

Poster Presentations

[MS14-P05] **The commensurately modulated structure of trimethyltin hydroxide at 220 K.** Somnath Dey, Andreas Schönleber and Sander van Smaalen,

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Trimethyltin hydroxide has been reported to crystallize at room temperature in a $2\mathbf{a} \times 2\mathbf{b} \times 8\mathbf{c}$ superstructure of a fictitious basic structure [1,2]. This superstructure has monoclinic \mathbf{b} -unique symmetry with space group Pn [1]. At $T = 120$ K the structure has been reported to be a disordered on a $1\mathbf{a} \times 1\mathbf{b} \times 2\mathbf{c}$ supercell in space group $P2_1/c$ [2]. Temperature-dependent single-crystal X-ray diffraction experiments at the HASYLAB/DESY (Hamburg, Germany) were performed to search for weak superstructure reflections, to perform full data collection and to explore the crystal structures between room temperature and $T = 100$ K. At $T = 220$ K superstructure reflections along \mathbf{a}^* and \mathbf{b}^* are not observed and superstructure reflections upto fourth order are found along \mathbf{c}^* . They can be indexed with a commensurate modulation wavevector $\mathbf{q} = (0, 0, \sigma_3)$ with $\sigma_3 = 3/8$. We thus propose a $1\mathbf{a} \times 1\mathbf{b} \times 8\mathbf{c}$ superstructure. Strong diffuse scattering is present in the $(\mathbf{a}^*, \mathbf{b}^*)$ planes defined by main reflections which reflects strong disorder in the crystal structure. The eightfold superstructure at $T = 220$ K is described in $(3 + 1)$ -dimensional superspace with orthorhombic superspace group $P2_1mn(00\sigma_3)0s0$ with disorder of hydroxy and methyl groups.

[1] N. Kasai, K. Yasuda, R. Okawara, *J. Organomet. Chem.* **3** (1965) 172–173.

[2] K. M. Anderson, S. E. Tallentire, M. R. Probert, A. E. Goeta, B. G. Mendis, J. W. Steed, *Cryst. Growth Des.* **11** (2011) 820–826.

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