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Potassium hydrogen disilicate: A possible model compound for ^{17}O NMR spectra of hydrous silicate glasses

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ABSTRACT

Oxygen-17 magic angle spinning, non-spinning, ^{1}H-decoupled, ^{1}H-^{17}O cross-polarization, and triple-quantum magic-angle spinning nuclear magnetic resonance (NMR) spectroscopy experiments were performed at two different magnetic fields on crystalline potassium hydrogen disilicate ($KHSi_2O_5$) and hydrous and anhydrous potassium tetrasilicate ($K_2Si_4O_9$), sanidine ($KAlSi_3O_8$), and haplogranite ($KAlSi_3O_8$-$NaAlSi_3O_8$-SiO_2) glasses. Crystalline $KHSi_2O_5$ has two bridging oxygen sites and one non-bridging oxygen site, and the NMR parameters for these two types of sites have been determined. The non-bridging oxygen (silanol) site is well-resolved and observed in a crystalline compound with an isotropic chemical shift (δ_{iso}) of 60 ppm, a quadrupolar coupling constant (C_Q) of 3.5 MHz, and an asymmetry parameter (η) of 0.35. Knowledge of the non-bridging-oxygen site parameters allows for comparisons to glassy or other materials that might have silanol-type structures. A similar peak can be found in the hydrous potassium silicate spectrum but not in the hydrous potassium aluminosilicate glass spectrum.