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Quantum effects in S=1/2 two-dimensional Heisenberg antiferromagnet in applied magnetic field

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Two-dimensional (2D) quantum antiferromagnets are of great fundamental interest because the presence of quantum fluctuations can lead to novel quantum excitations and novel ground states. Only little is known about the effects of applied magnetic fields on 2D square-lattice antiferromagnets. Using neutron scattering technique, we studied the magnetic excitation spectrum of the S=1/2 2D square-lattice Heisenberg antiferromagnet $Cu(pz)_2(ClO_4)_2$ [1] up to one third of saturation field. Inelastic neutron scattering measurements performed at zero field show 11.5(7)% dispersion along the antiferromagnetic zone-boundary and the existence of a magnetic continuum for wave-vectors around (π;0). Relatively small magnetic fields applied perpendicular to the square-lattice plane suppress the continuum and at H=14.9T the dispersion along the zone-boundary is inversed with respect to zero field with a minimum at (π/2;π/2). Due to quantum correlations magnetic fields strongly renormalize the entire excitation spectrum from factor Zc=1.19(2) at zero field to Zc=0.99(2) at H=14.9T. Renormalized spin wave theory describes the field dependence of the gap energy at the antiferromagnetic zone centre (π;π) with a small exchange anisotropy, but the dispersion of a well defined mode at high fields deviates from spin-wave theory, indicating the presence of quantum fluctuations.

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Keywords: quantum magnetism in low dimensions, inelastic neutron scattering, magnetic materials

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Assembling strategy of magnetic Mn complexes to design solid state multifunctional hybrid materials

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Two typical assembling or aggregation strategies to design multifunctional hybrid materials have been compared for modified chiral or single-molecule magnets based (SMM) of well-known magnetic Mn complex systems. Strategy I: Organic/inorganic hybrid materials of solid polymer films with photochromic azobenzene (AZ) and magnetic Mn complexes. It is valid for Mn12 SMM [1] forming structurally-determined compositions of photochromic AZ and magnetic moieties as well as mixed solutions in cast films [2,3], but it is limited for assembling or decomposition of coupled structures [4]. Strategy II: Stepwise assembling of potentially thermally-accessible crystalline Mn(III) complexes. Magnetic properties or ground spin states may be changed for mononuclear one [5]. It is partly valid for chiral Schiff base complexes of cyanide-bridged Mn-M'-Mn clusters [6], but the degree of distortion is small in cocrystals (Figure) [7].

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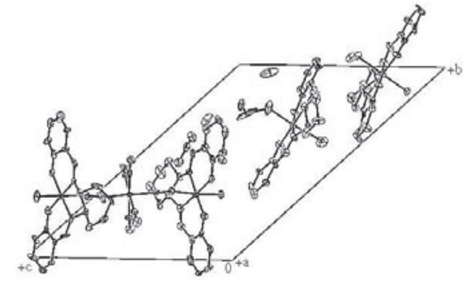

Keywords: materials chemistry, magnetochemistry, cocrystals

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Studies on some manganese-containing single-molecule magnets

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The synthesis, crystal structure, and magnetic properties of $[Mn_4O_2(OOCCMe_3)_6(bpy)_2]$ (**1**, bpy = 2,2'-bipyridine) and $[Mn_4O_2(OOCCMe_3)_6(phen)_2]$ (**2**, phen = 1,10-phenanthroline), are reported. Complexes **1** and **2** crystallize in the monoclinic P21/c space group and contain a known $[Mn^{III}_2Mn^{II}_2(\mu_3\text{-}O)_2]^{6+}$ core that can be considered as two edge-sharing, triangular $[Mn_3O]$ units. Peripheral ligation is by six $\mu_2\text{-}O_2CCMe_3$ and two terminal bipy/phen groups to yield a complex with imposed *C*i symmetry. The magnetic properties of Complexes **1** and **2** have been studied by direct current (DC) and alternating current (AC) magnetic susceptibility techniques.

Keywords: single-molecule magnets, manganese complexes, magnetic susceptibility studies

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Slow relaxation of the magnetization in rationally designed single chain magnets

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After the intense research activity in the field of slow dynamics of the magnetization in molecular clusters (SMMs) and the bistability related problem, the field of Molecular Magnetism is currently shifting towards more complicated systems. One direction has been opened by the observation of slow relaxation of the magnetization in 1D systems (called Single Chain Magnets or SCMs). Synthetic efforts are devoted to the development of new systems SCMs that can help us understanding the physical background that lies beneath this phenomenon. In this contest several groups have development new tools allowing for the engineering of both magnetic and structural properties. Here we discuss some opportunities offered by the Metal Nitronilnitroxyde strategy. In particular the experimental and theoretical work developed on finite-size effects revealed itself a key point. We describe the rational strategy that allowed creating the first rare-earth based SCMs. We show that we can freely substitute the metallic centres without structural alterations, thus tuning of the magnetic properties. This affords a useful information on the key parameters that rule SCMs.

Keywords: molecular magnets, superparamagnets, synthesis of new materials

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Synthesis, crystal structure, and magnetic properties of trioxotriangulene stable neutral radical

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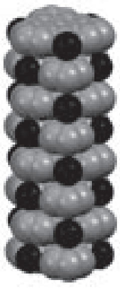
Synthesis and elucidations of molecular and electronic-spin structures of novel stable neutral radical derivatives are fundamentally important issues for the development of spin-mediated molecular functional materials. Oxophenalenoxyl derivatives are new persistent neutral radicals with two oxygen-atoms in the phenalenyl skeleton. Importantly, electronic-spin structures of these neutral radicals are intrinsically different in the topological symmetry from that of the phenalenyl. Furthermore, by controlling the redox process, these radicals show the reversible topological switching of the spin-delocalized nature. The electronic features enabled us to investigate the redox-based spin diversity and the molecular crystalline secondary battery. In this work, as the two-dimensional pi-extended derivative of 6-oxophenalenoxyls, we have synthesized and isolated trioxotriangulene neutral radical derivative having C_3-symmetric and 25pi-conjugated molecular/electronic structures. The electronic-spin structure and redox ability of this neutral radical have been revealed by X-ray crystal structure analysis (Figure), ESR and magnetic measurements, and DFT calculations.



Keywords: ESR, magnetic materials, radicals

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Hemidirected novel lead(II) azide complex of 2,6-diacetylpyridine dihydrazone

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The chelating behaviour of 2,6-diacetylpyridinedihydrazone (L) towards lead(II) with azide ion has been characterized by means of elemental analyses, FTIR and determined by single-crystal X-ray analysis. The title compound, $Pb(C_9H_{13}N_{11})$ (**1**), was crystallized in the monoclinic space group *C*2/*c*. Title complex exhibits the expected coordination sphere with five nitrogen atoms coordinated to the central lead(II) and shows distorted trigonal bipyramid coordination geometry. The coordination chemistry of title complex exhibits a gap around the lead(II) ion, occupied possibly by stereochemically active electron lone pair on lead(II) which results in a hemidirected lead complex. It has been obtained from the antimicrobial activities of the free ligand and its lead(II) complex that the antimicrobial activity of the complex is higher than the free ligand.

Keywords: biological activity, X-ray Diffraction, crystal structure

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Novel route to synthesis copper halide with Cu_2S_2 core and its crystal packing

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The novel route to synthesis of $[Cu_2\{\cdot\text{-}S{=}C(NH)_2(CH_2)_2\}2\{S{=}C(NH)_2(CH_2)_2\}_2Br_2]$ or (1) was simply. Single crystal X-ray structure analysis and FT-IR spectra confirmed its components. The structure revealed a dimeric monobromide bis(ethylenethiourea)copper(I) complex with in the monoclinic space group *C*2/*c*. The final residual factor (R) is 0.0285. The Cu_2S_2 core of the dimer is lozenge with C-S distances of 2.375(1) and 2.408(1) Å, a Cu-S-Cu angle of 70.81(3)°. The crystal packing is stabilized by extensive N-H•••Br interactions and weak N-H•••S interactions.

Keywords: X-ray crystal structure, Cu_2S_2 lozenged core, crystal packing

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Crystal structures of two new tetranuclear copper complexes based on Schiff-base ligands

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Two new double azido-bridged tetranuclear copper complexes were synthesized, namely Bis{μ-[bisN,N'-(salicilidene)-1,3-propane-diaminato-N,N'-diformamidecopper(**II**)]azido(μ-azido)copper(**II**)} (**I**) and Bis{μ-[bisN,N'-(salicilidene)-1,3-propanediaminato copper(**II**)]azido(μ-azido)copper(**II**)}dioxan (**II**),and their crystal structures were determined. In both compounds two doubly oxygen-bridged dinuclear Cu complexes are bridged in a head-to-head fashion via two azido groups. The terminal Cu ion in (**I**) and