s3.m11.p7 **Re-investigation of the incommensurate structure of HMT-Resorcinol in superspace.** Rodriguez M. Soraya and Chapuis Gervais, *LCr/EPFL, Switzerland. E-mail: soraya.rodriguez@epfl.ch*

Keywords: Incommensurate; Superspace; Diffuse scattering

HMT-Resorcinol, a 1:1 adduct with empirical formula $C_6H_{18}N_4O_2$ consists of resorcinol bonded to one nitrogen atom of HMT by an H atom bridging the hydroxyl group. According to the published structure [1] with orthorhombic cell parameters a=10.40(1) Å b=7.120(5) Å c=16.88(1) Å, 3 possible space groups were proposed: C2cm, Cm21 and Cmcm. Later [2], the structure was described as a superposition of two molecules of HMT and resorcinol related by a pseudo mirror plane in space group C2cm. Although some extra reflexions satisfying the condition k≈ n+1/3 were observed, they were not taken into account. Finally, a new investigation was published [3], describing the structure in the centrosymmetric space group Cmcm. In this model, the hydroxyl group bounding the two molecules is disordered.

In the present investigation, a single crystal X-ray diffraction study was carried out and clear signs of incommensurability were found. In addition to the main reflections, first order satellites could be observed in addition to strong diffuse scattering rods along **c***. The pattern was indexed with an orthorhombic cell and the modulation vector **q**=0**a***+0.37**b***+0**c***. The average structure, calculated from the main reflexions hkl0 has cell parameters a=10.3474(6) Å b=7.0763(6) Å c=16.8321(14) Å and Z=4. The anisotropic thermal parameters along a are very high for almost all atom. In superspace, the C centring extends to (1/2, 1/2, 0, 1/2). The most probable superspace group is X2cm(0,b,0)000. Results of the refinement will be discussed.

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[3] S.W.Ng. (2002). *Journal of Molecular Structure* **609**, 89-95.

s3.m11.p8 **Structural investigation of composite phases $Ba_{1+x}[(Na_xMn_{1-x})O_3]$ with x≈2/7, 5/17 and 1/3.** Pascal Roussel,[a] Eric Quarez,[a] Olivier Perez[b] and Olivier Mentre[a], [a]*Laboratoire de Cristallochimie et Physicochimie du Solide (CNRS UMR8012), ENSCL-Université de Lille, 59652 Villeneuve d'Ascq, France, and* [b]*Laboratoire CRISMAT (CNRS UMR6508), ISMRa-Université de Caen, 14050 Caen, France. E-mail: pascal.roussel@ensc-lille.fr*

Keywords: Composite structure; Hexagonal perovskite; Superspace formalism

The perovskite family is one of the most spread out series of oxides because of its ability to modify its crystal structure, dimensionality and properties from minor to drastic layers stacking modifications (for a review, see reference therein [1]). Iso-formulated ABO_3 compounds can thus adopt a arrangement going from tridimensional ideal 3C cubic perovskite (ABC stacking of $[A_3O_9]$ layers), to bidimensional hexagonal 2H form (AB stacking) through an infinity of intermediary forms (various stacking sequences) leading to the wide family of hexagonal perovskites. The title compounds, of trigonal symmetry, belong to the 2H series and are built up from metallic columns running along the ternary axis and delimiting channels where A cations (usually Ba, Ca and Sr) are located. These columns are formed by the stacking of face sharing octahedra (O) and trigonal prisms (P) occupied by B and A' metals respectively. Various sequence of the O and P polyhedra may be observed, often giving rise to large periods (or pseudo periods) along [001]. Different 3D space groups were found to describe the different structures, preventing to give an unified vision for it. A theoretical work was undertaken by some authors [2] to give an unified description of this family. Thus, those compounds can also be considered as composite crystals with two interpenetrating sublattices, a rhombohedral one $(A'_xB_{1-x}O_3)$ and an hexagonal one (A_{1+x}) exhibiting, in the general case, incommensurate c periodicities. This composite approach make it possible to describe the structure of all the family using an unique pair of super space group, i.e. a same 4D symmetry (super space groups : $R\,\bar{3}\,m(00\gamma)0s:P3c1(00\gamma^{-1})$). An original feature concerns the ration g=c1/c2 of the two component lattices which is related to the chemical composition through the relation g=(1+x)/2.

We report here a structural study of three different compounds of formula $Ba_{1+x}[(Na_xMn_{1-x})O_3$ with x≈2/7, 5/17 and 1/3 by single crystal X-ray diffraction. Super space formalism is used to obtain an unified description of the three phases, where the metallic columns are made of the alternation of MnO_6 octahedra and NaO_6 prisms. The insertion of this monovalent Na cation instead of usual divalent ones leads to the stabilization of "exotic" oxidation states ranging from 4.4 to 4.5 for the Mn atoms.

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