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Depolymerization effect of water in aluminosilicate glasses: Direct evidence from ^{1}H-^{27}Al heteronuclear correlation NMR

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ABSTRACT

We have applied one-dimensional (1D) ^{1}H MAS NMR, $^{27}Al \rightarrow {}^{1}H$ CP MAS NMR, as well as 2D ^{27}Al triple-quantum (3Q) MAS NMR, $^{27}Al \rightarrow {}^{1}H$ heteronuclear correlation (HETCOR) and high-resolution 3QMAS/HETCOR NMR techniques to $KAlSi_3O_8$ (Or), $NaAlSi_3O_8$ (Ab) and $NaAlSiO_4$ (Ne) glasses containing 0~2 wt% H_2O to shed light on the dissolution mechanisms of water in aluminosilicate melts (glasses). An Al Q^3-OH group, characterized by ^{1}H chemical shifts of 1.3–1.9 ppm, was identified for all hydrous glasses. Its abundance increases with bulk Al/Si ratio. The ^{27}Al chemical shifts (δ_i^{Al}) of this species are 64–68 ppm, larger than those of Al Q^4 by 3–6 ppm. Despite this difference, it is only through $^{27}Al \rightarrow {}^{1}H$ HETCOR and 3QMAS/HETCOR, but not ^{27}Al MAS or 3QMAS NMR that the peaks are resolved. This study has demonstrated that depolymerization and formation of AlOH/SiOH is a general water dissolution mechanism for polymerized aluminosilicate melts (glasses), and HETCOR NMR experiments involving ^{1}H are the key to its revelation.

Keywords: NMR, water, aluminosilicate glass, heteronuclear correlation, ^{1}H, ^{27}Al, depolymerization