phase relationships and detect phase mixtures in a complex multiphase system.

[1] PANalytical X'Pert HighScore Plus V2.x

Keywords: clustering, statistical analysis experimental data, phase analysis

P.03.02.1

Acta Cryst. (2005). A**61**, C165

Combined Experimental and Theoretical Studies of Solid State Proton Migration

David Martins[a], Carole A. Morrison[a], Colin R. Pulham[a], Chick C. Wilson[b], [a]*School of Chemistry, The University of Edinburgh, West Mains Road, Edinburgh, Scotland, UK.* [b]*Department of Chemistry, University of Glasgow, University Avenue, Glasgow, Scotland, UK*. E-mail: david.martins@ed.ac.uk

Hydrogen bonds are of great interest, due to their importance in structural, functional and dynamical properties of chemical systems, ranging from inorganic to biological chemistry [1]. The very strong hydrogen bonds are of current interest because they enable charge and energy to be transferred between molecules in the solid state.

Recent work has focused on urea-acid complexes, which contain a rich variety of short, strong hydrogen bonds in a relatively simple framework. It has been demonstrated that the combination of cutting edge computational techniques (MD/PW-DFT) with variable temperature neutron diffraction results was successful in showing the migration of the proton with increasing temperature and a plausible explanation for the effect has been presented [2].

A collaborative project with the aim of continuing this work has now begun. A series of hydrogen-bonded adducts have been prepared in a systematic manner for experimental and theoretical investigation. In particular, the effects of temperature and pressure on proton migration and disorder in these adducts are being explored to shed light on the factors that influence proton migration. In this poster presentation we will describe some of our most recent results, which include studies on periodic acid-urea and ammonium iodate.

[1] Steiner T., *Angew. Chem. Int. Ed.*, 2002, **41**, 48. [2] Morrison C. A., Siddick M. M., Camp P. J., Wilson C. C., *J. Am. Chem. Soc.*, *in press*.

Keywords: short hydrogen bonds, solid state, computational chemistry

P.03.03.1

Acta Cryst. (2005). A**61**, C165

EdMol: A Graphical Molecular Editor

Javier Gonzalez-Platas[a], Juan Rodriguez-Carvajal[b], [a]*Department of Physics II, University of La Laguna, Tenerife, Spain.* [b]*Laboratoire Léon Brillouin (CEA-CNRS), Saclay, France.* E-mail: jplatas@ull.es

EdMol is a graphical molecular editor tool for the input of molecular structures in 2D or 3D. The format of output coordinates (Z-Matrix, Spherical, Fractional or Cartesian are some of the options presently implemented) can be selected by the user as input for other programs, as FullProf [1], Expo2004 [2] or StructRes, in order to aid the structure solution, mainly from powder diffraction, using global optimisation as Simulated Annealing, Genetic algorithms or any other algorithm or method as Patterson or Direct Methods.

EdMol is written in Fortran95 using the CrysFML [3] (Crystallographic Fortran Module Library) and X/Winteracter [4] libraries for Linux (x86) and Windows 9X/NT/2K/XP versions. The use of EdMol is totally free for the scientific community and it is distributed within the FullProf Suite package or as a stand-alone program in the FullProf Suite Web site[5].

[1] Rodriguez-Carvajal J., *Physica B*, 1993, **192**, 55. [2] Altomare A., Caliandro R., Camalli M., Cuocci C., da Silva I., Giacovazzo C., Moliterni A. G. G., Rizzi R., *J. Appl. Cryst.*, *submitted*. [3] Rodriguez-Carvajal J., Gonzalez-Platas J., *Compcomm Newsletter*, 2003, **1**, 90. [4] *Winteracter. The Fortran 9X GUI Toolset* http://www.winteracter.com [5] *FullProf Suite Web* http://valmap.dfis.ull.es/fullprof

Keywords: computer applications, computer software, computer graphics molecular

P.03.03.2

Acta Cryst. (2005). A**61**, C165

DRAWxtl 5.1 - A Multi-Platform Computer Program to Display Crystal Structures

Martin Kroeker[a], Brian H. Toby[b], Larry W. Finger[c], [a]*Department of Inorganic Chemistry, University of Freiburg, Germany.* [b]*NIST Center for Neutron Research, Gaithersburg,USA.* [c]*Geophysical Laboratory,Washington D.C., USA(retired).* E-mail: martin@ruby.chemie.uni-freiburg.de

The computer program DRAWxtl is designed to display a crystal structure with minimal user input and maximum flexibility. It reads the description of a crystal structure, including unit-cell parameters, space group, atomic coordinates and thermal parameters, combines them with options that define the view, and outputs a geometry object that may contain polyhedra, planes, lone-pair cones, spheres or ellipsoids, bonds, and the unit-cell boundary lines.

Since the recently released version 5.0, the program presents an easy to use graphical user interface where the drawing can be previewed, and all parameters are accessible through conventient menues or direct interaction. A functionally identical command-line version is still available for easier integration into other program packages that provide their own user interface.

The most prominent new feature in version 5.1 is its ability to import electron density information from GSAS and JANA, which can be rendered as meshes and/or solid surfaces. Using a 3D cursor, local maxima in the electron density can be determined to aid in structure solution and refinement.

Both the complete source code and precompiled binaries for Linux, OSX, MS Windows and Irix are freely available from http://lwfinger.net/drawxtl.

Keywords: graphics, software, crystal structures

P.03.04.1

Acta Cryst. (2005). A**61**, C165

AFITT- Working with Good Chemistry

Thomas S. Peat, Jon Christopher, Kevin Schmidt, *OpenEye Scientific Software, Santa Fe, NM 87507*. E-mail: tom@eyesopen.com

AFITT is a new molecular graphics program developed by OpenEye Scientific Software for protein crystallographers. It runs on most operating systems, reads almost all data formats, easily connects to databases and will generate good chemical structures from a SMILES string. It has the most up to date rotomer library and Ramachandran plot to easily check the protein structure for outlying residues. It will create refinement dictionaries (either REFMAC or XPLOR format) for ligands and other small molecules automatically. Because AFITT uses the OEChem chemical library and OMEGA conformer generator, good chemistry is preserved even when starting from a SMILES string. Rapid docking into electron density is provided by OpenEye's Shape technology. To enhance communication with chemists, it also provides a 2D graphics window and automatic SMILES naming. Scripting is easily accomplished using Python. AFITT should be particularly useful for those involved in modeling large numbers of structures with small molecules.

Keywords: graphics, computational chemistry, drug design

P.03.04.2

Acta Cryst. (2005). A**61**, C165-C166

Molecular Dynamics Simulations of tetramethylketone p-tert-butyl calix[4]arene

Alexandre Suman de Araujo[a], Eduardo Ernesto Castellano, [a]*Instituto de Física de São Carlos*. E-mail: asaraujo@if.sc.usp.br

We describe the results of Molecular Dynamics simulations of the calixarene tetramethylketone p-*tert*-butyl calix[4]arene in vacuum, in pure acetonitrile and in the presence of Pb^{+2} ions solvated by acetonitrile. The mean goal of these calculations is to validate the parametrization of the system model using experimental thermodynamics and crystallographic data and to describe the process by which the calixarene traps one Pb^{+2} ion in its hydrophilic cavity and one acetonitrile molecule in its hydrophobic one. This information