

# BULK PROPERTIES OF ALKALI HYDRIDE CRYSTALS ON THE MOLECULAR BEHAVIOUR

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The hypothesis of identical ionic behaviour in the molecular and crystal state propounded by Kumar and Kachhava (1970) for alkali halides has been further applied to predict certain bulk properties of alkali hydride crystals. Computed values of equilibrium interionic distance, cohesive energy, compressibility, thermal expansion, Grüneisen constant, reststrahlen frequency, elastic constants, effective ionic charge and dielectric constants for the Born-Mayer, Hellmann and Logarithmic type of potentials have been reported. Logarithmic type of potential gives the best results of cohesive energy, interionic distance and dielectric constant and hence the other properties obtained on the basis of this potential are recommended.

## INTRODUCTION

Although alkali hydride crystals chemically appear to be very simple compounds but due to their reactive nature, a very few physical properties of these crystals could be measured and as such the experimental information about these crystals is very meagre. Owing to the non-availability of the experimental data for important practical applications, the theoretical estimates of the various properties of these hydrides will be useful. In this connection, efforts have already been made by the authors (Lachhman Dass & Saxena 1965a, 1970).

It is also well-known that the molecular properties of these substances have been more thoroughly examined (Varshni & Shukla 1963; and Lachhman Dass & Saxena 1965b) through the knowledge of the interatomic forces compared to the crystalline behaviour. Therefore, in this paper we aim to make use of the molecular properties for the investigation of crystal properties.

An interatomic potential in the molecular state is usually written as

$$\phi(r) = -\frac{e^2}{r} + v(r) \quad \dots (1)$$

In this  $\phi(r)$  is the interaction energy between two ions separated by a distance  $r$ ,  $e$  the electronic charge, and  $v(r)$  is the overlap term. This term usually involves two potential parameters. Three different forms for the overlap term shall be exploited to describe the various physical properties of these substances. The two potential parameters of Eq. (1) can be obtained from the equilibrium condition and the knowledge of the force constant as illustrated by Herzberg (1955). Taking identical ionic

behaviour in the molecular and crystal states, the interacting energy per cell,  $\phi(r)$ , in the crystal state assuming only the nearest neighbour interaction, can be written as

$$\Phi(r) = -\frac{\alpha e^2}{r} + M \nu(r) \quad \dots (2)$$

Here  $\alpha$  is the Madelung's constant and  $M$  is the co-ordination number. The form of Eq. (2) permits us to utilize molecular properties for predicting the various bulk physical properties of these substances. Such an approach also gets support from the work of Kumar and Kachhava (1970) on alkali halide crystals.

In this work the authors have utilised the following three forms for Eq. (2) :

$$\Phi(r) = -\frac{\alpha e^2}{r} + MA_1 e^{-r/\rho} \quad (Pot. I), \quad \dots (3)$$

$$\Phi(r) = -\frac{\alpha e^2}{r} + MA_2 (e^{-\lambda r}/r) \quad (Pot. II), \quad \dots (4)$$

and

$$\Phi(r) = -\frac{\alpha e^2}{r} + MA_3 \log_e \left( 1 - \frac{B}{r^9} \right) \quad (Pot. III), \quad \dots (5)$$

where  $A$ 's  $\rho$ ,  $\lambda$  and  $B$  are the potential parameters. Eqs. (3) and (4) are the well-known Born-Mayer and Hellmann potentials and have been found to be equally good for predicting the various bulk properties of alkali hydride crystals (Lachhman Dass & Saxena 1965a, 1970). Potential III of Eq. (5) has been found by Misra *et al.* (1971) to predict well a few crystal properties of alkali halides.

#### THEORETICAL FORMULATIONS

Applying equilibrium condition

$$\left[ \frac{d\Phi(r)}{dr} \right]_{r=r_0} = 0 \quad \dots (6)$$

to the potentials of Eqs. (3), (4) and (5), alongwith the equilibrium condition in the molecular state, we get the following expressions for  $r_0$  corresponding to the three potentials :

$$\log r_0 - \frac{r_0}{4.606\rho} + \frac{1}{2} \log \frac{6}{\alpha} + \frac{r_e}{4.606\rho} - \log r_e = 0, \quad \dots (7)$$

$$\log (1 + \lambda r_0) - (r_0 - r_e) \lambda + \log \frac{6}{\alpha} - \log (1 + \lambda r_e) = 0, \quad \dots (8)$$

and

$$r_0^9 - \frac{6r_e^8}{\alpha} \left( 1 + \frac{B}{r_e^9} \right) r_0 + B = 0. \quad \dots (9)$$

Here  $r_e$  is the equilibrium internuclear separation in the molecular state. No general method exists for finding  $r_0$  exactly from these transcendental equations.

TABLE I  
*r*<sub>0</sub> values of alkali hydride crystals in Å

Crystal	Expt.	Calculated					
		Pot. I	% ab. dev.	Pot. II	% ab. dev.	Pot. III	% ab. dev.
LiH	2.042	2.48	21.43	2.62	28.30	2.110	3.30
NaH	2.44	2.78	13.93	2.861	17.26	2.450	0.41
KH	2.85	3.14	10.17	3.213	12.74	2.869	0.67
PbH	3.0185	3.26	8.00	3.322	6.74	3.007	0.59
CsH	3.188	3.38	5.86	3.501	9.70	3.153	1.09
Average % ab. deviation			11.88		14.96		1.21

However, it is possible to compute *r*<sub>0</sub> to any desired degree of accuracy. These equations have been solved by the method of iteration (Scarborough 1964) and the values of *r*<sub>0</sub> so obtained have been recorded in Table I. Experimental values of *r*<sub>0</sub> reported by Lachhman Dass and Saxena (1965*a*) along with the average absolute deviation have also been given in this table.

The cohesive energy per mole, *W*<sub>0</sub>, is given by

$$W_0 = - [N\Phi(r_0) \div E_0]. \quad \dots (10)$$

In this  $\Phi(r_0)$  is the potential energy at equilibrium value of *r*, viz., *r*<sub>0</sub>. *N* is the Avogadro number and *E*<sub>0</sub> is the zero point energy per mole.

As no Debye temperature data for alkali hydride crystals are available, we have calculated *E*<sub>0</sub> from the well-known relation :

$$E_0 = \frac{9}{4} N h \nu_m \quad \dots (11)$$

In this equation *h* is the Planck's constant and  $\nu_m$  is the frequency corresponding to maximum absorption of energy.  $\nu_m$  has been found from the relation

$$\nu_m = \frac{1}{2\pi} \sqrt{\frac{A}{\mu}} \quad \dots (12)$$

Here  $\mu$  is the reduced mass of the two ions and *A* is the force constant and has the value (Born & Huang 1956) given by

$$A = \frac{M}{3} \left[ v''(r_0) \div \frac{2}{r_0} v'(r) \right], \quad \dots (13)$$

*v'*(*r*<sub>0</sub>) and *v''*(*r*<sub>0</sub>) being the first and second derivatives of *v*(*r*) at *r* = *r*<sub>0</sub>. The calculated values of *E*<sub>0</sub> for Born-Mayer type of potential have been used for all the three potentials as the values for the other potentials considered here are found to be of the same order. These values have been cited in Table II. The experimental and computed values of *W*<sub>0</sub> for the three potentials as well as the absolute deviation of the theoretical values from the experimental are shown in Table II.

Compressibility ( $\beta$ ), the thermal expansion ( $\alpha'$ ), and the Gruneisen constant ( $\gamma$ ) can be determined from  $\Phi(r)$  with the help of following relations given by Kachhaua and Saxena (1964, 1966a).

$$\frac{1}{\beta} = \frac{1}{18r_0} \left[ \frac{d^2 \Phi(r)}{dr^2} \right]_{r=r_0}, \quad \dots (14)$$

$$\alpha' = - \frac{C_v}{2r_0} \left[ \frac{d^3 \Phi(r)}{dr^3} \right]_{r=r_0} \left[ \frac{d^2 \Phi(r)}{dr^2} \right]_{r=r_0}^{-2} \quad \dots (15)$$

and

$$\gamma = - \frac{r_0}{6} \left[ \frac{d^3 \Phi(r)}{dr^3} \right]_{r=r_0} \left[ \frac{d^2 \Phi(r)}{dr^2} \right]_{r=r_0}^{-1} \quad \dots (16)$$

In Eq. (15),  $C_v$  is the specific heat per ion pair at constant volume.

TABLE II  
*Cohesive energy and zero-point energy of alkali hydride crystals in Kcal/mole*

Crystal	$E_0$	Cohesive energy $W_0$						
		Expt.	Calculated				Pot. III	% ab. dev.
			Pot. I	% ab. dev.	Pot. II	% ab. dev.		
LiH	6.02	215.98	165.35	23.44	141.83	34.31	235.22	8.91
NaH	4.88	191.25	164.80	13.83	151.50	31.67	203.67	6.50
KH	4.10	169.84	147.80	12.97	140.17	17.47	174.12	2.52
RbH	3.86	163.17	145.25	10.98	139.16	14.71	166.19	1.85
CsH	3.65	155.64	141.42	9.14	136.27	12.44	159.41	2.42
Average % ab. deviation				14.07		22.12		4.46

TABLE III  
 *$\beta$  and ( $\alpha'/C_v$ ) of alkali hydride crystals at 25°C*

Crystal	$\beta(10^{-12} \text{ cm}^2 \text{ dyne}^{-1})$			$\alpha'/C_v$ (in $10^{10}$ c.g.s. units)		
	Pot. I	Pot. II	Pot. III	Pot. I	Pot. II	Pot. III
LiH	1.05	1.13	0.94	1.82	2.01	2.74
NaH	2.33	2.39	1.88	2.80	2.79	2.96
KH	3.16	4.17	3.42	2.05	3.39	3.50
RbH	5.26	5.40	4.73	3.84	3.87	4.54
CsH	6.77	6.89	6.26	4.43	4.39	4.68

TABLE IV  
 $\gamma$  and  $\omega_0$  values of alkali hydride crystals at 25°C

Crystal	$\gamma$			$\omega_0$ in units of $10^{13}/\text{sec}$			
	Pot. I	Pot. II	Pot. III	Pot. I	Pot. II	Pot. III	Expt.
LiH	0.90	0.90	1.48	20.33	18.81	22.37	11.13
NaH	1.05	1.02	1.38	13.55	13.23	16.73	..
KH	0.91	1.13	1.42	14.26	11.13	13.36	..
RbH	1.21	1.18	1.58	10.10	9.83	11.19	..
CsH	1.28	1.24	1.46	8.96	8.79	9.72	..

The computed values of  $\beta$  and  $\alpha'/C_v$  as the experimental values of  $C_v$  for these substances (except LiH) are not known, are recorded in Table III and those of  $\gamma$  in Table IV.

According to the theories of Kellermann (1940), and Sharan and Tiwari (1964), the reststrahlen frequency,  $\omega_0$ , is given by the relation :

$$\omega_0^2 = \frac{e^2}{\mu v_a} \left( \frac{3v_a^2}{\beta e^2 r_0^2} - \frac{4\pi}{3} \right). \quad \dots (17)$$

In this equation  $v_a$  is the volume of the unit cell and  $\mu$  is the reduced mass. In conjunction with the  $\beta$  values of Table III values of  $\omega_0$  computed are given in Table IV. Only known experimental value is also given therein (Burstein 1963).

Knowing the potential, the elastic constants  $c_{11}$ ,  $c_{12}$  and  $c_{44}$  can also be calculated. According to Kellermann (1940), we have

$$c_{11} = \left( \frac{6r_0^4}{\beta e^2} - 1.395 \right) \frac{e^2}{2r_0^4}, \quad \dots (18)$$

and

$$c_{12} \approx c_{44} = \frac{0.3475e^2}{r_0^4}. \quad \dots (19)$$

Using the  $\beta$  values of Table III and other pertinent data, the computed values of  $c_{11}$  from Eq. (18) are recorded in Table V.  $c_{12} \approx c_{44}$  values which are independent of the form of the potential have also been given therein.

Krishnan and Roy (1952) from their theory of lattice vibrations of alkali halides deduced expressions for elastic constants for the Born-Mayer type of potential. We

TABLE V

Elastic constants  $c_{11}$ ,  $c_{12}$  and  $c_{44}$  of alkali hydride crystals on Kellermann and Krishnan and Roy (1952) model in units of  $10^{11}$  ergs/cm

$c_{12} \approx c_{44}$  is the same in both modes and for all potentials.

Crystal	Kellermann model			Krishnan and Roy model			$c_{12} \approx c_{44}$
	Pot. I	Pot. II	Pot. III	Pot. I	Pot. II	Pot. III	
LiH	19.46	17.32	22.54	15.09	12.75	16.21	4.61
NaH	8.32	8.03	11.47	6.18	5.89	10.93	2.26
KH	7.07	4.77	6.33	5.92	3.62	5.87	1.22
RbH	3.77	3.62	4.41	2.86	2.71	4.65	0.97
CsH	2.87	2.80	3.24	2.14	2.06	3.73	0.78

have also deduced expressions for the Pot. II and Pot. III. The general expression for  $c_{11}$  is

$$c_{11} = \left[ 2\alpha_1 (1 + \delta) - 6X \right] \frac{e^2}{12r_0^4} \quad \dots (20)$$

Here  $\alpha_1 = 1.75$  and  $X = 3.14$ .  $\delta$  has different form for each potential. For the three potentials its values in terms of the potential parameters and  $r_e$  are :—

$$\text{For Pot. I, } \delta = \frac{6r_0^3}{\rho\alpha r_e^2} e^{-(r_0 - r_e)/\rho}, \quad \dots (21)$$

$$\text{for Pot. II, } \delta = \frac{6(\lambda^2 r_0^2 + 2\lambda r_0 + 2)}{\alpha(1 + \lambda r_e)} e^{-(r_0 - r_e)\lambda} \quad \dots (22)$$

and

$$\text{for Pot. III, } \delta = \frac{6r_0(B + r_e^9)}{\alpha r_e} \frac{(B + 10r_0^9)}{(B + r_0^9)^2} \quad \dots (23)$$

Computed values of  $c_{11}$  from Eq. (20) in conjunction with Eqs. (21), (22) and (23) are displayed in Table V.

The high frequency dielectric constant,  $\epsilon_\infty$ , and low frequency dielectric constant,  $\epsilon_0$ , can be easily calculated by the theory of Mott and Gurney (1948) from the knowledge of the intermolecular forces. The corresponding expressions are :

$$\frac{\epsilon_{\infty} - 1}{4\pi} = \frac{\frac{8}{3} \pi N^2 \alpha_+ \alpha_- (\gamma' - 1) + N' (\alpha_+ + \alpha_-)}{1 - \frac{4\pi}{3} N' (\alpha_+ + \alpha_-) - \frac{16}{9} \pi^2 N'^2 (1 - \gamma'^2) \alpha_+ \alpha_-} \quad \dots (24)$$

and

$$\begin{aligned} \frac{\epsilon_0 - 1}{4\pi} = & \frac{\frac{4\pi}{3} N' \alpha_+ (\alpha_+ + \alpha_-) - \frac{32}{9} \pi^2 N'^2 (1 - \gamma') \alpha_+ \alpha_-}{1 - \frac{4\pi}{3} (\alpha_+ + \alpha_-) (1 - \gamma') + \frac{16}{9} \pi^2 N'^2 (1 - \gamma')^2 \alpha_+ \alpha_-} \\ & + \frac{\frac{4\pi}{3} \delta'}{1 - \frac{4\pi}{3} (1 - \gamma') \delta'} \quad \dots (25) \end{aligned}$$

In these equations  $N'$  is the number of ions pairs per unit volume,  $\alpha_+$  and  $\alpha_-$  the polarizabilities of the positive and negative ions respectively, and  $\gamma'$  a constant which varies between 0 and 1. Kachhava and Saxena (1966*b*) have shown that for the Born-Mayer potential it can be estimated from the following relation :

$$1 - \gamma' = \frac{r_0^2}{e^2 \rho} \frac{A_1}{6} e^{-r_0/\rho} \quad \dots (26)$$

However, the expressions for the three potentials, when identical ionic behaviour is assumed in molecular and crystal states, are respectively :

$$1 - \gamma' = \frac{r_0^2}{r_e} e^{-(r_0 - r_e)/\rho} \quad \dots (27)$$

$$1 - \gamma' = \frac{1 + \lambda r_0}{1 + \lambda r_e} e^{-(r_0 - r_e)\lambda}, \quad \dots (28)$$

and

$$1 - \gamma' = \frac{r_0}{r_e} \frac{B + r_e^9}{B + r_0^9} \quad \dots (29)$$

Further  $\delta'$  of Eq. (25) is related to  $A$  of Eq. (13) by the relation :

$$\delta' = \frac{N'e^2}{A} \quad \dots (30)$$

TABLE VI

*High frequency dielectric constant  $\epsilon_\infty$ , on the Mott-Gurney theory*

Substance	Expt.	$\gamma'=1$	$\gamma'=0$	Pot. I ( $\gamma'$ of Eq. 27)	Pot. II ( $\gamma'$ of Eq. 28)	Pot. III ( $\gamma'$ of Eq. 29)
LiH	3.61	3.45	3.40	3.42	3.42	3.43
NaH	..	2.20	2.13	2.26	2.16	2.18
KH	..	1.93	1.87	1.93	1.93	1.95
RbH	..	1.96	1.83	1.89	1.90	1.92
CsH	..	2.11	1.94	2.04	2.04	2.06

TABLE VII

*Low frequency dielectric constant,  $\epsilon_0$  on the Mott-Gurney model*

Substance	Expt.	Pot. I			Pot. II			Pot. III		
		$\gamma'=0$	$\gamma'=1$	$\gamma'$ of Eq. (27)	$\gamma'=0$	$\gamma'=1$	$\gamma'$ of Eq. (28)	$\gamma'=0$	$\gamma'=1$	$\gamma'$ of Eq. (29)
LiH	12.9	8.40	-50.31	16.57	11.07	-19.80	23.71	6.00	32.80	12.16
NaH	..	7.59	38.64	11.94	8.61	93.24	14.26	5.43	13.70	9.08
KH	..	6.03	14.39	8.49	6.61	17.76	9.38	4.98	9.67	7.35
RbH	..	6.02	30.37	8.60	6.53	44.16	9.78	5.31	19.95	8.46
CsH	..	6.20	18.93	10.06	6.65	23.30	10.91	5.70	15.34	10.18

In Tables VI and VII  $\epsilon_\infty$  and  $\epsilon_0$  computed from Eqs. (24) and (25) for the limiting values of 0 and 1 and also the value of  $\gamma'$  obtained from Eqs. (27), (28) and (29) are reported. Value of  $\delta'$  appropriate to the  $\gamma'$  has been calculated and used. The only experimental value available for LiH (Burstein 1963) has also been listed in Tables VI and VII.

Theory of Mott and Gurney (1948) has considerably been revised and many new theories have been given. One such theory is due to Dick and Overhauser (1958). They introduced a model known as shell model and tested their theory by calculating the effective ionic charge,  $s$ . We plan to check the theory by calculating dielectric constants  $\epsilon_0$  and  $\epsilon_\infty$  and  $s$  from the relations given by them. For alkali hydride crystal calculations, the procedure for calculating the constants like, number of electrons in the shell, the core-shell spring constant, the shell-shell spring constant, etc. has been outlined by Lachhman Dass and Saxena (1970). Neglecting exchange charge interaction effect which has been shown to be small by Dick and Overhauser for LiCl and NaCl on the basis of the overlap integrals of Lowdin (1948, 1956), one



has the following expressions for  $\epsilon_\infty$ ,  $\epsilon_0$ ,  $s$  and  $\beta^*/\beta$  :

$$\frac{\epsilon_\infty - 1}{\epsilon_\infty + 2} = \frac{4\pi N'}{3} e^2 \left[ \left( \frac{n_+^2}{k_+} + \frac{n_-^2}{k_-} \right) - \frac{A'}{1+A'\lambda} \left( \frac{n_+}{k_+} - \frac{n_-}{k_-} \right)^2 \right] \quad \dots (31)$$

$$\frac{\epsilon_0 - 1}{\epsilon_0 + 2} = \frac{4\pi N}{3} e^2 \left[ \frac{1 + A'\lambda}{A'} + 2 \left( \frac{n_+}{k_+} - \frac{n_-}{k_-} \right) + \left( \frac{n_+}{k_+} - \frac{n_-}{k_-} \right)^2 \right], \quad \dots (32)$$

$$s = \frac{e^*}{e} = 1 + A' \left( \frac{n_+}{k_+} - \frac{n_-}{k_-} \right) \cdot \frac{1}{1+A'\lambda}, \quad \dots (33)$$

and

$$\beta^*/\beta = 1 + A'\lambda. \quad \dots (34)$$

Here  $e^*$  is the effective ionic charge,  $\beta$  the compressibility value according the original theory of Szigeti (1949, 1950) given by the relation.

$$\beta = \frac{3}{N' r_0^2} \left( \frac{\epsilon_\infty + 2}{\epsilon_0 + 2} \right) \frac{1}{\mu \omega_0^2} \quad \dots (35)$$

and  $\beta^*$  the value of compressibility from the theory of Dick and Overhauser and is given by

$$\beta^* = 6r_0 \left( \frac{1 + A'\lambda}{A'} \right). \quad \dots (36)$$

Further,

$$A' = 6r_0/\beta, \quad \dots (37)$$

$$\lambda = \frac{1}{k_+} + \frac{1}{k_-},$$

and

$$k_\pm = (en_\pm)^2/\alpha_\pm. \quad \dots (38)$$

$n_+$  and  $n_-$  are the number of electrons in alkali and hydrogen shells respectively. The values of  $k_+$  and  $k_-$  have been reported by Lachhman Dass and Saxena (1970).

TABLE VIII  
 $\beta^*/\beta$  and  $s$  values from shell model

Substance	$\beta^*/\beta$				$s$		
	Pot. I	Pot. II	Pot. III	Expt.	Pot. I	Pot. II	Pot. III
LiH	1.185	1.172	1.205	0.53	0.660	0.683	0.631
NaH	1.063	1.097	1.194	..	0.804	0.814	0.783
KH	1.0869	1.066	1.080	..	0.847	0.882	0.858
RbH	1.056	1.054	1.062	..	0.907	0.909	0.897
CsH	1.046	1.046	1.046	..	0.931	0.936	0.926

TABLE IX  
 $\epsilon_0$  and  $\epsilon_\infty$  on the Dick and Overhauser model

Substance	$\epsilon_0$				$\epsilon_\infty$			
	Expt.	Pot. I	Pot. II	Pot. III	Expt.	Pot. I	Pot. II	Pot. III
LiH	12.9	6.20	7.21	5.27	3.6	2.87	2.91	2.82
NaH	..	6.05	6.80	5.02	..	2.07	2.08	2.07
KH	..	4.38	6.67	4.85	..	1.89	1.90	1.90
RbH	..	7.44	7.19	6.49	..	1.94	2.24	1.95
CsH	..	10.00	13.16	2.34	..	2.12	2.12	2.12

The calculated values of  $e^*/e$ ,  $\beta^*/\beta$ ,  $\epsilon_\infty$  and  $\epsilon_0$ , for the three potentials in the spirit of this paper are recorded in Tables VIII and IX. Calculated value of  $s$  for LiH from the theory of Szigeti (1949, 1950) is also given in Table VIII. Results of the theories of Hanlon and Lawson (1959) as well as Havinga (1960) are not encouraging for alkali hydride crystals and, therefore, these have not been reported here. However, we realize that more precise  $\alpha_\infty$  values are required for proper assessment of these theories.

#### RESULTS AND DISCUSSION

A comparison of the  $r_0$  values obtained through various potentials with the experimental data shows that the reproduction of values in the case of the logarithmic type is excellent. The average absolute percentage deviation in this case is only 1.21. In the case of cohesive energy, the analysis of Table II shows that the behaviour of logarithmic type of potential is much better than the other two. The superiority of this type of potential gets the support also from the calculations of Misra *et al.* (1971) and Thakur & Sarkar (1975), and also  $\epsilon_0$  and  $\epsilon_\infty$  and  $s$  values reported in this paper. No experimental data for  $\beta$ ,  $\alpha''C_v$ ,  $\gamma$  and  $\omega_0$  is available for comparison. However, the results for  $\beta$ ,  $\alpha''C_v$ ,  $\gamma$  and  $\omega_0$  obtained on the basis of logarithmic potential and given in Tables III and IV are, therefore, recommended as reliable values for future use.  $c_{11}$  values obtained for this potential with Krishnan and Roy model as this model is an improvement over the Kellermann model and  $c_{12} \approx c_{44}$  values displayed in the last column of Table V are recommended.

It is clear from Table VI that  $\epsilon_\infty$  values show only a weak dependence on  $\gamma'$ . Precise determination of  $\gamma'$  in this case is, therefore, not much useful. Although on the basis of  $\epsilon_\infty$  alone one cannot judge the adequacy of one potential over the other but the comparison of the only experimental value of LiH shows that the logarithmic type potential has a slight edge over the other two.  $\epsilon_0$  values, on the other hand from Mott and Gurney model found to be dependent on  $\gamma'$ ,  $\gamma' = 0$  as well as  $\gamma' = 1$  give absurd values for all the three potentials, but however,  $\gamma'$  determined from Eqs. (27), (28) and (29) give better values. Value of  $\epsilon_0$  for LiH with logarithmic potential is found to be in excellent agreement with the experimental

value. Thus we recommend  $\epsilon_0$  and  $\epsilon_\infty$  values of the last columns of Tables VI and VII respectively.  $s$  values of Table VIII show an increasing trend for all the potentials for the substances from LiH to CsH. In this case the comparison of the only value of LiH computed from Szigeti relation shows that logarithmic potential is superior than both the other two while Born-Mayer is found to be slightly better than Hellmann. As such we recommend  $s$  values given in the last column of Table VIII and  $\beta^*/\beta$  values given in 4th column of the same table. We have further tested the theory of Dick and Overhauser by calculating  $\epsilon_0$  and  $\epsilon_\infty$ . The values given in Table IX show that this model yields reliable values for  $\epsilon_\infty$  but does not seem to be suitable for predicting  $\epsilon_0$  values.

To be complete in our discussion we must realize that the whole structure of the present investigation is built upon one assumption, rather drastic, that the bond in alkali hydrides is almost ionic. Experimental data, whatever available, point to the fact that in practice there are substantial deviations from the pure ionic character. However, the potential parameters obtained on the basis of proposed scheme seem to assimilate these effects so as to reflect good agreement between theoretical values and existing experimental data. This agreement may therefore be also taken as an indication of the extent upto which the theoretical values of those properties for which there are no measurements can be relied upon.

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