

Accordingly the crystal was remounted so that [100] became the precession axis, and a series of precession photographs was taken for the levels 0, 1, 2, 3, and 4. The cell edge, computed from measurements on the zero level, was found to be  $a = 10.03 \text{ \AA}$ , as compared with  $10.02 \text{ \AA}$  of LLW.

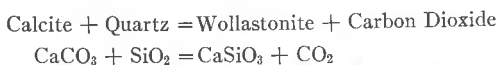
The plane symmetry of each of the levels proved to be  $4mm$ . This information combined with the symmetry  $3m$  of the [111] axis, shows that the diffraction effects of the crystal have symmetry  $4/m \bar{3} 2/m$ , which is consistent with any of the three crystal classes  $4/m \bar{3} 2/m$ ,  $\bar{4}3m$ , or  $432$ . The lattice proved to be face-centered, and there were no extinctions other than those required by the face-centered lattice. This fixes the space group as one of the three  $F4/m \bar{3} 2/m$ ,  $F\bar{4}3m$ , or  $F432$ . The symmetry adopted by LLW was the first of these.

The cell and symmetry of the structure proposed by LLW are therefore consistent with our findings by single crystal methods. It remained to check the particular structure proposed by LLW. This is in space group  $F4/m \bar{3} 2/m$ , with the 36 Fe and Ni atoms distributed at random over equipoints  $4b$  and  $32f$ , with  $x = \frac{1}{8}$ , and the 32 S atoms distributed over equipoints  $8c$  and  $24e$ , with  $y = \frac{1}{4}$ . We computed the amplitudes to be expected from such a structure, squared them, and multiplied by the Lorentz-polarization factor appropriate to the various levels of the precession photographs. These computed intensities were then compared with the degrees of blackness of the various corresponding spots on the precession photographs. All-around satisfactory agreement was found. From this it was concluded that the structure proposed by LLW for pentlandite is essentially correct.

#### A NOTE ON THE CALCITE-WOLLASTONITE EQUILIBRIUM

A. J. ELLIS AND W. S. FYFE, *Chemistry Department, University of Otago, Dunedin, New Zealand.*

The equilibrium pressure and temperature conditions of the reaction:



are important in limiting the conditions of formation of some broad groups of metamorphic rocks. Goldschmidt's original calculations have recently been improved by Danielsson (1) by the application of more recent thermodynamic data. At the time of Danielsson's calculations  $P$ - $V$ - $T$  data for carbon dioxide were not available for much of the region of interest. Kennedy (2) has recently published such data up to 1400 bars and  $1000^\circ \text{ C}$ . and these data have been used to check the calculations further.

Free energies of carbon dioxide from 50 bars to 1400 bars were obtained for each temperature from Kennedy's data by graphical integration using the relation:—

$$G_{(T, P)} = G_{(T, 50 \text{ bars})} + \int_{50 \text{ bars}}^P V_T dP$$

Free energies from 1–50 bars were obtained from the data of Sweigert, Weber and Allen (3).

The equations for  $\Delta G_0$  given by Danielson are correct and were used in the present calculation. The equilibrium pressures were then calculated from the relation:—

$$\Delta G_{(T, P)} = \Delta G_T^0 + \int_1^P V_g dP + \int_1^P \Delta V_s dP$$

Where  $\Delta G_T^0$  is the standard free energy change at temperature  $T$ ,  $\Delta V_s$  is the difference in molar volumes of the solid phases and  $V_g$  the molar volume of carbon dioxide. At equilibrium  $\Delta G_{(T, P)} = 0$ , and using the calculated free energies of carbon dioxide the equilibrium pressure was calculated by successive approximation. Thermal expansion and compressibility of the solid phases were neglected.

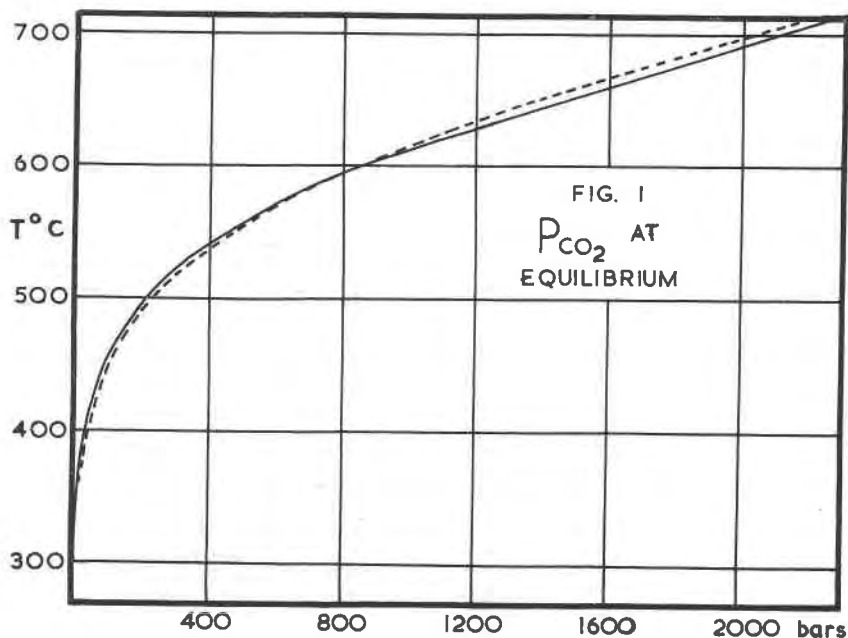


FIG. 1. Pressure-temperature curve for the reaction  $\text{CaCO}_3 + \text{SiO}_2 = \text{CaSiO}_3 + \text{CO}_2$ . Full curve, present calculation, dashed curve after Danielsson. The area under the curve is the field of calcite and quartz.

The results obtained with the improved  $P$ - $V$ - $T$  data are compared with those of Danielsson in Fig. 1. It is apparent that there are only small differences between the two curves. All points beyond 1400 bars necessitated extrapolation of Kennedy's data. The pressure of carbon dioxide is taken as the total pressure.

Little need be added to the many discussions of the geological significance of the reaction. The field of stability of the wollastonite bearing rocks of the hornfels and amphibolite facies may be very broad, especially when it is remembered that the partial pressure of carbon dioxide in a fluid phase may not be great compared with the partial pressure of water and that fluid and rock pressure may differ. At the same time the assemblage calcite-quartz could be stable into the region of partial melting in deep seated metamorphism.

#### REFERENCES

- (1) DANIELSSON, ALLAN (1950), Das Calcit-Wollastonitgleichgewicht: *Geochimica et Cosmochimica Acta*, **1**, 55-69.
- (2) KENNEDY, G. C. (1954),  $P$ - $V$ - $T$  relations in  $\text{CO}_2$  at elevated temperatures and pressures: *Am. Jour. Sci.*, **252**, 225-241.
- (3) SWEIGERT, R. L., WEBER, PAUL, AND ALLEN, R. L. (1946), Thermodynamic properties of gases, carbon dioxide: *Ind. Eng. Chem.*, **38**, 186-200.

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#### GEORGE FREDERICK KUNZ MEMORIAL PRIZE

At the March Meeting of the New York Mineralogical Club the George Frederick Kunz Memorial Prize was awarded to Mr. Davis Lapham, a graduate student in geology at Columbia University, for his paper entitled "Epidote from Hawleyville, Connecticut." This paper has been submitted for publication in *The American Mineralogist*. Mr. Lapham was the first recipient of this prize, established by the New York Mineralogical Club in 1955.

The Prize is made possible by a bequest of the late Dr. George Frederick Kunz, founder and first President of the New York Mineralogical Club. The prize is awarded annually for the most acceptable paper dealing with the study of a mineral locality or minerals from a deposit located within a 50 mile radius of New York City. The award is made by a Committee of three recognized mineralogists selected by the Board of Trustees of The New York Mineralogical Club. All papers for the next award must be submitted by February 15, 1957 for consideration. The rules governing the submission of papers or other information concerning the award can be obtained from Dr. Ralph J. Hoimes, Chairman of the George Frederick Kunz Memorial Prize Committee of the New York Mineralogical Club, Department of Geology, Columbia University, New York 27, N. Y.

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