

A New Form of Interaction Potential Energy Function of Diatomic Molecules

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Abstract : The present paper deals with a new Logarithmic potential function of the form

$$U(r) = - \left[e^2/r + G \log \left(1 + g/r^n \right) * m \right]$$

where G and g are potential parameters which are the characteristic of the molecules. This new form, though empirical, has been found to yield the acceptable behavior of the potential energy and force curve for diatomic molecules. Moreover, it has accurately reproduced the value of the parameters, r_e and potential parameters, P , Q , D , M and G in case of fifty-nine diatomic molecules of different series.

1. Introduction

The Interaction potential energy function has been a subject of extensive study for the last several decades for evaluating various properties of diatomic crystals. Various empirical and semiempirical interaction potential energy functions have been suggested to understand the binding of ions in the molecule.

Reference to literature¹⁻⁹ may be made previous work. A number of theoretical potential are also available, but they are inadequate for accurately reproducing the experimental results. It has been remarked earlier that exponential form of the interaction potential energy function fails to yield the properties of diatomic salts. Dobbs and Jones also claimed, "The exponential form for the repulsive potential makes calculations of the lattice properties rather complicated and in any case, is perhaps, not valid in the region near the minimum of the total potential which is of course the essential part in considering the properties of the lattice".

2. The logarithmic Potential Form : A Historic Background

It is worthwhile to give a new potential energy functions regarding the potential energy and force curves of diatomic molecule. The attention has been paid to the fact that the repulsion should be maximum (infinity) when the closest-shell electron clouds of anion and cation overlap in consequence of the Pauli's exclusion principle. In new

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functions, attempt has been made to enable the potential energy curve to show a potential well to infinite height when the electron clouds of cation and anion come in contact to each other. The following three interaction potential energy functions for 1 : 1 — diatomic molecules have been suggested to fulfill the purpose :

$$(1) \quad U(r) = -e^2/r + P \log(1 + p/r^4),$$

$$(2) \quad U(r) = -e^2/r + Q \log(2 + q/r^2),$$

$$(3) \quad U(r) = -e^2/r + D \log(4 + d/r)$$

where P , p , Q , q , D and d are the potential parameters which are characteristics of the molecule. Expanding the repulsive term of potential in power series as :

$$(4) \quad P \log(1 + P_p/r^4) = P_p/r^4 - P_p^2/2r^8 + P_p^3/3r^{12} - P_p^4/4r^{16} + \dots$$

The right side is equivalent to,

$$(5) \quad C_1/r^4 - C_2/r^8 + C_3/r^{12} - C_4/r^{16} \dots$$

Where C_1 , C_2 , C_3 and C_4 are constants. The terms are called Van der Waals dipole-dipole; dipole-quadrupole etc. interaction terms.

All these potential energy functions can be amalgamated to a general form :

$$(6) \quad U(r) = -e^2/r + P_n \log(4/n + p_n/r^n)$$

Where $n = 4, 2$ and 1 . The values of force $F(r)$ between two unlike ions according to pot (1), pot (2) and pot (3) are respectively as :

$$(7) \quad F(r) = -e^2/r^2 + 4P_p/r(r^4 + p)$$

$$(8) \quad F(r) = -e^2/r^2 + 2Q - q/r(2r^2 + q)$$

$$(9) \quad F(r) = -e^2/r^2 + D - d/r(4r + d)$$

The potential energy curves according to all these potential functions are similar in nature, unlike the exponential force curve of the ionic separation, which corresponds to the equilibrium ionic separation and approaches infinity in the positive side.

3. Potential Parameters and Their Physical Significance

Application of the interaction potential in order to calculate various properties of the molecules, we have to determine the various potential parameters. For which the molecule stability and the force constant conditions from following equations :

$$(10) \quad (dU/dr)_{r=r_e} = 0 \quad \text{and} \quad (d^2U/dr^2)_{r=r_e} = K_e$$

are used to pots (1)-(3). These conditions yield the following expression for the potential parameters :

$$(11) \quad P = e^2(r_e^2 + p) / 4pr_e$$

$$(12) \quad p = -r_e^4(k_e r_e^3/e^2 - 3) / (k_e - r_e^3/e^2 + 1)$$

$$(13) \quad Q = e^2(2r_e + q) / (2qr_e)$$

$$(14) \quad q = -2r_e^2(k_e r_e^3/e^2 - 1) / (k_e r_e^3/e^2 + 1)$$

$$(15) \quad D = e^2(4r_e + d) / dr_e$$

$$(16) \quad d = -4r_e^4 k_e / (k_e r_e^3 + e^2).$$

The values of both parameters P_n and p_n of equation (6) are negative. It is obvious from equation (5) that the potential energy curve should tend to infinity in the positive side at particular value of ionic separation r_e given by :

$$(17) \quad r_e = (-n / 4p_n)^{1/n}.$$

Since, the potential energy at $r = r_e$ is infinity in the positive side, i.e. the repulsive force is infinity in the positive side, i.e., at the repulsive force is infinity, the value of the internuclear separation can not be decreased than r_c . Thus, r_c may be called as the distance of the closest approach at two unlike gaseous ion in vacuum. This is the physical significance of the potential parameter p_n from which we are enable to evaluate the distance of closest approach r_c with the help of generalised equation (17).

Calculated values of pots (1)-(3) have been listed in Tables 1 to 5 for the first and second row diatomic molecules, heavy halides, diatomic hydrides, alkali halides and alkaline earth oxide molecules. Moreover, the value of r_c is less than r_e in all cases. We interpret r_c as the sum of radii of the unlike gaseous ions when they are highly compressed in vacuum. This type of physical significance cannot be associated with any other potential energy functions.

Table 1: The computed values of the distance of least approach, (r_c), according to the logarithmic potential energy functions for first and second row diatomic molecules.

S.No	Molecule	values of (r_c) $\times 10^{-8}$ cm				
		L1 Model	L2 Model	L3 Model	L4 Model	L5 Model
1.	LiH	1.2881	0.8558	1.0273	0.9588	0.5759
2.	BeH	0.8783	0.8540	0.9454	0.9081	0.5512
3.	BH	0.7686	0.8027	0.8776	0.8454	0.5152
4.	CH	0.5827	0.7622	0.8193	0.7944	0.4900
5.	NH	0.4348	0.7213	0.7691	0.7480	0.4650
6.	OH	0.3685	0.6927	0.7322	0.7146	0.4491
7.	HF	0.4415	0.6654	0.6999	0.6845	0.4334
8.	NaH	1.2924	1.1787	1.3118	1.2553	0.7591
9.	MgH	0.7558	1.2005	1.2815	1.2450	0.7736
10.	AlH	0.7120	1.1853	1.2505	1.2213	0.7698
11.	SiH	0.9263	1.1466	1.1924	1.1716	0.7579
12.	PH	0.9538	1.1027	1.1386	1.1222	0.7395
13.	SH	0.9600	1.0640	1.0937	1.0807	0.7258
14.	HCl	0.9354	1.0236	1.0483	1.0369	0.7028

Table 2. The computed values of the distance of least approach, (r_c), according to the logarithmic potential energy functions for HEAVY METAL HALIDES.

S.No.	Molecule	values of (r_c) $\times 10^{-8}$ cm				
		L1 Model	L2 Model	L3 Model	L4 Model	L5 Model
1.	TiF	1.8395	1.8681	2.6793	1.8749	1.4428
2.	TiCl	2.2016	2.2337	2.2464	2.2403	1.7349
3.	TiBr	2.2327	2.3637	2.3760	2.3701	1.8456
4.	TiI	2.5141	2.5459	2.5586	2.5525	1.9947
5.	InCl	2.1314	2.1616	2.1736	2.1678	1.6806
6.	InBr	2.2637	2.9442	2.3064	1.3005	1.7893
7.	InI	2.4622	2.4930	2.5053	2.4993	1.9448
8.	GaCl	1.9182	1.9545	1.9684	1.9617	1.4894
9.	GaBr	2.0544	2.0920	2.1064	1.0995	1.5979
10.	GaI	2.2710	2.8067	2.3200	2.3139	1.8707
11.	CuCl	1.7939	1.8260	1.8384	1.8324	1.3969
12.	BuI	2.0775	2.1065	2.1180	2.1124	1.6394

Table 3. The computed values of the distance of least approach, (r_c), according to the logarithmic potential energy functions for diatomic hydride molecules.

S.No.	Molecule	values of (r_c) $\times 10^{-8}$ cm				
		L1 Model	L2 Model	L3 Model	L4 Model	L5 Model
1.	KH	1.1526	1.5293	1.6427	1.5931	0.9832
2.	PbH	0.7351	1.6659	1.7697	1.7238	1.0762
3.	CsH	1.5994	1.9067	1.9756	1.9443	1.2688
4.	CuH	0.3368	1.0327	1.0959	1.0679	0.6676
5.	AgH	0.8605	1.1890	1.2459	1.2704	0.7776
6.	AuH	1.1391	1.2343	1.2618	1.2490	0.8530
7.	BaH	1.4538	1.7142	1.7742	1.7464	1.1436
8.	CaH	0.327	1.767	1.2478	1.2163	0.7611

Table 4. The computed values of the distance of least approach, (r_c), according to the logarithmic potential energy functions for alkali halide molecules.

S.No.	Molecule	values of (r_c) $\times 10^{-8}$ cm				
		L1 Model	L2 Model	L3 Model	L4 Model	L5 Model
1.	LiF	1.0749	1.2229	1.2601	1.2430	0.7501
2.	LiCl	1.5475	1.6564	1.6892	1.6739	1.3995
3.	LiBr	1.6915	1.7956	1.8279	1.8128	1.6121
4.	LiI	1.9129	2.0077	2.0385	2.0240	1.9176
5.	NaF	1.5124	1.5999	1.6275	1.6146	1.2395
6.	NaCl	1.9313	2.0086	2.0349	2.0225	1.8553
7.	NaBr	2.0681	2.1427	2.1685	2.1563	2.0458
8.	NaI	2.2493	2.3274	2.3546	2.3417	2.3189
9.	KF	1.7667	1.8413	1.8664	1.8546	1.6022
10.	KCl	2.2458	2.3117	2.3354	2.3241	2.2577
11.	KBr	2.3555	2.4316	2.4584	2.4457	2.4516
12.	KI	2.6000	2.6654	2.6894	2.6779	2.7296
13.	RbF	1.8809	1.9471	1.9701	1.9592	1.7445
14.	RbCl	2.3519	2.4193	2.4435	2.4319	2.0115
15.	RbBr	2.3519	2.5825	2.6048	2.5941	2.0056
16.	RbI	2.7423	2.8014	2.8236	2.8130	2.8840
17.	CaF	1.9601	2.0228	2.0450	2.0345	1.8557
18.	CsCl	2.5070	2.5615	2.5830	2.5722	2.5706

Table 5. The computed values of the distance of least approach, (r_c), according to the logarithmic potential energy functions for alkali halide molecules.

S.No.	Molecule	values of (r_c) $\times 10^{-8}$ cm				
		L1 Model	L2 Model	L3 Model	L4 Model	L5 Model
1.	LiF	1.0749	1.2229	1.2601	1.2430	0.7501
2.	LiCl	1.5475	1.6564	1.6892	1.6739	1.3995
3.	LiBr	1.6915	1.7956	1.8279	1.8128	1.6121
4.	LiI	1.9129	2.0077	2.0385	2.0240	1.9176
5.	NaF	1.5124	1.999	1.6275	1.6146	1.2395
6.	NaCl	1.9313	2.0077	1.0385	2.0240	1.9176
7.	NaBr	2.0681	2.1427	2.1685	2.1563	2.0458
8.	NaI	2.2493	2.3274	2.3546	2.3417	2.3279
9.	KF	1.7667	1.8413	1.8664	1.8546	1.6022
10.	KCl	2.2458	2.3117	2.3354	2.3241	2.2577
11.	KBr	2.3555	2.4316	2.4584	2.4457	2.4516
12.	KI	2.6000	2.6654	2.6894	2.6779	2.7296
13.	RbF	1.8809	1.9471	1.9701	1.9592	1.7445
14.	RbCl	2.3519	2.4193	2.4435	2.4319	2.0115
15.	RbBr	2.3519	2.5825	2.6048	2.5941	2.0056
16.	RbI	2.7423	2.8014	2.8236	2.8130	2.8840
17.	CaF	1.9601	2.0228	2.0450	2.0345	1.8587
18.	CsCl	2.5070	2.5615	2.5820	2.5722	2.5706
19.	CsBr	2.6648	2.7185	2.7389	2.7291	2.7694
20.	CsI	2.8963	2.9490	2.9692	2.9595	2.0541

Pandey *et al.* (29) have proposed a new potential by using 3/2 integer value to compute the ionic binding energy, which is found to be in good agreement with the experimental values for different groups of molecules.

The potential function for diatomic molecule is given by :

$$(18) \quad U(r) = -e^2/r + M \log \left(3/2 + m/r^{3/2} \right)$$

Where M and m are the potential parameters which are characteristics of the molecules. This potential function will be labeled as pot (4). The value of the force $F(r)$ is given by:

$$(19) \quad F(r) = -dU/dr$$

$$(20) \quad F(r) = -e^2/r^2 + 3Mm / \left(3r^{5/2} + 2mr \right)$$

The application of molecular stability and the force constant conditions of equation (10) to model pot (4) yields the following expression for the potential parameters :

$$(21) \quad m = 3/2 r_e^{3/2} \left(1/2 - k_e r_e^3 / e^2 \right) \left(k_e r_e / e^2 - 1 \right)^{-1}$$

and

$$(22) \quad M = \left[2/3 \left(3/2 + m / r_e^{3/2} \right) e^2 r_e^{1/2} \right] * m^{-1}.$$

4. A Newly Proposed Potential Energy Function

In the light of these facts we have suggested a new logarithmic potential energy function. This form of overlap repulsion obeys well-established Pauli's principle according to which short-range repulsion should become infinite when closed shell electron clouds of the anion and cations overlap. The present work is an attempt in the same direction.

We have seen that the potential parameters of various form of potential models depend on the experimental values of equilibrium internuclear distance, r_e and force constant, k_e , which vary from molecule to molecule. Keeping above facts we proposed a new logarithmic potential energy functions as :

$$(23) \quad U(r) = m \left[-e^2/r + G \log \left(1 + g/r^n \right) \right]$$

Where G , g , m and n are constants. The potential parameters G and g are characteristics of the molecules and would be determined using the stability and the force constant conditions as :

$$(24) \quad g = r_e^n (n - 1 - A/m) / (1 - A/m)$$

$$(25) \quad G = e^2/r_e (n - 1 - A/m)$$

where

$$(26) \quad A = 1 + k_e r_e^3 / e^2$$

$$(27) \quad m = 1 + 1.6e^2/k_e r_e^3$$

From the above expression we apply the condition $n < (1 + A/m)$, so that g should have negative values, for this we empirically consider,

$$(28) \quad n = 0.6 + A/m$$

It is obvious from (29) that the potential energy curve should tend to infinity in positive side at a particular value.

5. Features of g and G Used in New Potential Model

The potential parameter, g , is a dimensionally distance parameter such that (g/r^n) is a dimensionless quantity. Then $(1 + g/r^n)$ is a constant and log of that quantity is a constant, such that $(-1 < g/r^n < 0)$ and at $r = r_c$, $g/r^n = 1$. Hence, when $r = r_c$, it makes the term $\log(1 + g/r^n)$ undefined in the real domain.

Thus, g contributes the r_c which is closest approach distance such that r_c almost equal to the interionic radii $(r_+ + r_-)$ which are always less than r_0 i.e., interatomic distance in the crystalline state. Thus, the closest approach distance $r_c = (-g)^{1/n}$.

Potential parameter G is dimensionally an energy parameter of the the repulsive energy term. The expression of the repulsive energy term, $G \log(1 + g/r^n)$ shows that this is a repulsive energy term, which is infinity at a distance $r = r_c$, it becomes :

$$(29) \quad -G \log(1 - g/r^n) = G \log(0) \\ = +\infty.$$

But at $r = r_c$ the coulombian terms is $-r^2/r_c$, which is added to the repulsive term and the energy becomes infinity at $r = r_c$, thus ions can not come closer than $r = r_c$ which is approximately equal to the interionic radii $(r_+ + r_-)$.

6. Results and Discussion

The distance of closest approach of two unlike gaseous ions in vacuum has been evaluated with the help of the generalised equations (17) and the condition $r_c = (-g)^{1/n}$. The value of r_c calculated according to the potential models L_1, L_2, L_3, L_4 and L_5 have been listed in the Table 1 to 6. For all the first and second row diatomic molecules heavy metal halides, diatomic hydrides, alkali halides and alkaline earth molecules. Moreover, the value of r_c in all cases. We interpret r_c as the sum of radii of the unlike gaseous ions when they are highly compressed in vacuum. This type of physical significance cannot be associated with the other potential models.

Table 6. The computed values of the distance of least approach, (r_c) , according to the logarithmic potential energy functions for alkaline earth oxide molecules.

S.. No.	Molecules	values of $(r_c) \times 10^{-8}$ cm				
		L1 Model	L2 Model	L3 Model	L4 Model	L5 Model
1.	BeO	1.1405	1.1675	1.776	1.7281	0.8767
2.	MgO	1.5128	1.5445	1.5565	1.5507	1.1685
3.	SrO	1.7242	1.7440	1.7521	1.7482	1.3749
4.	BaO	1.7690	1.7840	1.7902	1.7872	1.4353
5.	CaO	1.6153	1.6387	1.6479	1.6435	1.2721

Table 7. The computed values of the potential parameters P, Q, D, M and G, according to the logarithmic potential models of first and second row diatomic molecules (in KJ mol⁻¹).

S.No	Molecule	P L1 Model $\times 10^{-32}$	Q L2 Model $\times 10^{-16}$	D L3 Model $\times 10^{-8}$	M L4 Model $\times 10^{-12}$	G L5 Model $\times 10^{-28}$
1.	LiH	2.7530	1.4650	4.1095	1.4082	0.6453
2.	BeH	0.5952	1.4723	3.7818	1.2981	1.4912
3.	BH	0.3413	1.2829	3.5106	1.6161	0.8940
4.	CH	0.1153	1.1621	3.2775	1.0621	0.2581
5.	NH	0.0357	1.0403	3.0764	0.9704	0.0365
6.	OH	0.0184	0.9597	2.9290	0.9062	0.1291
7.	HF	0.0380	0.8857	2.7997	0.8495	0.1896
8.	NaH	2.7898	2.7791	5.2472	2.1103	5.8726
9.	MgH	0.3263	2.8827	5.1260	2.0680	0.3322
10.	AlH	0.2571	2.8099	5.0008	2.0245	1.0592
11.	SiH	0.7364	2.6294	4.7699	1.9024	2.2839
12.	PH	0.8279	2.4322	4.5546	1.7832	2.5606
13.	SH	0.8496	2.2705	4.3751	1.6852	2.6653
14.	HCl	0.7657	2.0957	4.1933	1.5837	2.4583

Table 8. The computed values of the potential parameters P, Q, D, M and G, according to the logarithmic potential models of heavy halide molecules (in KJ mol⁻¹).

S.No	Molecule	P L1 Model $\times 10^{-32}$	Q L2 Model $\times 10^{-16}$	D L3 Model $\times 10^{-8}$	M L4 Model $\times 10^{-12}$	G L5 Model $\times 10^{-28}$
1.	TiF	11.4499	6.9800	7.5175	3.8480	27.1895
2.	TiCl	23.4958	9.9797	8.9859	5.0300	50.4734
3.	TiBr	29.6109	11.1744	9.5043	5.4732	61.7391
4.	TiI	39.9574	12.9638	10.2347	6.1171	79.9600
5.	InCl	20.6413	9.3455	8.6944	4.7877	45.2144
6.	InBr	26.2588	10.5275	9.2258	5.2341	55.6651
7.	InI	36.7576	12.4301	10.0213	5.9270	74.4655
8.	GaCl	13.5409	7.6406	7.8387	4.1215	31.1772
9.	GaBr	17.8156	8.7532	8.4257	4.5632	39.4966
10.	GaI	26.6034	10.6420	9.2826	5.2798	56.0082
11.	CuCl	10.3577	6.6690	7.3536	3.7209	24.8275
12.	CuI	18.6909	8.8751	8.4727	4.6055	41.4318

Table 9. The computed values of the potential parameters P, Q, D, M and G, according to the logarithmic potential models diatomic hydride molecules (in Kj mol^{-1}).

S.No	Molecule	P L1 Model $\times 10^{-32}$	Q L2 Model $\times 10^{-16}$	D L3 Model $\times 10^{-8}$	M L4 Model $\times 10^{-12}$	G L5 Model $\times 10^{-28}$
1.	KH	1.7652	4.6777	6.5709	3.0164	2.6037
2.	RbH	0.2920	5.5505	7.0789	3.3949	0.7895
3.	CsH	6.5441	2.2713	7.9033	4.0668	14.9480
4.	CuH	0.0128	2.1331	2.3836	1.6554	0.2324
5.	AgH	0.5485	2.8277	4.9830	2.0222	1.7166
6.	AuH	1.6837	3.0471	5.0472	2.0938	4.8637
7.	CaH	0.0107	2.7694	4.9913	0.2122	0.4427
8.	BaH	4.4674	5.8774	7.0970	3.4632	10.8029

Table 10. The computed values of the potential parameters P, Q, D, M and G, according to the logarithmic potential models alkali halide molecules (in Kj mol^{-1}).

S.No	Molecule	P L1 Model $\times 10^{-32}$	Q L2 Model $\times 10^{-16}$	D L3 Model $\times 10^{-8}$	M L4 Model $\times 10^{-12}$	G L5 Model $\times 10^{-28}$
1.	LiF	1.3351	2.9914	5.0403	2.0789	3.8808
2.	LiCl	5.7358	5.4877	6.7570	3.2486	14.0445
3.	LiBr	8.1872	6.4486	7.3119	3.6612	19.1930
4.	LiI	13.3910	8.0618	8.1542	4.3193	29.5984
5.	NaF	5.2328	5.1199	6.1502	3.0775	13.1117
6.	NaCl	13.9146	8.0679	8.1397	4.3145	30.9107
7.	NaBr	18.2957	9.1826	8.6741	4.7495	39.2818
8.	NaI	25.5993	10.8338	9.4184	5.3751	52.4863
9.	KF	9.7428	6.7813	7.4658	3.7885	22.7111
10.	KCl	25.4425	10.6888	9.3415	5.3148	52.6042
11.	KBr	3.7871	11.1825	9.8339	5.7372	61.6853
12.	KI	45.7014	14.2090	10.7576	6.5734	87.4954
13.	RbF	12.5164	7.5826	7.8805	4.1135	28.3986
14.	RbCl	30.6007	11.7061	9.7741	5.6889	61.6919
15.	RbBr	40.4750	13.3389	10.4192	6.2673	79.0084
16.	RbI	56.5611	15.6965	11.2946	7.0770	105.7001
17.	CsF	14.7617	8.1841	8.1802	4.3529	32.8559
18.	CsCl	39.5052	13.1233	10.3280	6.1880	77.6720
19.	CsBr	50.4232	14.7812	10.9557	6.7629	96.0377
20.	CsI	70.3735	17.3933	21.8769	7.6369	128.3045

Table 11. The computed values of the potential parameters P , Q , D , M and G , according to the logarithmic potential models alkaline earth oxide molecules (in KJ mol^{-1}).

S.No	Molecule	P L1 Model $\times 10^{-32}$	Q L2 Model $\times 10^{-16}$	D L3 Model $\times 10^{-8}$	M L4 Model $\times 10^{-12}$	G L5 Model $\times 10^{-28}$
1.	BeO	1.6919	2.7265	4.7104	1.9051	5.1935
2.	MgO	5.2379	4.7712	6.2260	2.8967	13.7553
3.	SrO	8.8383	6.0836	7.0085	3.4673	21.9920
4.	BaO	9.7944	6.3655	7.1610	3.5839	24.2321
5.	CaO	6.8094	5.3710	5.5919	3.1605	17.4571

The Potential parameters, P , Q , D , M and G respectively have been evaluated and listed in Table 7 to 11. These potential parameters enables us to evaluate the distance of closest approach r_c from the knowledge of equation (17) and the condition $r_c = (-g)^{1/n}$.

7. Conclusions

We have seen that previously proposed models for the potential energy function in the molecules are not entirely satisfactory, in that they are defined for a region where normal ionic forces no longer control the interaction between ions and the form of potential energy and force curves in unacceptably modified by the presence of attractive terms for the theoretically established dipole-dipole, dipole-quadrupole and hyperpolarizability force, for almost are leading repulsive interaction terms. In order to overcome these difficulties a new model has been proposed in which the interionic potential energy tends to infinity in the positive energy domain and it should come asymptotically to a finite value at $r \rightarrow \infty$ and minimum at $r = r_e$. It has been found that the new potential model gives a better representation of the experimental data for binding energy dissociation energy is comparable.

Although, the earlier models do not give realistic forms for the potential energy and force curve, they still yield satisfactory results for the various molecular parameter. However, this is because they are contained by known stability and force constant conditions thus all have a minimum at r_e . Under these conditions acceptable values for molecular properties particularly in view of the certainties in the experimental data, and for a model to be reliable it must be able to also predict satisfactory forms for the potential energy and force curves. Obviously this fundamental requirement. For once, a model has this merit, it will automatically predict accurate values of the crystal properties. The form for the potential proposed here is an improvement on previous models, although far from perfect, it may help in obtaining a better understanding of the nature of the ionic bond.

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