

LETTER

**Pressure-induced transformations in kaolinite**

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ABSTRACT

The compressional behavior of kaolinite (space group *C1*) from Keokuk, Iowa, has been studied to 7.8 GPa under static compression by synchrotron X-ray powder diffraction. Two phase transformations occur at  $\sim 3.7$  (kaolinite-I/II) and  $\sim 7$  GPa (kaolinite-II/III) that are registered by major changes in diffraction patterns. The layer shift involved in the I/II transformation preserves hydrogen-bonded contacts across the interlayer. This transformation removes cross-interlayer Al-Si superpositions and is analogous to the low-/high-dickite transformation, which occurs at  $\sim 2.6$  GPa (Dera et al. 2003). The 7 GPa transformation from kaolinite-II to “kaolinite-III” involves considerable contraction of the *a-b* plane (2.5%), marked shortening normal to the polyhedral layers, and a volume contraction of about 3%. Comparison of experimental patterns of kaolinite-III with those calculated for non-standard polytypes predicted by *ab initio* methods to 60 GPa by Mercier and Le Page (2009) allows the identification of kaolinite-III with their high-pressure, one-layer Model 18 polytype. Kaolinite-III can be quenched to room pressure, although significant transformation to kaolinite-I was observed at 0.5 GPa on decompression. At ambient conditions kaolinite-III is 6% more dense than kaolinite-I, nacrite, and low-dickite. Elastic moduli for kaolinite-I and kaolinite-III have been obtained that indicate that kaolinite-III is more compressible than kaolinite-I, due primarily to in-plane (**a-b**) softening. Both high-pressure polytypes encountered experimentally were predicted *ab initio* to be strong candidates for high-pressure structures by Mercier and Le Page (2008, 2009). This agreement between experimental and *ab initio* studies is encouraging for the application of *ab initio* methods to complex polytypic systems.

**Keywords:** Kaolinite, high pressure, transformations, polytypism