

Ordered and disordered environments in synthetic Ca-Tschermak clinopyroxene and variation with pressure, temperature and time.

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Aluminum content in pyroxene is known to increase with pressure, temperature, and cooling rate. Structural order-disorder will also vary. This has been examined in synthetic Ca-Tschermak pyroxene, CaAlAlSiO_6 , with changes in pressure (P), temperature (T), and reaction time (t). Samples were synthesized using a 4-post piston cylinder at U. of Alberta. Synthesis conditions ranged from 1300 - 1600 °C, 2.0 - 3.0 GPa, 4 - 164 h. Al environments in this aluminous clinopyroxene were examined by ^{27}Al 3Q MAS NMR at 21.1 Tesla on the Bruker Avance II 900 at the Ultrahigh-Field NMR Facility for Solids in Ottawa. For all samples, the octahedral region remains relatively unchanged. The tetrahedral region, however, changes as a function of P-T-t. At 2.0 GPa, 1400 °C, 24 h, two tetrahedral Al sites are resolved: A highly disordered but regular environment and an ordered but highly-distorted environment. The disordered environment appears to represent disequilibrium, as it disappears at longer reaction times (2.0 GPa, 1400 °C, 164 h) and higher P-T (e.g. 2.5 GPa, 1500 °C, 8 h). This has implications for thermobarometry. The highly-distorted environment has not been observed previously, in ^{27}Al NMR spectra acquired at lower field strength (≤ 14.4 Tesla).