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Insights of Solid State NMR: the Non-Linear Macroscopic Properties of Silica-Aluminophosphate Glasses

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The last three decades have seen the ongoing progress of glassy technologies, with the development of material engeneering and characterization methods, both crucial elements to this achievement. In this context the technique of Solid-State Nuclear Magnetic Resonance (NMR) Spectroscopy assumes a central role by its capability to probe the local environment of the nuclei in an element-selective fashion. (1) Exploring the potential of NMR, in the present work, we investigate optical fiber glass with the composition $(59-x)P_2O_3 - xSiO_2 - 13Al_2O_3 - 28Na_2O$ $(0 \leq x \leq 13)$, which shows non-linear behaviour of weathering stability, glass transition temperature, and thermal expansion coefficient as a function of x. While ^{31}P MAS-NMR results suggest that the phosphate units are dominantly of the $P^{(2)}$ (metaphosphate) type, ^{31}P(^{23}Na) and ^{31}P(^{27}Al) REAPDOR experiments (2) indicate two distinct environments with different strengths of the interaction with ^{23}Na and ^{27}Al nuclei. ^{29}Si NMR spectra are consistent with Si-O-Si and Si-O-P connectivities and the absence of six-coordinated silicon units that are observed in Al-free glasses with similar Na:Si:P ratios. (3) ^{31}P spin echo decay experiments confirm the decrease of P-O-P connectivity with increasing x, providing a rationale for the increase in weathering stability for the composition range $x \leq 6$. As none of the mentioned structural trends alone are able to explain the above-mentioned non-linear compositional evolution, it must be attributed to a superposition of multiple structural changes.

Palavras-chave: NMR. Phosphosilicate glass. Structure.

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Referências:

1 KROEKER, S. Nuclear magnetic resonance spectroscopy. *In:* AFFATIGATO,M. (ed.). **Modern glass characterization.** Hoboken: Wiley, 2015. p. 1-30

2 GULLION, T. Measurement of dipolar interactions between spin-12 and quadrupolar nuclei by rotational-echo, adiabatic-passage, double-resonance NMR. **Chemical Physics Letters,** v. 246, n. 3, p. 325, 1995.

3 REN, J.; ECKERT, H. Superstructural units involving six-coordinated silicon in sodium phosphosilicate glasses detected by solid-state NMR spectroscopy. **Journal of Physical Chemistry C,** v. 122, n. 48, p. 27620–27630, 2018.