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# Hydrogen-bond and cation partitioning in muscovite: A single-crystal neutron-diffraction study at 295 and 20 K

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## Abstract

The crystal chemistry of a pegmatitic Fe-bearing muscovite (with FeO ~5.1 wt%) from Val di Crana, Arvogno (Verbania, Nothern Italy) has been investigated by means of wavelength-dispersive X-ray spectroscopy and constant-wavelength [$\lambda$ = 0.9462(2) Å] single-crystal neutron diffraction at 295 and 20 K ($2\theta_{max}$ = 90°). The structure refinement at 295 K shows no significant deviation from the full occupancy of the K site (using the scattering length of potassium alone), and a disordered Si/Al-distribution in the two independent tetrahedral sites (i.e., T1 and T2) and Fe/Al-distribution in the M2 octahedral site. The difference Fourier map of the nuclear density shows that only one independent H site occurs in the muscovite structure, at both room and low temperature. No evidence of disorder in two sub-sites, as observed in a previous study, was found. The thermal displacement of the H site is here described anisotropically. A trifurcated hydrogen bonding scheme was found: the O6-H bond distance corrected for "riding motion" is ~0.984 Å at 295 K, and three significantly weak hydrogen bonds to the O atoms O2, O4, and O6 occur, with H···O2 = 2.635(5), H···O4 = 2.657(4), and H···O5 = 2.647(4) Å and O6-H···O angles all similar in value (~138°). The structure refinements show that the structure configuration of muscovite is maintained at least down to 20 K: the cation disordering in the tetrahedral and octahedral site and the H-bonding scheme are preserved. The structural evolution induced by decreasing temperature is governed by the contraction along a direction perpendicular to (001), mainly due to the compression of the "inner" K-O bonds, which leads to an increase of the tetrahedral rotation angle ($\alpha$) of the six-membered ring. A further effect in response to lowering the temperature is a significant reduction of the magnitude of the thermal displacement parameters.

**Keywords:** Muscovite, crystal chemistry, single-crystal neutron diffraction, hydrogen bonding