening possibility to extend some of protein techniques to this class of compounds.

[1] Petrícek, V., Dušek, K. & Palatinus, L. (2006). *Jana2006, the crystallographic computing system.* Institute of Physics ASCR, v.v.i., http://jana.fzu.cz
[2] Grishina, A., Stanchev, S., Kumprecht, L., Budešínský, M., Pojarová, M., Dušek, M., Rumlová, M., Krížová, I., Rulíšek, L. 7 Kraus, T. (2012). Chemistry - A European Journal, accepted for publication. DOI: 10.1002/chem.201201239

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