Workshop FOX, inorganics

$LiBH_4$ - HR synchrotron (SNBL) data (lambda=0.48562, zero = 0.0011, capillary 0.5 mm)
- Creation of XML file.
- Indexing, space group analysis.
- Solution without and with bond valence. Solution found after 12'000 moves (Max sintheta/lambda=0.16) without Bond valence cost, and after 12'000 moves with Bond valence cost scale 1'000.
- Solution from first 6 peaks (Max sintheta/lambda=0.16) can be obtained with a help of antibumps (scale=100) after 30'000 moves. The Bond valence cost only slow down the convergency.
- Solution with one excess Li or one excess BH_4. Solution with one excess Li found even with antibumps. Solution with one excess BH_4 found only without antibump.
- Manipulate geometry: Rotation around B-H1 (3-fold axis) bond by 45 deg, 8 rotations (=360 deg) needed to get the starting orientation. 3 rotations by 120 deg give also the starting orientation.
- Formula&Restraints: Remove one bond restraints (B-H1), also the bond angle restraints involving H1 will be removed. When starting the optimization H1 will be merged with other H atom, and BH_4 oriented so, that one H atom will be on general position.

$LiMg_2NiD_7$ - Two data sets, synchrotron and neutrons
- Combination of free atoms and polyhedra. Converges within 2'500'000 moves.
- Discussion of different cost-functions in Tracked data window.

$K_2V_3O_8$ - HR synchrotron (SLS) data (lambda=1.00097, zero = 0.0075)
- Comparison of the convergence speed with free atoms vs. with polyhedra. Faster with one tetrahedron VO_4 and one square pyramid VO_5 (obtained from VO_6 by editing the molecule and removing one oxygen).

$PbSO_4$ - MythenII synchrotron (SLS) data (lambda=1.00097, zero = 0.0075)
- Indexing with FOX. One impurity line in the powder pattern (12.67 deg 2theta). FOX finds double *b*-cell with this impurity line, and correct cell without this line. FOX finds the correct cell also as a triclinic.
- Solution from free atoms. Solution found with free atoms after 200'000 moves.
- Diff Fourier maps during the optimization (color yellow, contour +3).

$SrRuO_3$ - lab X-ray data (Cu Kalpha)
- Solution found with RuO_6 octahedra after 40'000 moves.
- s.g. non-constrained to the lattice: The s.g. setting is *Pnam*. You can model the orthorhombic structure also in *I*4/*m*.

Chalcanthite, $CuSO_4 . 5H_2O$
- Modra skalice.
- SLS2014 data, λ=0.77465, *P*-1, max Sintheta/lambda=0.3, 60 points in the background, two CuO_6 (Cu-O 1.95), one SO_4 (S-O 1.47) and one non-coordinating H_2O molecule in the a.s. Z=2
- CuO_6 octahedra are sitting in inversion centers, therefore we need two of them.
Four oxygens coordinating Cu are water, and two are oxygens shared with SO_4.
- Indexing works if you declare one spurious peak. Max V = 600, Max axis length 15.