

maximal subgroups of index ≤ 4 of a representative group of each type of magnetic group in the superfamilies of these groups.

MS38 P05

Magnetic structure of the Kagomé mixed compound

$(\text{Co}_{0.5}\text{Ni}_{0.5})_3\text{V}_2\text{O}_8$ N. Qureshi,^{a,b} H. Fuess,^a H. Ehrenberg^c, B. Ouladdiaf,^b T. C. Hansen,^b Th. Wolf,^d C. Meingast,^d Q. Zhang,^d W. Knafo,^{d,e} H. v. Löhneysen^{d,e} ^aInstitute for Materials Science, University of Technology, Darmstadt, Germany. ^bInstitut Max von Laue-Paul Langevin, Grenoble, France. ^cLeibniz Institute for Solid State and Materials Research, Dresden, Germany. ^dResearch Center Karlsruhe, Institute of Solid State Physics, Karlsruhe, Germany. ^ePhysics Institute, Karlsruhe University, Karlsruhe, Germany.

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$(\text{Co}_{0.5}\text{Ni}_{0.5})_3\text{V}_2\text{O}_8$ represents a mixed compound of the well investigated transition metal (M) orthovanadates $\text{Ni}_3\text{V}_2\text{O}_8$ (NVO) and $\text{Co}_3\text{V}_2\text{O}_8$ (CVO) labelled as Kagomé staircase structures, which are characterized by edge-sharing MO_6 octahedra isolated by nonmagnetic VO_4 tetrahedra. The crystallographic structure (orthorhombic space group Cmca) [1, 2] is interesting with respect to the magnetic properties as the magnetic ions form buckled planes of corner-sharing isosceles triangles representing an anisotropic variation of the ideal Kagomé net. Within these buckled planes, the Kagomé staircases, cross-tie ions on crystallographic (4a) sites link the linear chains of spine ions on (8e) sites. Due to the reduced symmetry of the Kagomé staircase geometry with respect to the ideal plane net the degree of frustration is lowered leading to interesting long range ordered magnetic structures. Magnetization and neutron diffraction experiments on a $(\text{Co}_{0.52}\text{Ni}_{0.48})_3\text{V}_2\text{O}_8$ powder sample [3] revealed only one magnetic phase transition into an antiferromagnetic ground state in contrast to the richness of magnetic phase transitions of its parent compounds [4, 5]. The magnetic structure is modulated by a composition dependent propagation vector $\mathbf{k}=(\delta, 0, 0)$ with δ being 0.491(4) for $(\text{Co}_{0.52}\text{Ni}_{0.48})_3\text{V}_2\text{O}_8$ where a similarity to the NVO type magnetic structure was assumed [3]. Neutron single crystal diffraction experiments followed by group theory analysis produced a more detailed picture. The magnetic structure of $(\text{Co}_{0.5}\text{Ni}_{0.5})_3\text{V}_2\text{O}_8$ exhibits features, which differ from the predominantly collinear alignment of its parent compounds NVO and CVO, which exhibit a variety of magnetic structures with magnetic moments mainly oriented along the a axis [4-7]. The averaged magnetic moments of the statistically distributed Ni^{2+} and Co^{2+} ions are oriented in the a - c plane. They point either towards or away from the centers of the respective isosceles triangles of the Kagomé staircase structure if viewed as a projection along the b axis. The spin arrangement is close to a 120° configuration as expected for antiferromagnetically ordering systems on a Kagomé lattice. This result shows once again that the competition of the exchange interactions along various coupling pathways in this particular crystallographic system results in a variety of different interesting magnetic structures.

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Magnetic structure of $\text{Ba}_7\text{Co}_6\text{BrO}_{17}$

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At the basis of the search for original electronic and magnetic behaviour, a number of studies focus on the prospecting for new complex structural types within "hot" topics such as cobaltites (strong competition between magnetic ground states, attractive thermoelectricity, superconductivity ...). In this context, we recently synthesized by solid state reaction the new $\text{Ba}_7\text{Co}_6\text{BrO}_{17}$ compound ($\text{P6}_3/\text{mmc}$: $a=5.6611(1)$ Å and $c=33.5672(8)$ Å) [1]. This cobaltite is built from a close-packing of $[\text{BaO}_3]$ and $[\text{BaOBr}]$ layers with a 14H stacking sequence (c' hhhcc')₂, which creates Co_4O_{15} tetramers of face-sharing octahedra connected to their extremities to isolated tetrahedra by corner-sharing. This material is strongly related to the 12H- $\text{BaCoO}_{2.6}$ [2] and 6H- $\text{Ba}_6\text{Co}_6\text{ClO}_{16}$ [3] cobaltites, with the existence of common blocks. Measurement of the magnetic susceptibility χ against T has been performed under applied magnetic field of 1 T. The experiment reveals the existence of two transitions at 60 K and 30 K. The curve was fitted to the Curie-Weiss law in the paramagnetic domain (above 60 K), leading to the values $p_{\text{eff}}=3.12$ $\mu\text{B}/\text{Co}$ and $\theta=55\text{K}$. This paramagnetic effective moment can be explained by assuming $\text{Co}^{3+} S=1$ and $\text{Co}^{4+} S=3/2$ i.e. cobalt atoms at the intermediate spin-state (considering the spin-only approximation). The positive θ value indicates important ferromagnetic exchanges among the structures. In order to understand the magnetic properties of this cobaltite, we collected neutron powder diffraction data on the G41 diffractometer (LLB Saclay, France). The pattern below 60 K revealed the onset of new reflections, this fact being ascribed to the occurrence of long-range magnetic ordering and confirming the magnetic transition previously reported. All those magnetic reflections were indexed in a commensurate lattice related to the crystallographic one by a propagation vector $\mathbf{k}=[000]$. Among all the possible magnetic models, only those for which the exchange interactions between two tetrahedral cobalt orders antiferromagnetically went to convergence with acceptable reliability factors. The magnetic structure can be described as the antiferromagnetic coupling of ferromagnetic blocks ($\text{Co}_4\text{O}_{15} + 2 \text{CoO}_4$ units). This kind of magnetic structure has been previously reported for 6H- $\text{Ba}_6\text{Co}_6\text{ClO}_{16}$ [4].

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