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Study of cohesion and thermodynamic properties of alkali halide crystals

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ABSTRACT

An interionic force model extended to the next nearest neighbours (NNN) and taking into account the contributions arising from van der Waals (vdW) dipole – dipole and dipole quadrupole interactions and three – body (TB) interactions is used to calculate cohesive energy (W), isothermal bulk modulus (B_T), Moelwyn – Hughes parameter (C_1), Debye temperature (θ_D), Grüneisen parameter (γ) and mode Grüneisen parameter (q) using slater, Dugdale and Mc Donald and free volume theories for alkali halide crystals. The calculated values compare well with available experimental data.

KEYWORDS

Interionic force model;
Alkali halide crystals;
Cohesive energy isothermal bulk modulus;
Debye temperature;
Moelwyn-Hughes parameter;
Grüneisen parameter;
Mode Grüneisen paramet.

INTRODUCTION

From time to time several workers[1-18] proposed and applied a number of empirical and semi-empirical interaction potential models (IPM) in which the short range (SR) repulsive part appears either as inverse power, exponential functions or logarithmic functions for evaluating the thermodynamic properties of ionic crystals. Among them the inverse power functions and logarithmic functions have a limited applications for ionic crystals as mentioned by earlier workers[19] on the other hand the exponential functions have been found suitable for ionic crystals[20].

It may be mentioned here that most of the previous workers considered only the nearest neighbour (NN) contributions and ignored the next nearest neighbour (NNN) contributions which are quite significant (contributing 30-40% to the cohesive energies of alkali halide crystals) Moreover these workers also neglected contributions due to the three body interaction (TBI), which have been found to play an important role in describing various static and dynamic properties of ionic solids[21-24].

In the present study we have used the short range repulsive potential (SRRP) of Ali and Hasan[25] which can be expressed in the generalized form as

$$W_{ij}^{SR}(r) = \frac{\beta_{ij} P}{r_{ij}^{m}} \exp(-b_{ij} r_{ij}^{N}) \tag{1}$$

where P and b are the repulsive strength parameter (RSP) and repulsive hardness parameter (RHP) respectively.

For NaCl strudcture $r_{ii} = r_{jj} = 1.4142$ r and for CsCl structure $r_{ii} = r_{jj} = 1.1547$ r. β_{ij} are Pauling Coefficients introduced to provide the appropriate weight for various ion pair interactions expressed as

$$\beta_{ij} = 1 + \frac{Z_i}{N_i} + \frac{Z_i}{N_i} \tag{2}$$

Where Z_i and Z_j are the valencies and N_i and N_j are the numbers of the outer most electrons of ions i and j .

In the present study we have taken into account the contributions of all types of interactions while calculating the various thermodynamic properties of all alkali halide crystals.

The essential requirements of an ideal potential as suggested by Varshni[26] are as follows:-

(i) It should be short range in nature i.e. it must fall sharply with increasing distances.
(ii) It should provide infinite repulsion at zero separation to avoid the mutual collapse of the ions into one another.

Unlike previous short range repulsion potentials (SRRP), Ali and Hasan form satisfies both conditions cited above.

The aim of the present work is to study the suitability of Ali and Hasan SRRP model in explaining the various thermodynamic properties of alkali halide crystals.

THEORETICAL APPROACH

For pure diatomic ionic crystals the interionic interaction potential model in generalized form can be expressed as

$$\mathbf{W(r) = W_c + W_v + W_{BT} + W_{SR}(r)} \qquad \mathbf{(3)}$$

Where W_c = long-range coulomb interaction energy
$= -AZ_1Z_2e^2/r$
W_v = van der Waals (vdw) interaction energy
$= -Cr^{-6} - Dr^{-8}$
C and D being vdW coefficients
W_{TB} = Three - body interaction energy
$= -nAZ_1Z_2e^2 f(r)/r$

Here n is a constant having values 6 and 8 respectively for NaCl and CsCl structures.

TBI arises from the charge transfer effect[21] between the adjacent ions and f(r) is TBI parameter dependent on overlap integrals[22,23]. This function is the measure of interionic size difference and its existence in ionic crystals is well established from Quantum mechanical theories[24]

$\mathbf{W_{SR}(r)}$ **= Short – range repulsive interaction (SRRI) energy which arises from the overlap of two combining ions due to like and unlike ion – pairs interaction.**

Considering the contributions of nearest neighbours (NN) and next nearest neighbours (NNN), SRRI is expressed as,

$$W_{SR}(r) = MP\beta_{ij}r_{ij}^{-2}\exp\left(-b_{ij}r_{ij}^{N}\right) + M'P\begin{bmatrix}\beta_{ii}r_{ii}^{-2}\exp\left(-b_{ii}r_{ii}^{N}\right)\\ +\beta_{jj}r_{jj}^{-2}\exp\left(-b_{jj}r_{jj}^{N}\right)\end{bmatrix} \qquad (4)$$

Here M and M’ are the number of NN and NNN having the values 6 and 12 for NaCl structure and 8 and 6 for CsCl structure.

METHOD OF EVALUATION OF POTENTIAL PARAMETERS

The repulsive strength parameter (RSP) is evaluated by applying crystal stability condition

$$\mathbf{(dW/dr)_{r=r0} = 0} \qquad \mathbf{(5)}$$

Where we get

$$\frac{P}{r_0^2} = \frac{2\begin{bmatrix}\left\{Ae^2r_0^{-1} + 6Cr_0^{-6} + 8Dr_0^{-8}\right\}\\ +nAe^2r_0^{-1}\{f(r_0) - r_0f'(r_0)\}\end{bmatrix}}{M\beta_{+-}\exp(-b_{+-}r_0^N)(3b_{+-}r_0^N + 4)} + \frac{M'}{2K_1^2}\begin{Bmatrix}\beta_{++}\exp(-b_{++}K_1^Nr_0^N)\times\\ (3b_{++}K_1^Nr_0^N + 4)\\ +\beta_{--}\exp(-b_{--}K_1^Nr_0^N)\times\\ (3b_{--}K_1^Nr_0^N + 4)\end{Bmatrix} \qquad (6)$$

The values of equilibrium interionic distance r_0 used in the above calculation have been taken from Smith et al[31] and Tosi[32] while those of van der Waals coefficienls C and D from Shanker et al[12].

The repulsive hardness parameter (RHP), (b_{+-}, b_{++} and $b\_$) are evaluated using relations proposed by Ali et al[25].

$$b_{+-} = (z_1z_2)^p\ (\rho_{+-}^{-N})/(k + 3.8) \qquad (7)$$

$$\mathbf{b_{++} = b_{+-}/K} \qquad \mathbf{(8)}$$

and

$$\mathbf{b\_ = 3b_{+-}/(k + m)} \qquad \mathbf{(9)}$$

where p = 0.12, m = 2, N = 1.5 and K = 2 for NaCl structure and 1.54 for CsCl structure. The values of ρ_{+-} have been taken from Shanker et al[27].

A detailed discussion on the justification of the relations (7-9) has been give in the paper[25].

The TBI parameter f(γ) and its derivalives have been evaluated using Cauchy relations (10, 11) and Cochran relation (12)

$$C_{12} - C_{44} = 2.3301\frac{e^2}{r_0^4}\left[r_0 f'(r_0)\right] \text{for NaCl structure.} \qquad \mathbf{(10)}$$

$$C_{12} - C_{44} = 12.2137\frac{e^2}{r_0^4}\left[r_0 f'(r_0)\right] \text{for CsCl structure.} \qquad \mathbf{(11)}$$

and

$$f(r) = f_0(r) \exp(-r/P_{+-}) \quad (12)$$

where $f_0(r)$ is a constant and ρ_{+-} is the repulsive hardness parameter for cation and anion interaction. The values of second order elastic constant (SOE) data used in the calculation have been taken from Gate[28].

The calculated values of P, (b_{+-}, b_{++} and b_) and f(r) are listed in TABLE 1.

TABLE 1 : Calculated values of repulsive hardness parameters (b_{+-}, b_{++} and b_{--}, all in 10^{12} cm^{-N}), repulsive strength parameter (P; 10^{-27}erg cm^2) and TBI parameter $f(r_0)$; 10^{-4} dimensionless.

Crystal	b_{+-}	b_{++}	b_{--}	P	$f(r_0)$
LiF	1.36289	0.68145	1.02217	4.19436	73.94750
LiCl	1.04403	0.52202	0.78302	6.84771	17.11130
LiBr	0.97521	0.48761	0.73141	8.46553	7.32297
LiI	0.88129	0.44065	0.66097	10.82556	-8.51766
NaF	1.30802	0.65401	0.98102	11.78326	41.54940
NaCl	1.01855	0.50958	0.76391	15.90201	1.27709
NaBr	0.98457	0.49229	0.73843	20.75542	-11.82260
NaI	0.86203	0.431015	0.64652	21.46000	-30.19490
KF	1.03371	0.51686	0.77528	10.76313	-22.64000
KCl	0.88522	0.44261	0.66392	20.06169	-9.73504
KBr	0.84713	0.42357	0.63535	24.89231	-13.88420
KI	0.77231	0.38616	0.57923	28.23037	-25.67140
RbF	0.96599	0.48300	0.72449	10.32218	-62.58110
RbCl	0.83983	0.41992	0.62987	21.38281	-34.63080
RbBr	0.79819	0.39910	0.59864	25.72627	-29.87530
RbI	0.75989	0.37995	0.56992	29.19258	-43.77970
CsF	0.86203	0.43102	0.64652	11.15497	-66.70540
CsCl	0.84230	0.54695	0.713812	46.82338	-7.12000
CsBr	0.79318	0.51505	0.67219	54.20648	-6.65630
CsI	0.74584	0.48431	0.63207	68.45457	-3.49932

Thermodynamic properties of alkali halide crystals

Once the potential parameters are known, we are able to evaluate various thermodynamic properties of alkali halide crystals extending the potential model upto the next nearest neighbours (NNN) and taking into account the contributions of vdW interaction and three body interaction.

Cohesive energy

The strength of a chemical bond in measured by the energy required to dissociate a solid into isolated atoms. This energy is generally known as cohesive energy.

The algebraic sum of all the interaction energies mentioned above gives the theoretical value of cohesive energy (W). Thus we have

$$W = -N_0 [W_c(r_0) + W_v(r_0) + W_{BT}(r_0) + W_{SR}(r_0)] \quad (13)$$

Substituting the values of each term under bracket W can be evaluated. The values thus obtained have been listed in TABLE 2 and compared with available theoretical[29] as well as experimental data[30]. In order to show the relative importance of the role played by various interactions we have computed their contributions separately which are also listed in TABLE 2.

TABLE 2 : Calculated values of coulomb energy (W_c), νdW energy (W_V), T.B.I energy (W_{TB}), short range repulsive energy (W_{SR}) and cohesive energy (W) [All in K cal mol^{-1}]

Crystal	Wc	W_v	W_{TB}	W_{SR}	W		
					Expt.[30]	Present Study	Other Work[29]
LiF	-288.2	-8.3	-12.8	61.4	246.7	247.9	253.8
LiCl	-225.7	-14.2	-2.3	42.1	203.2	200.1	203.3
LiBr	-210.9	-16.9	-0.9	39.7	194.2	189.0	192.1
LiI	-193.0	-20.9	+1.0	37.3	180.3	175.6	178.1
NaF	-250.4	-11.4	-6.2	45.4	219.5	222.6	211.3
NaCl	-205.7	-14.7	-0.2	34.1	187.1	186.5	188.6
NaBr	-194.1	-16.5	+1.4	31.0	178.5	178.2	179.4
NaI	-179.3	-19.0	3.2	29.2	167.0	165.9	167.4
KF	-217.0	-15.3	2.9	33.9	194.3	195.5	198.7
KCl	-184.4	-17.8	1.1	31.9	170.2	169.2	171.5
KBr	-175.8	-19.3	1.5	30.8	163.2	162.8	164.8
KI	-164.2	-20.9	2.5	29.1	153.6	153.5	155.3
RbF	-205.3	-16.4	7.7	27.3	185..8	186.7	189.5
RbCl	-176.3	-18.7	3.7	28.2	163.6	163.1	164.8
RbBr	-168.4	-20.0	3.0	28.5	157.2	156.9	158.6
RbI	-158.0	-16.5	4.2	22.8	148.5	147.5	147.9
CsF	-193.1	-19.6	7.7	28.7	177.0	176.3	181.6
CsCl	-163.9	-25.9	0.9	30.9	159.8	158.0	157.8
CsBr	-157.3	-30.0	0.8	33.8	154.1	152.7	153.2
CsI	-147.9	-29.3	0.4	32.1	146.1	144.7	144.1
Average % deviation						0.77	1.20

Isothermal bulk modulus and other allied properties

The isothermal bulk modulus is calculated using the relation.

$$B_T = \frac{r_0^2 W^{11}(r_0)}{9V} \quad (14)$$

The computed values of B_T are listed in TABLE 3 along with the available theoretical[29] and experimental[31,32] data.

The Moelwyn – Hughes parameter C_1, as reported by Moelwyn - Hughes[33] is given by

$$C_1 = [d(1/\beta)/dp]_T \tag{15}$$

where β is the isothermal compressibility, P the pressure and T the absolute temperature.

It may also be expened as-

$$C1 = [dB/dp]_T \tag{16}$$

where B is the isothermal bulk modulus of elasticity. This parameter is thus merely the pressure derivative of isothermal bulk modulus of elasticity at constant temperature.

The use of thermodynamic relations and application of crystal stability and compressibility conditions to an interionic potential model gives the following expression for C_1.

$$C_1 = 1 - \frac{r_0}{3}\frac{W^{11}(r_0)}{W^{11}(r_0)} \tag{17}$$

The computed values of C_1 from above eq. are listed in TABLE 3 along with the available theoretical[29] and experimental[31,32] data.

The Debye temperature has been evaluated using the relation

$$\theta_D = \frac{\hbar}{K_B}\left[\frac{5r_0B_T}{\mu}\right] \tag{18}$$

where K_B is the Boltzmann constant and μ is the reduced mass. The calculated values of θ_D are reported in TABLE 3 along with theoretical[34] and experimental[35] data.

TABLE 3 : Calculated values of bulk modulus B_T(10^{12} dyne cm^{-2}) Moelwyn - Hughes parameter, C_1 (dimensionless) and Debye temperature, θ_D (°k)

Crystal	B_T			C_1			θ_D		
	Expt[31,32]	Present Study	Other work[29]	Expt[31,32]	Present Study	Other work[29]	Expt[35]	Present Study	Other work[34]
LiF	0.674	0.637	0.836	5.30	4.18	4.27	730	663	835
LiCl	0.300	0.316	0.372	5.63	4.44	4.53	492	494	589
LiBr	0.238	0.236	0.300	5.68	4.63	4.63		421	522
LiI	0.175	0.194	0.232	6.15	4.82	4.62		391	473
NaF	0.471	0.180	0.539	5.25	4.73	4.70	422	432	503
NaCl	0.240	0.255	0.291	5.38	4.92	4.81	321	300	352
NaBr	0.197	0.225	0.243	5.44	4.98	4.90	224	256	293
NaI	0.151	0.169	0.186	5.58	5.14	4.96	164	217	255
KF	0.306	0.302	0.375	5.38	4.79	5.14	336	332	407
KCl	0.176	0.178	0.206	5.46	5.04	4.98	231	229	271
KBr	0.148	0.156	0.178	5.47	5.30	5.04	173	185	217
KI	0.117	0.126	0.142	5.56	5.22	5.10	131	156	188
RbF	0.271	0.264	0.323	5.69	5.19	5.14		289	352
RbCl	0.158	0.159	0.178	5.62	5.14	5.06	165	191	222
RbBr	0.134	0.137	0.154	5.59	5.20	5.10	131	141	165
RbI	0.106	0.106	0.116	5.60	5.37	5.12	103	113	133
CsF	0.235	0.206	0.300		4.88	5.91		255	
CsCl	0.180	0.184	0.225	5.76	5.52	5.89		202	
CsBr	0.159	0.164	0.192	5.71	5.58	5.75		146	
CsI	0.128	0.135	0.146	5.65	5.69	5.55		112	
Average % deviation		4.52	18.64		9.5	10.0		9.75	26.94

Anharmonic properties

Grüneisen parameter (γ) is an important solid state parameter which gives a measure of the an hormonicity of atomic vibration in crystals. The basic thermodynamic definition of this parameter of is given by

$$\boldsymbol{\gamma = -d(\ln \nu_i)/d(\ln V)} \qquad \textbf{(19)}$$

where ν_i is the frequency of ascillation of the crystal and V the crystal volume.

Different methods have been suggested for computing this parameter theoretically. However the basic theory for this parameter was proposed by Slater[36] on the basis of theory of elasticity. His expression for the vibration velocities are valid only if the solid is under zero external pressure. Dugdale and McDonald[37] derived a more general expression for by including the effect of perrssure. But these theories do not take into account the variation of Poisson's ratio with volume[38]. Vaschenko and Zubarov[39] developed a formulation of γ using free volume theory. Recently Migault and Romain[40] proposed a unification of these theories, taking into account the variation of Poisson's ratio with volume and deduced a general expression for γ given by

$$\gamma = -\frac{4-3S}{6} - \frac{V}{2}\frac{d^2(PV^s)/dV^2}{d(PV^s)/dV} \qquad \textbf{(20)}$$

where P is the perrssure at volume v and absolute temperature T. S is a parameter whose value is zero for all solids in slater's theory, 2/3 in Dugdale and McDonald (DM) theory and 4/3 in free volume (FV) theory.

The simplified form of the above eq. gives a direct relationship between γ and $[dB_T/dP]$ as

$$\gamma = -\frac{1}{6} + \frac{1}{2}\left[dB_T/dP\right] - \frac{S}{2} \qquad \textbf{(21)}$$

which further yields the following expressions

$$\gamma = -\frac{1}{6} + \frac{1}{2}\left[dB_T/dP\right] \qquad \textbf{(22)}$$

$$\gamma_{DM} = -\frac{1}{2} + \frac{1}{2}\left[dB_T/dP\right] \qquad \textbf{(23)}$$

and

$$\gamma_{FV} = -\frac{5}{6} + \frac{1}{2}\left[dB_T/dP\right] \qquad \textbf{(24)}$$

From the above equations

$$\gamma_{DM} = \gamma_S - \frac{1}{3} \qquad \textbf{(25)}$$

and

$$\gamma_{FV} = \gamma_S - \frac{2}{3} = \gamma_{DM} - \frac{1}{3} \qquad \textbf{(26)}$$

The first order volume dependence of Grüneisen parameter is commonly referred to as second Grüneisen parameter or mode Grüneisen parameter denoted by q. It is fundamental to the study of many basic phenomena accruing in solids. Knowledge of this parameter enables one to obtain information on the anharmonicity in a solid. The use of this parameter is also fundamental to the prediction of a variety of physical properties such as equation of state of a solid and its related thermodynamic properties. This parameter is also important in the study of thermoelastic properties in terms of shock waves[41,42]. The latter property is especially related to the study of the geophysics of earth's interior.

Davies and Parkes[45] were the first to explicity define the second Grüneisen parameter as

$$\boldsymbol{q = [d(\ln \gamma)/d(\ln V]_T} \qquad \textbf{(27)}$$

In the present study an attempt has been mode to compute this parameter based on higher order derivatives of an interaction potential within the frame work of theories proposed by slater[36], Dugdalekl and McDonald[37] and Vaschenko and Zubarov[39].

The mode Grüneisen parameter q is expressed as

$$q = \frac{1}{2\gamma}\left[S(1+S) - (1-S)V\frac{P^{II}}{P^{I}} - V^2\left\{\frac{P^{III}}{P^{I}} - \left(\frac{P^{II}}{P^{I}}\right)^2\right\}\right] \qquad \textbf{(28)}$$

Where

$$P = \frac{dW}{dV} \qquad \textbf{(29)}$$

upon differentiation

$$P^{I} = \frac{dP}{dV} = -\frac{1}{(3V)^2}\left[r_0 W^{II} - 2r_0 W^{I}\right] \qquad \textbf{(30)}$$

$$P^{II} = \frac{d^2P}{dV^2} = -\frac{1}{(3V)^3}\left[r_0^3 W^{III} - 6r_0^2 W^{II} + 10r_0 W^{I}\right] \qquad \textbf{(31)}$$

$$\begin{aligned}\mathbf{P^{III}} &= \mathbf{\frac{d^3P}{dV^3} = -\frac{1}{(3V)^4}\Big[r_0^4 W^{IV}} \\ &\quad \mathbf{-12r_0^3 W^{III} + 52r_0^2 W^{II} - 80r_0 W^{I}\Big]}\end{aligned} \qquad \textbf{(32)}$$

Here the primes denote the derivatives of w(γ) w.r.t γ at $\gamma = \gamma_0$ and P is the hydrostatic pressure. The calculated values of γs, γ_{DM}, γ_{FV}, q_S, q_{DM} and q_{FV} are listed in TABLE 4 and have been compared with available literature data[44,49].

TABLE 4 : Calculated values of Grüneisen parameters, γ_s, $_{DM}$ and γ_{FV} and mode Grüneisen parameters, q_S, q_{DM} and q_{FV} using slater Dugdale - McDonald and Free volume theories (all dimensionless).

Crystal	γ				q			
	Expt[46,47]	Present Study			Expt[48,49]	Present Study		
		γ_s	γ_{DM}	γ_{FV}		q_s	q_{DM}	q_{FV}
LiF		1.92	1.59	1.26	0.98	1.32	0.89	1.43
LiCl		2.05	1.72	1.39	1.46	1.46	1.02	0.79
LiBr	2.48	2.15	1.82	1.49	1.61	1.51	1.07	0.90
LiI	2.38	2.24	1.91	1.58	1.48	1.60	1.20	0.81
NaF	1.86	2.20	1.87	1.54	1.08	1.38	0.95	0.78
NaCl	1.69	2.29	1.96	1.63	1.14	1.25	0.75	0.73
NaBr	1.75	2.32	1.99	1.66	1.46	1.51	1.07	0.60
NaI	1.72	2.40	2.07	1.74	1.44	1.55	1.11	0.85
KF	1.71	2.23	1.90	1.57	1.34	1.45	1.02	0.45
KCl	1.59	2.35	2.02	1.69	1.53	1.53	1.08	0.71
KBr	1.69	2.48	2.15	1.82	1.14	1.56	1.10	0.92
KI	1.27	2.44	2.11	1.78	0.99	1.59	1.14	1.02
RbF	1.66	2.43	2.10	1.77	1.82	1.50	1.04	0.44
RbCl	1.45	2.40	2.07	1.74	1.84	1.57	1.10	0.93
RbBr	1.37	2.43	2.10	1.77	1.69	1.58	1.12	0.66
RbI	1.32	2.52	2.19	1.86	1.59	1.62	1.15	0.93
CsF		2.27	1.94	1.61		1.58	1.11	0.72
CsCl		2.59	2.26	1.93		1.70	1.28	0.95
CsBr		2.62	2.29	1.96		1.72	1.27	0.89
CsI		2.68	2. 35	2.02		1.76	1.30	0.91

RESULT AND DISCUSSION

TABLE 2 represents the various contributions to the cohesive energy separately and the net results based on our model taking into account the NNN interaction as well. The computed values are in reasonably good agreement with the experimental values[30] and are slightly better than the theoretical results obtained by Jain et al[29]. The computed values of B_T, C_1 and θ_D are reported in TABLE 3. It is seen that our computed values of B_T gives a very good agreement with the experimental data[31,32] and are superior to the theoretical results obtained by Jain et al.[29]. Fruther our computed values of C_1 also agree fairly well with the experimental data[31,32] and are slightly better than the theoretical results reported by Jain et al[29]. The values of θ_D evaluated on the basis of our model agree fairly well with the experimental data[36] and are far superior to the values reported by Agrawal et al[35]. The calculated values of γs, $_{DM}$, γ_{FV}, q_S, q_{DM} and q_{FV} are reported in TABLE 4 along with the experimental values[46-49]. It is remarkable to note that the calculated values of q_{DM} vary in a narrow band from 0.89 to 1.30 as well pass from LiF to CsI with an average equal to 1.08. Thus $q_{DM} \approx 1$ is a good approximation. This implies that Grüneisen parameter is directly proportional to the volume. This approximation ($q_{DM} \approx 1$) has been used in theories of shock wave propagation geophysical studies[43,44] and also in various descriptions of equation of state of solids[44,50].

Thus the present investigation is an attempt to compute various crystalline properties of alkali halide crystals using an interaction potential approach and taking into account all types of interactions. The close agreement of our theoretical results with the available experimental data is a sensitive test of our potential model and the method of analysis followed in the evaluation of properties of alkali halide crystals.

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REFERENCES

[1] M.Born, A.Lande; Verh, Deut.Phys.Ges., **20**, 210 **(1918)**.
[2] M.Born, J.E.Mayer; Z.Phys., **75**, 1 **(1932)**.
[3] Y.P.Varshni, R.C.Shukla; J.Chem.Phys., **35**, 582 **(1961)**.
[4] C.M.Kachhava, S.C.Saxena; Phil.Mag., **8**, 1429 **(1963)**.
[5] L.Das, S.C.Saxena; J.Chem.Phys., **43**, 1747 **(1965)**.
[6] M.M.Patel, V.B.Gohel, M.D.Trivedi; Indian J.Phys., **41**, 235 **(1967)**.
[7] V.K.Mathur, S.P.Singh; J.Phys.Chem.Solids, **29**, 959 **(1968)**.
[8] S.Prakash, J.Behari; Indian J.Pure Appl.Phys., **7**, 709 **(1969)**.
[9] L.V.Woodcock; J.Chem.Soc.Faraday Trans., **2(70)**, 1405 **(1974)**.

[10] **(a)** K.P.Thakur; Acta Cryst.A, **32**, 363 **(1996)**; **(b)** J.Inorg.Nucl.Chem., **38**, 1433 **(1976)**; **(c)** J.Chim. Phys., **75**, 300 **(1978)**.

[11] M.J.I.Sangster, R.M.Atwood; J.Phys.C, **11**, 1541 **(1978)**.

[12] J.Shanker, G.G.Agrawal, R.P.Singh; J.Chem.Phys., **69**, 670 **(1978)**.

[13] J.C.Jain, J.Shanker; Indian J.Pure Appl.Phys., **132**, 99 **(1979)**.

[14] J.Shanker, K.Singh; Phys.Status Solidi b, **109**, 411 **(1982)**.

[15] V.P.Gupta, C.P.Agrawal; Phys.Status Solidi b, **114**, 265 **(1982)**.

[16] J.Shanker, G.G.Agrawal; Phys.Status Solidi b, **123**, 11 **(1984)**.

[17] V.P.Gupta, S.K.Sipani; J.Phys.Chem.Solids, **51**, 141 **(1990)**.

[18] S.K.Sipani, V.P.Gupta; Phys.Rev.B, **43**, 9924 **(1991)**.

[19] A.J.Kaur, P.C.Jan, P.S.Bakhshi, J.Shanker; Ind.J. Chem., **22A**, 595 **(1983)**.

[20] W.A.Harrison; Phys.Rev.B, **23**, 5230 **(1981)**.

[21] R.K.Singh; Phys.Rep., **85**, 259 **(1982)**.

[22] **(a)** S.O.Lundqvist; Ark.Fys.(Sweden), **9**, 435 **(1955)**; **(b)** **12**, 263 **(1957)**.

[23] M.P.Verma, R.K.Singh; Phys.Status Solidi b, **33**, 769 **(1969)**.

[24] R.K.Singh, P.Khare; Phys.Status Solidi b, **103**, 337 **(1981)**.

[25] M.S.Ali, M.M.Hasan; Ind.J.Phys., **63B**, 486 **(1989)**.

[26] Y.P.Varshni; Rev.Mod.Phys., **29**, 664 **(1957)**.

[27] J.Shanker, M.Kumar; Phys.Status Solidi b, **142**, 325 **(1987)**.

[28] P.B.Gate; Phys.Rev., **139(A)**, 1666 **(1965)**.

[29] V.C.Jain, J.Shanker; Ind.J.Pure Appl.Phys., **17**, 713 **(1970)**.

[30] M.F.C.Ladd; J.Chem.Phys., **60**, 1954 **(1974)**.

[31] S.C.Smith, L.S.Cain; J.Phys.Chem.Solids, **36**, 205 **(1975)**.

[32] M.P.Tosi; Solid State Phys., **16**, 1 **(1964)**.

[33] **(a)** E.A.Moelwyn-Hughes; J.Phys.Chem., **55**, 1246 **(1951)**; **(b)** Physical Chemintry, 2nd Edition, Pergamon, London, 26 **(1964)**.

[34] S.C.Agrawal, O.P.Sharma, J.Shanker; Ind.J.Phys., **59A**, 46-54 **(1985)**.

[35] N.W.Aschroft, N.D.Merwin; Solid State State Physics, Holl Sanders International Edition, N.Y., **(1976)**.

[36] J.C.Slater; Introduction to Chemical Physics, McGraw Hill, New York, **(1939)**.

[37] J.C.Dugdate, D.K.McDonald; Phys.Rev.B, **9**, 832 **(1953)**.

[38] D.J.Pertine; Phys.Rev., **138A**, 767 **(1965)**.

[39] V.Vaschenko, V.N.Zubarov; Sov.Phys.Solid State, **5**, 653 **(1963)**.

[40] A.Magault, J.P.Romain; J.Phys.Chem.Solids, **38**, 555 **(1977)**.

[41] B.J.Alder; Solid under Pressure, W.Paul, D.M.Warshhauer, (Eds); McGrow Hill, New York, 385 **(1963)**.

[42] G.E.Duvall, G.R.Fowles; High Pressure Physics and Chemistry, R.S.Bradley, (Ed); Academic Press, London, **2**, 193 209.

[43] N.Soga, E.Schreeber, O.L.Anderson; J.Geophys. Res., **71**, 5315 **(1966)**.

[44] C.A.Swenson; J.Phys.Chem.Solids, **29**, 1337 **(1968)**.

[45] R.C.Davies, S.Parkes; Phil.Mag., **4**, 341 **(1959)**.

[46] H.H.Demarest Jr.; J.Phys.Chem.Solids, **35**, 1396 **(1974)**.

[47] V.V.Palciauskas; J.Phys.Chem.Solids, **36**, 611 **(1935)**.

[48] K.O.McLean, C.S.Smith; J.Phys.Chem.Solds, **33**, 279 **(1972)**.

[49] **(a)** R.W.Roberts, C.S.Smith; J.Phys.Chem.Solids, **31**, 619 **(1970)**; **(b)** **31**, 2397 **(1970)**.

[50] S.P.Singh, V.K.Mathur; Phys.Lett.A, **28**, 317 **(1968)**.