

TABLE 2. X-RAY DIFFRACTION PATTERN OF CALCITE AT 61 KBAR

High-pressure polymorph (d Å)	Assignment (d Å— I/I ASTM value)
4.26	vaterite (4.26-75)
3.87	calcite (3.86-12)
3.64	vaterite (3.58-100)
3.35	vaterite (3.30-100) and aragonite (3.40-100) (?)
3.04	calcite (3.04-100)
2.72	vaterite (2.73-100) and aragonite (2.70-46) (?)
2.32	vaterite (2.33-50) and calcite (2.285-18) (?)
	2.30

sary to initiate a repulsive force for an in-plane bending mode (v_4) of this nature without considerably affecting the symmetric stretching (v_1) mode. The production of a new polymorphic transition produced by a change in pressure is extremely complex in that kinetic as well as potential energies are involved. A complete structural picture of the new polymorphic transition will require consideration of these energies. Hopefully, this will be accomplished when all the infrared data below 400 cm^{-1} has been collected. Due to the correlative features of the high pressure polymorph with known vaterite as evidenced by both infrared and X-ray data, it is believed that "vaterite-type" structure is a stable polymorph of calcium carbonate under pressure of 60 kbar to 65 kbar. High pressure experiments on the vaterite polymorph indicate that it is very stable under high pressure. Only minor frequency shifts of the bands are noted, with no evidence of new band production.

However, to even remotely suggest that calcium carbonate vaterite is a high pressure polymorph of calcite is precarious, McConnel's (1962) density of 2.60 for vaterite makes it thermodynamically impossible for vaterite to form from calcite I, II, or III at high pressure as a reversible equilibrium product unless it is sufficiently compressible so as to overcome the density difference and thus Gibb's Free Energy differences among these phases. Bridgman's compression data give an increase in density of 10 percent at 50-60 kbar for CaCO_3 . Jamison (1957) has also shown that vaterite is less compressible than calcite at about 20 kbar.

As suggested by Davis (1964), many calcite polymorph structures may be isostructural with various nitrate structures. Confirmation of these suggestions are beyond the scope of data collected in the mid-infrared spectral region (5000 to 400 cm^{-1}). Studies in the far-infrared spectral region (750 - 33 cm^{-1}) will be attempted to obtain insight into the lattice vibrations of this high-pressure polymorph.

ACKNOWLEDGMENT

The author gratefully acknowledges the financial support of the Wright-Patterson Air Force Materials Laboratory under contract number F 33 615-69-C-1247.

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Manuscript received, July 24, 1969; accepted for publication, January 26, 1970.