FA5-MS45-P01

ICSD Web – One year and beyond. Stephan Rühl, *FIZ Karlsruhe, Eggenstein-Leopoldshafen.*
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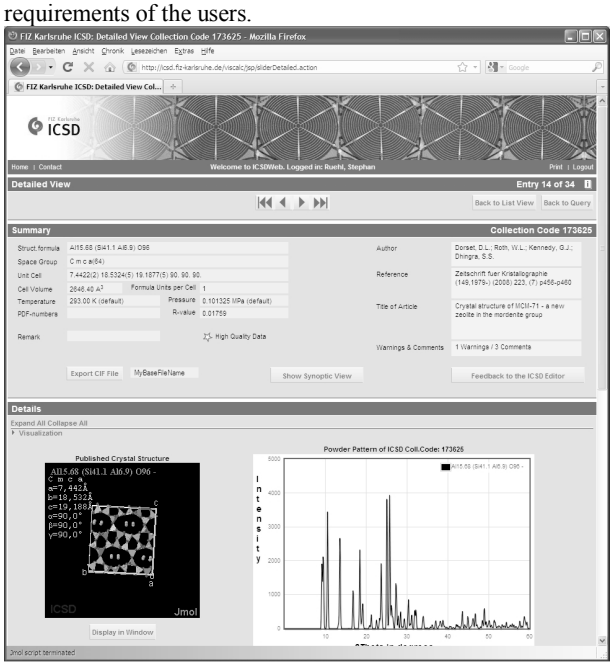
The new ICSD Web [1] has been available since mid 2009. It offers both the flexibility of a browser-based interface and the functionality of a modern graphical user interface. ICSD Web is developed by FIZ Karlsruhe in order to meet the increasing requirements of the users.



The user-friendly interface is easy to navigate with up-to-date features for retrieval and visualization and flexible export of data. A modern query management system offers options to save and load queries. An Online help is available for all features.
The visualization is realized as an interactive web browser applet (Jmol [2]) which offers suitable features for displaying crystal structures and is highly customizable. A very convenient tool for the comparing similar entries is the so-called synoptic view. It simultaneously shows up to six crystal structures after they have been standardized following the rules given by Gelato and Parthé [3] or up to six powder pattern diagrams generated on the fly from the CIF files.
The current version of the ICSD [4] contains 132,526 entries including 117,389 fully determined crystal structures derived from experimental data and 15,137 crystal structures with atom coordinates derived from the corresponding structure types.

[1] ICSD is available online at http://icsd.fiz-karlsruhe.de. More details can be found on http://www.fiz-karlsruhe.de/icsd_web.html. [2] Jmol: an open-source Java viewer for chemical structures in 3D. http://www.jmol.org/. [3] Gelato L.M., Parthé E., *J. Appl. Cryst.* 1987, 20, 139-143. [4] Bergerhoff G., Brown I.D., „*Crystallographic Databases*“, 1987, Allen F.H. (Editor) Chester, International Union of Crystallography.

Keywords: ICSD, web interface, databases

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DRAWxtl 5.5 An open-source program for crystal structure drawings. Martin Kroeker[a], Brian H. Toby[b], Larry W. Finger[c]. [a]*Inorganic Chemistry, University of Freiburg, Germany.* [b]*Advanced Light Source, ANL, Argonne, USA* [c]*retired from the Carnegie Institution, Washington DC, USA.*
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DRAWxtl is a versatile drawing program that supports all the conventional elements of crystal structure drawings such as atomic spheres, thermal ellipsoids and polyhedra of arbitrary complexity. Although it is mainly designed for the rendering of inorganic crystal structures, with import filters for CIF, CSD, Fullprof, GSAS, JANA and Shelx format, it is equally well suited for displaying the results of DFT calculations done with the popular VASP, WIEN2k and ELK codes.
While the focus of the preceding versions was on adding support for modulated and composite structures[1], ELF and AIM plots, and voids or surface mapping respectively, the upcoming 5.5 release will provide more options for Fourier map drawing, including arbitrary cross sections and color mapping. General usability improvements include automatic adaption to small (netbook) screens and new output formats, including rotatable 3D scenes embedded in pdf documents.
The program is freely available under the GPL license from http://www.lwfinger.net/drawxtl/ in the form of ready-to-run binaries for Linux, OS X and Microsoft Windows, as well as C++ source code for building on other platforms.

[1] Finger L.W., Toby B.H., Kroeker M., *J.Appl.Cryst.*, 2007, 40, 188.

Keywords: computer graphics, computer programs, linux crystallographic computing

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On the use of single crystal diffractometer data necessary for performing the 2nd and 4th restricted moment method. Prabal Dasgupta*, Bholanath Mondal. *Indian Association for the Cultivation of Science, Kolkata-700032, India.*
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With the advent of epoch-making paper [1,]renaissance of 2^{nd} & 4^{th} restricted moment method for evaluation of crystallite size has taken place, particularly for nano-sized crystals.Above mentioned authors have reported that they have made use of high resolution XRD data. Present work aims to explore if the same technique may be applied to commonly used single crystal diffractometer data? To probe this,background & instrumental broadening corrected 111 & 200 lines of commercial grade Ni were subjected to such analysis. M_2 & M_4/q^2 plots suggest that peak broadening in these materials are mainly crystallite size-related broadening. Different step-widths and scan rates were tried so as to ascertain the quality of data that yields more or less same crystallite size(within 5%) from the 2^{nd} & 4^{th} moment plot. It was revealed that XRD data with stepwidth of 0.01 deg and scan speed of 2.0 sec step $^{-1}$ in the continous mode yields satisfactory converegence.