

## I. PHYSICS

### Chemical Physics

# AN EXPONENTIAL FUNCTION FOR REPULSIVE INTERACTION FOR METAL HALIDES

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The suitably modified Varshni-Shukla (V-S) potential energy function has been applied to study the thermodynamic properties of some metal halides. The potential parameters have been evaluated at room temperature ( $T$ ) and atmospheric pressure ( $p = 0$ ). The computed values of thermodynamic properties viz., lattice energy ( $W$ ), infrared eigen frequency ( $\nu_0$ ), Debye characteristic temperature ( $\Theta_D$ ), the Grüneisen parameter ( $\gamma$ ), and the recently discovered Anderson-Grüneisen parameter ( $\delta$ ), compare well with the experimental values and exhibit a marked improvement over calculated results of other workers. It has been inferred that the suitably modified V-S model is also a good choice for understanding the behaviour of heavier ionic crystal lattices.

**Keywords :** Varshni-Shukla Potential Energy Function; Lattice Energy; Infrared Eigen Frequency; Debye Characteristic Temperature; Grüneisen Parameter; Anderson-Grüneisen Parameter.

## INTRODUCTION

THE macroscopic properties of alkali halide crystals employing the interaction approach have attracted the attention of various workers viz., Born and Mayer (1932), Huggins and Mayer (1933), Huggins (1937, 1947), Born and Huang (1954), Cubicciotti (1959), Sharma and Madan (1964a), Gchel (1968) and Koski (1972), from time to time as they yield interesting and valuable information regarding the forces operating in the solids. However, little attention has been paid to study the thermodynamic properties of heavier ionic crystals e.g., metal halides. Although few forms of potential models have been suggested to study the lattice properties of metal halides, they have achieved only limited success (cf. Mayer, 1933; Mayer & Levy, 1933; Bleick, 1934; Sharma & Madan, 1964b; Saxena & Kachhava, 1964; and Gupta & Sharma, 1969, 1970, 1971).

Recently, an exponential form of potential energy function suggested by Varshni and Shukla (1961) and subsequently modified by Patel *et al.* (1967) for repulsive interaction energy term of the form  $\lambda \exp(-\mu r^{3/2})$  was applied, in conjunction with the expression for Coulomb energy, dipole-dipole and dipole-quadrupole interaction energy terms, by Misra *et al.* (1974) for some alkali halides and good results were obtained. For the heavier ionic solids, the inclusion of the dipole-quadrupole interaction energy term in the expression for the potential energy makes the potential

more realistic and suitable (Born & Huang, 1954). Considering the success of the applicability of modified V-S potential in the case of alkali halides (Misra & Sharma, 1972; Sharma & Tripathi, 1975; Gupta *et al.*, 1975; and Shanker *et al.*, 1978), the present authors have extended this model for studying the various thermodynamic properties of metal halides and have achieved good results.

### THEORY

Assuming the modified V-S repulsion energy form of the type  $\lambda \exp(-\mu r^{3/2})$ , the expression for the potential energy per unit cell may be expressed as :

$$\psi(r) = -\frac{\alpha e^2}{\gamma} + \lambda e^{-\mu r^{3/2}} - \frac{C}{r^6} - \frac{D}{r^8}, \quad \dots(1)$$

where  $\alpha$  is the Madelung constant,  $e$  the electronic charge,  $r$  the interionic distance,  $\lambda$  and  $\mu$  are the potential parameters,  $C$  and  $D$  are the van der Walls constants. The parameters  $\lambda$  and  $\mu$  can be evaluated by applying the suitable thermodynamic equilibrium conditions.

#### *Evaluation of Potential Parameters*

The parameters  $\lambda$  and  $\mu$  of equation (1) have been evaluated by applying the following well-known room temperature ( $T$ ) (thermodynamic equilibrium) conditions at atmospheric pressure ( $p=0$ ) (Born & Huang, 1954):

$$r_0 [\psi'(r)]_{r=r_0} = \frac{3vT\alpha_v}{\beta} \quad \dots(2)$$

and

$$r_0^2 [\psi''(r)]_{r=r_0} = \frac{9v}{\beta} F_{T,P} \quad \dots(3)$$

where  $v$  is the volume of the unit cell,  $\alpha_v$  the volume thermal expansion coefficient,  $r_0$  the equilibrium interionic distance,  $\beta$  the compressibility and  $F_{T,P}$  a correction factor. Combining equations (2) and (3) in conjunction with equation (1), one obtains

$$\lambda = \frac{\left( \frac{\alpha e^2}{r_0} + \frac{6C}{r_0^6} + \frac{8D}{r_0^8} - \frac{3vT\alpha_v}{\beta} \right)^2 e^{\mu r_0^{3/2}}}{\frac{5\alpha e^2}{2r_0} + \frac{45C}{r_0^6} + \frac{76D}{r_0^8} - \frac{3vT\alpha_v}{2\beta} + \frac{9v}{\beta} F_{T,P}} \quad \dots(4)$$

and

$$\mu = \frac{\frac{5\alpha e^2}{3r_0} + \frac{30C}{r_0^6} + \frac{152D}{3r_0^8} - \frac{vT\alpha_v}{\beta} + \frac{6v}{\beta} F_{T,P}}{r_0^{\frac{3}{2}} \left[ \frac{\alpha e^2}{r_0} + \frac{6C}{r_0^6} + \frac{8D}{r_0^8} - \frac{3vT\alpha_v}{\beta} \right]} \quad \dots(5)$$

The parameters  $\lambda$  and  $\mu$  have been evaluated employing equations (4) and (5) and are presented in Table I. The experimental input data for the computation of  $\lambda$  and  $\mu$  and other thermodynamic properties of the crystals investigated in the present work are presented in Table II.

TABLE I  
Potential parameters and the cohesive energy of heavier halides

Crystals	$\lambda(10^{-12})$	$\mu(10^{+12})$	Cohesive Energy (KCal/mole)			
			Exptl.*	Theoretical eqns. (1) & (6)	Theoretical*	Theoretical**
AgCl	3466.241	1.582	203	207.39	197.5	197.9
AgBr	3897.645	1.526	197	199.77	190.2	190.5
AgI	3931.178	1.585	190	193.74	183.9	—
CuCl	717.197	1.569	221.9	224.88	211.0	216.9
CuBr	765.911	1.987	216	212.36	201.9	—
CuI	742.895	1.414	213.4	203.70	195.6	194.5
TlCl	1449.505	1.065	167	172.27	161.5	168.2
TlBr	1630.463	1.032	164	167.55	157.6	162.4
NH <sub>4</sub> Cl	1042.474	1.039	—	166.19	—	—
NH <sub>4</sub> Br	1704.676	1.069	—	160.54	—	—

\*Saxena *et al.* (1964).

\*\*Mathur and Singh (1967).

### Calculation of Crystal Properties

(a) *Cohesive Energy*: Once the parameters of the potential energy function are evaluated, the cohesive energy per mole ( $W$ ) can be determined by the relation:

$$W = - [N\psi(r_0) + \epsilon] \quad \dots(6)$$

where  $N$  and  $\epsilon$  are the Avogadro's numbers and the zero point energy per mole respectively. Theoretical values of  $W$  on the basis of equation (6) for some heavier halides are presented in Table II. The values so obtained have been compared and discussed in the light of the observed values and other calculated values.

(b) *Force Constant and Infrared Eigen Frequency*: Krishnan and Roy (1951) and Born and Huang (1954) have derived a general expression for the force constant ( $f$ ). Their expression can be re-expressed as :

$$f = \frac{1}{3} \left[ \phi''(r_0) + \frac{2}{r_0} \phi'(r_0) \right] \quad \dots(7)$$

Where  $\phi'(r_0)$  and  $\phi''(r_0)$  are the first and second derivatives of the  $\phi(r)$  with respect to  $r$  at  $r = r_0$ , the function  $\phi(r)$  takes into account, all the terms of equation (1) except the Coulombian energy term  $\left( -\frac{\alpha e^2}{r} \right)$

For the Varshni-Shukla potential, equation (7) yields:

$$f = \frac{P(36r_0^{\frac{3}{2}} - 5)}{6r_0^2} - \frac{10C}{r_0^8} - \frac{56D}{3r_0^{10}} \quad \dots(8)$$

TABLE II  
Input data for heavier halides

Crystal	Geometry	$K$	$\alpha$	$r_0$ ( $10^{-8}$ cm)	$\beta$ ( $10^{-13}$ cm <sup>2</sup> dyne <sup>-1</sup> )	$\alpha_v$ ( $10^{-6}$ deg <sup>-1</sup> )	$C$ ( $10^{-40}$ erg cm <sup>4</sup> )	$D$ ( $10^{-72}$ erg cm <sup>8</sup> )	$m^{-1}$ $10^{-23}$ gm <sup>-1</sup>	$\epsilon_0$	$\epsilon_\infty$
AgCl	NaCl	2.00	1.7476*	2.772*	2.40*	98.9*	767*	1065*	0.2250	12.30*	4.60*
AgBr	NaCl	2.00	1.7476*	2.884*	2.75*	104.0*	967*	1410*	0.1312	13.10+	4.62+
AgI	ZnS	3.20	1.6381*	2.812*	4.11*	113.3*	850*	1467*	—	—	—
CuCl	ZnS	3.20	1.6381**	2.340**	2.51**	65.4**	146**	150**	0.2645	10.00+	3.57+
CuBr	ZnS	3.20	1.6381**	2.460**	2.93**	62.1**	198**	220**	0.1702	8.00+	4.08+
CuI	ZnS	3.20	1.6381**	2.620**	2.81**	73.5**	330**	420**	—	—	—
TlCl	CsCl	1.54	1.7626*	3.330*	4.90*	163.8*	2270*	3665*	0.1992	31.90+	5.10+
TlBr	CsCl	1.54	1.7626*	3.440*	5.03*	153.4*	2785*	4820*	0.1049	29.80+	5.10+
NH <sub>4</sub> Cl	CsCl	1.54	1.7626***	3.342***	5.76***	142.0***	1251***	1898***	0.5043	6.96+	2.62+
NH <sub>4</sub> Br	CsCl	1.54	1.7626***	3.514***	6.13***	161.0***	1597***	2681***	—	—	—

\*Mayer (1933).

\*\*Mayer and Levy (1933).

\*\*\*Bleick (1934).

+Born and Huang (1954).

where

$$P = \frac{\alpha e^2}{r_0} + \frac{6C}{r_0^6} + \frac{8D}{r_0^8} - \frac{3\nu T \alpha_\nu}{\beta}$$

The values of  $f$  computed using equation (8) have been reported in Table III. The theoretical values of  $f$  thus obtained can be utilised to evaluate the infrared eigen frequency  $\nu_0$  from the following relation (Born & Huang, 1954):

$$\nu_0 = (2\pi)^{-1} \left( \frac{f}{m} \right)^{1/2} (\epsilon_\infty + 2)^{1/2} (\epsilon_0 + 2)^{-1/2} \quad \dots(9)$$

where the symbols have their usual significance. The  $\nu_0$  values obtained from equation (9) are also reported in Table III where they have been compared with the observed as well as with theoretical values of other workers.

(c) *Debye Characteristic Temperature*  $\Theta_D$ : Blackmann (1955) obtained the relations for  $\Theta_D$  from the lattice theory of specific heat and also from the elastic constants. Mitra and Joshi (1960a,b) derived the relation on the basis of model considerations. In the present treatment, the authors have chosen the following relation for  $\Theta_D$

$$\Theta_D = \frac{h\nu_0}{k} \quad \dots(10)$$

The values of  $\Theta_D$  on the basis of equation (10) are presented in Table IV along with the experimental as well as theoretical values of other workers.

(d) *The Grüneisen Parameter*  $\gamma$ : Sharma and Jain (1973) have developed a general relation for  $\gamma$  which can be written as:

$$\gamma = -\gamma_0 [\psi^{11}(\gamma_0)] [6\psi^{11}(\gamma_0)]^{-1} \quad \dots(11)$$

(f) *The Anderson-Grüneisen Parameter*  $\delta$ : The recently introduced Anderson-Grüneisen parameter  $\delta$  is important as it yields useful information about the macroscopic behaviour of thermodynamic properties of crystals for which the experimental data is inadequate. Anderson (1966) related  $\delta$  with adiabatic bulk modulus  $B_s$  and  $\alpha_\nu$  by the following relation:

$$\delta = -\frac{1}{\alpha_\nu} \left[ \frac{d(\ln B_s)}{dT} \right]_P = - \left[ \frac{\partial \ln B_s}{\partial \ln \nu} \right]_P \quad \dots(12)$$

Later, Chang (1967) related  $\delta$  with the variation of isothermal and adiabatic bulk modulus against pressure as:

$$\delta = \left( \frac{dB_T}{dP} - 1 \right) \approx \left( \frac{dB_S}{dP} - 1 \right) \quad \dots(13)$$

Chang (1967) also derived two simple expressions for  $\delta$  in terms of  $\gamma$  which can be written as:

$$\delta = 2\gamma - \frac{2}{3} \quad \dots(14)$$

and

$$\delta = 2\gamma \quad \dots(15)$$

Recently, Misra (1974), Sharma and Tripathi (1975), Tripathi *et al.* (1975), Sharma and Gupta (1975), Sharma *et al.* (1976) have also developed some relations

TABLE III  
*Values of  $f$ ,  $\nu_0$ ,  $\gamma$  and  $\delta$  for heavier halides*

Crystal	$f$ ( $10^6$ ) Eqn. (8)	$\nu_0$ ( $10^{12}$ cm Sec $^{-1}$ )		$\gamma$		$\delta$			
		Exptl. Eqn. (9)	Theoret. Eqn. (9)	Theoret.***	Exptl.+	Theoret. Eqn. (11)	Exptl.	Theoret. Eqns. (11) & (15)	Theoret. Eqns. (11) & (14)
AgCl	7.067	3.09*	3.98	4.17	2.22	2.02	2.62	4.44	4.04
AgBr	6.422	2.40**	3.06	3.09	2.23	2.09	2.67	4.46	4.18
AgI	—	—	—	—	—	2.10	2.70	—	4.20
CuCl	9.298	5.67*	5.38	5.34	—	1.33	2.38	—	2.66
CuBr	8.259	5.27*	4.66	4.69	—	2.04	2.43	—	4.08
CuI	—	—	—	—	—	2.09	2.90	—	4.18
TlCl	3.241	1.89**	1.85	1.91	2.21	1.71	2.36	4.42	3.42
TlBr	2.829	1.43**	1.32	1.59	—	2.64	2.44	—	5.28
NH $_4$ Cl	2.756	—	4.26	—	—	1.76	2.31	—	3.52
NH $_4$ Br	—	—	—	—	—	1.94	2.29	—	3.88

\*Born and Huang (1954).

\*\*Jones *et al.* (1961).

\*\*\*Srivastava and Madan (1967).

+Gupta and Sharma (1971).

\*\*Obtained by doubling the corresponding values of  $\gamma$  of column VIII.

for the evaluation of  $\delta$  in terms of various thermodynamic properties of crystals and the potential energy function. For the lighter ionic crystals sufficient work has been done on the studies of  $\delta$  but for the heavier ionic crystals very little attention has been paid. Thus it was thought to study the  $\delta$ -property for the metal halides and to study how far the suitably modified V-S potential model is useful for the evaluation of  $\delta$ . In the present work,  $\delta$  has been evaluated employing Chang's relation [equation (15)] connecting  $\gamma$  and  $\delta$ . We can rewrite this equation in terms of the derivatives of the potential energy function. Combining equations (11) and (15), we get :

$$\delta = -\gamma_0 [\psi'''(\gamma_0)] [3\psi''(\gamma_0)]^{-1} \quad \dots(16)$$

#### RESULTS AND DISCUSSION

The theoretical values of  $W$  using eqns. (1) and (6) are presented in Table II show a close agreement with the observed ones. Present results are superior to those given by Saxena *et al.* (1964) (Col. VI) using Born-Mayer potential and also to those of Mathur and Singh (1967) (Col. VII) using Varshni-Shukla potential. The reasons for the superiority over the latter values is evident where no account of Van der Waals interaction terms, which play an important role particularly in heavier salts, has been taken (Born & Huang, 1954). But the superiority over the Saxena *et al.* (1964) renders us to think that Born-Mayer potential which yields equally and sometimes even better results in alkali halides cannot estimate the cohesive energy of heavier salts upto that mark which may be achieved with the aid of modified V-S potential.

The calculated values of Reststrahlen frequencies  $\nu_0$  given in Table III are quite close to the experimental ones. These values are better than those by Srivastava and Madan (1967) (Col. V) obtained using the B-M potential. In case of CuBr and TlCl latter ones are of course slightly better than present values but the difference is too small to be taken as an important factor which may effect the conclusion. Consequently it may be inferred that the modified V-S potential satisfies the requirements of alkali as well as heavier halides in estimating the values of  $\nu_0$  with reasonable accuracy.

The theoretical values of  $\gamma$  and  $\delta$  for heavier halides have also been reported in Table III. The experimental values of  $\gamma$  are known for only three crystals out of ten as given by Gupta and Sharma (1971). The experimental values of  $\delta$  have been obtained directly by substituting the respective values of  $\gamma$  in the relation  $\delta = 2\gamma$ . One set of theoretical values has also been reported. It may be observed from Table III that in two out of three cases where observed values of  $\gamma$  are available (Silver halides) present results are better than those of Gupta and Sharma (1971). However, in TlCl their values are slightly better than the present ones. It may be noted that the values given by Gupta and Sharma (1971) using Lennard-Jones model are invariably higher while the present results are always lower than the experimental values of  $\gamma$ .

A general agreement between the calculated values of  $\Theta_D$  (Table IV) and those estimated from experiment is evident from the table. However, for the heavier salts

TABLE IV  
 Values of Debye characteristic temperature  $\Theta_D$  ( $^{\circ}\text{K}$ )

Crystal	Exptl.*	Theoret. eqn. (10)	Theoret.**	Theoret.+	Theoret.**
AgCl	183	191	188	136	—
AgBr	144	147	147	128	—
CuCl	—	258	265	—	—
CuBr	—	223	222	—	—
TlCl	—	89	89	—	157, 123, 125, 164
TlBr	—	67	65	109	123, 114, 117
NH <sub>4</sub> Cl	—	204	—	—	—

\*Readdy (1963).

\*\*Sharma (1969).

+Mitra and Joshi (1960*b*).

++Bleick (1934).

except AgCl and AgBr observed values of  $\Theta_D$  are not available and hence we can infer that the present approach which yields most satisfactory results for all other lattice properties should provide a fair estimate of  $\Theta_D$  for these salts.

It is evident from the analysis of the theoretically obtained values presented in this investigation that the suitably modified V-S potential is a good choice for heavier halides among all other potentials discussed in the present work.

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