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The compression pathway of quartz

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Abstract

The structure of quartz over the temperature domain (298 K, 1078 K) and pressure domain (0 GPa, 20.25 GPa) is compared to the following three hypothetical quartz crystals: (1) Ideal α-quartz with perfectly regular tetrahedra and the same volume and Si-O-Si angle as its observed equivalent (ideal β-quartz has Si-O-Si angle fixed at 155.6°). (2) Model α-quartz with the same Si-O-Si angle and cell parameters as its observed equivalent, derived from ideal by altering the axial ratio. (3) BCC quartz with a perfectly body-centered cubic arrangement of oxygen anions and the same volume as its observed equivalent.

Comparison of experimental data recorded in the literature for quartz with these hypothetical crystal structures shows that quartz becomes more ideal as temperature increases, more BCC as pressure increases, and that model quartz is a very good representation of observed quartz under all conditions. This is consistent with the hypothesis that quartz compresses through Si-O-Si angle-bending, which is resisted by anion-anion repulsion resulting in increasing distortion of the *c*/*a* axial ratio from ideal as temperature decreases and/or pressure increases.

Keywords: Crystal structure, ideal quartz, model quartz, BCC quartz, high-pressure studies, high-temperature studies, Brazil law twins, Dauphiné twin