

08.4-7 THE INCOMMENSURATELY MODULATED STRUCTURE OF AN ANDESINE An_{38} . By W. Steurer and H. Jagodzinski, Inst. f. Kristallographie und Mineralogie der Universität, Theresienstraße 41, D-8000 München 2, FRG.

The modulated structure of the intermediate plagioclase $Ca_{.38}Na_{.62}Al_{1.38}Si_{2.62}O_8$ 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 $P_{I}^{PI}(.080(9), .031(8), -.261(10))$ with additional centering translations. $a=8.151(3)$, $b=12.829(5)$, $c=14.206(7)$ Å, $\alpha=93.62(3)$, $\beta=116.21(2)$, $\gamma=89.70(2)^\circ$, $U=1329.7$ 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 sequel ...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...Ab...An*... which can be found in Ca-rich intermediate plagioclases.

08.4-8 POLYTYPISM IN THE HYDROCALUMITE AND RELATED SYNTHETIC PHASES. By M. Sacerdoti, Istituto di Mineralogia, Università di Ferrara, Ferrara, Italy.

Hydrocalumite is the only natural counterpart of several synthetic compounds with schematical chemical formula $Ca_4M_2^{3+}(OH)_{12}(X.nH_2O).4H_2O$, where M^{3+} is normally Al but also Fe, Cr and Ga, X is $2Cl^-$, $2Br^-$, $2I^-$, $2(OH)^-$, $2(NO_3^-)$ or $(CO_3)^{2-}$, $(SO_4)^{2-}$, and n ranges from 0 to 2 depending on the charge of the anion group. The structure consists in main portlandite-like layers (8 Å thick) containing an ordered arrangement of Ca and Al cations in the 2:1 ratio, alternating with intermediate layers containing $(X.nH_2O)$. The Al cations are coordinate by six (OH), and Ca ones by six (OH) and one H_2O . 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 $R\bar{3}2/c$; Allmann (N. Jb. Min., Mh., 1968, 140-144) (X = (SO_4) ; n=2), $R\bar{3}$; Le Bel and Grasland (Proc. 5th Int. Symp. Chem. Cement, Tokyo, 1968 2, 79-83), $R\bar{3}$. 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 = $\frac{1}{2}(CO_3) + Cl$, n=0.8), with space group $C2/c$ for the subcell and $P2/c$ for the cell (doubling the cell parameter b). The difference in space group may be understood if: i) in $R\bar{3}$ (or $R\bar{3}$) space group the structure consists in the superposition of three layers isooriented R , R' , R'' ; ii) in the $C2/c$ space group the structure consists in the superposition of two layers of type R and L, L being related to R by a diad axes parallel to the sheet in the interlayer zone. $P2/c$ is due to the ordering of anions in the interlayer zone, causing the doubling of the b parameter; iii) $R\bar{3}2/c$ 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.