

**DIFFERENCES BETWEEN NEAR-SURFACE AND BULK PREFERRED
ORIENTATION WITH POWDER DIFFRACTION DATA OF
MOLYBDITE (MOO₃) AND CALCITE (CACO₃)**

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Correcting of crystallographic preferred orientation in crystalline materials is of critical importance in powder diffraction analysis - for structure refinements and in the determination of bulk descriptors such as phase composition. A comparative evaluation of the March and the generalized spherical harmonic preferred orientation models using X-ray powder diffraction data for undiluted (100%) and diluted (50% by weight silica gel) molybdate (MoO₃) and calcite (CaCO₃) powders uniaxially-pressed at five different pressures was originally conducted by the authors. It was shown that as the uniaxial pressure (and, therefore, the level of preferred orientation) increases, the refinements for the diluted powders all provided lower preferred orientations compared with those undiluted samples; and the generalized spherical harmonic description generally provided superior figures-of-merit compared with the March model results [Sitepu, O'Connor and Li. (2005). *J. Appl. Cryst.* **38**, 158-167; Sitepu. (2009). *Powder Diffr.* **24**, 315-326]. In the present study, the generalized spherical harmonic description has been extended to determine the preferred orientation of the same undiluted molybdate (MoO₃) and calcite (CaCO₃) powders uniaxially pressed at five different pressures. Subsequently, a combined neutron and X-ray structural refinement was conducted to determine the differences between near-surface and bulk preferred orientation with the same undiluted samples.