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LETTER

Si-Al distribution in high-pressure $CaAl_4Si_2O_{11}$ phase: A ^{29}Si and ^{27}Al NMR study

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ABSTRACT

High-resolution ^{29}Si and ^{27}Al NMR techniques have been applied to resolve the Si-Al distribution and coordination in the high-pressure $CaAl_4Si_2O_{11}$ (CAS) phase, a potentially important mineral in subducted crustal materials in the deep mantle that has a unique hexagonal ferrite structure containing two octahedral (M1; M2) and one trigonal bipyramidal sites. The ^{29}Si MAS NMR spectra of the CAS phase synthesized at 20 GPa and 1400~1600 °C show two broad, asymmetric peaks near –92.7 and –182.7 ppm with an intensity ratio of 1:3, suggesting that 1/4 of the Si are in tetrahedral coordination and 3/4 in octahedral coordination. Therefore, the trigonal bipyramidal and M1 octahedral sites are each occupied by equal proportions of Si and Al, and the former are effectively half-occupied face-sharing tetrahedra (at least for Si). The ^{27}Al MAS and 3Q MAS NMR spectra contain only one unresolved peak typical of octahedral Al with a range of quadrupolar coupling constants.

Keywords: NMR spectroscopy, Al and Si coordination, CAS phase, Si-Al disorder, high pressure