

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). A61, C165

Combined Experimental and Theoretical Studies of Solid State Proton Migration

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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). A61, C165

EdMol: A Graphical Molecular Editor

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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). A61, C165

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

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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 convenient menus 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). A61, C165

AFITT- Working with Good Chemistry

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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 rotamer library and Ramachandran plot to easily check the protein structure for outlying residues. It will create refinement dictionaries (either REFMAC or XPLO 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). A61, C165-C166

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

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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 main 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

allows us to determine the relevance of several structural parameters in the process of complexation, thus adding to the rational building of more efficient ligands. The initial state of the simulations is taken from X-ray diffraction results^[1] which are also used to verify that the simulations predictions are in agreement with experimental data.

[1] de Namor A.F.D., Chahine S., Kowalska D., Castellano E.E., Piro O.E., *J. Am. Chem. Soc.*, 2002, **124**, 12824-12836.

Keywords: molecular dynamics, calixarene complexes, small molecules

P.03.04.3

Acta Cryst. (2005). A61, C166

Structural Properties of Pt-based Anti-cancer Drugs; Computational Studies

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It is generally accepted that *cis*-[PtCl₂Pyr₂] is cytotoxic while *trans*-[PtCl₂Pyr₂] is not. Although original empirical structural-activity studies indicated *trans* Pt complexes as being inactive as anti-cancer drugs, it has subsequently been found that *trans*-[PtCl₂Pyr₂] is in fact active, both *in vitro* and *in vivo*, and that for the latter the compound is even more active than the corresponding *cis* form. A more likely explanation for the lack of antitumour activity is instead that the *trans* isomer is kinetically more reactive and more susceptible to deactivation than the corresponding *cis* form [1].

We have in the current work investigated both isomers and their corresponding step-wise activation (aquation) processes in order to provide more detailed insights into their mechanisms. The results are also compared to corresponding data for the parent compounds *cis* and *trans*-platin [PtCl₂(NH₃)₂]. Implicit as well as explicit solvent effects have previously been shown to be important for these types of reactions [2,3], and thus included in the study.

[1] Wong E., Giandomenico M., *Chem. Rev.*, 1999, **99**, 2451. [2] Raber J., Zhu C., Eriksson L.A., *Mol. Phys.*, 2004, **102**, 2537. [3] Zhu C., Raber J., Eriksson L.A., *J. Phys. Chem. B*, 2005, *in press*.

Keywords: anticancer compounds, DFT, platinum antitumour agents

P.03.05.1

Acta Cryst. (2005). A61, C166

Effect of Nanoscale Surface Modification on Interfacial Adhesion: a Theoretical Modelling Study

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The effects of modification of polyester surfaces on adhesion to carbonaceous solids are investigated using theoretical techniques. Fully atomistic models are constructed of cross-linked polyester and glassy carbon surfaces. Polyester surface modifiers of both the hydrophilic and hydrophobic nature are introduced and simulations are then performed to obtain qualitative and quantitative measures of interfacial strength between the polyester and carbon thin layers [1].

Our studies indicate that Van der Waals forces contribute significantly to the interfacial strength between the thin layers while atomic scale surface roughness is found to significantly reduce adhesion. Interfaces formed from rigid surface models provide general information on structural and chemical effects but such rigid models tend to overestimate the magnitude of these effects. Relaxed interfacial models provide more realistic representations on interactions between the layers. Flexible chain-based modifiers on the surface of the polyester films tend to migrate away from the interface and flatten the surface thereby decreasing the roughness effects on interfacial strength. Both hydrophilic and hydrophobic surface modifications resulted in reduced adhesion at the interface.

[1] Henry D. J., Lukey C. A., Evans E., Yarovsky I., *Mol. Sim.*, *in press*.

Keywords: adhesion, surface modification, molecular modelling

P.03.05.2

Acta Cryst. (2005). A61, C166

Modeling of Crystal Structures of Materials: Which Goals can be Achieved?

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Ability to predict structures of crystalline materials is important in many cases for practical applications. For instance, second harmonic generation by crystalline nonlinear optical materials necessarily require acentric structure of their crystals. Crystal structure is also important for high-energy materials, where molecular packing defines crystal density. Some other properties such as fluorescence, conductivity and even potency of drugs are also related to their crystal structure.

We analyzed effectiveness of different force fields for crystal structure prediction for group of organic nonlinear optical, high-energy and conductive materials. It was shown that for non-planar molecules improvement of a force field could bring to a significant improvement of results. On the other hand crystal structure of planar molecules is difficult to predict, and in this case some new approaches for instance implementation of "stacking forces" should be introduced.

Keywords: crystal structure modeling, force fields, crystalline materials

P.03.05.3

Acta Cryst. (2005). A61, C166

A Global Search for the Optimal Bandstructure for Thermoelectric Applications

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The best thermoelectric (TE) materials over the last 30 years has been Bi₂Te₃ and its alloys. However recent discoveries have renewed the interest in finding a better TE material. We've decided to use a global search genetic algorithm to try and determine the optimal bandstructure for materials with TE applications. This project involves bandstructure analysis and transport property calculations of known materials with interesting TE properties. We want to employ a genetic algorithm to try and locate general features in a bandstructure which have importance for the TE effect of the material.

Keywords: density functional theory, band structure, transport properties

P.03.06.1

Acta Cryst. (2005). A61, C166-C167

Computer Modeling of Local Structure and Properties of Oxide Solid Solutions with NaCl Type Structure

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Atomistic semi-empirical potentials were applied to calculate the structural, thermodynamic, elastic properties and phase equilibrium of MgO-CaO, MgO-MnO, MnO-CaO, CaO-SrO, BaO-SrO disordered solid solutions by using of the GULP code [1]. The calculations were performed with partially covalent approximations for 7:1, 3:1, 1:1, 1:3, 1:7 randomly mixed cation compositions. It was used 256-ion primitive supercell with quadrupled parameters of the unit cell for all compositions. It was demonstrated that such supercell allows to imitate random distribution of cations.

On the basis of the calculated values of free energy the component fields of stability, mixing limits and critical temperature were predicted. The values are in a good agreement within the temperature range 298 – 1800 K with the available data and results of other theoretical investigation. For 1:1 composition the analyses of the local