

Molecular structure of tangdanite from the Jánská vein, Příbram (Czech Republic) - a vibrational spectroscopy study

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Abstract

We have undertaken a study of the copper arsenate sulphate mineral tangdanite from the Jánská vein, Příbram, central Bohemia (Czech Republic). Tangdanite has been found on a few specimens and forms individual radial aggregates up to 3 mm in size composed of platy crystals with perfect cleavage. Tangdanite aggregates usually grow on chrysocolla, or more rarely on hematitized rock. The quantitative chemical analyses of tangdanite agrees well with the proposed ideal composition and corresponds to the following empirical formula: $\text{Ca}_{1.96}\text{Cu}_{9.01}\text{Zn}_{0.02}(\text{AsO}_4)_{4.06}(\text{PO}_4)_{0.01}(\text{SO}_4)_{0.51}(\text{OH})_{8.76} \cdot 9\text{H}_2\text{O}$ (on the basis of 11 cations *pfu*). Tangdanite is monoclinic, space group *C2/c*, with unit-cell parameters: *a* 54.3218(8), *b* 5.5685, *c* 10.469 Å, β 96.294°, *V* 3147.7 Å³; due to strong preferred orientation on sample, only a parameter was refined. Raman bands at 3486, 3046 and 2907 cm⁻¹ and infrared bands at 3475, 3310 and 3015 cm⁻¹ are assigned to the ν OH stretching of structurally distinct differently hydrogen bonded water molecules and hydroxyls. A Raman band at 1621 cm⁻¹ and infrared bands at 1662 and 1611, 1601 cm⁻¹ are assigned to the ν_2 (δ) H₂O bending vibrations of structurally distinct hydrogen bonded water molecules. Infrared bands at 1120, 1083, 1065 and 1027 cm⁻¹ are assigned to the ν_3 (SO₄)²⁻ antisymmetric stretching and the ν_1 (SO₄)²⁻ symmetric stretching vibrations. Raman band at 997 cm⁻¹ and infrared band at 981 cm⁻¹ are connected with the ν_1 (SO₄)²⁻ symmetric stretching vibration. Infrared band at 946 cm⁻¹ may be connected with (to) the δ M-OH bending vibration. A dominant Raman band at 850 cm⁻¹ is attributed to (with) the ν_1 (AsO₄)³⁻ symmetric and a Raman band at 801 cm⁻¹ and an infrared band at 791 cm⁻¹ to (with) the ν_3 (AsO₄)³⁻ antisymmetric stretching vibrations. Infrared bands at 668 and 610 cm⁻¹ may be connected to libration modes of water molecules and to the ν_4 (δ) (SO₄)²⁻ bending vibrations. A Raman band at 509 cm⁻¹ and an infrared band at 543 cm⁻¹ are assigned to the ν_4 (δ) (SO₄)²⁻ triply degenerate bending vibrations, Raman bands at 467 and 415 cm⁻¹ and infrared bands and shoulders at 481, 465 and 422 cm⁻¹ are connected with the ν_2 (δ) (SO₄)²⁻ bending and to the ν_4 (δ) (AsO₄)³⁻ bending vibrations. Raman bands at 382, 366 and 314 cm⁻¹ may be related to the ν_2 (δ) (AsO₄)³⁻ bending vibrations. A Raman band at 268 cm⁻¹ may be assigned to the ν (O-H×××O) stretching vibration. Raman bands at 171, 154, 127, 92 and 55 cm⁻¹ are assigned to lattice modes. Raman and infrared spectroscopy confirms absence of (CO₃)²⁻ groups in the crystal structure of studied tangdanite.

Key words: tangdanite, unit-cell parameters, chemical composition, Raman spectroscopy, infrared spectroscopy, Jánská vein, Příbram, Czech Republic

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