

Re-investigation of the incommensurate structure of HMT-Resorcinol in superspace

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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 Cmcn. 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 $k \approx n+1/3$ were observed, they were not taken into account. Finally, a new investigation was published [3], describing the structure in the centrosymmetric space group Cmcn. 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 $q=0a^*+0.37b^*+0c^*$. 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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[2] M.M.Mahmoud (1979) *Acta Cryst.* B35.2370-2374

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