

LETTER

Water speciation in hydrous silicate and aluminosilicate glasses: Direct evidence from ^{29}Si - ^1H and ^{27}Al - ^1H double-resonance NMR

XIANYU XUE*

Institute for Study of the Earth's Interior, Okayama University, Misasa, Tottori 682-0193, Japan

ABSTRACT

Through a combination of ^1H MAS NMR, $^1\text{H} \rightarrow ^{29}\text{Si} \rightarrow ^1\text{H}$ double cross-polarization (CP) MAS NMR and $^{27}\text{Al} \rightarrow ^1\text{H}$ CP MAS NMR, different OH species [SiOH, AlOH, and (Ca,Mg)OH (free OH)] have been unambiguously identified for hydrous Ca,Mg-(alumino)silicate glasses. This confirms my earlier speciation assignments made partially on the basis of ^1H chemical shift arguments. The dissolution mechanisms of water in both Al-free silicate and aluminosilicate glasses (quenched melts) are fundamentally similar. For relatively polymerized compositions, it involves dominantly the formation of TOH species (T: Si, Al) through the rupture of T-O-T linkages, in addition to molecular H_2O ; for more depolymerized compositions containing network-modifying cations of large field strength (e.g., Ca, Mg), free OH species are also important.

Keywords: Aluminosilicate, silicate, glass, melt, NMR, water speciation, structure