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

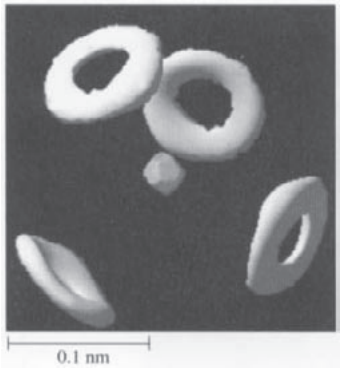
MS.67.5

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