INORGANIC AND MINERALOGICAL CRYSTALLOGRAPHY

08.4-7

THE INCOMMENSURATELY MODULATED STRUCTURE OF AN ANDESINE An38.

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The modulated structure of the intermediate plagioclase Ca38Na62Al138Si262O8 has been determined by single-crystal X-ray methods. The structure has been refined using general sinusoidal density and displacement waves because main reflections and first order satellites were observable only. Starting values for the amplitudes and phases of the modulation functions have been derived from (3+1)-dimensional Patterson maps (Steurer, W. Acta Cryst., 1987, A43, in the press). Crystal data: super-space group equivalent to P1211 with additional centering translations. a=8.151(3), b=12.829(5), c=14.206(7) Å, a=93.62(3), β=116.21(2), γ=89.70(2)°, U=1329.7 Å³, Z=8, half period of the modulation wave T=26.7(3) Å. The overall wR=0.047, wR=0.044 for 1176 main and wR=0.151 for 2343 satellite reflections. The analysis of the mean T-O bond lengths reveals incomplete Al/Si-ordering on the T-sites. The displacive modulation of the extraframework cations is strongly correlated with the periodic distortion of the framework structure. There is no Ca/Na-substitutional modulation. The modulated structure can be characterized by the sequence An...An...An, where An and An* represent regions with I-anorthite-like structure being in antiphase relation to each other. The disordered boundary zones correspond to the average structure of the andesine. The absence of second order satellites excludes any Al/Si- and Ca/Na-long-range order as An...An...Ab...An*, which can be found in Ca-rich intermediate plagioclases.

08.4-8

POLYTYPISM IN THE HYDROCALUMITE AND RELATED SYNTHETIC PHASES.

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Hydrocalumite is the only natural counterpart of several synthetic compounds with schematic chemical formula Ca32+(OH)12(X.nH2O).4H2O, where M3+ is normally Al but also Fe, Cr and Ga, X is 2Cl-, 2Br-, 2I-, 2(OH)-, 2(NO3)2 or (CO3)2-, (SO4)2-, and n ranges from 0 to 2 depending on the charge of the anion group. The structure consists in main porindantite-like layers (8 Å thick) containing an ordered arrangement of Ca and Al cations in the 2:1 ratio, alternating with intermediate layers containing (X.nH2O). The Al cations are coordinate by six (OH) and one H2O. The layers are linked by interlayer anions through hydrogen bonds of water molecules. The structure has been approximately solved by Ahmed and Taylor (Nature, 1967, 215, 622-623) (X = 2(OH); n=1); space group R 3 2/c; Allmann (N. Jb. Min., Hh., 1968, 160-164) (X= Cl; n=2), R 3; Le Bel and Grassland (Proc. 5th Int. Symp. Chem. Cement, Tokyo, 1968, 70-79, 83), R 3. The first complete solution of a natural hydrocalumite has been made by Sacerdoti and Passaglia (14th Gen. Meet. Int. Min. Ass., Stanford, 1986, 219) (X= 3(CO3)+ Cl, n=0.8), with space group C 2/c for the subcell and P 2/n for the cell (doubling the cell parameter). The difference in space group may be understood if: i) in R 3 (or R 3) space group the structure consists in the superposition of three layers isorotated R, R', R''; ii) in the C 2/c space group the structure consists in the superposition of two layers of type R and L, L being related to R by a 2a axes parallel to the sheet in the interlayer zone. The doubling of the unit cell parameter; iii) R 3 2/c must be due to the superposition of six layers R, L, R', L', R'', L''. The different nets of hydrogen bonds for the two models are discussed.