

Leverage analysis and structure refinement of minerals

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ABSTRACT

Leverage analysis allows detection of the reflections that have the greatest influence on the estimate of a refined variable. We have applied leverage analysis in the structure refinement of some rock-forming minerals, in the attempt of settling the best procedures to obtain accurate and reliable results. Attention has been focused on those variables (e.g., the refined site-scatterings) which are fundamental to the determination of site populations, which in turn are the basis for the study of order-disorder processes and petrogenetic modeling. A garnet (pyrope) and an amphibole (tremolite) were used to test the procedure, being illustrative of different symmetries and structural complexity. As the omission of reflections with high leverage on a particular variable may strongly decrease the accuracy in its estimate, the results indicate that systematic procedures for data truncation [either on the basis of (low or high) $\sin \theta/\lambda$, high $\Delta F/\sigma F_o$ or of low I/σ_I] are potentially dangerous.

The choice of a correctly ionized model is shown to be critical to obtain accurate estimates of the refined site-scatterings. The set of reflections with the highest leverage value with respect to a peculiar group of variables was found to be nearly invariant within isomorphous solid-solutions; this implies that the results of this work are valid throughout the amphibole and garnet compositional spaces. The warnings proposed to the treatment and refinement of X-ray diffracted data may be of general utility in the structure refinement of minerals.