

at 200K (Cubic, $P2_13$) and at 100K (Orthorhombic, $P2_12_12_1$) respectively were collected and analyzed by using XD2006 package (4). The topological analysis and calculation of relevant properties bring out the salient features which allow for a clear distinction in bond paths, Laplacian maps and electrostatic potential isosurfaces in both metal coordination and sulfate tetrahedra across the phase transition.

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Keywords: charge density, mineral structures, sulfates

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Tartaric acid gyration tensor components from charge density distribution

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L-tartaric, (+)-(2R,3R)-2,3-dihydroxybutanedioic, acid crystallizes in non-centrosymmetric space group $P2_1$. Experimentally determined principal components of the gyration tensor [1] and the optical rotation calculated from the structural data using Pauling's atom volume polarizabilities [2] differed significantly. Since the contribution of the molecule itself to optical activity of the crystal was estimated as relatively small, the predominating intermolecular effects were expected to be responsible for the high gyration tensor components. To get necessary information, charge density analysis was performed [3] using the program package XD [4] and low-temperature (80 K) X-ray diffraction data. The results of the topological analysis of $\rho(r)$ at the bond critical points gave a quantitative description of the hydrogen bonds whereas the properties of charge density distribution enabled the derivation of atom volume polarizabilities [5,6] which in turn were utilized for the determination of gyration tensor components. This work is partially supported by the Polish Ministry of Education and Science (grant No. N204 124 32/3169).

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Keywords: charge density distribution, optical rotation, atom volume polarizability

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Chemical bonding in energetic RDX: An experimental and theoretical study

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Accurate X-ray diffraction data at 20K and 120K were obtained for the alpha-form of the 1,3,5-trinitrohexahydro-1,3,5-triazine (RDX) crystal using a Rigaku R-Axis Rapid high-power rotating anode diffractometer with a curved image plate detector. Data were integrated with the program VIIPP [1] using the predicted reflection positions from the program HKL2000 [2], scaled and averaged with SORTAV [3], and the multipole refinements performed with the XD program package [4]. The experimental electron density (ED) obtained at two temperatures has been analyzed in terms of the Quantum Theory of Atoms in Molecules, and compared with the ED calculated theoretically. Features of the intra- and inter-molecular bond critical points and the oxygen atom lone-pair locations are discussed. Hydrogen bonding, O · · · O, O · · · N and N · · · N intermolecular interactions are reported. Atomic charges, features of the electrostatic potential and the molecular dipole moment are discussed.

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Keywords: experimental charge density, topological analysis, Image plate

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Application of the aspherical scattering formalism on the refinement of macromolecules

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The conventional modelling of an X-ray diffraction experiment makes use of the "Independent Atom Model (IAM)", which ignores a priori electron density asphericities caused by the interaction of atoms. The Hansen&Coppens multipole model allows for a non-spherical atomic description but may require more than 40 parameters per atom and therefore needs high resolution diffraction data ($d < 0.5 \text{ \AA}$), which is mostly far beyond the scattering power of macromolecules. The recently introduced invariom model overcomes this limitation by assignment of individual aspherical scattering factors (multipoles) to each chemically unique atom in a structure. This permits to refine only atomic positional and vibrational parameters and thus to use data sets of medium resolution ($d < 0.9 \text{ \AA}$). The invariom library covers all bonding situations in polypeptides. Numerous tests on small molecules showed that this approach improves the accuracy of the molecular geometry, yields a better description of the displacement parameters and more accurate Flack parameters even in the case of limited resolution. But so far

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 Mn₃ cluster determined by polarised neutron diffraction

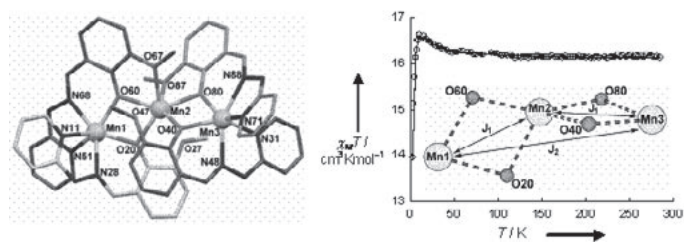
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The self-assembly between metal centres and selected ligands into predetermined molecular architectures is especially relevant in the field of magnetic materials, since remarkable metal-metal interactions may be achieved.[1] The compound studied here 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_xPd₃ single crystals

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Materials based on gadolinium are prospective for applications in magnetic refrigeration cycles. Magnetocaloric properties of polycrystalline Gd₇Pd₃ were investigated by Canepa et al. [1]. Wide investigations of the Gd₇T₃ (T = Rh, Pd) single crystals were performed [2, 3]. They crystallize in Th₇Fe₃ type hexagonal structure with $c/a=0.63$. Gd₇Rh₃ orders antiferromagnetically at 140 K while Gd₇Pd₃ 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_xPd₃ 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 Gd³⁺ ions and itinerant ferromagnetism from 4d- and 5d-electron bands. The magnetic behaviour of the Gd_{7-x}Y_xPd₃ 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_xPd₃ series is consistent with change in the RKKY-interaction strength, while the spin-reorientation are probably governed by the vanishing of the magnetic frustration. Acknowledgements The work is supported by the Ministry of Science and Higher Education in Poland within Grant No. N202 149 31/2727. SQUID magnetometer partially financed by European Regional Development Fund.

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Spin form factors of the samarium ions in SmAl₂

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We have tried spin-form factor measurements on SmAl₂ 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, PrAl₂ and DyAl₂ [3]. In this presentation, the newly measured results on SmAl₂ will be shown and discussed.

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