an intermediate phase of space group \( I4/1/acd \) between \( T_c = 910 \) K and \( T_c = 960 \) K. This was further confirmed by a measurement in narrower temperature intervals of the \( c/a \)-ratio (using the \((400)\)-reflection) showing an abrupt change of the sign at \( T_c \) as well as by the intensity variation of a superstructure reflexion (503) (extinct in \( Ia\overline{3d} \)), which becomes diffuse approaching \( T_c \) 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 explained by the T-point and in \((\xi, 0, 0)\)-directions observed by inelastic neutron scattering (Boyen, Eckold, Symm. on Neutron Scattering, Berlin 1984). The tridymite transition is characterized by a rotational rearrangement of \( (51, A_1)_{0} \) tetrahedra combined with an ordering of \( B_1 \) and \( A_1 \), the extent of which is probably due to the decrease of the rate of cooling and the formation of twins separated by \((11\overline{2})\) interfaces.

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

Tridymite is known to have 6 modifications at room temperature. Through the experimental studies under high temperatures and pressures, \( N_C \) (monoclinic \( C_c \); \( a = 17.21, b = 4.991, c = 25.833 \) and \( \beta = 117.75^\circ \)) \( P_O -10 \) (triclinic \( P_I \); \( a = 17.21, b = 9.93 \) and \( c = 81.868 \)) and \( M_X -2 \) (monoclinic; \( a = 8.6, b = 15.026, c = 16.434 \) 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 \((N_C, P_O -10 \) and \( M_X -2 \)) 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 \( M_X + \) cristobalite and \( M_X + P_O + \) 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] 113, 351) as well as [111] of cristobalite. These facts can be understood: a) the stability relationships between tridymite and cristobalite, b) the polymorphic relationships among these, 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. Pobedinskaja, T.N. K. R. 24, 25, 26, 27, Leningrad, USSR.

The structure of barenitsite \( \text{Na}_3\text{Al}(\text{CO}_3)\hspace{1cm} (\text{HCO}_3)_2 \) \( F_2 \) \( (a=8.806, b=6.735, c=6.472A, \beta=119.32, \gamma=99.73, \alpha=92.50^\circ, \gamma=1, P1) \) is based on brucite-like layers alternating with distorted ones of double columns of Na-octahedra. The hydrogen atom makes connection between neighbouring \( \text{CO}_3 \)-groups. The structure of bontstedtite \( \text{Na}_4\text{F}(\text{PO}_4)\hspace{1cm} \text{CO}_3 \) \( (a=8.955, b=6.029, \gamma=5.149A, \beta=99.55^\circ, \gamma=1, P2_1/m) \) consists of complex sheets of \( \text{Fe}-\)octahedra, \( \text{PO}_4 \)-tetrahedra and Na-polyhedra. The \( \text{CO}_3 \)-groups connect polyhedra of cations. In the structure of donnayite-like carbonate \( \text{Na}_7\text{Y}(\text{PO}_4)\hspace{1cm} \text{Sr}(\text{CO}_3)\hspace{1cm} \text{H}_2\text{O} \) \( (a=8.535, b=6.816, c=5.212A, \gamma=105.28^\circ, \gamma=2, \text{Pn} \) Sr has coordination 10, and Na and TR are seven-coordinated. The layers consisting of Sr-polyhedra are alternating with ones other by \( \text{CO}_3 \)-groups.

The structure of three members of isomorphous series of phlogopite-tetraferriphlogopite \( \text{K}_0\text{Na}_{0.4}(\text{K}_0\text{Na}_{0.4})_4\text{Fe}_{1.37}\hspace{1cm} (\text{Al}_1\text{Fe}_{1.37})\text{Si}_4\text{O}_{10}\text{OH}_2 \) \( (\text{sample } 3) \) and tetraferriphlogopite \( \text{K}_0\text{Na}_{0.4}\hspace{1cm} (\text{K}_0\text{Na}_{0.4})_4\text{Fe}_{1.37}\hspace{1cm} (\text{Al}_1\text{Fe}_{1.37})\text{Si}_4\text{O}_{10}\text{OH}_2 \) \( (\text{sample } 4) \) have been refined:

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Single crystal investigations were carried out using a X-ray four-circle diffractometer with \( \text{Mo } K_{\alpha} \)-radiation. The refinement of the structures was carried out in space group \( \text{C} 2/\text{m} \) in an anisotropic approach. It was determined that \( \text{Al} -\text{Fe}^3+ \) substitution in tetrahedral sheets significantly influenced upon all the structural parameters of minerals. Tetrahedral sheets. The incorporation of large \( \text{Fe}^{3+} \) cations leads to the linear increasing of the tetrahedral bond lengths from \( \text{d}_{4}=1.66A \) in phlogopite structure up to \( 1.665, 1.680 \) and \( 1.695 \) \( A \) in intermediate and tetraferriphlogopites and tetraferriphlogopite respectively.
Phlogopite-tetraferriphlogopite series it also leads to the displacement of tetrahedral cation from the spical 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 is 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 (α=8.96°) 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...=2.932 Å) are closer than in phlogopite (2.969 Å). The height of interlayer space increases from 3.461 Å (phlogopite) to 3.607 Å (tetraferriphlogopite). In tetraferribiotite structure K-O bond length along inner oxygens (K-O...=2.974 Å).

Octahedral sheet. The larger is the substitution of M(1) Fe432cu0.014) into M(1) [1-1,1(1)] and M(2) [2-1,1(2)] in phlogopite and tetraferriphlogopite respectively and its enashing edges from 3.074 Å in phlogopite to 3.097 Å 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).