American Mineralogist, Volume 82, pages 479–482, 1997

MAS NMR study of pentacoordinated magnesium in grandidierite

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ABSTRACT

The 11.7 T ^{25}Mg, ^{27}Al, ^{29}Si, and ^{11}B MAS NMR spectra are reported for well-characterized grandidierite, $(Mg,Fe)Al_3SiBO_9$, which contains both Al and Mg in fivefold coordination with oxygen. The ^{25}Mg spectrum is the first to be reported for ^{5}Mg, and exhibits a quadrupolar lineshape from which the nuclear quadrupolar coupling constant (3.8 ± 0.1 MHz), the asymmetry parameter (0.6 ± 0.05), and the isotropic chemical shift (55 ± 2 ppm) were derived by spectral simulation. These spectroscopic parameters are discussed in terms of the crystallographic geometry of the fivefold-coordinated site.