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# Structure of Mixed Anion Salt Glasses from Synchrotron X-Ray Pair Distribution Functions

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## Abstract

This study seeks to understand the melt structure of molten salts in relation to the low temperature reactions and melts that occur during the vitrification of Hanford Low Activity Waste (LAW). Salts (such as nitrates, sulfates, carbonates, halides, etc.) play a key role in these low temperature reactions as they form complex eutectic mixtures during early stage melting. Sulfates are of particular interest as they have limited solubility in the final glass waste form and can be detrimental to its long-term durability as they form a water soluble salt phase on the glass surface. To better understand these low temperature processes, melts of several simple binary and ternary salt systems are studied. In one example, salt melts consisting of varied amounts in the ternary  $K_2SO_4$ - $ZnSO_4$ - $NaCl$  were melted and rapidly quenched to retain the amorphous melt structure. Synchrotron x-ray diffraction pair distribution function (PDF) data was obtained for these systems. Empirical Potential Structure Refinement (EPSR) was used to model the PDF. From this model, the individual atom pair distribution functions and coordination numbers were determined. Additional information was determined from infrared absorption spectroscopy and thermal analysis.

**Keywords:** mixed salt, pair distribution function, salt glass

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