American Mineralogist, Volume 84, pages 983–986, 1999

LETTERS

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

JONATHAN F. STEBBINS,* SUNG KEUN LEE, AND JANE V. OGLESBY

Department of Geological and Environmental Sciences, Stanford University, Stanford, California 94305-2115, U.S.A.

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) ≈ 1.8 MHz. The latter contains several peaks with δ_{iso} ranging from 39 to 87 ppm and C_Q ≈ 1.5 to 2.4 MHz. Triple-quantum MAS (3QMAS) spectra of sodium and calcium aluminosilicate glasses with Si/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.