1,2-benzoquinone, formed by electron transfer between metal d and semiquinonate π* orbitals.

X-ray crystal structure analysis of **1** was performed at 302 and 56 K using synchrotron radiation at BL02B1 beamline at the SPring-8 facility. Compound **1** only consists of linear chains of [Rh(3,6-DBDiox-4,5-Cl_2)$(CO)_2$] molecules and these complex molecules form trimer units in the linear chain at 302 K. At 56 K, the trimer units in the linear chain dimerized and form hexamer units. Compound **1** shows a significantly large conductivity (17–34 S cm^{-1}) at room temperature regardless of the neutral molecule. The temperature dependence of the electrical conductivity shows a semiconducting behavior. The observed dimerization of trimers in the 1-D chain is considered to originate from Peierls distortion.

[1] Tanaka H., Okano Y., Kobayashi H., Suzuki W., Kobayashi A., *Science*, 2001, **291**, 285–287.

Keywords: conducting molecular crystals, mixed-valence compounds, synchrotron X-ray diffraction

MS95.30.5

Acta Cryst. (2005). A**61**, C121

In Field Incommensurate-Commensurate Phase Transition in the Multiferroic $TbMnO_3$

Nadir Aliouane, D.N. Argyriou[a], J. Strempfer[b], S. Langesell[a], C.J. Milne[a,c], M.v. Zimmerman[c], [a]*HMI Berlin, Germany.* [b]*MPI-FSK Stuttgat.* [c]*Hasylb-Hamburg, Germany*. E-mail: aliouane@hmi.de

Orthorhombic $TbMnO_3$[1] is a multiferroic compound that exhibits a flop in the electrical polarization from c to the a-direction with a applied magnetic field either along a or b axis. We have studied the magnetic field dependence of the incommensurate wave vectors (q_{Mn} q_{Tb}) associated with the polarization and the magnetic ordering by neutron and x-ray single crystal diffraction with H||a and b. The polarization flop transition corresponds to first-order transition from an incommensurate multi-q-structure to a commensurate single q-structure with q=1/4 at H||a, H>9T T_C~28K. In our X-ray measurements, the induced magneto-elastic coupling is observed as a structural modulation at twice the magnetic wavevector ($2q_{Mn,Tb}$). The temperature and field dependence of the magnetic and superlattice reflections are consistent with a soliton formalism which predicts a stable commensurate single q=1/4-phase.

[1] Kimura et al., *Nature*, 2003, **426**, 55.

Keywords: 1/4-phase, polarization flop, soliton formalism

MS96 CRYSTALLOGRAPHIC TEACHING

Chairpersons: Åke Oskarsson, Randy Read

MS96.30.1

Acta Cryst. (2005). A**61**, C121

Crystallography Boot Camp at Cold Spring Harbor Laboratory

James W. Pflugrath, *Rigaku/MSC, Inc., The Woodlands, TX, USA.* E-mail: jwp@rigakumsc.com

A theoretical and practical course teaching the fundamentals of macromolecular crystallography has been held at Cold Spring Harbor Laboratory for the last 16 years. This course exposes participants to basic diffraction theory, crystallization (proteins, nucleic acids and complexes), crystal characterization, X-ray sources and optics, synchrotrons, crystal freezing, data collection, data reduction, multiple isomorphous replacement, multiwavelength anomalous diffraction, molecular replacement, solvent flattening, non-crystallographic symmetry averaging, electron density interpretation, molecular graphics, structure refinement, structure validation, coordinate deposition and structure presentation. Participants learn through extensive hands-on experiments in which one or more proteins are crystallized and the structure(s) determined by several methods, in parallel with lectures on the theory and informal discussions behind the techniques.

Several core tenets have served to make this course well-regarded. First, extremely experienced instructors both lecture and run practicals. For example, the mathematical theory of crystallography and the practical side of growing crystals is anchored by the irreplaceable Alex McPherson. Another core feature of the course is a dedicated fully equipped laboratory with bench space, microscopes, and computer workstations which are always available during the long hours of the course. Finally, the extraordinary venue with nearby housing and dining facilities keeps the participants fully focused on the demanding, yet flexible, training schedule.

Keywords: education, teaching, training

MS96.30.2

Acta Cryst. (2005). A**61**, C121

Introducing Twinning

Simon Parsons, *School of Chemsitry, The University of Edinburgh, Scotland.* E-mail: S.Parsons@ed.ac.uk

Twinning is a relatively common phenomenon in crystallography, but it has long been considered to be amongst the most serious obstacles to successful structure determination. A twinned crystal is an aggregate in which different domains are joined together according to a specific symmetry operation - the twin law. Reflections from different domains may overlap, and twinned crystals fall broadly into two categories in which either all reflections or only certain zones of reflections are affected by overlap. The former occurs when a crystal lattice belongs to a higher point group than the crystal structure itself, the latter frequently occurs when the twin law is a symmetry operation belonging to a higher symmetry supercell.

Software has now developed to such an extent that some twin problems can now be tackled using a black-box approach. More commonly, successful use of these tools depends of some understanding of twinning and its basis in symmetry. This talk will describe some of my experiences in teaching students about twinning.

Keywords: crystallographic education, twins, software for crystallography

MS96.30.3

Acta Cryst. (2005). A**61**, C121

Real versus Virtual aids in Teaching Crystallography

Mariusz Jaskolski, Elzbieta Bartoszak-Adamska, *Department of Crystallography, Faculty of Chemistry, A. Mickiewicz University, Poznan, Poland.* E-mail: mariuszj@amu.edu.pl

Crystallography is a special discipline, impossible without models. Our macroscopic models of the microscopic world are only crude approximations of the atomic reality. Those artificial "reflections" of the real world can be expressed using material "substance" or as virtual reality. The explosive development of computer graphics tools has provided a tremendous boost to both structural research and teaching. Without the use of computers it would be impossible to teach about the expanding frontiers of biocrystallography. In addition to being the scenes and tools for displaying and manipulating molecular models, computers are also invaluable in modernizing the teaching/learning process, facilitating distance education, individual learning pace, exchange of teaching aids, etc. Despite the possibilities offered by computer tools, many educators believe that the use of traditional "real" models is essential. Classroom experience shows that some aspects of space and symmetry, almost intuitively obvious with solid models, are complicated or inconvenient when handled on the computer screen. At the introductory level, where simple models and hand-waving can be very appealing, there is no need to strive to recreate three dimensions in the computer. There is also a psychological aspect of using solid objects as material models, even if not perfect, seem to have some physical properties that make them closer to the real world than the idealized computer representation. Besides, computer models can only display what had been foreseen by the programmer, while the use of pliers, plasticine, glue, and imagination can lead to almost unlimited creativity.

Keywords: computer graphics, models, teaching aids

MS96.30.4

Acta Cryst. (2005). A**61**, C121-C122

Towards a Web-Based Interactive Environment for the Teaching of Crystallography

Gervais Chapuis, Nicolas Schoeni, *Laboratoire de cristallographie,*