

## Pressure-controlled polytypism in hydrous layered materials

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### ABSTRACT

An isosymmetric displacive structural transformation in the hydrous layer silicate dickite [Al<sub>2</sub>Si<sub>2</sub>O<sub>5</sub>(OH)<sub>4</sub>, monoclinic *Cc*,  $a = 5.161(3)$ ,  $b = 8.960(6)$ ,  $c = 14.459(10)$  Å,  $\beta = 96.77(1)^\circ$ ], occurring under hydrostatic compression above 2.0 GPa, has been studied using single-crystal X-ray diffraction and diamond-anvil cell techniques. The structure of the high-pressure phase, determined in situ, is monoclinic with space group *Cc* with unit-cell parameters  $a = 5.082(3)$ ,  $b = 8.757(6)$ ,  $c = 13.771(9)$  Å, and  $\beta = 89.60(2)^\circ$  at 4.1 GPa. The positions of all hydrogen atoms at both ambient and high pressure have been determined by a combination of simulated annealing and energy minimization. The mechanism of the transformation, which may be general for other hydrous layered materials, involves a shift of the 1:1 layers with respect to each other by the vector  $[1/6, 1/6, 0]$  and is accompanied by the formation of new hydrogen bonds.