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SPIN DENSITY INVESTIGATION FOR A BETTER DETERMINATION OF THE MAGNETIC STRUCTURE

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The TPV molecule is a planar molecule built of a verdazyl ring surrounded by three phenyl groups. It is a stable free radical carrying a spin S=1/2. It crystallizes in an orthorhombic cell (space group $P2_12_12_1$) and the molecules form zigzag chains along the c axis. Below T_N = 1.78K, it presents a long range magnetic order : it becomes antiferromagnetic, but a weak ferromagnetism develops at the same time.

Two low temperature, non polarized, neutron diffraction investigations(1,2) have been already performed to determine the exact magnetic structure of this molecular compound. Both agreed on the antiferromagnetic nature of the chains but an ambiguity persisted about the direction of the magnetic moments. In the analysis of these investigations, it was assumed for the form factor of the different reflections that the spin of the molecule was equally shared by the 4 nitrogen atoms of the TPV molecule.

In order to improve the analysis of the former investigations, we have performed an experimental study of the spin density of this molecule. We have used the same crystal at higher temperature, in the paramagnetic state, aligned the magnetic moments by a strong magnetic field, and measured the magnetic contributions to the amplitude of the Bragg reflections with polarized neutrons. The spin density distribution obtained this way yields the form factors for the magnetic structure investigations.

References
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MANGANESE CLUSTERS AS SINGLE-MOLECULE MAGNETS

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Many present and future specialized applications of magnets require monodisperse, nanoscale magnetic particles, and the discovery that individual molecules can function as nanoscale magnets was therefore a significant development. Each molecule functions as a nanoscale, single-domain magnetic particle that, below its blocking temperature, exhibits the classical macroscale property of a magnet, namely magnetization hysteresis. Such single-molecule magnets (SMMs) straddle the interface between classical and quantum behavior by also exhibiting quantum tunneling of magnetization (QTM). The first SMMs discovered were the $[Mn_{12}O_{12}(O_2CR)_{16}(H_2O)_4]$ family with a ground state of S = 10. This large spin value and a significant easy-axis (Ising-type) anisotropy (negative zero-field splitting parameter, D) lead to a significant barrier to magnetization reorientation and are thus the origin of the SMM property. The Mn_{12} family of complexes has been extended by chemical reduction to the one- and two-electron reduced species $[Mn_{12}]^-$ and $[Mn_{12}]^{2-}$ with S = 19/2 and 10, respectively. Both are SMMs, providing a family of related species for detailed comparison. Other variations of the Mn_{12} family include the introduction of non-carboxylate ligands, either organic ($Ph_2PO_2^-$) or inorganic (NO_3^-), with retention of the SMM properties.

Another well-studied SMM family are the related $[Mn_4O_3X(O_2CR)_3(dbm)_3]$ and $[Mn_4O_3Cl_4(O_2CR)_3(py)_3]$ complexes (X^- = Cl^-, Br^-, F^-, MeO^-, etc ; dbm^- = the anion of dibenzoylmethane; py = pyridine) with S = 9/2. These Mn_4 SMMs have been a particularly rich source of data on the sensitivity of QTM to small structural perturbations, the solvation environment, and exchange interactions with neighbouring molecules.

Keywords: MANGANESE, CLUSTERS, MAGNETISM

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A HISTORY THUS FAR OF OVERSAMPLING AND SINGLE PARTICLE IMAGING

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A methodology is described which is very close to that of x-ray crystallography, but in which the specimen is general and need not be a crystal. Important facts concerning the method are: 1. The often limiting problem of crystallization does not arise. Specimens may be amorphous or defect structures in materials science, single large biomolecules, single biological cells or cellular subunits, etc. Single microcrystals are a further possibility. 2. Diffraction patterns are continuous, not discrete, and by fine sampling yield more information than the classical Bragg-spot pattern, making the phase problem in many respects simpler than in the crystallographic setting. 3. Diffraction patterns are weak and require the use of large x-ray exposure while avoiding excessive damage to the specimen.

Current status is: (A) images of radiation-resistant specimens in 2D and 3D have been obtained by use of the method, (B) FEL flash x-ray 3D single-molecule imaging of the large protein rubisco at atomic resolution has been carried out by computer simulation of the method, (C) a project aimed at 3D imaging of a cryo-protected yeast cell at 20 nm resolution is underway. A brief history will be given, with some details of (C). Details of (A) and (B) will be given in the talk by John Miao later in the symposium.

Keywords: NON-CRYSTAL SPECIMENS SINGLE-PARTICLE IMAGING OVERSAMPLING

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3-D IMAGING BASED ON X-RAY MICROSCOPE IMAGES

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X-ray microcopy has resolved 30 nm structures in biological cells. To protect the cells from radiation damage caused by X-rays, imaging of the samples has to be performed at cryogenic temperatures, which makes it possible to take multiple images of a single cell. Due to the small numerical aperture of zone plates, X-ray objectives have a depth of focus on the order of several microns. By treating the X-ray microscopic images as projections of the sample absorption, computed tomography (CT) can be performed. Since cryogenic biological samples are resistant to radiation damage, it is possible to reconstruct frozen-hydrated cells imaged with a full-field X-ray microscope. This approach is used to obtain three-dimensional information about the location of specific proteins in cells. To localize proteins in cells, immunolabelling with strongly X-ray absorbing nanoparticles was performed. With the new tomography setup developed for the X-ray microscope XM-1 installed at the ALS, we have performed tomography of immunolabelled frozen-hydrated cells to detect protein distributions inside of cells. As a first example, the distribution of the nuclear protein, male specific lethal 1 (MSL-1) in the *Drosophila melanogaster* cell was studied.

Keywords: X-RAY MICROSCOPY, TOMOGRAPHY, PROTEIN LABELING