Coates *J. Mol. Biol.* **2010**, *396*, 1070-1080 [2] S.J. Tomanicek, K.K. Wang, K.L. Weiss, M.P. Blakeley, J. Cooper, Y. Chen, L. Coates *FEBS Letters* **2011**, *585*, 364-368

Keywords: beta lactamase, neutron diffraction, toho-1

MS.82.5

Acta Cryst. (2011) A**67,** C182

Deuteration of oleic acid, lipids and other molecules for neutron studies

Tamim Darwish, Emily Luks, Greta Moraes, Marie Gillon, Taavi Hunt, Tracey Hanley, Michael James, Peter Holden, *National Deuteration Facility, Australian Nuclear Science and Technology Organisation (ANSTO), Locked Bag 2001, Kirrawee DC, NSW, 2232 (Australia).* E-mail: tamim.darwish@ansto.gov.au

In this paper, the synthesis and application of a range of deuterated organic molecules for the investigation of complex systems in the fields of structural biology, biotechnology and nanotechnology will be discussed. In chemical reactions, deuterium (^{2}H) behaves similarly to hydrogen (^{1}H); however, the different physical properties of the hydrogen and deuterium nuclei mean that they scatter neutrons quite differently. Techniques such as Small Angle Neutron Scattering, Neutron Reflectometry and Neutron Crystallography exploit this difference in scattering length densities to obtain data for properties such as: atomic and molecular structure, the precise location of hydrogen atoms in organometallic systems, and highlighting molecular components in complex nanostructured systems.

In studies where one may wish to observe the interaction between hydrocarbon-based chemicals or biological molecules with lipids or surfactants, there is often a lack of neutron scattering contrast in the system which can be overcome by deuteration of the tail component of these lipids or fatty acids. Oleic acid forms an unsaturated tail component in many phospholipid molecules that are fundamental to the structure and functioning of cellular membranes. We have recently produced deuterated oleic acid on a gram scale in our laboratories from deuterated fatty acid molecules with the appropriate mono- and bi-functional terminal groups; prepared using a multi-step reaction scheme. This involved hydrothermal heterogeneous catalytic H/D exchange reactions in D_2O followed by synthetic reactions. Conjugating the two deuterated alkyl chains using the Wittig reaction afforded purely a *cis*-conformation around the carbon-carbon double bond, essentially producing deuterated oleic acid. This facilitated the synthesis of deuterated glycerol monooleate through esterification of the prepared d-oleic acid with a glycerol fragment. Similar reactions were also used to prepare lipids with hydrophobic (different alkyl chain lengths) and hydrophilic (ethylene oxide) moieties where the head group is conjugated to a sulfur- or alkene-containing anchoring ligands for surface modification and self-assembly (i.e., on gold or silicon surfaces).

The strategies used for deuteration and synthesis of oleic acid, lipids, surfactants, sugars, bioactive small organic molecules, heterocyclic and aromatic compounds will be presented. We will also demonstrate how the availability of these deuterated compounds greatly increases the scope of some neutron scattering, reflectometry and diffraction experiments. For example, deuterated trehalose was used to determine the localisation of sugar molecules with respect to lipid head groups using neutron diffraction, to provide insight into the molecular mechanisms of cryoprotection by sugar molecules. Using neutron scattering, deuterated oleic acid and glycerol monooleate allowed investigation of surfactant interaction with cubosome and hexosome liquid crystal nanoparticles forming 3D structures with intertwining aqueous channels. Deuterated organic light emitting diode (OLED) molecules facilitated investigation of the morphology of thin-film multilayer organic light emitting devices using neutron reflectometry [1].

[1] A.R.G. Smith, J.L. Ruggles, H. Cavaye, P. Shaw, T.A. Darwish, M. James, I. R. Gentle, P.L. Burn, *Advanced Functional Materials*, **2011**, Published Online. DOI: 10.1002/adfm.201002365.

Keywords: deuteration, deuterated oleic acid, deuterated lipid

MS.83.1

Acta Cryst. (2011) A**67,** C182

Cyber-enabled learning and practice in crystallography: educating the next generation

Katherine A. Kantardjieff, *Departments of Chemistry, University, Center for Molecular Structure, and Center for Macromolecular Modeling and Materials Design, California State Polytechnic University Pomona (USA).* E-mail: kantardjieff@csupomona.edu

This talk will describe the current state of crystallographic science and new pedagogy made possible by Web 3.0. In the last fifteen years, academic crystallography has largely migrated from a research specialty to a technique employed by a broad user community. Yet, the knowledge gained from analysis of its structures is a key underpinning of modern science and technology. Crystallography has gained importance for researchers in disciplines where it has not previously appeared, such as engineering and solar energy technology. Technical advances, however, now enable users with little or no training, or deeper understanding, to often but not always produce quality results, as revealed by recent high profile and embarrassing retractions in the peer reviewed literature, many the result of pathological science or inadequate review. The absence of crystallography in many curricula has led to growth of and dependence on independently funded workshops and summer schools, as well as other, non-traditional curricular resources for crystallography instruction, such as Web pages and online courses, which allow crystallography to be self-taught. Implementing modern Web technologies with sound pedagogy requires skilful integration of relevant, often disparate resources into useful and usable frameworks, enabling learners to interact, explore new situations, and use scientific reasoning skills such as hypothesis testing and model-based reasoning. The evident disproportion in implementing contemporary technologies into our global crystallography education resources requires that we shift our focus from simply imparting content knowledge to empowering students with the fundamental processes and skills needed for on-demand learning and practice in crystallography.

Acknowledgements: California State University Program for Education and Research in Biotechnology; W.M. Keck Foundation; National Science Foundation; The Boeing Company.

Keywords: teaching crystallography, Web 3.0, elearning pedagogy

MS.83.2

Acta Cryst. (2011) A**67,** C182-C183

Promoting crystallography: using crystal structures in chemical education

Frank H. Allen, *CCDC, 12 Union Road, Cambridge, (UK).* E-mail: allen@ccdc.cam.ac.uk

Crystallography is truly interdisciplinary. It has its roots in physics, mathematics and computer science, and has practitioners and beneficiaries from chemistry, biology, materials science and many other disciplines. Despite its pre-eminence as *the* preferred method for

structure determination, and despite its involvement in 25 Nobel Prize awards, crystallography is poorly represented in University teaching curricula; at best, it is simply noted at high school level. As a consequence, there is sometimes a limited understanding of crystallographic results, e.g. some medicinal chemists regard all conformational information as being tainted by crystal packing forces, precision indicators are misunderstood, and so on. One way of improving this situation is to promote the use of crystal structures in high school and undergraduate teaching. By taking crystallography to its beneficiary subjects in an educational way, we may hope to generate a greater familiarity with the results and a deeper interest in the experimental aspects of the technique.

The Cambridge Structural Database (CSD) contains a wealth of chemical information, and a subset of around 500 entries is freely available for teaching purposes at http://www.ccdc.cam.ac.uk/free_services/teaching/ [1]. Chemistry is a 3D subject, too often introduced and taught using 2D and 2.5D representations. However, the fully interactive exploration of crystal structures (e.g. via JMOL or Mercury) provides fundamental understanding at both school and undergraduate level, making students think and learn in 3D. Comparing the conformations of ethane and *n*-butane, studying chirality in L- and D-alanine, or exploring important structure types such as alkaloids, steroids, and metal-organics with various coordination geometries, brings chemistry to life. The teaching area of the CCDC website also contains a series of modules that use both the subset and the complete CSD to address specific chemical topics [2]. These include (teaching subset): aromaticity, rings strain and conformation, valence shell electron pair repulsion, and hapticity, as well as (full CSD): mean molecular dimensions, halonium ions as reaction intermediates, metal-carbonyl back bonding, and geometrical interconversions in four-coordinate metal complexes. This set of modules is now being extended to include, among others, studies of reaction pathways and studies of hydrogen bonding and other intermolecular interactions.

[1] G.M. Battle, F.H. Allen, G.M. Ferrence, *J.Chem.Educ*. **2010,** *87*, 809-812 and *87*, 813-818. [2] G.M. Battle, G.M. Ferrence, F.H. Allen, *J.Appl.Cryst.* **2010***, 43*, 1208-1223.

Keywords: database, teaching

MS.83.3

Acta Cryst. (2011) A**67,** C183

Experimental determination of chemical structure in the undergraduate curriculum

Dean H. Johnston, *Department of Chemistry, Otterbein University, Westerville, Ohio (USA).* E-mail: djohnston@otterbein.edu.

Exercises in experimental structural chemistry have been introduced into the first and second-year chemistry laboratory at Otterbein University. In the first-year laboratory, student groups were assigned one of twelve amino acids. Students researched crystallization methods using the web-based Cambridge Structural Database (WebCSD) and grew crystals for X-ray analysis. Selected crystal samples were analyzed using the Bruker SMART X2S diffractometer. Using the Mercury software package, students analyzed molecular geometry, hydrogen bonding, unit cells, density and crystal packing. This activity serves as an integrated exercise to teach and reinforce concepts of chemical bonding, molecular structure, intermolecular forces and the nature of crystalline materials. In the second-year inorganic chemistry laboratory, students used X-ray diffraction as a significant tool for structural characterization of products from a multi-week independent synthesis project.

Keywords: education, database

MS.83.4

Acta Cryst. (2011) A**67,** C183

Writing crystal structure reports in collaboration with undergraduate students

Joseph M. Tanski, *Department of Chemistry, Vassar College, Poughkeepsie, NY 12604 (USA).* E-mail: jotanski@vassar.edu.

An approach for increasing the impact of undergraduate scientific training with chemical crystallography through a laboratory report writing exercise has been developed. In an introductory chemistry curriculum, one of the first things we teach our students is the structure of atoms and molecules in order to help them develop a "molecular understanding". With drawings or models, students learn to answer questions such as, "What is the angle between these three atoms?" or "What is the shape of this molecule?" In organic chemistry, students are then introduced to chirality and stereochemistry. With modern instrumentation, molecular structures, and often the absolute structure of resolved compounds, may be experimentally determined in a matter of hours, adding another means to depict realistic molecules for students that also links learning to the experimental laboratory. The speed and ease of use of such instrumentation today is exceptional, such that it may be introduced more widely to undergraduate students in coursework, even when there is limited time available for a crystallography module.

As scientific educators, it is also important to mentor students in the communication of new knowledge. Just as chemical crystallography can be a fast, effective tool to experimentally observe the structure of molecules and enhance student learning of structure, it can also provide an inspiring opportunity for students to write short, scientific journal style reports that may be edited and published in collaboration with a crystallographer. This contribution will focus on a course module used to expose undergraduate students to small molecule crystallography, and in particular to the preparation of the resulting crystal structures for publication. With examples of both published and unpublished structures, topics will include: compound choice, structure validation, literature and database searching, and the writing of descriptions of crystal and molecular structures, absolute structure, packing and intermolecular interactions.

This work was supported by grants from the U.S. National Science Foundation, No. 0521237 & 0911324.

Keywords: crystallography teaching aids, journal publications, technical writing

MS.83.5

Acta Cryst. (2011) A**67,** C183-C184

"Applied crystal chemistry" for chemists and materials scientists

Elena V. Boldyreva, Vasily S. Minkov, *REC-008 Novosibirsk State University, ul. Pirogova, 2, Novosibirsk, (Russia). Institute of Solid State Chemistry and Mechanochemistry SB RAS, ul. Kutateladze, 18, Novosibirsk, (Russia).* E-mail: eboldyreva@yahoo.com

The contribution describes a 30-year experience of teaching a general course in solid-state chemistry for undergraduates, which introduces at the same time the main concepts of crystallography, gives an introduction into structure analysis techniques and makes links to the courses in inorganic chemistry, organic chemistry, and biochemistry. Such a combination can be beneficial for bringing the fundamental crystallography (basics and techniques) closer to its "users" – chemists, materials scientists, biologists, and can be considered as an attempt of a course in "applied crystallography". The aim of the course is to teach chemists, which chemical information can be retrieved from a crystal structure, and how. This is complementary to more generally