***Ab-intio* Structure Determination of a Metal Complex from Laboratory X-ray Powder Data**

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The crystal structure of Praseodymium tartrate, $Pr(C_4H_4O_6)_2.H_2O$, has been determined *ab initio* from laboratory X-ray powder diffraction data. Diffraction data were collected using monochromatized Cu Kα1 radiation (λ=1.5406Å) in the 2θ range 7.00-86.26º with a step width 0.02º and Bruker D8 Advance X-ray powder diffractometer. Indexing of the pattern was carried out using the program *NTREOR*. The solution with highest figure of merit [M_{20}=47.0, F_{20}=100.0] in the orthorhombic system having a=21.98(4), b=7.59(3), c=5.96(3) Å, agreed with the possible solutions obtained from the *DICVOL91* and *TREOR90* programs. Fitting the pattern with different possible space groups and a pseudo-Voigt function for the peak shape, the integrated intensities of 498 reflections were extracted based on the best fitted space group $P2_12_12_1$ using the program *TOPAS*. The position of the heavy atom was found from the Patterson map calculations. Attempts to build the structure with successive Fourier method were not successful. Finally the direct space approach using the program *FOX* with different input options led to a model structure containing one Praseodymium, two tartrate ions and one water molecule in the asymmetric unit. Rietveld refinement of the model structure with restraints using the program *EXPO2004* converged to Rp = 0.088, Rwp = 0.113, Re = 0.074 and GoF = 1.543, respectively. The final structure reveals that the Praseodymium atom is coordinated by nine O atoms of the ligands lying in the range 2.30 to 2.95 Å.

Keywords: ab-initio powder structure determination, direct space method, Rietveld refinement