approaches I will also outline the progress we have made with regard to computational methods in multicomponent crystal prediction as well as property prediction/rationalization.

Keywords: multicomponent crystals, cocrystals, crystal structure prediction

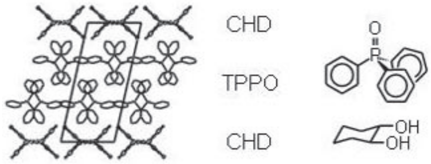
MS.66.4

Acta Cryst. (2008). A**64**, C115

An unexpected molecular co-crystal with a variable degree of order

Carolyn P. Brock, Maxime A. Siegler, Yigang Fu, Greg H. Simpson, Daniel P. King, Sean Parkin
University of Kentucky, Department of Chemistry, 505 Rose Street, Lexington, KY, 40506-0055, USA, E-mail：cpbrock@uky.edu

A 1:1 co-crystal of rac-trans-1,2-$C_6H_{10}(OH)_2$ (hereafter, CHD) and triphenylphosphine oxide (or, TPPO) has been found that is unusual because there are no strong interactions between the two components. Neither CHD nor TPPO has any obvious packing problem that would make formation of an inclusion complex likely. The TPPO layers are very much like those in two of the four known polymorphs of pure TPPO. The H-bonded ribbons of CHD are similar to those found in other vic-diol crystals. The co-crystals are triclinic (*P*1-bar), with the very small deviations from monoclinic symmetry (*C*2/*c*) arising from incomplete enantiomeric disorder of the R,R and S,S diols. The sizes of the deviations depend on the solvent from which the crystal is grown. Individual CHD layers seem to be at least mostly ordered. Information about R,R/S,S ordering is transmitted from one diol layer to the next through the almost centrosymmetric TPPO layer. The degree of order is unlikely to change with crystal heating or cooling. Thermal data suggest the existence of the co-crystal is a consequence of kinetic factors. Reasons for this surprising failure of fractional crystallization will be discussed.



Keywords: co-crystal, incomplete ordering, crystal growth

MS.66.5

Acta Cryst. (2008). A**64**, C115

In-situ cocrystallisation combined with Raman spectroscopy

Michael T. Kirchner, Roland Boese, Dieter Bläser
Universitaet Duisburg-Essen, Institut f. Anorg. Chemie, Universtitaetsstr. 5, Essen, NRW, 45117, Germany, E-mail：michael.kirchner@uni-due.de

Fast characterization of the products from cocrystallisation experiments is highly important since there are no general rules for appropriate growth conditions. Therefore a large number of experiments have to be performed to find the right conditions which favor the growth of a cocrystal over the growth of the individual components. For in-situ crystallization on a single crystal diffractometer this is especially important as characterization by diffraction is time consuming. We therefore incorporated a Raman probe into our in-situ laser zone melting apparatus. First results from systems containing acetylene, dioxane, formamide, formic acid and formaldehyde are highly promising. Already in the Raman spectra of the liquid mixtures we found hints to the formation of molecular aggregates which might be precursors of the cocrystals. After solidification and zone melting growth we used Raman spectroscopy to identify the formation of a cocrystal. Basic research in cocrystal formation is of increasing interest to pharmaceutical science as cocrystals of active pharmaceutical ingredients can have advantageous properties.

Keywords: crystal growth, ocrystallization and complexation of small molecul, raman spectroscopy

MS.67.1

Acta Cryst. (2008). A**64**, C115

Magnetic and structural transitions in frustrated magnets

Seung-Hun Lee
University of Virginia, Physics, Department of Physics, University of Virginia, Charlottesville, VA, 22904, USA, E-mail：shlee@virginia.edu

I will review recent neutron and synchrotron X-ray scattering studies of frustrated spinels and kagomes. The main focus will be to investigate what kinds of magnetic transitions, and lattice and magnetic states can arise when frustrated spins are coupled with lattice in the highly frustrated antiferromagnets.

Keywords: frustrated magnets, neutron scattering, X-ray scattering

MS.67.2

Acta Cryst. (2008). A**64**, C115-116

E/*T*-scaling behavior in the magnetic quasicrystal Zn-Mg-Ho

Taku J Sato[1], An Pang Tsai[2]
[1]University of Tokyo, Neutron Science Laboratory, Institute for Solid State Physics, 106-1 Shirakata, Tokai, Ibaraki, 319-1106, Japan, [2]Tohoku University, Katahira, Aoba-ku, Sendai, Japan, E-mail：taku@issp.u-tokyo.ac.jp

Quasicrystals have distinct (quasiperiodic) spatial symmetry characterized by a hidden translational invariance in higher dimensional space, and thus differs both from the periodic crystals and random glasses. Ordering and dynamics of spins in the quasiperiodic structures have been one of fundamental issues. Despite a variety of theoretically expected anomalous properties, earlier macroscopic experiments only exhibited rather normal spin-glass-like behavior. Recently, using the neutron scattering technique, we have revealed non-trivial spin dynamics --temperature independent spin excitation spectrum-- in the magnetic quasicrystal Zn-Mg-Ho, which is, we believe, the most prominent feature ever found. Magnetic excitation spectrum in the Zn-Mg-Ho quasicrystal has only a quasielastic component centered at the elastic position. The quasielastic signal for the positive energy-transfer side is found to be temperature-independent in a wide temperature range $1.5 < T < 200$K; it may be noteworthy that the excitation spectrum shows little change even below the spin-glass-like freezing temperature $T = 1.95$K. In the low-energy region $E<1.5$meV, imaginary part of generalized susceptibility obtained from the scattering function shows scaling behavior: $\mathrm{Im}\ \chi\ (Q,\ E/k_BT)(k_BT)^{1/3} \propto (E/k_BT)^{-1/3} \tanh(\alpha E/k_BT)$. This is a typical *E*/*T*-scaling function, where the susceptibility is scaled only by *E*/*T*, except for the weak prefactor $T^{1/3}$. This *E*/*T*-scaling is frequently observed in the non-Fermi-liquid (NFL) compounds, such as UCu_4Pd, being in vicinity of a quantum critical point. At the present moment we are not sure what mechanism is responsible for the *E*/*T*-scaling in the magnetic quasicrystal, however, there must be interesting common background in the two seemingly different systems.

Keywords: quasicrystals, magnetic neutron scattering, magnetic structure and excitations

MS.67.3

Acta Cryst. (2008). A**64**, C116

Quantum critical points and nematics: The ruthenate $Sr_3Ru_2O_7$

Santiago A Grigera
School of Physics and Astronomy, University of St Andrews, St Andrews, FIfe, KY169SS, UK, E-mail:sag2@st-and.ac.uk

$Sr_3Ru_2O_7$ is an interesting strongly correlated metal that can be tuned to show a zero temperature metamagnetic transition. In its vicinity, there is experimental evidence supporting the existence of a novel quantum phase, with anisotropic transport properties. In this talk, I will discuss this topics and describe an extensive follow-up project to characterise and understand this phase.

Keywords: magnetic phase transitions, magnetic properties, magnetic and transport behaviours

MS.67.4

Acta Cryst. (2008). A**64**, C116

Exotic superconductivity in crystals without inversion center

Youichi Yanase[1], Manfred Sigrist[2]
[1]University of Tokyo, Department of Physics, 7-3-1, Hongo, Bunkyo-ku, Tokyo, Tokyo, 113-0033, Japan, [2]Theoretische Physik, ETH Honggerberg, 8093 Zurich, Switzerland, E-mail:yanase@hosi.phys.s.u-tokyo.ac.jp

I am planning to talk about some exotic properties in noncentrosymmetric superconductors which have no inversion symmetry in the crystal structure.
The breakdown of inversion symmetry induces
(i) the admixture of spin singlet and spin triplet order parameters,
(ii) helical superconductivity,
(iii) magneto-electric effect,
(iv) anomalous paramagnetic effect, and so on.
Our microscopic theory on the noncentrosymmetric heavy fermion materials, namely CePt_3Si, CeRhSi_3 and CeIrSi_3 will be reviewed. The possibility of s+P-wave superconductivity is pointed out. I will discuss the relationship and common physics with FFLO superconductivity in heavy fermion superconductor CeCoIn_5, organic superconductors, cold fermion atoms and high density quark matters.

Keywords: superconductivity, noncentrosymmetry, magnetic properties

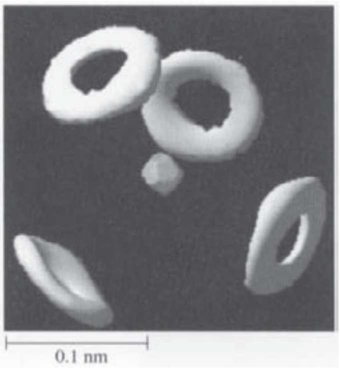
MS.67.5

Acta Cryst. (2008). A**64**, C116

Quantum mechanical delocalization of hydrogen atoms in $(NH_4)_2PtCl_6$

Takasuke Matsuo[1], Yoshio Kume[2], Noriko Onoda-Yamamuro[3], Osamu Yamamuro[4], Akira Inaba[1], Ryouji Kiyanagi[5], Hiroyuki Kimura[5], Yukio Noda[5]
[1]Osaka University (retired), Chemistry, Graduate School of Science, Ao-Shinke 5 Chome 17-17, Minoo, Osaka, 562-0024, Japan, [2]Azabu University, Fuchinobe, Sagamihara, Japan, [3]Tokyo Denki University, Hiki, Japan, [4]ISSP, The University of Tokyo, Kashiwa, Chiba, Japan, [5]IMRAM, Tohoku University, Katahira, Sendai, Miyagi, Japan, E-mail : tmatsuo@bc4.so-net.ne.jp

We performed neutron diffraction on $(NH_4)_2PtCl_6$ using the JAEA single crystal diffractometer FONDER. The crystal was essentially in the ground state at 7 K. 59 (hkl) intensity data were MEM-analyzed. The resulting nuclear density is shown in the figure for the NH_4^+ portion of the structure. The four rings represent the protons forming an NH_4^+ ion. The hydrogen atom is delocalized on the ring of ca.0.08 nm in diameter. The orientation of the NH_4^+ ions is thus distributed over the ring in the ground state of the crystal. The distribution is evidence for rotational tunneling of NH_4^+ in the cubic environment, explaining the different low temperature behavior of $(NH_4)_2PtCl_6$ and $(ND_4)_2PtCl_6$.



[1] T. Matsuo, Pure & Appl. Chem., 75 (2003) 913.

Keywords: proton delocalization, ammonium ion, deuteration-induced phase transition

MS.68.1

Acta Cryst. (2008). A**64**, C116-117

On the evaluation of energy densities with aspherical pseudoatoms: A model study

Anatoliy Volkov, Tibor Koritsanszky
Middle Tennessee State University, Chemistry, 239 Davis Science Bldg., MTSU Box 68, Murfreesboro, TN, 37132, USA, E-mail : avolkov@mtsu.edu

There is an increasing number of X-ray charge density studies reporting local and integrated kinetic-energy densities (KED) based on the pseudoatom model. These calculations utilize approximate KED functionals and invoke the local virial theorem to derive the potential-energy density. Such a procedure thus combines a formalism of limited applicability with a density model lacking a physical soundness, through a relation that is known to be valid only for the exact properties in question. The purpose of this model study is to trace the propagation of errors associated with each step of the calculation. We evaluate a number of approximate KED's using ab initio densities and their pseudoatom representations. The results are compared with the wave-function-based KED's locally, as well as in terms of integrated values for atomic basins. We also test theoretical densities against the local virial relationship. In line with earlier observations, our analysis shows that KED's obtained via functionals closely resemble exact KED's only in regions of low and flat density. The discrepancy between exact and approximate KED