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Temperature variation of the Debye-Waller factors of metal and halide ions in CsCl and CsBr powders by X-ray diffraction. I. Debye-Waller factors of Cs^+ and Cl^- ions in CsCl from room temperature to 90°K

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Abstract. The temperature variation of the Debye-Waller factors of Cs^+ and Cl^- ions in CsCl powder has been studied using X-ray powder diffraction. A continuous flow cryostat has been used to record the diffractograms and the integrated intensities of the Bragg peaks at different temperatures have been obtained. The integrated intensities of the odd and even reflections have been analysed following the structure of the CsCl compound and the Debye-Waller factors of the Cs^+ and Cl^- ions have been estimated. The results have been verified by structure factor least squares refinement. Theoretical shell model lattice dynamical calculations have been done using a 7-parameter model in the harmonic approximation and the values compared with the present X-ray measurements.

Keywords. Cryostat; powder diffraction; Debye-Waller factor; structure factor least square; lattice dynamics; caesium chloride; thermal diffuse scattering correction.

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1. Introduction

Lattice dynamics of caesium chloride has been studied in the past both theoretically and experimentally. The phonon dispersion relations in CsCl have been studied by neutron inelastic scattering (Ahmed *et al* 1972) and the parameters for a shell model fit of the dispersion relations are given by Jindal and Mahesh (1975). Thermal expansion in this compound has been measured by interferometric (Bailey and Yates 1967) and X-ray diffraction (Ganesan and Girirajan 1986) methods over the temperature range 90–298°K. The Debye-Waller (D-W) factors of the metal and chlorine atoms in this compound and their temperature variation have not been measured and it was therefore considered worthwhile to undertake this study by analysing and calculating the powder X-ray diffractograms by employing theoretical lattice dynamics techniques. Section 2 describes the experiments for getting the diffractograms of CsCl and § 3 deals with an analysis of the experimental data and the results on the temperature variation of the D-W factors of caesium and chloride ions. Section 4 details the theoretical calculations on a shell model lattice dynamics and a comparison between theory and experiment.