

USE OF THE RIETVELD METHOD FOR DESCRIBING STRUCTURE AND TEXTURE IN X-RAY DIFFRACTION DATA OF HUNTITE [CaMg₃(CO₃)₄], DOLOMITE [CaMg(CO₃)₂] AND MAGNESITE [MgCO₃] POWDERS

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Crystallographic preferred orientation, *i.e.* texture in crystalline materials, is a common feature of experimental powder diffraction patterns and can cause serious systematic errors in both quantitative phase analysis and crystal structure determination. Recently, the author reviewed the mathematics of two commonly used models for preferred orientation — the March-Dollase and the generalized spherical-harmonic models, and applied each individually to X-ray diffraction data [Sitepu *et al.* (2005). *J. Appl. Cryst.* **38**, 158-167] and neutron diffraction data [Sitepu. (2002). *J. Appl. Cryst.* **35**, 274-277; Sitepu. (2009). *Powder Diff.* **24**, 315-326] from uniaxially pressed molybdate (MoO₃) and calcite (CaCO₃) powders in Rietveld analyses. The results indicated that the generalized spherical-harmonic (GSH) description provided better Rietveld fits than the March model for the molybdate and calcite, and therefore, the GSH description was recommended for correction of preferred orientation in X-ray and neutron diffraction analysis for both crystal structure refinement and quantitative phase analysis.

In the present study, the GSH description has been extended to describe crystal structure and texture in X-ray diffraction data of the as-received powders, as well as the uniaxially pressed huntite [CaMg₃(CO₃)₄], dolomite [CaMg(CO₃)₂] and magnesite [MgCO₃] powders. Then, the structural refinement parameters along with the cation-oxygen distances results obtained from the Rietveld refinement with the GSH description will be compared with the corresponding single crystal structures and distances. Additionally, the present study will describe the general applicability of GSH description with particular reference to X-ray diffraction data of overlaps peaks and/or highly oriented huntite, dolomite and magnesite specimens. Finally, quantitative phase analysis from X-ray powder diffraction data of mixtures of huntite, dolomite and magnesite using the Rietveld method will be described.