Al^{3+} Coordination in Cryolitic Melts: A Computer Simulation Study

Michael J. Castiglione, Mauro C. C. Ribeiro, Mark Wilson, and Paul A. Madden

Physical and Theoretical Chemistry Laboratory, Oxford University,
South Parks Road, Oxford OX1 3QZ, U.K.

Reprint requests to Prof. P. A. M.; e-mail: madden@physchem.ox.ac.uk

Z. Naturforsch. **54 a,** 605–610 (1999); received August 23, 1999

The structures of melts containing cryolite have proved difficult to confirm, despite decades of study, on account of the high temperatures and corrosiveness of these melts. Raman spectroscopy has so far provided the majority of the insight into the aluminium coordination environments, but some of its interpretations are still debated.

In this paper we present the results of MD simulations on various NaF-AlF_3 liquid mixtures using published potentials developed for the solid state and published Raman spectra.

Key words: Cryolite; Raman Spectra; MD Simulation; Complex Ions.