

Universidade de São Paulo
Instituto de Física de São Carlos

Semana Integrada do Instituto de Física
de São Carlos

13ª edição

Livro de Resumos

São Carlos
2023

Ficha catalográfica elaborada pelo Serviço de Informação do IFSC

Semana Integrada do Instituto de Física de São Carlos
(13: 21-25 ago.: 2023: São Carlos, SP.)
Livro de resumos da XIII Semana Integrada do Instituto de
Física de São Carlos – Universidade de São Paulo / Organizado
por Adonai Hilário da Silva [et al.]. São Carlos: IFSC, 2023.
358p.

Texto em português.

1.Física. I. Silva, Adonai Hilário da, org. II. Título.

ISSN: 2965-7679

PG169

Study of structural and dynamic properties in Li phosphate glasses by solid state NMR and impedance spectroscopySCHNEIDER, José Fábian¹; FERREIRA, Matheus José¹; MORGUETTO, Gabriel Felipe¹

gabriel.morguetto@usp.br

¹Instituto de Física de São Carlos - USP

With the addition of a mobile ion species, ionic conductivity is introduced in a glass matrix, which makes these materials interesting for applications in batteries and sensors. However, when a second mobile ion species is added to the system, strong anomalies in the conductivity might be observed, reducing the values by orders of magnitude below the expected additive behavior. (1) This phenomenon is known as the mixed ion effect (MIE). The extent of the deviation is usually correlated with the size mismatch between the mixed ions, attaining several orders of magnitude for pairs such as Li-Na or Li-Rb. Other properties of the material dependent on ion diffusion also exhibit nonlinear behavior. A model that tries to explain the MIE is the Random Ion Distribution Model (RIDM) (2), whose hypothesis is the random mixture of mobile species and the presence of structurally different sites of occupation for each ion. To study the validity of the model, the random mixture of ions will be frustrated by manipulating the structural properties of the matrix or by the introduction of a third mobile specie, with high Colombian potential. Therefore, a vitreous system with intense MIE (Li-Cs metaphosphate) was disturbed by the addition of a third non-mobile specie (Sr), looking for conditions to inhibit MIE associated with the mixture of alkaline ions, according to the composition $(50 - x - y)\text{Cs}_2\text{O} - x\text{Li}_2\text{O} - y\text{SrO} - 50\text{P}_2\text{O}_5$, varying x from 0 to 37.5 mol% and y from 0 to 40 mol%. A second vitreous system, without MIE (Li-Ca metaphosphate), had its vitreous matrix distorted by leaving the metaphosphate composition for the polyphosphate, according to the composition $x\text{Li}_2\text{O} - y\text{CaO} - (50 - x - y)\text{P}_2\text{O}_5$, varying x from 20 to 60 mol% and y from 0 to 30 mol%. With solid-state NMR, we measured average isotropic chemical shifts and line widths of the nucleus ^{31}P , ^7Li and ^{133}Cs as a function of their ionic density. For all Li-Cs and Li-Ca ratios, we observed linear behaviors, indicating that variations of any of the ions do not affect the dilution of the others, indicative of the random mixture of ions, in accordance with the RIDM. In addition, through impedance spectroscopy and static NMR with variation on temperature, we show that MIE is still present after the addition of Sr, which acts as blocking ion in the diffusion of Li and Cs, decreasing the conductivity globally.

Palavras-chave: NMR. Ionic glasses. Phosphorus glasses. Mixed ions effect.**Agência de fomento:** CNPq (140808/2020-5)**Referências:**

1 ISARD, J. O. The mixed alkali effect in glass. **Journal of Non-Crystalline Solids**, v. 1, n. 3, p. 235-261, 1969.

2 SWENSON, J. *et al.* Random ion distribution model: a structural approach to the mixed-alkali effect in glasses. **Physical Review B**, v. 63, n. 13, p. 132202-1-132202-4, 2001.