Structure and elastic properties of quartz at pressure

**LOUISE LEVIEN**, **CHARLES T. PREWITT** AND **DONALD J. WEIDNER**

*Department of Earth and Space Sciences*
*State University of New York*
*Stony Brook, New York 11794*

**Abstract**

Unit cells and crystal structures were determined on a single crystal of quartz at seven pressures from 1 atm to 61.4 kbar. Unit-cell parameters are $a = 4.916(1)$ and $c = 5.4054(4)$Å at 1 atm, and $a = 4.7022(3)$ and $c = 5.2561(2)$Å at 61.4 kbar. Structural changes observed over this pressure range include a decrease in the Si–O–Si angle from 143.73(7)° to 134.2(1)°, a decrease in the average Si–O bond distance from 1.6092(7) to 1.605(1)Å, and an increase in distortion of the silicate tetrahedron. Several O–O distances show very large changes (11%) that can be related to the unit-cell-edge compression. As pressure is increased, the geometry of the SiO$_2$ (quartz) structure approaches that of the low-pressure GeO$_2$ (quartz) structure.

The structural changes that take place with increased temperature are not the inverses of those that occur with increased pressure; changes in the Si–O–Si angle and the tetrahedral tilt angle control thermal expansion, whereas smaller changes in the Si–O–Si angle and tetrahedral distortion control isothermal compression.

By constraining the zero-pressure bulk modulus to be equal to that calculated from acoustic data [$K_T = 0.371(2)$ Mbar], the pressure derivative of the bulk modulus at zero pressure [$K_T = 6.2(1)$] has been calculated by fitting the $P–V$ data to a Birch-Murnaghan equation of state. The anomalously low value of Poisson's ratio in quartz can be explained by the low ratio of the off-diagonal shear moduli to the pure-shear moduli. This small ratio reflects the easily expanding or contracting spirals of tetrahedra that behave like coiled springs.

**Introduction**

The literature on the crystal structure and compressibility of quartz leaves many questions about its changes with pressure. As high-pressure structural refinements have not been as precise as those performed under ambient conditions, these studies report large changes (e.g., the Si–O–Si interbond angle); however, subtle ones have not been previously resolvable. Recent experimental developments in our laboratory offer the potential of providing improved resolution in high-pressure structural data.

The crystal structure of quartz at room temperature and pressure has been refined many times (Young and Post, 1962; Smith and Alexander, 1963; Zachariasen and Plettinger, 1965; Le Page and Donnay, 1976; Jorgensen, 1978; d’Amour et al., 1979).

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1 Present address: Division of Geological and Planetary Sciences, California Institute of Technology, Pasadena, California 91125.

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