

Unravelling the Internal Complexities of Molten Salts

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Much experimental and theoretical effort has gone into revealing the internal complexities of molten salts for the past two decades. In this paper we shall show how neutron diffraction and computer simulation techniques have helped in gaining a better understanding of these systems at the microscopic level. Firstly, a short review on the structure of molten halide systems as revealed by these techniques will be presented. Complementarity of using X-rays with neutrons and, some recent results on the structure of molten DyCl_3 obtained by combining neutron and X-ray diffraction with molecular dynamic simulations will be discussed. Neutron diffraction isotopic substitution techniques have played an important role in elucidating the interatomic structure of a diversity of molten salts. Pair distribution functions (PDFs), determined for a number of 1 : 1 and 2 : 1 halide melts, provided theorists with a critical test of their model potentials. It is now clear that for 1 : 1 molten systems theoretical models based on Fumi-Tosi potentials can adequately describe many of the structural features. Nevertheless, the challenge is two fold: (i) to determine real interatomic potentials for 2 : 1 and 3 : 1 molten systems capable of reproducing not only the microscopic structural details obtained at the partial PDF, $g_{\alpha\beta}(r)$ level, but also their macroscopic behaviour and, (ii) to characterise the structure in binary molten salt mixtures.

Key words: Molten Salts; Structure; Neutron and X-ray Diffraction; Computer Simulations; Liquid State Structural Theory; Molten Halides.

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