MS15-04 | Structural Behavior of the sII Clathrasil Chibaite at Low Temperatures and High Pressures

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Clathrasils are built up from a framework of corner-sharing [SiO_4]-tetrahedra that entraps guest atoms and molecules in cages. They have gained interest because of their potential application for gas storage and separation [1]. The behavior of the structure of the clathrasil chibaite and the influence of guest components at low temperatures as well as pressures was investigated using single-crystal X-ray diffraction and Raman spectroscopy. Chibaite is isotypic with the sII-gas hydrate characterized by larger [$5^{12}6^4$]-cages and smaller [5^{12}]-cages [2]. The natural sample of this study contains the hydrocarbons C_2H_6, C_3H_8, *i*-C_4H_{10} in both cage types, and additionally CH_4 molecules only in the small cages. With decreasing temperature to 100 K, the cubic *Fd*-3*m* room-temperature structure shows a continuous symmetry-lowering transformation to a monoclinic *A*2/*n* structure [3]. High-pressure experiments up to 10.3 GPa were performed in diamond-anvil cells using 4:1 methanol-ethanol mixture, helium and neon as pressure-transmitting media [4]. Compressed in the non-penetrating methanol-ethanol mixture, the *Fd*-3*m* framework undergoes a first transformation between 1.7 and 2.2 GPa with monoclinic metric and a second between 3.9 and 4.3 GPa with monoclinic or tetragonal metric. Using neon and helium the structure is stiffened during compression. The high-pressure behavior is characterized by a distortion of the lattice without leading to a pressure-induced amorphization.

[1] Navrotsky, A. et al. (2003). Am. Mineral. 88, 1612–1614.
[2] Momma, K. et al. (2011). Nat. Commun. 2, 196.
[3] Scheidl, K.S. et al. (2018). IUCrJ 5, 595-607.
[4] Scheidl, K.S. et al. (2019). Microporous Mesoporous Mater. 273, 73-89.