ABSTRACT

On the basis of matrix formalism of method of moments developed by Perlin and Tsukerblat [20], we have calculated theoretically the second and third moments of A→T absorption band in U-centre of KBr and NaI. The electron-phonon interaction was expressed in a point-lattice model in linear approximation and the phonon sum appearing in the formulae for the moments was taken in Debye's approximation for acoustical and Einstein's approximation for optical phonons with cut off wave vector $\chi_D = \frac{(3\pi^2)^{1/3}}{a_0}$, where a_0 is the nearest neighbour distance. The calculated values of second moment, σ_2, are 8.01×10^{-3} eV^2 and 14.43×10^{-3} eV^2 at 7 K and $78^{\circ}K$ respectively, and that of third moment, σ_3, which is temperature independent, is 10.30×10^{-5} eV^3 for KBr. While the experimental values for the second and third moments are $\sigma_2(7^{\circ}K) = (12.50 \pm 0.8) \times 10^{-3}$ eV^2, $\sigma_2(78^{\circ}K) = (17.2 \pm 0.9) \times 10^{-3}$ eV^2 and $\sigma_3 = 10.90 \times 10^{-5}$ eV^3 [34]. Similar calculations were done for NaI crystal and they are found to be $\sigma_2(7^{\circ}K) = 7.18 \times 10^{-3}$ eV^2, $\sigma_2(78^{\circ}K) = 12.82 \times 10^{-3}$ eV^2 and $\sigma_3 = 8.97 \times 10^{-5}$ eV^3. With the help of Edgeworth Series, where the band shape function is expressed in terms of Gaussian Curve as trial function and the moments of the spectrum, we have calculated the half-widths of the absorption spectra, which are found to be 0.21 eV and 0.28 eV at $7^{\circ}K$ and $78^{\circ}K$ respectively for KBr, while the corresponding

experimental values are 0.25eV and 0.30eV. For NaI crystal, the half-widths are found to be 0.20eV and 0.27eV at 7^{o}K and 78^{o}K respectively. These results show that the point-ion model for crystal field and the Extended Brillouin Zone scheme for phonon sum are applicable to the absorption spectrum by p-electron of U-centre in alkali halide crystals.