Orientation of OH dipole and crystal structure in topaz at high temperature

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In this study, The crystal structure and the orientation of OH dipole moment of natural topaz sample [composition, Al2.01Si1.00O4F1.57(OH)0.43; space group, Pbnm] from Gilgit division, Pakistan were determined under high temperature.

The unit cell parameters and X-ray diffraction intensities data were collected at high temperature up to 900C by an imaging plate X-ray diffractometer with rotating anode (MoKa, 50kV, 80mA) using a U-shaped resistance heater (Huber: High temperature attachment 231). The U-shaped resistance heater was calibrated for temperature by melting points of three standard materials (NaNO3: 307C, NaCl: 801C, Au: 1062C), unit cell parameters and alpha-beta phase transition (573C) of quartz. Polarized infrared spectra were measured by Fourier transform infrared spectrometer (FTIR, JEOL: Diamond20 and Perkin Elmer: SPECTRA GX) with a heating stage (Linkam: LK-1500).

Thermal expansion coefficient of the unit cell parameters and volume are alpha a=6.4(7) x10-6C-1, alpha b=5.5(6) x10-6C-1, alpha c=8.1(6) x10-6C-1, and alpha V =2.0(1) x10-5C-1. The results of structure refinement at each temperature point with anisotropic displacement parameters yielded R factors of 2.48, 2.60, 2.56 and 2.70% at 25C, 300C, 600C and 900C, respectively. Focusing attention on around H atom in the crystal structure at high temperature, O-H...O or O-H...F distances have the large thermal expansion coefficients, comparatively. The anisotropy of thermal vibration of the (OH, F) site perpendicular to the direction bonds to Al is showed from thermal vibration ellipsoids. In order to refine the polarized infrared spectra, the absorbance to the polarizer angle for the optical system of our laboratory was formulated. The refinement of obtained polarized infrared spectra by derived formulation shows that the orientation of OH dipole moment at room temperature is inclined about 35 degrees from c-axis in (010) plane. The OH dipole moment changes it's orientation so as to decreases the angle between c-axis with increasing temperature.