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# Distribution of Li, P, and F Atoms in phosphate-fluoride glasses investigated by solid-state NMR and atomistic simulations

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Abstract: Lithium phosphate-fluoride glasses are of interest to optical thermometry applications. As a phosphate-fluoride system, these glasses are complex from a structural stand point. For the study of the structural aspects of the glasses, several single and double resonance advanced NMR techniques were employed, namely, $^{7}$Li SATRAS, $^{31}$P SED, $^{19}$F SED, $^{31}$P{$^{19}$F} REDOR, $^{19}$F{$^{31}$P} REDOR, $^{7}$Li{$^{19}$F} REDOR/CT-REDOR, $^{19}$F{$^{7}$Li} REDOR/CT-REDOR, $^{6}$Li{$^{31}$P} REDOR, $^{31}$P INADEQUATE, and j-resolved. The consistent analysis of all the results reveals that the phosphate and fluoride regions exist separately with very small amount of P–F bonds. Moreover, phosphate units form short dimer and trimer chains. The analysis of $^{31}$P SED based on Monte-Carlo simulations reveal phosphate clustering. The ab initio molecular dynamics simulations are also in agreement with the experimental NMR data.

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