Spectroscopic Constants & Potential Energy Function for Diatomic Molecules

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Abstract

The interionic interaction potential energy functions consisting of an attractive term within the framework of 'effective charge model along with a short range repulsive interaction (SRRI) term incorporating the near values of molecular state polarizability, van der Waals dipole-dipole and dipole-quadrupole interaction and repulsive interaction of the Born-Mayer, Hellmann, Varshni-shukla and Ali-Hasan types have been used to compute the dipole moment, binding energy, rotation-vibration coupling constant and vibrational anharmonicity. The values of binding energies have been calculated with and without the inclusion of polarization. The inclusion of polarizable terms in the interaction-energy makes significant improvement in the result. This shows the interaction model must be dependent on this effect. The obtained values are in good agreement with the observed values available in the literature. The results are capable enough to establish the reliability and superiority of the interaction models.

Keywords: - Anharmonicity constant, Binding energy, Dipole moments, dipole-dipole and dipole-quadrupole interaction constants, vdWenergies

1. Introduction

Studies of interaction potential energy function in diatomic molecules play an important role in molecular physics as well as in the problems of astrophysical importance [1].Recently there have been several investigations [2-5] on the potential energy function using the interaction originally due to Morse [6], Kratzer [7] and Rydberg [8]. Raghubanshi and Sharma [2] and Verma and Jha [5] have developed new potentials by combining Morse and Kratzer function and Rydberg and Kratzer functions respectively. The rotational vibrational constants α_e for diatomic molecules were calculated by using Morse-Kratzer (MK) and Rydberg-Kratzer (RK) potentials. But the results were far from satisfactory [1]. Rittner [9], for the first time proposed a polarizable ion model for alkali halide molecules by which interaction terms could be understood. Later on, Brumer and Karplus [10] modified Rittner model known as truncated Ritter model known as T-Rittner model expressed as.

$$U(r) = -\frac{z^z e^z}{r} - \frac{(\alpha_1 + \alpha_2)}{2r^4} - \frac{C}{r^6} - \frac{D}{r^8} + U_R(r) \dots\dots\dots\dots\dots\dots\dots\dots. (1)$$

The first term is the electrostatic attraction between two point charges z(+e) and z(-e) separated by a distance r and known as Coulomb interaction. The second term is the polarization energy, the third and the fourth terms are the vander waals (vdw) dipole-dipole and dipole-quadrupole interaction energy and the last term is the short range repulsive interaction (SRRI). There are various repulsive interactions proposed by different theoretical workers from time to time to describe the structure and properties of ionic molecules [11].The repulsive interactions in logarithmic functions [12-13] are also available in literature not free from error. In the present calculations, we introduce the modification in the previous work in order to improve the interaction potential model for calculating the spectroscopic constant of diatomic molecules. Four repulsive interactions namely, Born-Mayer [14] Hellmann [15], Varshni-Shukla [11] and Ali-Hasan [16] have been chosen as the short range repulsive interaction to investigate their validity for alkali halide molecules as the results obtained from other potential models are far from errors.

A generalized formula for short range repulsive interactions can be expressed as

$$U_R(r) = \frac{B}{r^m} \quad \exp \quad (-r/\rho) \dots\dots\dots\dots\dots\dots\dots\dots.. (2)$$

which takes the form of Born-Mayer repulsive potential when m=0, Hellmam repulsive potential when m=1 and Varshni-Shukla potential when m=2. Ali-Hasan empirical repulsive potential is given by

$$U_R(r) = \frac{S}{r_m} \exp \left(-br^n\right) \dots\dots\dots\dots\dots\dots. (3)$$

In this potential m=2 and n =3/2. In eq[ns] (2) and (3) B, S, ρ and b are repulsive potential parameters

2. Methods Of Calculation

The repulsive potential parameters are determined by applying the equilibrium criteria;

$$\left(\frac{dU(r)}{dr}\right)_{r=r_e} = 0 \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots . (4)$$

and

$$\left(\frac{d^2U(r)}{dr^2}\right)_{r=r_e} = K_e = 4\pi^2\omega_e^2 C^2\mu_A \ldots \ldots \ldots \ldots \ldots . (5)$$

K_e is the molecular force coustant, ω_e is the equilibrium vibrational frequency, C is the speed of light in vacuum and μ_A is the reduced mass and r_e is the equilibrium interionic separation. The electronic polarizabilities of ions in the molecular state or bonded state differ from the free state polarizabilities. This is mainly due to the existence of the Coulomb interaction. Wilson and Curtis [17] have shown that the polarizability of cation remains unchanged where as that of anion decreases significantly in the bonded state due to the effect of Coulomb interaction. The molecular state polarizability of anion (α_m) is calculated from the relation based on ruffia energy analysis [18] given by

$$\alpha_2 = \alpha_m = \frac{e^2h^2n_0}{4\pi^2m\,(E_f + e\varphi)^2} \ldots \ldots \ldots \ldots \ldots \ldots (6)$$

Where $\varphi = e/r$

The values of E_f, known as energy parameter are calculated from free-ion polarizabilities α_f as reported by Cocker [19] given by.

$$E_f^2 = \frac{e^2h^2n_0}{4\pi^2m\,\alpha_f} \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots (7)$$

where m is the electron mass, n_o is the total no. of electrons in the ions and h is the planck's constant. The molecular state polarizability of anions calculated from eq (6) and the free state polarizability of cations taken from Pauling [20] are used to estimate the dipole moment μ from the relation given by

$$\mu = er - \frac{e\,(\alpha_1 + \alpha_2)}{r^2} \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots (8)$$

and vdW dipole-dipole constant C and dipole – quadrupole constant D taken from Slater Kirkwood variational method [21] are expressed as

$$C = \frac{3\,eh}{4\pi\,m^{\frac{1}{2}}} \frac{\alpha_1\alpha_2}{\left(\frac{\alpha_1}{N_+}\right)^{\frac{1}{2}} + \left(\frac{\alpha_2}{N_-}\right)^{\frac{1}{2}}} \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots . . (9)$$

and

$$D = \frac{\frac{27h^2\alpha_1\alpha_2}{32\pi^2m}\left(\left(\frac{\alpha_1}{N+}\right)^{\frac{1}{2}} + \left(\frac{\alpha_2}{N-}\right)^{\frac{1}{2}}\right)^2}{\left(\frac{\alpha_1}{N+}\right) - \frac{20}{3}\left(\frac{\alpha_1\alpha_2}{N_+N_-}\right)^{\frac{1}{2}} + \left(\frac{\alpha_2}{N_-}\right)} \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots . . (10)$$

Where N_+ and N_- are the effective no. of electrons in the ions and are defined by

$$N_+ = N + Z_+ \quad\quad \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots (11)$$
$$N_- = N - Z_- \quad\quad \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots (12)$$

Here N is the total no of electrons in the outer two shells.

The rotation vibration coupling constant (α_e) and vibrational anharmonicity consant ($\omega_e x_e$) are calculated from the relations [22]

$$\alpha_e = -\left(\frac{x_3 r_e}{3} + 1\right)\frac{6B_e^2}{\omega_e} \ldots \ldots \ldots \ldots \ldots . (13)$$

$$\omega_e x_e = \left(\frac{5}{3}x_3^2 - x_4\right)\frac{h}{64\,\pi^2 c\mu} \ldots \ldots \ldots \ldots \ldots . (14)$$

and $$x_p = \left(\frac{d^p U(r)}{dr^p}\right)_{r=r_e} \Big/ \left(\frac{d^2U(r)}{dr^2}\right)_{r=r_e} \ldots \ldots \ldots \ldots \ldots . (15)$$

where p stands for order of derivative.
The binding energy D_i per mole of a diatomic molecule is given by

$$D_i = -NU\,(r_e) \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots (16)$$

Where N is the Avogadro's Number and r_e is the molecular equilibrium distance.

3. Results & Discussion

The molecular state polarizabilities for diatomic molecules have been calculated by using eq[ns]. (6) and (7). They are calculated to obtain the improved values of polarization energies and vdWenegies. Table – 1 shows their calculated values. The values of N_+N_- and r_e are taken from Mandal and Ghatak [23] and Huber and Hertzberg [1]. The different potential parameters have been computed with the help of molecular equilibrium

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equations (4) and (5). Their values have been used to calculate spectroscopic constants.The constants C and D known as dipole-dipole, dipole quadrupole van der waals interaction constants have been obtained with the help of eq^{ns} (9) and (10) given by Slater Kirkwood variational method. These values have been used in the evaluation of binding energy (D_i) and dissociation energy(D_e.)

Table – 1 Calculated values of electronic polarizablities $\alpha_1(A^{03})$ and $\alpha_2(A^{03})$, N+ and N- (total no. of electrons in the outer two shells) and values of $r_e(A^o)$,

Molecules	$\alpha_1(A^{03})$	$\alpha_2(A^{03})$	N+	N-	r_e
LiF	0.036 1.564	0.741	3	9	
LiCl	0.034 2.021	2.202	3	15	
LiBr	0.036 2.170	3.350	3	25	
Li I	0.033 2.392	5.224	3	25	
NaF	0.190 1.926	0.821	11	9	
NaCl	0.184 2.361	2.372	11	15	
NaBr	0.182 2.502	3.534	11	25	
Na I	0.180 2.711	5.455	11	25	
KF	1.143 2.172	0.865	17	9	
KCl	1.078 2.667	2.498	17	15	
KBr	1.063	3.680	17	25	2.821
K I	1.045 3.048	5.659	17	25	
RbF	1.805 2.270	0.881	27	9	
RbCl	1.718 2.787	2.543	27	15	
RbBr	1.693 2.945	3.731	27	25	
Rb I	1.673 3.177	5.728	27	25	
CsF	3.154 2.345	0.893	27	9	
CsCl	2.989 2.906	2.534	27	15	
CsBr	2.952 3.072	3.779	27	25	
CsI	2.908 3.315	5.880	27	25	

Table- 2 shows the obtained values of the dipole moments of diatomic molecules. These calculation are based on the eq(8), Column (2) of this table shows the present calculation with possible errors Column(b) and (c) denote values of dipole moments for the mentioned molecules obtaiend by Rittner model [9] and point ion model the experimental values of μ have been taken from Brumer and karplus [10]. The average percentage errors obtained by us and Ali-Hasan & Shankar et al are respectively 2.79, 13.58 and 31.29. The higher percentage errors in their values may be attributed to the omission of molecular polarizablities. The values of μ obtained simply indicate the significance of molecular state polarizabities.

Table2. calculated values of dipole moments μ in debye

Molecules	Expt. (1,22)' %error	present	%error	b calculation	%error	c
LiF	6.284 19.5	5.982	4.8	5.311	15.5	7.511
LiCl	7.085 36	7.07	0.2	5.241	26	9.706
LiBr	7.226 44.2	6.967	3.6	5.406	25.2	10.422

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Li I	7.429 54.6	7.0703	4.8	5.375	27.5	11.488
NaF	8.123 7.77	8.387	3.25	7.492	13.8	9250
NaCl	8.972 26.4	9.132	1.78	7.773	13.4	11.339
NaBr	9.092 24.2	9.361	2.95	7.96	12.45	12.017
Nal	9.21 41.36	9.332	1.32	7.992	13.2	13.02
kF	8.558 21.8	8.383	2.04	8.074	5.6	10.432
KCl	10.238 25.1	10.389	1.47	9.181	10.3	12.809
kBr	10.603 27.78	10.68	0.73	9.575	9.69	13.549
KI	11.05 32.47	11.199	1.35	9.921	13.3	14.369
RbF	8.513 18.1	8.359	1.8	8.001	6	10.902
RbCl	10.483 32.3	10.745	2.49	9.469	9.8	13.885
RbBr	- -	11.131	-	-	-	14.144
RbI	- -	11.729	-	-	-	15.259
CsF	7.489 50.4	7.723	3.12	7.278	2.8	11.268
CsCl	10.858 28.5	10.782	0.69	9.364	13.7	13.957
CsBr	- -	11.322	-	-	-	14.754
CsI	12.1 31.57	10.756	11.1	10.61	12.3	15.921
Average % deviation 30.70882			2.793529		13.56118	

Table- 3 (a) & 3 (b) Show the calculated values of binding energy (D_i) of molecules with and without the inclusion of molecular polarization energy. The calculation have been done for all the four short range repulsive interaction models. The average percentage errors in both cases for all the models are also very revealing. BM and VS interaction models give better results of binding energy in comparision to HM & AH models. The result indicates that the BM & VS interaction models are to be considered to be exact potention energy functions for the prediction of binding energy of these molecules. Results show that BM>VS>HM>AH. Thus the polarization energy has to be taken a reality for the evaluation of binding energy for halide molecules.

Table-3a Calculated Values of Binding Energy (Di) in K. Calorie/mole (With Polarization)

Molecules	Expt .(1,22) %Error	B.M With	%Error	Hell. With	%Error	V.S. With	%Error	A & H. With	
LiF	184.1	199.95	8.6	197.8	7.4	197.9	7.49	199.8	8.5
LiCl	153.3	159.6	4.1	157.1	2.4	160.3	4.5	161.45	5.2
LiBr	147.4	157.5	6.8	156.6	6.2	156.6	6.2	157.8	7.1
LiI	138.7	147.6	6.4	146.9	5.9	146.9	5.9	147.8	6.5
NaF	153.9	156.1	1.4	155.3	0.9	154.3	0.26	156.2	1.89
NaCl	132.6	133.8	0.9	134.8	1.6	132.8	0.15	134.1	1.13
NaBr	127.7	129.13	1.1	128.7	0.7	128.25	0.73	129.3	1.25
NaI	120.3	122.7	1.9	122.5	1.8	113.09	5.9	124.48	3.4
KF	139.2	152.4	9.5	151.9	8.6	151.5	8.8	167.4	20.2
KCl	118	128.4	8.8	123.2	4.4	134.4	13.8	133.4	13
KBr	113.6	121.8	7.2	110.5	2.7	110.4	2.8	111.24	2.07
KI	106.1	108.2	1.9	107.9	1.7	107.6	1.4	124.4	17.2
RbF	133.6	142.7	6.8	142.2	6.4	141.9	6.2	156.3	16.9

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RbCl	113.4	114.2	0.7	114	0.4	113.6	0.17	124.7	9.96
RbBr	109	109.96	0.8	111	1.9	110.75	1.6	121.8	11.7
RbI	101.9	104.2	2.2	104.7	2.7	104.5	2.5	114.9	12.7
CsF	130.5	147.9	1.3	147.6	13.1	147.2	12.7	151.1	18.7
CsCl	112.3	114.45	1.9	114.1	1.6	113.95	1.46	111.9	.35
CsBr	130.5	109.4	16.1	109.1	9.65	109.1	9.6	107.6	17.6
CsI	101.1	104.06	2.9	103.9	2.8	102.2	1.1	100.6	.49

AVERAGE% DEVIATION 4.565   9.475   4.658   13.642

Table-3b Calculated Values of Binding Energy (Di) in K. Calorie/mole (Without Polarization)

Molecules	Expt. .(1,22) %Error	B.M Without	%Error	Hell. Without	%Error	V.S. Without	%Error	A & H. Without	
LiF	184.1 2.7	179.2	2.6	177.2	3.7	177.7	3.5	179.2	
LiCl	153.3 10.6	138.2	9.8	139	9.3	138.7	9.5	137	
LiBr	147.4 9.2	134.7	8.6	133.7	9.3	131.6	10.7	133.9	
LiI	138.7 12.1	146.9	2.9	121.2	12.6	121.1	12.6	121.9	
NaF	153.9	143.9	6.5	143.2	6.9	142.2	7.2	144.1	6
NaCl	132.6 9.12	128.8	2.9	121.24	8.5	122.8	7.4	120.5	
NaBr	127.7 10.94	113.48	11.1	113.1	11.4	112.59	11.9	113.72	
NaI	120.3 10.83	105.5	12.3	105.3	12.4	95.36	20.7	107.26	
KF	139.2 9.5	137.5	1.2	137.1	1.5	136.6	1.86	152.5	
KCl	118 3.2	111.7	5.3	111.5	5.5	122.8	4.06	121.8	
KBr	113.6 12.9	110.5	2.7	98.2	13.6	98.04	13.6	98.9	
KI	106.1 5.18	95.4	10.1	95.1	10.36	94.76	10.6	111.6	
RbF	133.6 4.4	126.1	5.6	126.1	5.6	125.2	6.3	139.5	
RbCl	113.4 0.32	102.6	9.5	101.3	10.6	101.9	10.1	113.03	
RbBr	109 5.32	98.2	1.1	99.2	8.9	98.9	9.26	103.6	
RbI	101.9 1.66	92.94	9.3	93.5	8.2	93.2	8.5	103.6	
CsF	130.5 4.99	125.9	3.5	125.6	3.7	125.13	4.11	137.02	
CsCl	112.3	101.6	9.5	101.3	9.7	101.2	9.8	112.3	0
CsBr	130.5	96.9	25.7	96.5	26.1	91.1	30.1	130.5	0
CsI	101.1	92.1	8.9	91.92	1.1	89.68	11.2	101.1	0

AVERAGE% DEVIATION 7.455   8.948   10.145   5.948

Table 4 & 5 present the calculated values of α_e and $\omega_e x_e$ for halide molecules in the case of well-known four repulsive interaction models along with their experimental values. From the table it is evident that α_e for BM, HM, VS & AH are respectively 8.4, 10.21, 7.57, 6.28. The order of suitability of the models are

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AH>VS>BM>HM. Similarly the percentage deviations of $\omega_e x_e$ for the above models are 5.57, 7.81, 6.27, 5.71 for BM, HM, VS & AH. Here VS and AH models give still more approximate values of anharmonicity. The small discrepancy between the observed and experimental values of the calculated quantities may be attributed due to overlap of electron clouding between anion & cations and hence the dependence of potential model on interionic separations.

Table-4 Calculated Values of Rotational constant α_e (in 10^{-4} cm)

Molecules	Expt.(1,22)	B.M	%Error	Hell.	%Error	V.S.	%Error	A&H	%Error
LiF	202.7	187.2	7.6	198.7	1.97	211.9	4.5	196.9	2.8
LiCl	80	87.6	9.5	91.5	14.3	97.7	2.1	74.6	6.7
LiBr	56.4	66.7	18.2	71.5	26.7	72.5	8.5	87.6	5.3
LiI	40.9	44.4	8.5	54.7	33.7	53.3	3.3	44.8	9.5
NaF	45.6	47.1	3.2	34.08	25.2	48.3	5.9	36	21
NaCl	16.3	15.5	4.9	16.4	0.6	17.2	5.5	15.4	5.5
NaBr	9.4	9.1	3.19	9.5	1.06	9.5	1	10.8	4.8
NaI	6.47	6.21	4	6.45	0.31	6.71	3.7	6.3	2.6
KF	28.3	23.28	17.7	22.5	10.9	24.6	13	23.7	16.2
KCl	7.89	9.8	24.2	10.2	9.8	7.38	6.4	4.3	5.5
KBr	4.05	4.03	0.5	5.1	5.9	3.75	7.4	3.5	3.5
KI	2.68	3.52	3	3.5	0.5	3.52	1.3	2.88	1.4
RbF	15.2	14.9	1.9	15.4	1.3	16.1	5.9	15.9	4.6
RbCl	4.53	4.42	2.48	4.18	7.6	4.76	5	3.54	1.8
RbBr	1.86	1.89	1.61	1.98	6.4	2.16	6.1	1.86	0
RbI	1.09	1.04	4.58	1.06	2.7	10.4	4.5	1.05	3.6
CsF	16.8	14.19	15.5	14.05	16.3	14.04	16.4	14.1	16
CsCl	3.39	3.64	7.3	3.75	10.6	4.2	23.8	3.6	0.61
CsBr	1.24	1	19.3	1.41	13.7	1.03	16.9	1	9.3
CsI	0.68	0.6	11.7	0.78	14.7	0.61	10.2	0.51	5
AVERAGE % DEVIATION			8.443		10.212		7.57		6.2855

Table- 5 Calculated values of Vibrational anharmonitity constant $\omega_e x_e$ (in cm^{-1})

Molecules	Expt. (1,22)	B.M	%Error	Hell.	%Error	V.S.	%Error	A&H	% Error
LiF	8.1	8.3	0.24	8.17	0.86	7.4	8.6	8.46	4.4
LiCl	4.5	5.11	13.5	5.22	16	5.77	8.2	2.56	31
LiBr	3.53	4.54	8.6	2.12	9.9	4.89	8.5	8.68	5.8
LiI	3.39	3.9	15	3.7	9.6	3.7	9.1	3.8	12
NaF	3.83	4.24	10.7	3.05	20.3	4.4	4.8	3.51	8.3
NaCl	1.76	1.6	9	1.61	8.5	1.65	6.2	1.5	4.7
NaBr	1.16	1.13	2.5	1.15	8.5	1.1	5.1	1.57	5.3
NaI	0.96	0.94	2	1.1	4.5	1.95	1	1.93	3.1
KF	0.56	0.53	5.3	0.52	7.1	0.54	3.5	0.61	3.9
KCl	1.17	1.34	4.5	1.29	10.2	1.18	8.5	1.19	1.7
KBr	0.76	0.82	7.8	0.71	6.5	0.79	3.9	0.69	9.2
KI	2.43	2.46	1.2	1.35	4.4	2.45	8.2	2.26	6.9
RbF	1.8	1.79	5.5	1.89	5	1.64	8.8	1.95	8.3
RbCl	0.86	0.78	1.4	0.76	11.6	0.9	4.6	0.86	4.6
RbBr	0.46	0.44	4.3	0.42	3.6	0.49	6.5	0.47	2.8
RbI	0.34	0.34	0	0.36	3.8	0.36	5.8	0.33	2.9
CsF	1.62	1.6	1.2	1.3	9.7	1.75	8	1.69	4.3
CsCl	0.74	0.77	4	0.79	6.7	0.79	6.7	0.69	6.7
CsBr	0.36	0.37	2.7	0.38	0.38	5.5		0.33	8.3
CsI	0.25	0.22	12	0.24	4	0.24	4	0.27	8
AVERAGE % DEVIATION			5.572		7.813		6.275		5.715

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