

**m30.p13****New 1D, 2D and 3D chiral MOF's based on cyclohexane-1,2-diamine**

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*Institut de Chimie, Université de Neuchâtel, Rue Emile-Argand 11, CH-2009 Neuchâtel, Switzerland. E-mail: olha.sereda@unine.ch***Keywords: crystal structure, cyano compounds, paramagnetism**

Cyanide-bridged bimetallic systems, prepared from assembling cyanometallates and transition metal complexes, have been shown to exhibit fascinating structures with interesting magnetic, electrochemical, magneto-optical and zeolite-like properties [1]. The design and synthesis of nanoporous metal-organic frameworks (MOF's), mimicking zeolites, is drawing a great deal of attention due to the application of these materials as catalysts, adsorbents and ion exchangers. Chiral structures are a new target for the lattice architecture in the field of magnetic materials. There are only a very few examples where cyclohexane-1,2-diamine has been incorporated into cyanide-containing complexes resulting in the formation of ferromagnets [2], [3], [4]. We will present some new one-, two- and three-dimensional chiral cyanide-bridged bimetallic MOF's,  $[M_1(\text{chxn})_n]_n[M_2(\text{CN})_6]_m$  (where  $M_1 = \text{Cu, Ni}$ ;  $M_2 = \text{Ru, Cr, Co}$ ;  $n = 2, 3$ ;  $m = 1, 2$ ;  $\text{chxn} = \text{trans-1S,2S}$  or  $1R,2R$ -cyclohexane-1,2-diamine), and their structural features, magnetic and zeolite-like properties will be discussed.

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**m30.p14****Atomic and domain structure of the low temperature phase of barium metagermanate**Daniel Maria Töbrens,<sup>a</sup> Volker Kahlenberg,<sup>a</sup> Christian Gspan<sup>b</sup>, Gerald Kothleitner<sup>b</sup>*<sup>a</sup>Institute of Mineralogy and Petrography, University of Innsbruck, Austria, and <sup>b</sup>Research Institute for Electron Microscopy, Graz, Austria. E-mail: daniel.toebrens@uibk.ac.at***Keywords: domain structure, layered structures, electron microscopy**

The crystal structure of the low temperature form of barium metagermanate ( $\text{BaGeO}_3$ ) has been determined from laboratory X-ray powder diffraction data collected at 25.5(5) °C. The compound is monoclinic with space group  $C2/c$  and unit cell parameters of  $a = 13.1877(2) \text{ \AA}$ ,  $b = 7.6222(1) \text{ \AA}$ ,  $c = 11.7190(1) \text{ \AA}$ ,  $\beta = 112.295(1)^\circ$ ,  $V = 1089.9(1) \text{ \AA}^3$  and  $Z = 12$ . The structure was found to consist of alternating layers of barium atoms and three-membered  $[\text{GeO}_3]_3$ -rings showing a twofold positional disorder. Apart from the disorder the structure is very similar to the one of  $\text{SrGeO}_3$  [1]; both are six-layer structures build from the same type of layers. The same structure type also appears in pseudo-wollastonite, forming four- or six-layer polytypes [2]. Careful studies of possible structural variations using simulated annealing [3] did not reveal any deviation from symmetry  $C2/c$ .

The disorder of the ternary rings can be summarized as follows: ternary  $[\text{GeO}_3]_3$ -rings appear in only one out of two possible orientations and occupy only 2/3 of the positions compatible with this orientation. Following [2], for six-layered structures of this type there is only one distinct polytype with the inherent symmetry  $C2/c$ . There are, however, two non-congruent enantiomorphs of this structure. The disorder observed in  $\text{BaGeO}_3$  can be described as the simultaneous appearance of both possibilities.

Electron microscopy reveals in SAED patterns the existence of twins; the twin law can be described as a mirror plane normal to  $\mathbf{a}$ . Diffuse scattering within the lattice rods parallel  $\mathbf{c}^*$  indicates disorder within the layers of the structure. HRTEM shows fully ordered domains, which are separated by narrow disordered regions; the domain borders observed are normal to  $\mathbf{c}^*$ . Larger disordered regions are observed as well.

Based on these observations the disorder in the structure can be addressed as stacking fault disorder, a behaviour also found in polytypes of pseudo-wollastonite [2]. The stacking, however, is not random but can be rationalized by a twinning mechanism mapping the enantiomorphic polytypes onto each other.

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