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A neutron diffraction study of KCl. A correction. By M. J. Cooper and K. D. Rouse, *Materials Physics Division, AERE, Harwell, Oxfordshire, England*

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The previously published result for the anisotropic fourth-order anharmonic thermal vibrations in KCl, determined from neutron diffraction measurements, contained an error in sign. The parameter δ_{Cl}, which characterizes the appropriate term in the effective one-particle potential, should be negative, indicating the predominance of Coulombic attractive forces between the ions in determining this contribution.

The paper of the above title (Cooper & Rouse, 1973) reports the analysis of accurate neutron diffraction measurements on KCl in terms of anharmonic thermal vibrations of the constituent ions. In particular it was shown that the data indicated a significant anisotropic fourth-order anharmonic component in the thermal vibration of the chlorine ions, corresponding to a value of $\delta_{Cl} = 0{\cdot}13\ (5) \times 10^{-12}$ erg Å^{-4}, where δ_{Cl} is the parameter defining the anisotropic fourth-order term in the effective one-particle potential for the chlorine ions. Unfortunately an error in the computer program resulted in this value being given the wrong sign. The result should be negative, *i.e.* $\delta_{Cl} = -0{\cdot}13\ (5) \times 10^{-12}$ erg Å^{-4}.

Consideration of the definition of the effective one-particle potential shows that a negative value of δ_{Cl} indicates that the chlorine ions are vibrating preferentially along the six ⟨100⟩ directions, *i.e.* towards the nearest-neighbour potassium ions. This is in contradiction to the prediction of Willis (1969) based on the assumption that the ions will always prefer to vibrate in directions away from their nearest neighbours. Whilst such an assumption is justifiable for atoms having point masses and zero charge, Coulombic forces must certainly be considered for a highly ionic compound such as KCl. The repulsive core–core interaction will cause the atoms to vibrate along ⟨111⟩ directions, towards atoms of the same type, and hence tend to make δ_J positive. However, Coulombic forces will inhibit such motion, causing preferred vibration along ⟨100⟩ directions, towards atoms of the opposite type, with resulting negative δ_J values as observed for the chlorine ions. The experimental results therefore indicate that, in the case of the chlorine ions in KCl, the Coulombic forces have greater influence on the anisotropic fourth-order vibrations than do the repulsive forces between cores. A similar result has since been observed for both types of ion in SrF_2 (Mair, Barnea, Cooper & Rouse, 1974).

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