

^{29}Si CPMAS NMR investigations of silanol-group minerals and hydrous aluminosilicate glasses

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ABSTRACT

One-pulse magic angle spinning (MAS) ^{29}Si and ^1H - ^{29}Si cross-polarization (CP) MAS nuclear magnetic resonance (NMR) spectroscopy was performed on minerals with OH groups and on hydrous aluminosilicate glass samples. The silanol-group samples used were krauskopffite, rosenhahnite, thaumasite, ussingite, and KHSi_2O_5 with known Si to H distances and ellenbergerite, the proton positions of which are not as well defined. The Si-H distances from the minerals can be compared with the cross-polarization time constants (τ_{SiH}) and the proton spin-relaxation times in the rotating frame [$\tau_{1\rho}(\text{H})$], and a rough correspondence exists between a mineral's shortest Si-H distance and its τ_{SiH} value. Also, fast [$\tau_{1\rho}(\text{H})$] values correspond to large bulk H densities. The CP spectra of the hydrous aluminosilicate glass samples were fitted with two peaks, representing two different Si environments within the glass structure. The contact-time curves of the higher frequency peak imply τ_{SiH} similar to the mineral samples with short Si-H distances, and this suggests that the glasses could contain a large fraction of either Si-OH groups or protonated bridging O atoms.