

LETTERS

Al-O-Al oxygen sites in crystalline aluminates and aluminosilicate glasses: High-resolution oxygen-17 NMR results

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ABSTRACT

We report ^{17}O magic-angle spinning (MAS) NMR data for crystalline NaAlO_2 and CaAl_2O_4 at external magnetic fields of 9.4 and 14.1 T, as model compounds for Al-O-Al sites in tetrahedral networks. The former contains one peak with isotropic chemical shift (δ_{iso}) = 30.9 ppm and quadrupolar coupling constant (C_Q) \approx 1.8 MHz. The latter contains several peaks with δ_{iso} ranging from 39 to 87 ppm and $C_Q \approx$ 1.5 to 2.4 MHz. Triple-quantum MAS (3QMAS) spectra of sodium and calcium aluminosilicate glasses with $\text{Si}/\text{Al} < 1$ show clearly resolved peaks for Al-O-Al sites, removing ambiguity in the use of such spectra to explore the extent of aluminum avoidance in both glassy and crystalline materials. We also report ^{23}Na and ^{27}Al NMR data for the crystalline phases.