Lattice Dynamics of Alkali Halides (LiF and NaCl).

M. S. KUSHWAHA

*Department of Physics, Banaras Hindu University - Varanasi 221005, India**(Nuovo Cimento B, 60, 187 (1980))*

The total potential energy per unit cell $\varphi(r)$ for the NaCl structure in the framework of BBFM (see sect. 4) is written as

$$\varphi(r) = \{6\varphi_1(r_I) + 6(\varphi_1^{++}(r_{II}) + \varphi_1^{--}(r_{II}))\} + \varphi_2(\delta\theta) - \alpha_m \frac{Z^2 e^2}{r_I}.$$

In case the cation-cation interactions $\varphi_1^{++}(r_{II})$ are treated equal to the anion-anion interactions $\varphi_1^{--}(r_{II})$, eq. (10) should read

$$(10) \quad \varphi(r) = \{6\varphi_1(r_I) + 12\varphi_1(r_{II})\} + \varphi_2(\delta\theta) - \alpha_m \frac{Z^2 e^2}{r_I}.$$

And thus eq. (12) should read

$$(12) \quad \beta_1 + 4\beta_2 = -0.29126 Z^2$$

as a consequence of eq. (11).

The use of eq. (12) now enables us to explain the Cauchy discrepancy ($C_{12} - C_{44}$), from eqs. (8b) and (8c), such that

$$(C_{12} - C_{44}) = \frac{e^2}{2a^4} (-6y'_1 - 4y'_2 - 6y'_3).$$

It may thus be concluded that the bond-bending forces do explain the Cauchy discrepancy.