

HIGH-PRESSURE BEHAVIOR OF KALSILITE-*OI* PHASE

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Several polymorphs of KAlSiO_4 are known to exist. The “*KAlSiO}_4*-*OI*” phase is structurally closely related to the stuffed derivatives of tridymite, however, the topology of the Si/Al-ordered framework is different. The tridymite-framework exhibits UDUDUD rings whereas the framework of the “*OI*”-phase shows two different types of six-membered rings with UUDUD and UUDDDD configuration that are occurring in a ratio of 2:1. A similar arrangement has been found in the structure of megakalsilite (KAlSiO_4 ; KHOMYAKOV et al., 2002) where the same two types of rings appear in a ratio of 1:3.

The crystal structure of the “*OI*”-phase has been solved and refined from synthesized material (GREGORKIEWITZ et al., 2008; KREMENOVIC et al., 2013). Recently, the first natural crystals of “*KAlSiO}_4*-*OI*” have been found in the pyrometamorphic rocks of the Hatrurim Complex, Negev Desert, Israel (KRÜGER et al., 2016).

In this study we present the high pressure (HP) behaviour of kalsilite, performing in-situ high-pressure single-crystal diffraction and Raman spectroscopic investigations in the diamond anvil cell on a natural grown crystal from ambient conditions up to 6.3 GPa. Raman spectra indicate a phase transition between 0.5 GPa and 1.6 GPa on pressure increase. On decreasing pressure the HP-phase was observed on pressures as low as 1.1 GPa. For the HP-phase full-intensity X-ray diffraction data collections have been collected at 1.1, 2.4, 3.0, 4.0 and 5.2 GPa.

In contrast to the HP-behaviour of trigonal kalsilite (GATTA et al., 2011) kalsilite-*OI* performs a HP-phase transition to a larger unit cell with lattice parameter $b_{HP} = 3 \times b_{LP}$ while maintaining monoclinic symmetry. The unit cell dimensions of HP kalsilite “*OI*”-phase at 5.2 GPa are $a=15.277(4)$ Å, $b=26.606(6)$ Å, $c=8.1511(16)$ Å, $\beta=90.18(2)^\circ$, $V=3313(1)$ Å³. The pressure induced structural phase transition in kalsilite “*OI*”-phase appears to be completely reversible.

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