

MS23-P06 | ON THE PUZZLING CASE OF SODIUM SACCHARINATE 1.875-HYDRATE: STRUCTURE DESCRIPTION IN (3+1)-DIMENSIONAL SUPERSPACE

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Sodium Saccharinate hydrate is an artificial sweetener. Despite its extensive use in the food industry, its structure has been first reported relatively recently [1,2]. The reason for that may be the unusual complexity of this solid phase. It comprises a large unit cell in $P2_1/n$ space group with $Z'=16$. However, a considerable pseudosymmetry can be noted hinting that this high- Z' structure can be described in a higher dimensional space.

In this study superspace approach has been used to describe Sodium Saccharinate 1.875-hydrate structure in (3+1)-dimensional superspace. Reconstruction of the hkl planes in the reciprocal space indicates for an 8-fold substructure in a base-centered lattice. Examination of the raw diffraction data has revealed commensurability of this modulated structure which has been later proven also during the refinement. The structure has been described in the superspace group $C2/c(0, \frac{1}{4}, 0)s0$ with $Z'=2$. Unit cell parameter b is $\frac{1}{4}$ of that of the supercell structure in $P2_1/n$. The other parameters being equal to those of the 3-dimensional structure description. In addition to positional modulation there is also a complex occupational modulation present in a crenel function fashion.

[1] Naumov P., Jovanovski, G., Grupce, O., Kaitner, B., Rae, A. D., Ng, S. W. *Angew. Chem. Ed.*, 2005, 44, 1251

[2] Banerjee, R., Bhatt, P. M., Kirchner, M. T., Desiraju, G. R. *Angew. Chem. Ed.*, 2005, 44, 2515