Reasons for reduction of perfect symmetry on the example of rondorfite

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In our study the molecular structure of the magnesium silicate chlorine mineral rondorfite about empirical formula $Ca_8Mg(SiO_4)_4Cl_2$ has been investigated by the infrared and Raman vibrational spectroscopy and XPS measurements. The structure of rondorfite was refinement using powder and single crystal X-ray analysis and also has been carried out the fluorescence measurements on the solid state of this mineral.
Rondorfite is the mineral, which belong to a group of silicate. The orange brown various was first discovered at the Bellberg volcano in Germany and analyzed by us, sample of rondorfite comes from the Upper Chegem volcanic structure from Russia [1]. This mineral forms anhedral grains sizes up to 0.3mm, crystallized in a cubic structure and space group is $Fd\overline{3}$.
The Raman measurements have been carried out on the grain in the section using a Nicolet Almega XR Dispersive Raman equipped with a 780nm diode laser at 50x objective. The spectra were accumulated in the range between 100 and 3600cm^{-1}. The infrared transmittance spectra were measured on the powder material using BioRad FTS-6000 spectrometer, a standard source and DTGS Peltier-cooled detector in the range 380-4000cm^{-1}. X-ray photoelectron spectroscopy (XPS) was performed on the single 10μm crystal using multi-technique electron spectrometer; model PHI 5700/660 from Physical Electronics. Measurements were made using monochromator Al Kα radiation (1486.6eV) with energy resolution of about 0.1eV.
The infrared and correspond Raman bands attributed to M-OH or SiOH stretching vibrations of OH units are observed in the 3700-3200cm^{-1} range and deformation modes are found out in the 1800-1300cm^{-1} range. In turn, infrared and Raman bands connected to the water molecule stretching vibrations are observed in the 3200-2800cm^{-1} range [2]. XPS studies confirm that the hydroxyl units and water molecules are present in the structure of rondorfite. The presence these groups might indicate to the lower crystallinity than originally expected based on the ideal chemical pattern [3]. Distortion of the structure provide to the phenomenon of fluorescence. The observation of hydroxyl bands and weakly water molecules indicate to the concept that the empirical formula of rondorfite is not so, as microprobe analysis originally shown
$(Mg_{0.90}Al_{0.04}Fe^{3+}_{0.04}Ti^{4+}_{0.02})_{\Sigma1}(Ca_{7.99}Na_{0.01})_{\Sigma8}(Si_{3.97}Al_{0.03})_{\Sigma4}O_{16.06}Cl_{1.96}$ but as
$(Mg_{0.90}Al_{0.04}Fe^{3+}_{0.04}Ti^{4+}_{0.02})_{\Sigma1}(Ca_{7.99}Na_{0.01})_{\Sigma8}(Si_{3.97}Al_{0.03})_{\Sigma4}O_{16.00}(Cl_{1.96}[OH]_{0.04})_{\Sigma2} \cdot xH_2O$.

References:
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