

phlogopite-tetraferriphlogopite series it also leads to the displacement of tetrahedral cation from the apical oxygen in direction of the geometrical centre of tetrahedron. The decreasing of tetrahedron length along c^* and approaching its form to the ideal one in the structure of end tetraferriphlogopite are observed. The tetrahedral rotation angle α changes from 8.97° in phlogopite to 11.75° in end tetraferriphlogopite. In the structure of tetraferribiotite the distortion of individual tetrahedron along with tetrahedral sheet ($\alpha=8.96^\circ$) is similar to that observed in phlogopite structure.

Interlayer cation. In all the structures due to the large ditrigonal distortion the coordination of interlayer cation approaches to an octahedral group. In the tetraferriphlogopite the inner oxygens ($K-O_{in}=2.932 \text{ \AA}$) are closer than in phlogopite (2.969 \AA). The height of interlayer space increases from 3.446 \AA (phlogopite) to 3.461 \AA (tetraferriphlogopite). In tetraferribiotite structure $K-O$ bond length with inner oxygens is 2.974 \AA .

Octahedral sheet. The larger is the substitution of Al on Fe in tetrahedra the larger are the degree of flattening of octahedral sheet ($h_o=2.164 \text{ \AA}$, $\psi=58.6^\circ$; $h_o=2.146 \text{ \AA}$, $\psi=59.0^\circ$ in phlogopite and tetraferriphlogopite respectively) and its ensharing edges from 3.074 \AA in phlogopite to 3.097 \AA in tetraferriphlogopite. The distortion of octahedral sheet in tetraferribiotite is similar to that in phlogopite structure. The positional parameters of H atom were obtained from difference Fourier map. In all structures the O-H axis is normal to (001).

tings of 25 reflections with high θ -angle:

	Thulite	Piemontite
a [Å]	16.2051(37)	8.8739(11)
b [Å]	5.5488(12)	5.6156(8)
c [Å]	10.0329(18)	10.1484(13)
β [°]	90.0	115.488
S.G.	Pnma	$P2_1/m$

For thulite (corresponding piemontite values in parentheses) a total of 2142 (3027) reflections were collected, for the idiomorphic thulite crystal an absorption correction gave minimum and maximum transmission factors of 0.858 and 0.908, the piemontite data were not corrected for absorption because of the irregular shape of the crystal fragment. The programs SHELX (Sheldrick, University of Cambridge, 1976) and RFINTE (Finger and Prince, Natl. Bur. Stand. (U.S.) Tech. Note 854, 1975) were used for the refinement which included the variation of anisotropic temperature factors and of occupancy factors of possible M^{3+} -sites and resulted in residuals of 0.037 (0.029) for 1456 (2462) observed reflections. The chemical compositions obtained from EMP-analyses were used as a constraint for the site occupancy refinement, which in the case of thulite led to an Al-content of 7.96(3) atoms in the 8-fold M(1,2) position and of 3.47 in the 4-fold M(3) position. Al-distribution in piemontite is 3.80(2), 3.91(2) and 2.00 atoms in the three 4-fold positions M(1), M(2) and M(3). As expected for the piemontite structure most M^{3+} atoms are situated in the M(3) position but significant amounts are also present in M(1) and M(2), a result which confirms the interpretation of the ν_{OH} -bands in synthetic piemontites with $p>1.0$ Langer et al., Z. Krist. (1976) 144, 334).

08.4-42 CRYSTAL STRUCTURE REFINEMENTS OF COEXISTING THULITE AND PIEMONTITE, $Ca_2Al_3-pM^{3+}[OH/O/SiO_4/Si_2O_7]$ ($M^{3+}=Mn^{3+}+Fe^{3+}$).

By E. Tillmanns, Univ. Mainz, K. Langer and R. Arni, TU Berlin and K. Abraham, RU Bochum

Coexisting thulite (Mn^{3+} orthozoisite) and piemontite from Lom/Norge have been analysed by microprobe (EMP) and structurally refined with the following aims:

(i) evaluation of the inter- and intra-crystalline partitioning of $M^{3+}=(Mn^{3+}+Fe^{3+})$, and (ii) solution of the discrepancy between the spectroscopic results of Burns and Strens (Mineral. Mag. (1967) 36, 204), i.e. $M(3) \gg M(2) \gg M(1)$ in piemontites and structural results of Dollase (Am. Min. (1968) 53, 1882) who found $M(3) \gg M(1) \gg M(2)$.

Optically clear, inclusion-free crystals with homogeneous and sharp optical extinction were selected for data collection. EMP-results on these crystals (Cameca Camebax, Program MISO) yielded the crystallochemical formulae:

Thulite (TUPILA 19-Thu2)

$(Ca_{1.970}Mg_{0.002}Zn_{0.010})^{[7-8]}(Al_{2.857}Mn^{3+}_{0.030}Fe^{3+}_{0.096}Cu^{2+}_{0.009})^{[6]}[OH/O/SiO_4/Si_{2.018}O_7]$

Piemontite (TUPILA 19-Pie 1)

$(Ca_{1.975}Mg_{0.012}Zn_{0.008})^{[7-8]}(Al_{2.428}Mn^{3+}_{0.143}Fe^{3+}_{0.432}Cu_{0.014})^{[6]}[OH/O(SiO_4/Si_{1.994}O_7)]$

Lattice constants were refined from the set-

08.4-43 THE CRYSTAL STRUCTURE OF NEW MINERAL FROM DELCHAEILITE FAMILY AND THE CRYSTAL CHEMISTRY FEATURES OF TR-SILICATES. By K.G.Ragimov, M.I.Chiragov. The Institute of Inorganic and Physical Chemistry Academy of Sciences of the Azerbaijan SSR and The Azerbaijan State University, Baku, USSR.

The structure of K-delchaelite discovered in the Khibina massif of the USSR has been determined by single-crystal X-ray analysis. K-delchaelite- $K_4Na_2[Ca_2(Si_6Al_2O_{19})(F,Cl)_2]H_2O$ is orthorhombic with $a=6.598(2)$, $b=24.655(2)$, $c=7.080(2) \text{ \AA}$, space group $Pn2_1m$, $z=2$. The structure was refined up to $R=0.07$. The structure is similar to that of delchaelite- $K_3Na_2[Ca_2(Si,Al)_8O_{19}(F,Cl)_2]$. The crystal structure consists of layers formed by the Ca- and Na-polyhedra parallel to (010), which is held together by the doubled sheets of tetrahedra with the formula $(Si_6Al_2)O_{19}$. The formation of these doubled sheets may be considered as a condensation of the wollastonite chains and additional Al_2O_7 groups. Atoms K and molecules H_2O are localized in the mixed framework cavities.

The crystal structure of monteredgianite - $K_2Na_4Y_2Si_{16}O_{38} \cdot 10H_2O$ is closely related to that of delchaelite. Monteredgianite is orthorhombic with $a=2x7.02$, $b=23.91$, $c=2x6.598 \text{ \AA}$, space group $Bmab$. This structure is very probably based on a mixed framework made up of delchaelite (Si_8O_{19}) sheet and octahedrally coordinated Y and Na. It is supposed that iso-