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MoleCoolQt – A Molecule Viewer for Charge Density Related Science. Christian B. Hübschle,
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MoleCoolQt is a molecular viewer designed to be a useful tool for charge-density science. Features include the visualization of local-atomic coordinate systems in multipole refinements based on the Hansen and Coppens formalism [1]. Residual peaks and holes show up next to the atoms of the asymmetric unit if they are calculated by the refinement software. Critical points from the topological analysis of the charge density could also show in the structure visualization. Color-mapped iso-surfaces like in Moliso [2] can be generated with an easy to use user interface.
Beside of its visualization features it interactively helps the user in assigning local coordinate systems and local symmetry for the multi-polar refinement. It can automatically detect the local symmetry, but the user can easily reduce symmetry on demand. Dummy atoms are calculated and inserted into the model. When using data bases, rarely occurring Invariom [3], [4] name assignment problems can be solved by the use of an interactive dialog. Currently only the XD [5] package is fully supported, but other programs will follow in future. Currently the subsequent file formats are supported: XD, SHELX, GAUSSIAN (com, FChk, cube), CIF, PDB.
MoleCoolQt is written in C++ using the Qt library, has an user friendly GUI and is available for several flavors of Linux and Windows. A Mac version is currently being tested. After its final release it will be licensed under GPL. Since November 2009 test versions can be downloaded at http://www.molecoolqt.de after registration.

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Keywords: charge density, computer graphics, databases

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Crystal structure analysis using integrated X-ray powder diffraction software suite PDXL. Götz Schuck[a], Akihiko Iwata[a], Akito Sasaki[b], Akihiro Himeda[b], Hisashi Konaka[b], Norihiro Muroyama[b],
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The integrated X-ray powder diffraction software suite PDXL allows the user to perform many types of analysis (e.g.: automatic peak search, phase identification, quantitative analysis and Rietveld refinement) using a single platform, making it possible to obtain a diverse array of analysis results from one single X-ray powder diffraction (XRPD) pattern. PDXL has been developed as a comprehensive software package for the analysis of XRPD data. Recently Rigaku Corporation has included the easy-to-use PDXL Structure Analysis Package into PDXL software suite.
Initial crystal structure model construction routines (like parallel tempering and charge flipping) can be used within PDXL Structure Analysis Package. EXPO2009 is included in order to perform direct method or simulated annealing method. PDXL Structure Analysis Package offers three methods for initial structure determination: a) Direct method, b) Direct space method and c) Charge flipping method.
Direct method using EXPO2009 calculates phases from diffraction intensity by using theoretical probability equation [1]. Direct space method is searching the molecule configurations in a unit cell, in which simulated XRPD pattern is fit to observed one. The direct space method places a molecular structure in a unit cell and optimizes its position, Euler angles and several internal degrees of freedom to determine the initial crystal structure. The charge flipping method obtains electron density and phase using iteration between Fourier and inverse Fourier processes [2].
PDXL Structure Analysis Package is working together with other PDXL software suite features like indexing programs (DICVOL, ITO, N-TREOR), software tools for space group determination (both used before initial crystal structure determination) and an easy-to-use Rietveld analysis package (refinement of the crystal structure after solving the initial crystal structure with PDXL Structure Analysis Package). The PDXL Rietveld Analysis Package is designed to allow even a novice user to easily perform Rietveld analysis. PDXL automatically estimates the initial values of required parameters (e.g.: peak-profile parameters, etc.) prior to performing Rietveld refinement. After Rietveld refinement electron density distribution analysis such as Fourier/difference Fourier synthesis or MEM (Maximum Entropy Method) can be performed using PDXL Structure Analysis Package. PDXL suite also offers export functions to other software packages (e.g.: FOX, GSAS or FullProf).
The number of scientists and engineers using XRPD for materials characterization is growing rapidly and PDXL software suite including PDXL Rietveld Analysis Package and PDXL Structure Analysis Package make it possible for those who are not specialists in the field of X-ray diffraction to easily perform Rietveld analysis and ab-initio crystal structure analysis.

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Keywords: ab-initio structure determination, Rietveld method, X-ray powder diffraction

FA5-MS44-P04

POLYGON and other tools: model validation at a glance. Alexandre Urzhumtsev[a,b], Pavel V. Afonine[c], Ludmila Urzhumtseva[d], Paul D. Adams[c]. [a]*Department of Structural Biology, IGBMC-CERBM, 67404 Illkirch, France.* [b]*Nancy University, 54506 Vandoeuvre-lès-Nancy, France.* [c]*LBNL, Berkeley, CA 94720, USA.* [d]*ARN, IBMC-UdS-CNRS, 67084 Strasbourg, France.*
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A quality of a crystallographic model is typically reflected by a list of numbers such as *R*-factors, deviations from ideal stereochemistry, average B-factors and other. A presentation of these values by a single plot instead of a traditional table simplifies a quick model quality evaluation [1]. Each model

characteristic is shown by a point at its own ruler, and the rulers are plotted together as a set of lines with the same origin, forming a hub and spokes. The points for a given model marked on these lines are connected to form a polygon. A polygon strongly compressed or dilated along some axes reveals unusually low or high values of corresponding characteristics. Different parts of the rulers are colored differently to reflect the frequency (red color for a low frequency, blue for a high frequency) with which the corresponding values are observed in a reference set of structures determined previously. Polygon vertices in 'red zones' indicate parameters which lie outside typical values. The reference set of structures can be selected by the resolution, by their size of structures or by other characteristics. The list of model characteristics to be shown in the polygon is also variable. In particular, in addition to (or instead of) the average values of distortion of stereochemical parameters it may include their maximal values to indicate local problems if they exist. Both the stand-alone Tcl/tk version of the program for macromolecules and the python version incorporated into *PHENIX* [2] are available. As an extra control tool and independently of the POLYGON, the typical values for the *R*- and R_{free}-factors and for their difference at a given resolution can be obtained as linear functions of the logarithm of the resolution [3].

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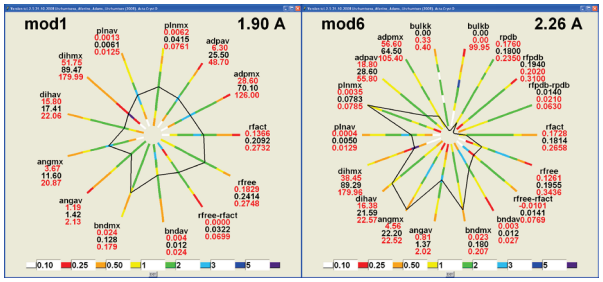
Keywords: model validation, graphics, computer analysis



FA5-MS44-P05

Self-organizing Crystal Structure. Mahendhran Arumugam[a], Georg Roth[b], Heike Emmerich[a], Stefaan Cottenier[c]. [a]*Institute of Minerals Engineering, RWTH Aachen University, Germany.* [b]*Institute of Crystallography, RWTH Aachen University, Germany.* [c]*Center for Molecular Modeling, Ghent University, Belgium.*
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We introduce a self-organizing classification method to classify the structure types of Silica polymorphs using scaled powder diffraction intensities and the Kohonen neural network. The classification results show not only that the isopointal and isoconfigurational structure types are automatically recognized and classified, but also that the acquired classification knowledge in the neural network can be used for performing the classification of yet unclassified or newly determined crystal structures. Additionally, we show the possibility of classifying structures irrespective of their chemical composition, by replacing all atoms by unit scatterers in a combined group of SiO2, GeO2, GaPO4 and AlPO4 polymorphs. The developed method is believed to be applicable to arbitrary types of inorganic crystal structures.

Keywords: classification of crystal structures, neural networks, powder diffraction data.

FA5-MS44-P06

Advanced Shape Descriptors for Identification of Ligands in Electron Density. Ciaran Carolan, Gerrit Langer, Victor Lamzin, *European Molecular Biology Laboratory, Hamburg Outstation, Notkestr. 85, 22607 Hamburg, Germany.*
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Numerous descriptors have been developed in fields as diverse as computer graphics, physics and biology that allow the comparison of the shapes of complex bodies. Many of these are moments-based descriptors that encode the shape of an object as a series of numbers that contain variable levels of information and allow reconstruction of the object to varying degrees of accuracy. As these moments can be rapidly calculated and quickly compared, they appear to be especially suitable for parametrising a cluster of electron density and identifying ligands which best fit the shape of that cluster. They may also be useful for building the identified ligands into a macromolecular model. We have tested various methodologies based on shape description, including third order moment invariants, spherical harmonic moments, Zernike moments and moments of inter-atomic distance matrices, in order to identify which might be most suitable for the convenient identification of ligands in electron density. In essence, after the shape descriptors for the mystery electron density are computed, they are slid through the database of molecular shapes which includes the ligand molecules of interest present in a variety of alternative feasible conformations. The top hits are ranked based on shape similarities as well as predicted binding energy in the protein as assessed using typical docking scores. Excellent results have been obtained to date using several of the methods noted above. In order to develop the methods further, we have begun to investigate the possibility of incorporating protein residue and charge information into the search templates where this is possible. We are also examining whether the developed methods may be applied to the characterization and analysis of electron density isosurfaces of protein clefts and gorges. By screening large databases of potential drug molecules, such as the ZINC database, it should be possible to identify new leads for drug development even in the absence of crystallographic data for that ligand in the protein. All developed methods will be applicable to drug development research, allowing for the soaking of multiple ligands into a protein and for the subsequent automated identification of the ligands binding at the site of interest, as well as for high-throughput computational drug screening.

Keywords: ligand recognition, model building, methods macromolecular crystallography