s7.m26.p10 **Structural aspects of the metal-insulator transition in BaVS₃.** S. Fagot[1], P. Foury[1], J.-P. Pouget[1], S. Ravy[2], E. Elkaim[2], G. Popov[3], M.V. Lobanov[3], M. Greenblatt[3], M. Anne[4], *[1]Laboratoire de Physique des Solides (CNRS-UMR 8502), Université Paris-Sud, Bât. 510, 91405 Orsay, France, [2]Synchrotron SOLEIL, L'Orme des Merisiers, Saint-Aubin - BP 48, 91192 GIF-sur-YVETTE, France, [3]Dpmt of Chemistry and Chemical Biology, Rutgers, State Univ. of New Jersey, Piscataway, NJ08854,USA, [4]Laboratoire de Cristallographie, CNRS, Bât. F, 25 Av. des martyrs, 38042 Grenoble cedex 9, France. E-mail: sylvain.ravy@synchrotron-soleil.fr*

Keywords: Phase transition; Charge-density wave; Charge ordering

This study presents structural transitions of the one dimensional system BaVS₃ at low temperature by means of high resolution synchrotron powder diffraction. At room temperature the structure is hexagonal ($P6_3/mmc$) with face sharing VS_6 octahedral chains along the c axis separated by Ba atoms leading to a V-V intrachain distance of 2.808(1)Å and an interchain distance 6.714(1)Å. The hexagonal structure at room temperature becomes orthorhombic ($Cmc2_1$) at 240K with a V straight chains transformed into uniform zigzag but without significant change in the electronic properties. At 70K a metal-insulator transition occurs with the appearance of a superstructure which doubles the chain periodicity. The structure refined at 40K revealed a weak monoclinic distorsion (β= 90.046(1)°) with 4 nonequivalent V sites. A valence bond analysis shows no evidence for charge disproportion on these sites. However at 5K, the faces of the VS6 octahedra are stretched (site V1) or compressed (V3) inducing a 0.5e- charge disproportionation between the V1 and V3 sites.

s8.m27.p1 **Towards an understanding of molecular crystals from powder X-ray diffraction techniques.** Eugene Y. Cheung, Andrew J. Hanson, Scott Habershon, Fang Guo and Kenneth D.M. Harris, *School of Chemistry, Cardiff University, PO Box 912, Cardiff CF10 3TB, UK. E-mail: eyc@struct.chem.cf.ac.uk*

Keywords: Powder X-ray diffraction; Structure solution; Molecular crystals

With the advances of direct space strategies for structure solution from powder data [1,2], and in particular the success of the Genetic Algorithm method [3,4], a fundamental question on what structural information can be extracted from the diffraction data of increasingly poor diffraction data must be addressed. Structural problems which have the complexity of more than one molecule in the asymmetric unit present new challenges to powder X-ray diffraction [5], and recent developments in the structure solution of complicated structures using powder diffraction techniques will be highlighted [6].

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