## LETTER

## Water speciation in hydrous silicate and aluminosilicate glasses: Direct evidence from <sup>29</sup>Si-<sup>1</sup>H and <sup>27</sup>Al-<sup>1</sup>H double-resonance NMR

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## ABSTRACT

Through a combination of <sup>1</sup>H MAS NMR, <sup>1</sup>H  $\rightarrow$  <sup>29</sup>Si  $\rightarrow$  <sup>1</sup>H double cross-polarization (CP) MAS NMR and <sup>27</sup>Al  $\rightarrow$  <sup>1</sup>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 <sup>1</sup>H 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<sub>2</sub>O; 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