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Compressibility and pressure-induced amorphization of guest-free melanophlogite: An in-situ synchrotron X-ray diffraction study

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ABSTRACT

Melanophlogite, a clathrasil, possesses a framework of corner-linked silica tetrahedra forming framework cavities that can enclose small guest molecules. Synchrotron X-ray diffraction experiments of the guest-free melanophlogite have been conducted at pressures up to 12 GPa and temperatures up to 1473 K. Upon compression at room temperature, melanophlogite gradually lost its crystallinity and became completely X-ray amorphous at ~8 GPa. The amorphization process was similar to those of denser silica polymorphs, but it reached completion at a much lower pressure (e.g., quartz becomes X-ray amorphous at ~30 GPa). The decreased amorphization pressure of melanophlogite may be attributed to its lower framework density and the ease of bending of its Si-O-Si linkages, thereby accelerating the collapse of the structure under high pressure. Determination of cell volumes of melanophlogite prior to its amorphization yielded a room-temperature bulk modulus of 26.3 ± 1.7 GPa, which is consistent with the relatively large compressibilities reported for the structurally similar zeolites. When heated at ~8 GPa, the amorphous phase started to crystallize at 873 K into coesite, the stable silica phase at these pressure and temperature conditions. Thus the occurrence of pressure-induced amorphization in melanophlogite appears to result from the kinetic hindrance to its transformation to the thermodynamically stable coesite.

Keywords: Melanophlogite, clathrasil, pressure-induced amorphization, compressibility, synchrotron X-ray diffraction