Magnetic Order in Er^{3+} Halides

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Magnetic structures of a variety of Er^{3+} halides were investigated by neutron diffraction. The aim of the investigation was to establish correlations between the crystallographic and magnetic structures, and finally to predict magnetic properties from easy accessible crystal-structure data.

From those compounds two structural families show very interesting properties: the binary halides ErX_3, and the ternary cesium halides $Cs_3Er_2X_9$, where X represents the heavier halides Cl, Br and I.

The binary halides have layer structures of the $AlCl_3$ ($ErCl_3$) and the BiI_3 ($ErBr_3$, ErI_3) type. The Er^{3+} ions form two-dimensional (2D) honey-comb layers, well separated from each other by halide ions. The magnetic order within these layers is identical for all three compounds. They show a new type of two sublattice 120° antiferromagnetic order. Upon cooling the magnetic interactions in $ErBr_3$ and ErI_3 occur gradually from short range, over 2D, to 3D order at 280 mK with a limited correlation length of 15 Å perpendicular to the layers. In $ErCl_3$ on the other hand, a 3D magnetic order replaces the short range correlations below 350 mK. In the BiI_3 structure the rhombohedral layer stacking introduces geometrical frustration and prevents long-range 3D order, whereas 3D order occurs for the non-frustrated $AlCl_3$ type stacking.

The $Cs_3Er_2X_9$ compounds show two structure types, too. $Cs_3Er_2I_9$ crystallizes in the $Cs_3Cr_2I_9$ type structure, whereas $Cs_3Er_2Cl_9$ and $Cs_3Er_2Br_9$ adopt the $Cs_3Tl_2Cl_9$ type structure. Both structures contain Er_2X_9 units built from two face-sharing octahedra. In the magnetically ordered state those Er_2 units are ferromagnetically coupled and the spins are aligned parallel to the hexagonal or rhombohedral c-axis for X=I or Cl/Br, resp. The rhombohedral lattice introduces frustration which results in 1D ferromagnetic order for $Cs_3Er_2Br_9$. A transition to the 3D ferromagnetically ordered state can easily be induced by a magnetic field of 0.3 Tesla along the c-axis. The hexagonal $Cs_3Er_2I_9$ on the other hand shows a transition to 3D antiferromagnetic order with $\mathbf{k}$ = (¼, ¼, 0) below 230 mK.

Er^{3+} is an ideal subject for magnetic studies due to its Kramers ground state and its rather big moment. Erbium halides offer a variety of crystal structures and open a rich field for the investigation of 1D, 2D and 3D magnetic phenomena.