CONCLUSIONS

In this investigation the thermal expansion and Debye temperatures of the alkali halides KI, RbI, and CsI have been determined at different temperatures from room temperature up to about melting point.

It has been shown probably for the first time that a single equation cannot explain the entire plot of the cell constant \( a_t \) versus temperature for the halides studied. Two equations are found necessary, one from room temperature to about the temperature corresponding to the 'knee' of electrical conductivity versus \( 1/T \) plot and other for higher temperatures. At high temperature the deviations from the extrapolated initial part of the \( \Delta \alpha - t \) curve are found to increase exponentially according to the equation

\[
\Delta \alpha = A e^{-U/KT}
\]

where \( A \) is a constant. The energy \( U \) has been identified with the energy of formation of a vacancy.
The values of $U$ obtained for the halides agree closely with the experimental and theoretical values of other workers. The plot of $\alpha/\alpha_{m/2}$ versus $1/T$ for all these halides closely coincides with the similar curve for NaCl, KCl and CsBr obtained by Pathak and Vasavada (1970), showing that these halides also follow the general law of corresponding states. The frequency spectra of these halides are examined and it is shown that in the range of temperatures from 300 to 900°K the geometric mean of the frequency ratio $\nu_i/\nu_{ic}$ decreases from 13 to 22% for the halides studied.

The Debye characteristic temperatures of KI, RbI and CsI have been determined from room temperature up to about their melting points. The temperature variation of $\Theta$ has been calculated by three different methods. It is found that the values of $\Theta$ determined by Maradudin and Flinn's method are consistently lower than those obtained by the other two methods. Only in the case of KI experimental study of temperature variation of $\Theta$ up to 600°C has been made by Pearson and Tompson (1967). Their results are in complete agreement with ours at all temperatures. For
RbI and CsI unfortunately there is hardly any reliable experimental data available and hence no comparison is possible. High temperature data for RbI and CsI are obtained for the first time. It is shown that the anharmonic contribution to Debye $\Theta$ arises essentially from thermal expansion up to about $650^\circ K$ establishing the validity of quasiharmonic theory of lattice vibrations. Above this temperature higher order terms viz. quartic in the potential energy function of the crystals would be required to explain the deviations of experimental points.

It was interesting to find that the plot of the reduced expansion $\alpha / \alpha m^2$ versus $T/\alpha m^2$ gives a common curve for KI and RbI. A common equation between $\alpha$, $T$ and $\Theta$ is established for these halides.

The results of these investigations together with those of Pathak and Vasavada (1970) show that the thermal expansion of alkali halides is intimately associated with the creation of Schottky defects. A more detailed study of this phenomenon as well as variation of Debye $\Theta$ with temperature especially at
High temperature may lead to a better understanding of various processes occurring in solids e.g. it may give deeper insight into the nature of anharmonic forces, role of lattice defects, and the mechanism of melting.