heat measurements. Spin glasses provide an important class of frustrated magnets. Typically based on disordered systems, they have found relevance in diverse areas of research, such as neural networks, the origin of life, and algorithm theory. Despite the theoretically prediction that these materials have a non-zero residual entropy, there have been no clear experimental studies of the entropy of a spin glass. This presentation describes an experimental study of the magnetic properties and zero point entropy of a series of S=1/2 spin glasses. Diamagnetic dilution in the spinel systems $CuAl_2O_4$ and $CuGa_2O_4$ forms isomorphic solid solutions $Zn_xCu_{(1-x)}Ga_2O_4$ and $Zn_xCu_{(1-x)}Al_2O_4$ that provides an opportunity to investigate the effect that non-magnetic substitution has on the spin glass properties of $CuGa_2O_4$ and on the entropy of the related spin glass states. Low temperature specific heat measurements were carried out on both $CuGa_2O_4$ and $CuAl_2O_4$ in order to determine the magnetic entropies, and compare them with the value theoretically predicted for S = 1/2 spin glasses. Both spinels were found to possess a non-zero magnetic entropy at 0K, with values that are significantly greater than the predicted value. These studies also indicate that the ground state degeneracy of these frustrated magnets can be controlled by chemical substitution.

Keywords: magnetic frustration, specific heat, magnetic ordering

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Polaronic behavior of Mn_4O_4 heterocubane clusters in $LiMn_2O_4$ spinel

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Crystals of $LiMn_2O_4$ undergo a structural phase transition near the room temperature. The high temperature (HT) form adopts a normal spinel-type structure (cubic, *Fd*-3*m*) with the octahedral sites populated statistically with heterovalent Mn^{III} and Mn^{IV} in the equal ratio. The low temperature (LT) form adopts a 3x3x1 superstructure (orthorhombic, Fddd) with respect to the HT form, containing Mn^{III}, Mn^{IV}, and the intervalent Mn atoms. The synchrotron X-ray single-crystal electron-density analysis, carried out at the beamline 14A, Photon Factory, Tsukuba, revealed a large anisotropy of the atomic displacement parameters for part of O atoms, suggesting a possible occurrence of the bond-length fluctuation along the pseudo-tetragonal Jahn-Teller distortion parallel to the a-axis in the heterocubane Mn_4O_4 cluster. The cluster presumably shares three electrons among four e-parentage orbitals of Mn and behaves as a core of Zener-type polaron. The heterocubane Mn_4O_4 clusters are isolated from each other and embedded in an orbitally-ordered way in the charge-ordered matrix containing Mn^{III} and Mn^{IV}. The transition between the LT and HT forms of $LiMn_2O_4$ can thus be regarded as an order-disorder transition of the Zener-type heterocubane polarons.

Keywords: zener polaron, synchrotron X-ray diffaction, phase transition

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Magnetic structure of the quasi-one-dimensional, frustrated, spin-1 antiferromagnet CaV_2O_4

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We present the magnetic structure determination of the quasi-one-dimensional, frustrated, spin-1 chain material CaV_2O_4 by means of neutron diffraction. This material crystallizes in the post-spinel-type $CaFe_2O_4$-type structure at room temperature (orthorhombic Pnam) and contains zig-zag chains of edge-sharing VO_6 octahedra along the crystallographic **c** direction. Nearest and next nearest neighbour V^{3+}-ions (spin-1) are almost equally spaced leading to competing antiferromagnetic exchange interactions and resulting in considerable geometrical frustration. The non-magnetic Ca^{2+}-ions act as spacers between the chains minimizing the interchain exchange coupling and making this system a low-dimensional quantum magnet. Upon cooling the material undergoes two phase transitions. A structural transition from orthorhombic to monoclinic occurs at T_s=140K. This distortion partially lifts the frustration of the system thus assisting the onset of long-range antiferromagnetic order below T_N=71 K. By performing neutron diffraction experiments on CaV_2O_4 in the magnetically ordered phase, we found that it consists of two collinear antiferromagnetically coupled sub-chains, which are canted with respect to each other. The canting is a result of the distorted octahedral environment of the V^{3+}-ions, which lifts the orbital degeneracy of the Vanadium $3d^2$ electrons. Furthermore, the ordered magnetic moment of the V^{3+}-ions turned out to be is strongly suppressed, possibly due to strong quantum fluctuations caused by geometrical frustration and low-dimensional interactions. The analysis was challenging because the small monoclinic splitting resulted in twinned peaks whose intensity could only be separated by measuring a single crystal on a four-circle diffractometer.

Keywords: neutron diffraction, magnetic frustration, magnetic neutron scattering

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Federated repositories of X-ray diffraction images

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