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New insight into crystal chemistry of topaz: A multi-methodological study

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Abstract

The crystal chemistry of a natural topaz [with OH/(OH + F) < 0.5] was reinvestigated by means of laser ablation inductively coupled plasma mass spectroscopy, single-crystal X-ray diffraction (at 298 K) and neutron diffraction (at 298 and 10 K), and polarized infrared spectroscopy to define unambiguously the real symmetry of topaz, the location of the proton and its thermal displacement parameters at room and low temperatures, the hydrogen-bonding and the vibration modes (stretching and bending) of the OH dipole. X-ray and neutron structural refinements allow us to infer that the crystal structure of natural topaz with OH/(OH + F) < 0.5 can be described with the *Pbnm* space group. Violating reflections, found in the previous investigations and in this study, are likely due to Renninger effect (double diffraction phenomenon). The nuclear density Fourier map shows that the proton is located at Wyckoff 8*d* position and the refined coordinates are: $x = 0.495(2)$, $y = 0.252(1)$, $z = 0.1629(7)$. The O-H bond lies on the (010)-plane and forms an angle of about 28.9° with the *c*-axis. Neutron structural refinements at 298 and 10 K show that the displacement ellipsoid of the proton is highly anisotropic. The H-bonding arrangement appears to be complex, with at least four potential H···O/F interactions (distances < 2.38 Å). The topological configuration of the O-H group described by the neutron structural refinements is confirmed by the infrared investigation: the OH stretching mode (at 3640 cm^{-1}) has no component of vibration parallel to the *b* axis (i.e., the O-H direction is perpendicular to [010]). The OH bending mode (at 1161 cm^{-1}) shows components along the three crystallographic axes, which appear to be more prominent along the *a* and *b*-axes. The possible distribution into the crystal structure of topaz of the minor/trace elements found (Na, Ca, Fe Cr, V, Ti, B), and the implied topological effects, is discussed.

Keywords: Topaz, crystal chemistry, plasma mass spectroscopy, X-ray and neutron diffraction, infrared spectroscopy