

## **Determination of site population in olivine: Warnings on X-ray data treatment and refinement**

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### **ABSTRACT**

Leverage analysis enables identification of reflections with the greatest influence on the estimate of each refined variable, and thus may be an important tool to improve standard structure-refinement procedures, especially in the case of minerals with complex composition. In this work, leverage analysis was used to investigate in detail the influence of each reflection in high-resolution X-ray diffraction data collected from olivine, a mineral often used to model order-disorder processes and to calculate temperatures of closure and cooling rates of host rocks. Particular attention was paid to the estimate of the scattering power at the cation sites, that are crucial for the above studies. Various procedures for data correction and refinement were also investigated, and the different possible choices were compared to choose the strategy that provides the best results.

The presence of high-leverage weak reflections in olivine strongly suggests that systematic data truncation according to intensity threshold should be avoided. The estimates of the site-scatterings obtained under the different conditions tested are very close (always  $\leq 3 \sigma$ ); they are often smaller than those which may be obtained from electron-microprobe analysis under different experimental conditions or on inhomogeneous (zoned) crystals. Chemical data should thus not be routinely used to constrain the refinement procedure and/or to optimize final site-populations, provided that appropriate errors are given; on the other hand, they are valuable to appreciate the presence and the amounts of very minor, sometimes unexpected, substituents. Our tests show that precision better than 0.001 in site-occupancy determination (sometimes claimed in the literature) is probably not achieved.