

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 tetraferriphlogopite 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 tetraferriphlogopite 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 tetraferriphlogopite 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 [\AA] | 16.2051(37) | 8.8739(11) |
| b [\AA] | 5.5488(12) | 5.6156(8) |
| c [\AA] | 10.0329(18) | 10.1484(13) |
| β [$^\circ$] | 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, $Ca_2Al_3-pM^{3+}[OH/O/SiO_4/Si_2O_7]$ ($M^{3+}=Mn^{3+}+Fe^{3+}$).

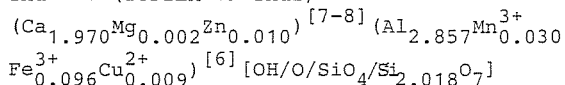
By E. Tillmanns, Univ. Mainz, K. Langer and R. Arni, TU Berlin and K. Abraham, RU Bochum

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

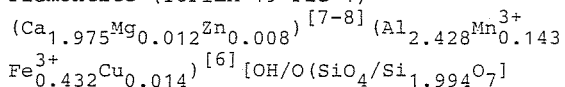
(i) evaluation of the inter- and intra-crystalline partitioning of $M^{3+}=(Mn^{3+}+Fe^{3+})$, and (ii) solution of the discrepancy between the spectroscopic results of Burns and Strens (Mineral. Mag. (1967) 36, 204), i.e. $M(3) \gg M(2) \gg M(1)$ in piemontites and structural results of Dollase (Am.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



Piemontite (TUPILA 19-Pie 1)



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-

morphous replacement of $2Ca \rightleftharpoons Na^+Y^{3+}$ takes place. The large cavities in this framework are occupied by K, Na and H_2O , which are most probably responsible for pseudo-cell. K-delchaelite is the first known member of the delchaelite family, the end member of which is hydrodelchaelite. The mentioned and related TR-, Ca- silicates are given.

Fe-bearing hornblendes ($0.75 \leq X_{Fe^{2+}} \leq 0.85$) have the highest value of ΔV_{mix} ($\sim 4 \text{ cm}^3/\text{mol}$).

The behaviour of structural characteristics and molar volumes of natural solid solutions Ca-rich pyroxenes and amphiboles allows to make some critical estimations of given in literature calculations of excess thermodynamical mixture functions of solid solutions of the same composition.

08.4-44 CRYSTAL STRUCTURES OF NATURAL SOLID SOLUTIONS OF Ca-RICH PYROXENES AND AMPHIBOLES. By A.V.Maslenikov, Institute of Precambrian Geology and Geochronology USSR Academy of Sciences, nab. Makarova, 2, Leningrad 199164 USSR.

The structures of four natural Ca-rich pyroxenes of diopside-hedenbergite series (with Fe^{2+} content from 0.04 up to 0.81 per form. unit) have been refined. The nonadditive variation in M1-O and M2-O distances and their relationship with Fe^{2+} content are determined. Deviation from Vegard's law is negative. Unit cell parameters of the natural pyroxenes of the same composition are calculated on the X-Ray powder diffraction data. Concentration relationship of the molar volume is similar to variation of structural characteristics and shows the nonideality of natural solid solutions of Ca-pyroxenes. Maximum value of ΔV_{mix} is equal to $-0.5 \text{ cm}^3/\text{mol}$ when $0.25 \leq X_{Fe^{2+}} \leq 0.4$ per form. unit.

Values of molar volumes of 120 natural amphiboles of isomorphous series tremolite-ferroactinolite (Al_{IV} content up to 0.10 and R_{YI}^{3+} up to 0.05 per form. unit), actinolitic hornblende (Al_{IV} up to 0.75, R_{YI}^{3+} up to 0.20 per form. unit) and hornblende are calculated on the X-Ray powder diffraction data. Concentration relationship of molar volume of natural amphiboles has the positive deviation from Vegard's law that indicates the nonideality of this solid solutions. The samples of

08.5-1 THE MAGNETIC STRUCTURE OF FAYALITE FROM ^{57}Fe MÖSSBAUER RESONANCE. By G. Amthauer¹, H. Fuess², S.S.Hafner¹ and W.Lottermoser² Institut für Mineralogie der Universität Marburg¹ and Institut für Kristallographie und Mineralogie der Universität Frankfurt², W.Germany

Fayalite Fe_2SiO_4 (Pnma) is antiferromagnetic below $T_N=65K$. Two somewhat different magnetic structures were reported (Cox et al., Abstracts Am.Cryst.Assoc.Meet. (1965) 47; Santoro et al., J. Phys. Chem. Solids (1966) 27, 655). We studied the magnetic Mössbauer spectra of ^{57}Fe in a powdered single-crystal fragment of synthetic fayalite at 5.5 and 40K. The spectra were fitted by a direct solution of the Hamiltonian for the ^{57}Fe magnetic and electrostatic interactions, using the least-squares procedure. The assignment of the two subspectra to 4a and 4c is possible from the somewhat different temperature dependence of the ^{57}Fe quadrupole interaction Δ at 4a and 4c between 5.5 and 700K: $\partial\Delta(4a)/\partial T < \partial\Delta(4c)/\partial T$. The values obtained from the fits of the spectrum at 5.5K are (the first value corresponds to 4a, the second one to 4c): 320 and 117 kOe for the local magnetic field H_{eff} , +3.09 and +3.04 mm/s for Δ and 0.19 and 0.75 for the asymmetry parameter η ; at 40K we got 152 and 72 kOe for H_{eff} , +3.08 and +3.01 mm/s for Δ and 0.26 and 0.83 for η . The values for 4a are in good agreement with the previous data of Kündig et al. (J.Appl.Phys. (1967) 38, 947). However, at 4c we find a small inclination θ between H_{eff} and the eigenvector Z of Δ of 5-8 degrees. This is inconsistent with the crystallographic space group Pnma which was assumed by Kündig et al. for their early spectra ($\theta=0$). The results will be discussed in connection with recent neutron diffraction single-crystal data.