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Synthesis of Niobium Phosphate Glasses and Structural Characterization by Solid State NMR

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Phosphate glasses are used in a wide range of applications such as optical communications, three-dimensional displays, optical switching devises and solid lasers owing to their high solubility with active metal ions. (1) The incorporation of transition metal ions, such as Nb_2O_5, not only improves the chemical durability of phosphate glasses, but also significantly contributes to increase both their linear and non-linear indexes of refraction. (2) As a result, they were hence proposed as host matrix of rare-earth elements for optical applications. However, a fundamental understanding about the structural role of niobium, which can serve as a network modifier or as a network former, into these glasses has not been achieved. Solid-state nuclear magnetic resonance (NMR) has been proven to be a powerful tool in addressing structural elucidation, especially for disordered materials, due to its well-proven ability to provide structural information. (1) In this context and as a first step, we synthetize and study glasses in the ternary system $Na_2O - Nb_2O_5 - P_2O_5$ from two compositional series through advanced multinuclear NMR experiments with the aim to obtain new structural insights towards the development of new structure-function correlations. While the NMR of ^{31}P and ^{23}Na is relatively straightforward, the nuclear isotope ^{93}Nb poses significant challenges owing to its large nuclear electric quadrupole moment, resulting in excessive line broadening and resolution. These challenges can be addressed by new single and double resonance techniques involving various wideband excitation and dipolar recoupling technique. (3) An important objective of the project will be the development of a generally applicable magnetic resonance strategy that can be extended to other quadrupolar nuclei with similar characteristics, such as ^{25}Mg, ^{45}Sc, ^{47}Ti, and $^{69/71}Ga$, and ^{139}La, featuring similar spin dynamics.

Palavras-chave: Phosphate glasses. Niobium oxide. NMR.

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Referências:

1 ZHANG, R. *et al.* Structural studies of $Bi_2O_3 - NaPO_3$ glasses by solid state nuclear magnetic resonance and x-ray photoelectron spectroscopy. **Journal of Physical Chemistry,** v. 121, n. 18, p. 10087–10094, 2017.

2 KOUDELKA, L. *et al.* Structure and properties of barium niobophosphate glasses. **Journal of Non-Crystalline Solids,** v. 459, p. 68-74. 2017.

3 KOPPE, J. *et al.* Minimizing lineshape distortions in static ultra-wideline nuclear magnetic resonance of half-integer spin quadrupolar nuclei. **Journal of Physical Chemistry A,** v. 124, n. 21, p. 4314-4321, 2020.