

Geochemical, MCX and neutron diffraction in situ analyses of high OH blue topaz, Padre Paraíso (BR)

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The aim of this work is to deeply investigate the role of OH/F substitution in topaz. We focused on the crystal structure and crystal chemistry of natural (OH,F)-topazes occurring in Padre Paraíso municipality (PadPar), Minas Gerais State (Brazil) combining the potentiality of both synchrotron and neutron facilities. Solid and biphasic inclusions have been observed as well as a high R.I. Temperature-dependent variation of the unit cell parameters upon heating were set in the 298-1300K temperature range. On the basis of the neutron diffraction data, the F-amount gives rise to ~1.03 a.p.f.u. so the chemical composition can be inferred as $\text{Al}_{1.92}\text{Si}_{0.96}\text{O}_4\text{F}_{1.032}\text{OH}_{0.968}$ ($\text{OH}/(\text{OH}+\text{F})=0.484$). The fluorine content (10.94%wt) appears to be in very good agreement with that measured by means of SEM-EDAX (9.98%wt). Unit-cell parameters increase at increasing temperature (up to 1010K), indicating that the thermal expansion is the dominant mechanism at this stage of the experiment. Above this temperature, this trend suddenly changes as result of the structural modifications induced by the fluorine departure. A rapid decomposition of the the main diffraction peaks associated with the topaz is reported at 1181° K and a second phase appeared to grow. This reveals the topaz transformation in mullite. At 1272°K Rietveld refinement indicated ~30 and 70% in weight of topaz and mullite, respectively. At the same time, the fluorine content goes from 0.768 to 0.63 a.p.f.u The fluorine fugacity [expressed as the ratio $\log(f\text{H}_2\text{O}/f\text{HF})$] of possible fluids (or H₂O-F saturated silic melt) indicated that PadPar topaz was stabilized by H₂O saturated fluids- a H₂O saturated peraluminous, low-Ca compositions melt/fluid(s) with F contents not exceeding 1 wt% [1].

[1] Lukkari *et al.*(2007) *Contrib. Mineral. Petrol.*, 153, 273-288