

**A PDF-4 ORGANICS 2006 APPLICATION NOTE
CALCIUM TARTRATE TETRAHYDRATE WINE CRYSTALS**

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White crystals isolated from the bottom of a glass of red wine were identified as calcium tartrate tetrahydrate while the powder pattern was being measured, by a 3-line "long line" search in the PDF-4 Organics 2006. The crystal structure was refined using the Rietveld method, and the hydrogens were located by a quantum chemical calculation (which was also used to quantify the hydrogen bonding). The accuracy and precision of the structural parameters were nearly as good as those of the three single crystal refinements of this structure. Comparing bond distances, angles, and torsions to those obtained from MOGUL and bond valence calculations provides good tests of the chemical reasonableness of the refined structure. The utility of the various sorts of Rietveld plots in determining the quality of the refinement is discussed. An improved powder pattern of calcium tartrate tetrahydrate has been generated and submitted to the PDF.