no protein structure has been refined using the invariom model. The proteins under examination are lysozyme, insulin and myoglobin -- macromolecules with molecular weights of 6 to 17kDa. They all have important biological functions, so it is desirable to improve their refinement and to obtain a high quality electron density distribution. The latter allows to derive e.g. Bader's bond and atomic descriptors, electrostatic potentials and lattice energies. To achieve the necessary atomic resolution for the invariom refinement high intense synchrotron beamlines (Swiss Light Source, Diamond Light Source) were utilized.

Keywords: macromolecules, invariome, electron charge density

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Internal magnetic structure of a Mn_3 cluster determined by polarised neutron diffraction

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The self-assembly between metal centres and selected ligands into predetermined molecular architectures is especially relevant in the field of magnetic materials, since remarkable metal-metal interactions may be achieved.[1] The compound studied here exhibits fascinating features from the supramolecular and magnetism point of view.[2] It results from the fusion of two double-stranded helicates by 'click self-assembly' to form an unprecedented trinuclear helical structure(See figure). The magnetic response of the compound reveals that this is a rare lineal trinuclear MnII compound showing weak ferromagnetic interactions. Here we present the results of a polarized neutron experiment aiming to determine the spin density in the Mn atoms and to elucidate the magnetic interaction model. The understanding of the delicate interactions intra- and inter-clusters is crucial to permit in future the design of new magnetic interesting compounds.

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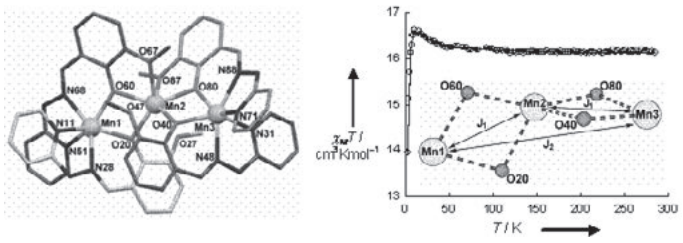

Keywords: molecular magnetism, spin density, self-assembly

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Magnetic frustration in $Gd_{7-x}Y_xPd_3$ single crystals

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Materials based on gadolinium are prospective for applications in magnetic refrigeration cycles. Magnetocaloric properties of polycrystalline Gd_7Pd_3 were investigated by Canepa et al. [1]. Wide investigations of the Gd_7T_3 (T = Rh, Pd) single crystals were performed [2, 3]. They crystallize in Th_7Fe_3 type hexagonal structure with c/a=0.63. Gd_7Rh_3 orders antiferromagnetically at 140 K while Gd_7Pd_3 becomes ferromagnetic at about 334 K. The aim of this work is to examine the influence of substitution of nonmagnetic yttrium into gadolinium sublattice. Single crystals of $Gd_{7-x}Y_xPd_3$ were grown by the Czochralski method from a levitated melt. The X-ray Berg-Barrett topography confirmed a good quality of the obtained crystals. The observed XPS, magnetic and electrical resistivity behaviour points to the coexistence of localized magnetism from the magnetic Gd^{3+} ions and itinerant ferromagnetism from 4d- and 5d-electron bands. The magnetic behaviour of the $Gd_{7-x}Y_xPd_3$ solid solutions in terms of three competition mechanisms: RKKY-interaction, magnetic frustration and spin-fluctuation is discussed. The change in TC across the $Gd_{7-x}Y_xPd_3$ series is consistent with change in the RKKY-interaction strength, while the spin-reorientation are probably governed by the vanishing of the magnetic frustration.

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Keywords: Czochralski method, ferromagnetics, magnetization

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Spin form factors of the samarium ions in $SmAl_2$

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We have tried spin-form factor measurements on $SmAl_2$ using the synchrotron radiation and established the method of analyzing the data using the operator-equivalent technique before [1]. It was, however, difficult to interpret the experiment and we have subsequently improved the experimental procedure and instrumentation. After that, a quantitative agreement with the theoretical estimates has been observed for, for example, $PrAl_2$ and $DyAl_2$ [3]. In this presentation, the newly measured results on $SmAl_2$ will be shown and discussed.

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