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High-pressure behavior of bikitaite: An integrated theoretical and experimental approach

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ABSTRACT

Pressure-induced structural modifications in the zeolite bikitaite are studied by means of in situ synchrotron X-ray powder diffraction and ab initio molecular dynamics. The experimental cell parameters were refined up to 9 GPa, at which pressure we found reductions of 4.5, 4.5, 6.3, and 15% in *a*, *b*, *c*, and *V*, respectively. Minor variations were observed for the cell angles. Complete X-ray amorphization is not achieved in the investigated *P* range, moreover the *P*-induced effects on the bikitaite structure are completely reversible. Because it was possible to extract only the cell parameters from the powder patterns, the atomic coordinates at 5.7 and 9.0 GPa were obtained by means of Car-Parrinello simulations using the unit-cell parameters experimentally determined at these pressures. Analysis of the computational results for increasing pressures showed that the volume contraction is essentially due to rotations of the tetrahedra; the 8-ring channels become more circular; the pyroxene chain becomes more corrugated in the *b*-*c* plane; and the mean Li-O bond distances and coordination polyhedral volumes decrease with increasing pressure without significant distortion of the internal angles. The peculiar aspect of the bikitaite structure, i.e., the presence in the channels of a "floating" one-dimensional water chain, is only partially maintained at high pressure; the compression brings framework O atoms close enough to water hydrogen atoms to allow the formation of host-guest hydrogen bonds, without, however, destroying the one-dimensional chain.