

an intermediate phase of space group  $I4_1/acd$  between  $T_{c1} \sim 910$  K and  $T_{c2} \sim 960$  K. This was further confirmed by a measurement in narrower temperature intervals of the  $c/a$ -ratio (using the (400)-reflexion) showing an abrupt change of the slope at  $T_{c1}$ , as well as by the intensity variation of a superstructure reflexion (503) (extinct in  $Ia3d$ ), which becomes diffuse approaching  $T_{c2}$  from below. These latter reflexions are also visible on X-ray photographs using longer exposure times. Together with these changes there appears a strong increase of the diffuse background in the powder diagrams showing a characteristic modulation, which can be connected with overdamped soft modes at the  $\Gamma$ -point and in  $(\xi\xi 0)$ -directions observed by inelastic neutron scattering (Boysen, Eckold, Symp. on Neutron Scattering, Berlin, 1984). In conclusion the transition is characterized by a rotational rearrangement of (nearly) rigid  $(Si, Al)O_4$ -tetrahedra combined with an ordering of Si and Al, the extent of which is probably due to the rate of cooling and the formation of twins separated by (110)-interfaces.

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08.4-39 COEXISTENCE OF TRIDYMITE POLYMORPHS AND CRISTOBALITE IN TRIDYMITE CRYSTALS. By A. Nukui and O.W. Flörke\*, National Institute for Research in Inorganic Materials, Namiki 1-1, Sakura-mura, Ibaraki, 305 Japan. \*Institut für Mineralogie, Ruhr-Universität Bochum, D-4630 Bochum 1, Germany-B.R.D..

Tridymite is known to have 6 modifications at room temperature. Through the experimental studies under high temperatures and pressures, MC (monoclinic Cc;  $a=17.21$ ,  $b=4.991$ ,  $c=25.83A$  and  $\beta=117.75^\circ$ ), PO-10 (triclinic F1;  $a=17.21$ ,  $b=9.93$  and  $c=81.86A$ ) and MX-2 (monoclinic;  $a=8.6$ ,  $b=15.026$ ,  $c=16.434A$  and  $\beta=91.496^\circ$ ) modifications are suggested to be low-temperature phases (e.g. Nukui et al., J. Mineral. Soc. Japan (1980) 14, 364). A variety of diffraction patterns of tridymite crystals were obtained by the X-ray precession method in this study, which can be explained by some combinations of the three modifications (MC, PO-10 and MX-2) and cristobalite. For these four, 15 combinations are possible; single (4), two (6), three (4) and four phases (1). 13 of them have so far been observed in crystals with different formation conditions. The patterns of MX + cristobalite and MX + PO + cristobalite phases are not observed. Because the three tridymite modifications are superstructures with a common fundamental cell, their stacking direction is parallel to the  $c$ -direction of the high-temperature form of tridymite (Gibbs, Proc. Roy. Soc. London (1927) A113, 351) as well as [111] of cristobalite. These facts can be used to understand: a) the stability relationships between tridymites and cristobalite, b) the polymorphic relationships among them, and c) their coexistence mechanism.

08.4-40 THE CRYSTAL STRUCTURES OF ALKALINE CARBONATES: BARENTSITE, BONSHTEDTITE AND DONNAYITE. By Trinh Thi Le Thi, E.A. Pobedimskaja, T.N. Nadezhina, A.P. Khomjakov. Geological Faculty, Moscow State University, Moscow, USSR.

The structure of barentsite  $Na_7Al(CO_3)(HCO_3)_2F_4$  ( $a=8.806$ ,  $b=6.735$ ,  $c=6.472A$ ,  $\alpha=119.32$ ,  $\beta=97.33$ ,  $\gamma=92.50^\circ$ ,  $Z=1$ ,  $P\bar{1}$ ) is based on brucite-like layers alternating with distorted ones of double columns of Na-octahedra. The hydrogen atom makes connection between neighbouring  $CO_3$ -groups. The structure of bonshtedtite  $Na_3F(PO_4)(CO_3)$  ( $a=8.955$ ,  $b=6.029$ ,  $c=5.149A$ ,  $\beta=89.55^\circ$ ,  $Z=1$ ,  $P2_1/m$ ) consists of complex sheets of Fe-octahedra,  $(PO_4)$ -tetrahedra and Na-polyhedra. The  $CO_3$ -groups connect polyhedra of cations. In the structure of donnayite-like carbonate  $(Na, Y, TR)Sr(CO_3)_2 \cdot H_2O$  ( $a=8.535$ ,  $b=6.818$ ,  $c=5.212A$ ,  $\gamma=109.29^\circ$ ,  $Z=2$ ,  $Pn$ ) Sr has coordination 10, and Na and TR are seven-coordinated. The layers consisting of Sr-polyhedra are alternating with ones of Na, TR-polyhedra and connected with ones other by  $CO_3$ -groups.

08.4-41 THE STRUCTURAL CHARACTERISTICS OF MICAS WITH TETRAHEDRAL IRON CONTENT REGARDING ISOMORPHOUS SUBSTITUTIONS. By T.F. Semenova (a), I.V. Rozhdestvenskaya (b) and V.A. Frank-Kamenetskii (a), Faculty of Geology, Leningrad State University, University Embankment 7/9, Leningrad, USSR (a), NPO "Burevestnik", Stahanovtsev 1, Leningrad, USSR (b).

The structures of three members of isomorphous series of phlogopite-tetraferriphlogopite  $(K_{0.9}Na_{0.1})(Mg_{2.85}Fe_{0.15}^{2+})[Al_{1-x}Fe_x^{3+}Si_3O_{10}(OH)_2]$  (samples 1-3) and tetraferriphlogopite  $(K_{0.9}Na_{0.1})(Mg_{1.64}Fe_{1.37}^{2+})[Al_{0.03}Fe_{0.87}^{3+}Si_3O_{10}(OH)_2]$  (sample 4) have been refined:

	x	a (Å)	b (Å)	c (Å)	$\beta$ (°)	R
1.	0	5.319	9.220	10.288	99.93	0.031
2.	0.45	5.341	9.259	10.297	99.95	0.057
3.	0.85	5.358	9.297	10.318	100.02	0.042
4.	0.87	5.373	9.311	10.306	100.10	0.079

Single crystal investigations were carried out using a X-ray four-circle diffractometer with  $Mo K\alpha$ -radiation. The refinement of the structures was carried out in sp.gr. C 2/m in anisotropic approach. It was determined that  $Al \leftarrow Fe^{3+}$  substitution in tetrahedral sheets significantly influenced upon all the structural parameters of micas. Tetrahedral sheet. The incorporation of large  $Fe^{3+}$  cations leads to the linear increasing of the tetrahedral bond lengths from  $d_t=1.660$  Å in phlogopite structure up to 1.665, 1.680 and 1.676 Å in intermediate, end tetraferriphlogopites and tetraferriphlogopite respectively. In