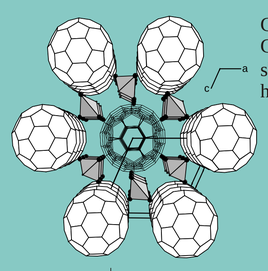
Max-Planck-Institut für Festkörperforschung

X-Ray Diffraction Service Group

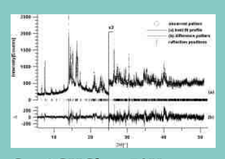
MAX-PLANCK-GESELLSCHAFT

Robert Dinnebier

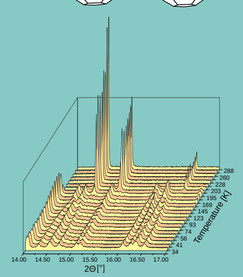
C_{60} derivative



Crystal structure of low Temp C_{60}.2$CHCl_3$ in a view along b axis showing the close relationship to the hexagonal room T phase.



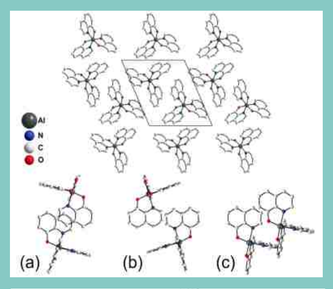
$C_{60} \cdot 2CHCl_3$ at 50K



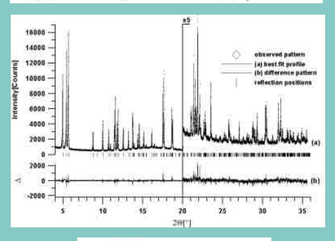
Hexagonal → Monoclinic → Triclinic

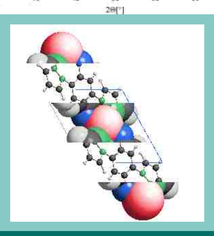
Heating-cooling cycles showed pronounced hysteresis and co-existence of the different phases over a large temperature range.

Blue luminescent polymers



Crystal structure and Rietveld plot of facial-Alq_3. (a), (b) and (c) are projections perpendicular to the planes of the hydroxyquinoline-ligands 1, 2 and 3, respectively, showing the overlap between ligands of neighbouring Alq_3 molecules.Different degrees of overlap of the pi-orbitals of hydroxyquinoline ligands belonging to neighboring Alq_3 molecules are likely to be the origin of the significantly different electro-optical properties.





one-dimensional Heisenberg spin chain: dipyhydroquinone-copper

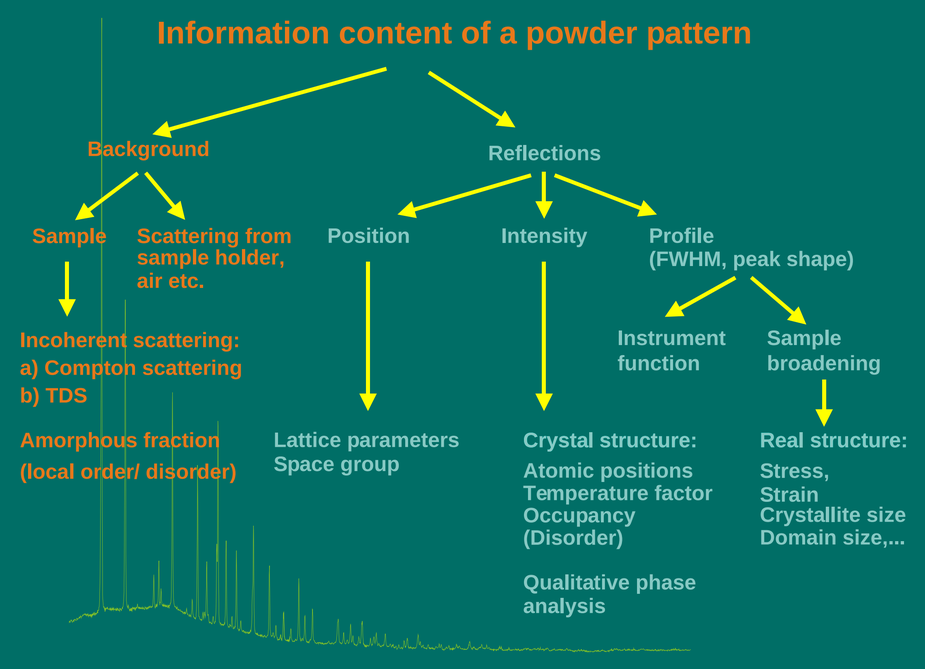
The X-ray diffraction service group provides X-ray diffraction measurements of single crystals and powders in the laboratory at room and low temperature.

Research within the X-ray diffraction service group is mainly concerned with the determination of crystal structures and microstructural properties (strain, domain size) of condensed matter from powder diffraction data. In addition, methodological development within this area is pursued. Special expertise in the field of solution and refinement of crystal structures from powder diffraction data can be provided.

Scientific cooperation in the field of non-routine structure determination (phase transitions, disorder, anisotropic peak broadening etc.) from powders is offered. This includes the performance of experiments at synchrotron and neutron sources at ambient and non-ambient conditions.

Materials currently under investigation include organometallic precursors, binary and ternary oxides, ionic conductors, electronic and magnetic materials, and rotator phases.

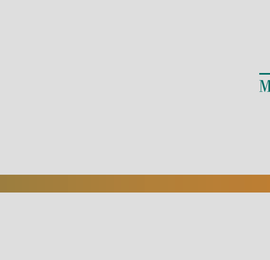
Information content of a powder pattern

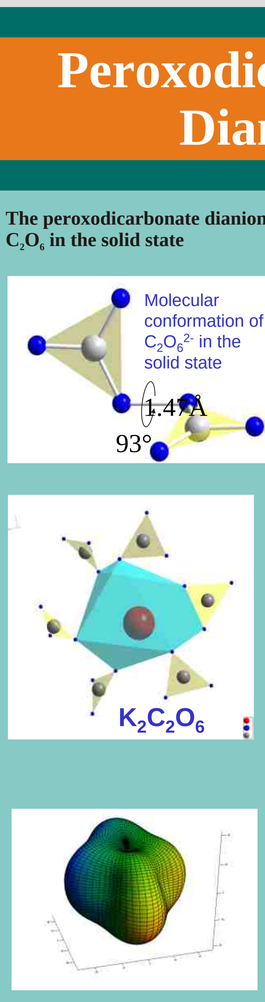


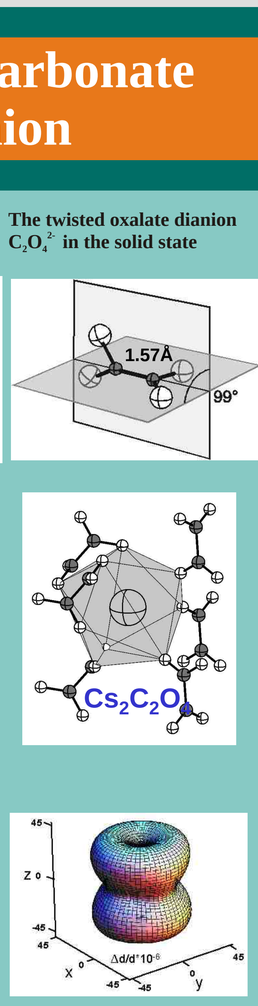
Peroxodicarbonate Dianion

The peroxodicarbonate dianion C_2O_6 in the solid state

The twisted oxalate dianion $C_2O_4^{2-}$ in the solid state

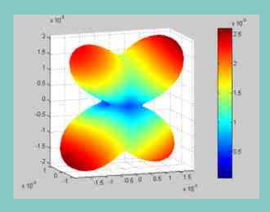






Iisosurface of anisotropic microstrain of of $K_2C_2O_6$ (left) and â-$Rb_2C_2O_4$ (right)

Anisotropic Microstrain

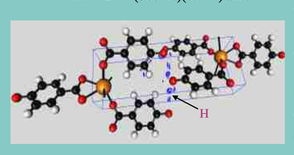


Anisotropic strain distribution for Na *para*-OH benzoate. Shading and distance from origin represents degree of microstrain (d/d) as a function of direction.

$S^2 = S_{400}h^4 + S_{301}h^3l + ... + S_{004}l^4$

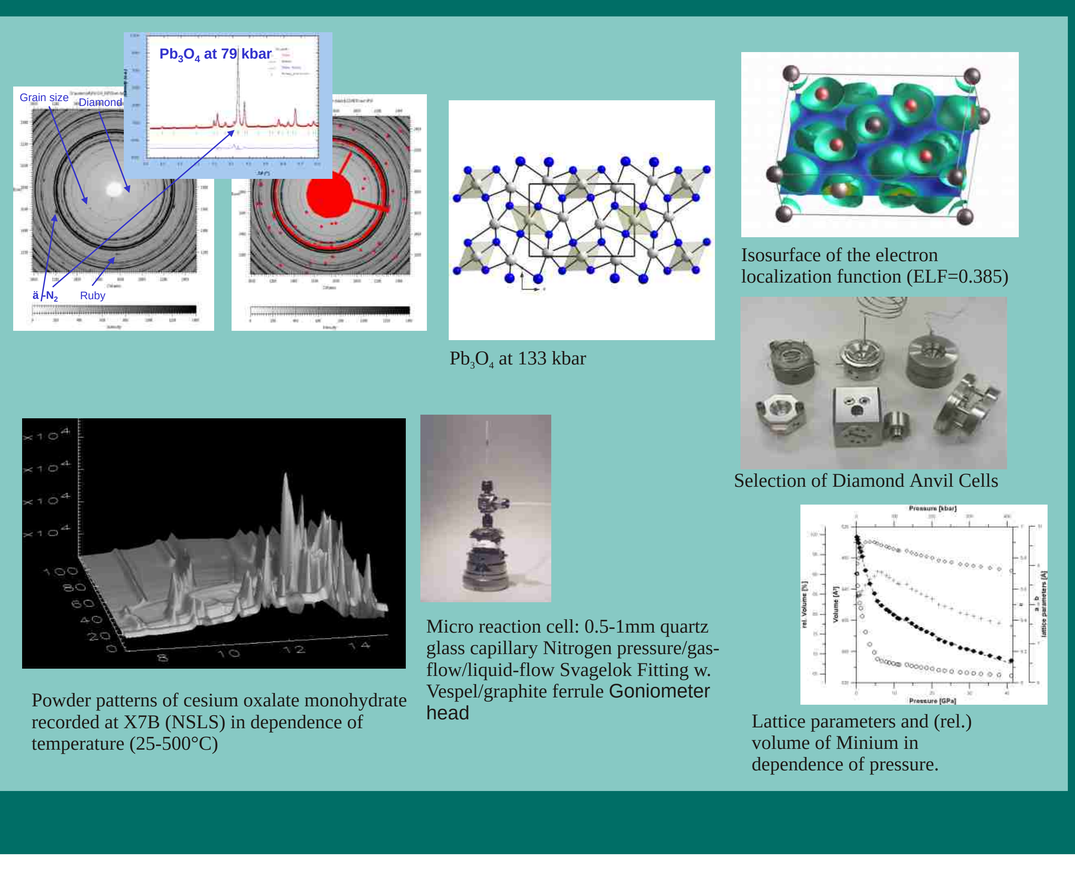
$\delta d/d = \pi(S^2)^{1/2} d^2/180$

FWHM in $2\theta = (360/\pi)(\delta d/d)\tan\theta$.



3-dimensional difference-Fourier plot of $NaC_7O_3H_5$ after applying the anisotropic FWHM model. The missing hydroxy-hydrogen atoms are clearly visible between the hydroxy-oxygen atoms.

Pharmaceuticals



Powder patterns of cesium oxalate monohydrate recorded at X7B (NSLS) in dependence of temperature (25-500°C)

Micro reaction cell: 0.5-1mm quartz glass capillary Nitrogen pressure/gas-flow/liquid-flow Svagelok Fitting w. Vespel/graphite ferrule Goniometer head

Lattice parameters and (rel.) volume of Minium in dependence of pressure.