HMT-Resorcinol: An Example of Modulated Structure in Substituted HMT Adducts

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Hexamethylenetetramine (HMT) has a tendency to create modulated structures when forming adducts with hydroxyl moieties. Many examples have been reported recently [1], [2], [3], [4], [5]. We report here a model of the incommensurately modulated structure of HMT-Resorcinol solved at room temperature, in the superspacegroup Xmcm(0b0)s0s (where the X centering corresponds h+k+m=2n). The model consists mainly in an occupation modulation of the Resorcinol, which can adopt two different positions related by a mirror plane. This compound undergoes a lock-in phase transition of second order at about 278K yielding a commensurate structure. X-ray diffraction data have been collected at 120K, with LT cell parameters related to the room temperature ones by $(\mathbf{a}_{LT}=\mathbf{a}_{RT}, \mathbf{b}_{LT}=2\mathbf{b}_{RT}, \mathbf{c}_{LT}=4\mathbf{c}_{RT})$. A comparison of the supercell model and a commensurate model derived from the superspace formalism will be presented.

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