

# HIGH-RESOLUTION POWDER X-RAY DIFFRACTION STUDY OF COMPLEX MINERALS

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Synchrotron high-resolution powder X-ray diffraction (HRPXR) data and Rietveld structure refinements were used to examine the crystal structures of many minerals [e.g., quartz, sodalite, tremolite, scapolite, nepheline, etc] and comparison of the results with those obtained from single-crystal X-ray diffraction (SXTL) data was carried out. This comparison indicates that results from the two methods agree quite well, but some important and significant differences occur between the structures obtained by the two methods. The cell parameters obtained by Rietveld refinements using HRPXR data are of superior quality to those obtained by SXTL. This is illustrated by comparison of data across the scapolite series.

Using HRPXR data, weak satellite reflections are sharp and are easily observed. In the case of nepheline, antiphase domains cause unrealistic bond distances for the framework atoms. Using minerals that have similar structure types, we can deduce Al-Si order and site occupancies of the framework T (=Al-Si) atoms.

The  $\langle \text{Si-O} \rangle$  distances in pure  $\text{SiO}_4$  tetrahedron in quartz, sodalite, and tremolite are 1.6081(3), 1.6100(2), and 1.620(1) Å, respectively. These values are affected by interstitial cations. In scapolite  $\text{Me}_{79.6}$ , the average  $\langle \text{T1-O} \rangle$  and  $\langle \text{T2-O} \rangle$  distances are 1.647(1) and 1.670(1), respectively and they indicate that the occupancies are  $(\text{Al}_{0.28}\text{Si}_{0.72})$  for T1 where the atoms are partially ordered and  $(\text{Al}_{0.45}\text{Si}_{0.55})$  for T2 site where the atoms are nearly disordered, based on sodalite Si-O and Al-O distances of 1.6100(2) and 1.7435(2) Å, respectively.