75. *Thermal Expansion of Aragonite and its Atomic Displacements by Transformation into Calcite between 450°C and 490°C in Air, II.*

By Shukusuké KÔZU and Kô-ichi KANI.

Institute of Mineralogy, Petrology and Economic Geology,
Tohoku Imperial University, Sendai.

(Comm. by S. KÔUZ, M.I.A., April 12, 1934)

In order to see the displacements of atoms and atomic groups of aragonite by the transformation into calcite structure, the projections of the calcite structure at 500°C on the a-b and b-c planes were drawn, as is seen in Fig. 4, and the same projections of aragonite at 450°C are given in Fig. 5.

The calcite structure is obtained from the aragonite structure by

Fig. 4. Calcite structure at 500°C, projected on the a-b and b-c planes.

Fig. 5. Aragonite structure at 450°C, projected on the a-b and b-c planes.

Fig. 6. The a-stage during the transformation of aragonite into calcite, when two kinds of CO_2 were rotated $\pm 30^\circ$ respectively, projections being on the a-b and b-c planes.

Fig. 7. The b-stage during the transformation of aragonite into calcite between 450°C and 490°C .

the following procedures:—a) Rotate 30° in counter-clockwise the A-group of CO_2 (Fig. 5) and rotate 30° in clockwise the B-group of CO_3 , the result being shown in Fig. 6. b) Transform the A-groups of CO_3 on the b and e layers along the c-axis $-\frac{1}{12}c_0 \text{ Å}$ and the B-groups of CO_3 on the c and f layers $+\frac{1}{12}c_0 \text{ Å}$. By these procedures, the transformed structure projected on the b-c plane is shown in Fig. 7, in which two layers of CO_3 and those of Ca occur in coincidence with those in the unit cell of calcite, as is seen in Fig. 8.

Fig. 8. Comparison of the calcite structure at 500°C with the b-stage of transforming aragonite structure, projection being on the b-c planes.

c) In order to compare the structure of aragonite thus transformed with the calcite structure at 500°C , Fig. 8 is given. We can see in Fig. 8 that the CO_3 group and Ca in the layers of 0, 1, 6, 11 and 12 coincide in their centers to each other and the atom groups and atoms in the other eight layers are still in different positions. However by slight and regular displacements of these atoms (Table V), the centers of the CO_3 group and Ca of aragonite perfectly coincide with those of calcite. d) Slight difference is the positions of 3O surrounding C still remaining. In calcite, 3O are arranged at the apexes of a regular triangle whose edge is about $1.23 \text{ \AA}$ and, in aragonite, they are at the apexes of an isosceles triangle which shows practically a regular triangle whose edge is about $2.27 \text{ \AA}$.

TABLE V.

No. of layer	Atom or atom group	Displacement along a-axis	Displacement along b-axis
0	CO_3	0.0	0.0
1	Ca	0.0	0.0
2	CO_3	$2.4 \text{ \AA}$	$1.5 \text{ \AA}$
3	Ca	2.4 ,,	-1.5 ,,
4	CO_3	2.4 ,,	-1.5 ,,
5	Ca	2.4 ,,	-1.5 ,,
6	CO_3	0.0	0.0
7	Ca	2.4 ,,	1.5 ,,
8	CO_3	2.4 ,,	1.5 ,,
9	Ca	2.4 ,,	1.5 ,,
10	CO_3	2.4 ,,	-1.5 ,,
11	Ca	0.0	0.0
12	CO_3	0.0	0.0

From the transformed structure stated above, we also notice that Ca in the layers 1 and 11 of aragonite always remains in the same position with that of calcite at any temperature, while the positions of 3O forming CO_3 must rotate $\pm 30^{\circ}$ by the transformation. Hence, referring only to Ca, the a-axis of calcite can be taken for the same direction of the a-axis of aragonite, but the same conclusion can not be made from the arrangement of O.