
Investigation of Structure-Property Relationships of Ionic Glasses

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Abstract

Unlike conventional glass formers, ionic glasses, whose behaviour is determined by majority cation-anion interactions, contain few network bonds.(1) Three ionic glass series: potassium-zinc sulphate, potassium-zinc phosphate, and zinc sulfophosphate are synthesised, and characterized using Raman, FTIR, and ³¹P solid-state MAS NMR for structural information. The dependence of ionic conductivity and mechanical properties on glass structure is investigated. To perform ¹⁷O solid-state MAS NMR, the glass raw materials are enriched using the conventional ¹⁷O -enrichment process via chemical reactions with H₂¹⁷O (2). Through the analysis of ¹⁷O solid-state MAS NMR spectra, bridging and non-bridging oxygens from different chemical environment can be distinguished, respectively (3-5). The aim is to predict quantitatively preferential bonding between different cations and anions (6); The whole structure of these glass series could be analysed thoroughly, which could provide great potential and convenience in understanding the structure of glasses without conventional network bonding. References

(1) C. Calahoo and L. Wondraczek, "Ionic glasses: Structure, properties and classification," *Journal of Non-Crystalline Solids: X*, vol. 8, p. 100054, 2020.

(2) A. Flambard, L. Montagne, and L. Delevoye, "A new ¹⁷O-isotopic enrichment method for the NMR characterisation of phosphate compounds," *Chemical communications*, no. 32, pp. 3426-3428, 2006.

(3) H. K. C. Timken, N. Janes, G. L. Turner, S. L. Lambert, L. Welsh, and E. Oldfield, "Solid-state oxygen-17 nuclear magnetic resonance spectroscopic studies of zeolites and related systems. 2," *Journal of the American Chemical Society*, vol. 108, no. 23, pp. 7236-7241, 1986.

(4) Z. Xu and J. Stebbins, "Oxygen site exchange kinetics observed with solid state NMR in a natural zeolite," *Geochimica et Cosmochimica Acta*, vol. 62, no. 10, pp. 1803-1809, 1998.

(5) M. Zeyer-Düsterer, L. Montagne, G. Palavit, and C. Jäger, "Combined ¹⁷O NMR and ¹¹B-³¹P double resonance NMR studies of sodium borophosphate glasses," *Solid state nuclear magnetic resonance*, vol. 27, no. 1-2, pp. 50-64, 2005.

(6) N. Da, O. Grassmé, K. H. Nielsen, G. Peters, and L. Wondraczek, "Formation and structure of ionic (Na, Zn) sulfophosphate glasses," *Journal of non-crystalline solids*, vol. 357, no. 10, pp. 2202-2206, 2011.

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