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MoleCoolQt – A Molecule Viewer for Charge Density Related Science. Christian B. Hübschle, *Georg-August-University Göttingen, Germany.* E-mail: chuebsc@gwdg.de

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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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], [a]*Rigaku European Headquarters Berlin, Germany,* [b]*Rigaku Corporation , Japan.* E-mail: schuck@rigaku.co.jp

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.

[1] Altomare et al., *J. Appl. Cryst*, 42 (2009) 1197-1202. [2] G. Oszlányi and A. Sütő, Acta Cryst., A64 (2008) 123-134.

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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.* E-mail: sacha@igbmc.fr

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