Available online at http://www.journalcra.com

INTERNATIONAL JOURNAL
OF CURRENT RESEARCH

International Journal of Current Research
Vol. 14, Issue, 02, pp.20871-20874, February, 2022

DOI: https://doi.org/10.24941/ijcr.43099.02.2022

ISSN: 0975-833X

RESEARCH ARTICLE

ESTIMATION OF BINDING ENERGY, DISSOCIATION ENERGY AND ELECTRON AFFINITY OF FIRST AND SECOND ROW DIATOMIC MOLECULES USING VARIOUS INTERACTION POTENTIALS

[1]Pandey, J.D., [1]Tripathi, S.B., Soni, N.K.[2] and Singh, V.K.[3]*

[1]Department of Chemistry, University of Allahabad, Allahabad
[2]DepartmentofChemistry, Govt. P.G. College, Charkhari, Mahoba
[3]Department of Physics, V.S.S.D. College, Kanpur

ARTICLE INFO

Article History:
Received 14th November, 2021
Received in revised form
19th December, 2021
Accepted 15th January, 2022
Published online 28th February, 2022

Keywords:

Interaction Potentials, Binding Energy, Dissociation Energy, Electron Affinity.

Corresponding author:
Singh, V.K.,

ABSTRACT

The binding energy and dissociation energy of fourteen first and second row diatomic molecules (twelve hydride molecules and two hydrogen halide molecules) have been computed using Börn-Mayer, Gaussian, Woodcock and Logarithmic (L_5) potential models. The Woodcock and Logarithmic models are also used to compute the electron affinity of halogen atoms and hydrogen atom. The estimated values are compared with the experimental findings. The Logarithmic (L_5) and Woodcock models provide the better results in comparison to other proposed models.

Citation: Pandey, J.D., Tripathi, S.B., Soni, N.K. & Singh, V.K.. *"*Estimation of binding energy, dissociation energy and electron affinity of first and second row diatomic molecules using various interaction potentials", *2022. International Journal of Current Research, 14, (02), 20871-20874.*

INTRODUCTION

The nature of binding in diatomic molecules is very important to predict various spectroscopic properties of the molecules. The knowledge of interatomic potential energy function is of fundamental importance. The evaluation of binding energy of diatomic molecules using appropriate form of interaction potential energy functions has been a subject of extensive studies for the last several decades (1-7). The binding energy in the molecules arises from purely electrostatic interaction between ions, which includes charge-charge interaction, charge-dipole interaction and dipole -dipole interaction and quasi-elastic energy stored in the induced dipoles. The chemist deals with the matter in bulk and determines the heat required to dissociate a gram molecule of diatomic gas at standard temperature (usually 25° C) to monoatomic gases at the same temperature. Direct measurement of this quantity is never possible, and the heat of dissociation defined in this way must be regarded as a constant, which comes into certain calculations and has a simple physical interpretation. Determination of heat of dissociation is done by several workers (8-14). The electron affinity of an atom can be defined as the energy difference between the anion and the neutral atom in their ground electronic states. It is, of course, equal to the first ionization potential of the anions. In order to know the better insight of atoms' electronic structures, which equally determine the magnitude of their electron affinities, one should formulate theexperimental and theoretical techniques for evaluation of these quantities. The determination of the electron affinity of hydrogen atom has been a subject of extensive study for many years and several experimental and theoretical methods have been developed with varying degree of success. These methods include electron attachment, equilibrium measurement, calculation from lattice energy, heat of salvation of ions, the kinetics of electrode processes, quantum mechanical, spectral and extrapolation methods. From the literature, it appears that, experimentally an exact determination of the electron affinity of hydrogen atom is rather difficult and usually indirect methods are adopted(15).

On the theoretical side, a number of attempts have been made to derive the electron affinity from Spectro static data, many of them depending on extrapolation and interpolation methods. One of the most widely used extrapolation methods for the estimation of electron affinities of atoms depend on the knowledge of the ionization potential of a series of isoelectronic positive ions. This method of calculation has been utilized by Glocker, Bates (16), Pritchard (17) and Varshni & Srivastava. The electron affinity of halogen and hydrogen atoms has been compiled by Pandey (18).

The accuracy of the result depends upon

- The nature of interaction potential, and
- The accuracy of the molecular constants used in the calculation.

In the present work, expressions for the binding energy, dissociation energy and electron affinity of diatomic molecules have been derived by considering the different potential functions including the recently proposed potential function (L_5). The potential functions have been assumed to be consist of the following terms:

- Eletrostatic term, e^2/r
- Repulsion of the form (a)Exponential, (b)Gaussian, and Logarithmic

Theory: The binding energy D_i, can be obtained by applying the following condition to the potential model

$$D_i = -U(r_e) \tag{1}$$

In the present study, we have considered the following previously proposed interaction potential models possessing the different kinds of repulsive terms

Woodcock Potential$^{(4)}$

$$U(r) = Ar^{-m}e^{[-B(r^n-1)]} - \frac{e^2}{r} \tag{2}$$

Börn-Mayer potential$^{(5)}$

$$U(r) = -\frac{e^2}{r} + Ae^{-(r/\rho)} \tag{3}$$

Gaussian Potential$^{(6)}$

$$U(r) = -\frac{e^2}{r} + Pe^{-(kr^2)} \tag{4}$$

Logarithmic (L_5) Model $^{(7)}$

$$U(r) = m\left[\frac{-e^2}{r} + G\log\left(1 + \frac{g}{r^n}\right)\right] \tag{5}$$

In Eqs.2,3,4 &5, A, B; A, ρ; P, k; G, g respectively are the potential parameters. These parameters can be determined by using the following molecular stability and force constant conditions:

$$U'(r_e) = 0 \tag{6}$$

$$U''(r_e) = k_e \tag{7}$$

where $U'(r)$ and $U''(r)$ refer to the first and second derivatives of U(r) and r_e, is the intermolecular distance. On imposing conditions (6) and (7) to potentials (2) to (5),we get the following expressions respectively for the binding energy D_i:

$$D_i = \frac{e^2}{r_e}\left[1 - \frac{1}{(m + nBr_e^n)}\right] \tag{8}$$

$$D_i = \frac{e^2}{r_e}\left[1 - \left(\frac{k_e r_e^3}{e^2} + 2\right)^{-1}\right] \tag{9}$$

$$D_i = \frac{e^2}{r_e}\left[1 - \left(\frac{k_e r_e}{e^2} + 3\right)^{-1}\right] \tag{10}$$

$$D_i = m\frac{e^2}{r_e}\left[1 - \frac{1}{\left(n - 1 - \frac{k_e r_e^3}{me^2}\right)}\log\left(\frac{n}{1 + \frac{k_e r_e^3}{me^2}}\right)\right] \tag{11}$$

It has been found from Eq. (8) that D_i is very sensitive to n. Thus, while working with the Woodcock potential, the choice of n should be made very carefully. We have computed the values of binding energy, D_i, for n=1(0.5)20 for all the diatomic molecules considered under the present study. The methodology used to compute the dissociation energy is the interaction potential energy function. The dissociation energies of first and second row diatomic molecules have been deduced with the help of skeleton relation [Eq. (1)] and

$$D_e = D_i + E - I \tag{12}$$

Where E is the electron affinity and I, the ionization potential. On substituting the expressions for binding energy in Eq.(12),we have corresponding expressions for the dissociation energy as:

$$D_e = E - I + \frac{e^2}{r_e}\left[1 - \left(\frac{1}{m + nBr_e^n}\right)\right] \tag{13}$$

$$D_e = E - I + \frac{e^2}{r_e}\left[1 - \left(\frac{k_e r_e^3}{e^2} + 2\right)^{-1}\right] \tag{14}$$

$$D_e = E - I + \frac{e^2}{r_e}\left[1 - \left(\frac{k_e r_e}{e^2} + 3\right)^{-1}\right] \tag{15}$$

$$D_e = E - I + m\frac{e^2}{r_e}\left[1 - \frac{1}{\left(n - 1 - \frac{k_e r_e^3}{me^2}\right)}\log\left(\frac{n}{1 + \frac{k_e r_e^3}{me^2}}\right)\right] \tag{16}$$

The expressions for electron affinity obtained from conditions of stability and force constant in continuum to Eq.(12) for Woodcock potential and L_5 model respectively is given by

$$E = D_e + I - \frac{e^2}{r_e}\left[1 - \left(\frac{1}{m + nBr_e^n}\right)\right] \tag{17}$$

$$E = D_e + I - m\frac{e^2}{r_e}\left[1 - \frac{1}{\left(n - 1 - \frac{k_e r_e^3}{me^2}\right)}\log\left(\frac{n}{1 + \frac{k_e r_e^3}{me^2}}\right)\right] \tag{18}$$

The values of E have been calculated from Eqs. (17& 18).The average values of E for atoms obtained by such calculations have been compiled in Tables III & IV respectively with the recent experimental (19, 20) and theoretical values (5,18).

RESULTS AND DISCUSSIONS

The binding energy of fourteen diatomic molecules (twelve different hydride molecules and two hydrogen halide molecules) have been computed using four forms of the potential energy functions including the generalized pair potential.

The necessary data for the computation have been taken from different sources (1,21,22). A comparative study has been made and it is found that the generalized pair potential (Woodcock) model yields the best results for the binding energies of all the fourteen diatomic molecules. These molecules include LiH, BeH, BH, CH, NH, OH, HF, NaH, MgH, AlH, SiH, PH, SH and HCl. Börn-Mayer(5) and Gaussian(6) potential models have been found highly successful in reproducing the various properties of most commonly investigated alkali halide molecules(3). However, in the present study, these models have not been found so successful irrespective of these hydrides.

Table 1. Experimental and calculated values of binding energy (Di), and the mean deviations for first and second row diatomic molecules (KJmole-1)

Molecule	$D_i(exp.)$	$D_i(Wood$ cock)	$D_i(Börn - Mayer)$	$D_i(Gaus$ sian)	$D_i(L_5)$	$D_i\%(Wood$ cock)	$D_i\%(Börn - Mayer)$	$D_i\%(Gaus$ sian)	$D_i\%(L_5$)
LiH	0667.20	0752.27	0641.26	0688.76	0703.31	12.75	03.89	03.23	05.41
BeH	1015.00	0976.82	0797.65	0841.50	0948.97	03.76	21.41	17.09	06.51
BH	1035.20	1014.87	0874.34	0920.32	1046.87	01.96	15.54	11.10	01.13
CH	1341.70	1172.69	0976.97	1022.75	1183.83	12.60	27.18	23.77	11.77
NH	1633.50	1268.16	1064.77	1111.45	1296.00	22.37	34.82	31.96	20.66
OH	1660.80	1356.31	1149.76	1196.01	1404.60	18.33	30.77	27.99	15.43
HF	1544.40	1435.15	1224.08	1270.58	1497.40	07.07	20.74	17.73	03.04
NaH	0616.30	0626.37	0563.77	0596.20	0665.61	01.63	08.52	03.26	08.00
MgH	0853.30	0759.65	0637.18	0665.35	0775.16	10.97	25.33	22.03	09.16
AlH	0779.90	0778.39	0678.45	0705.10	0829.38	00.19	13.01	09.59	06.34
SiH	1044.30	0866.80	0751.04	0775.41	0918.88	17.00	28.08	25.75	12.01
PH	1272.00	1272.52	0968.56	1055.15	0950.77	00.04	23.86	17.05	25.25
SH	1226.60	0986.22	0873.85	0895.54	1060.90	19.60	28.76	26.99	13.51
HCl	1631.00	1037.02	0924.73	0946.22	1119.44	36.42	43.30	41.99	31.36
Average						09.70	23.23	19.50	09.13

Table II. Experimental and calculated values of dissociation energy (De), and the mean deviations for first and second row diatomic molecules (KJmole-1)

Molecule	$D_e(exp.)$	$D_e(Wood$ cock)	$D_e(Börn - Mayer)$	$D_e(Gaus$ sian)	$D_e(L_5)$	$D_e\%$ $(Wood$ cock)	$D_e\%(Börn - Mayer)$	$D_e\%(Gaus$ sian)	$D_e\%(L_5)$
HF	564.42	450.95	239.88	286.38	513.20	20.10	57.50	49.26	9.08
OH	426.67	117.81	088.74	042.49	166.10	72.39	79.20	90.04	61.07
PH	338.90	335.73	031.77	118.36	013.98	0.94	90.63	65.07	95.87
NH	309.62	059.04	262.43	215.75	031.20	80.93	15.24	30.32	89.92
CH	334.73	161.42	034.30	011.48	172.56	51.77	89.75	96.57	48.45
BH	327.18	289.37	148.84	194.82	321.37	11.56	54.51	40.46	1.78
HCI	427.60	078.89	033.40	011.91	161.31	81.55	92.19	97.21	62.27
SH	340.58	061.57	050.80	029.11	136.25	81.92	85.09	91.45	59.99
BeH	221.75	152.16	027.01	016.84	124.31	31.38	87.82	92.41	43.94
SiH	294.97	155.11	039.35	063.72	207.19	47.42	86.66	78.40	29.76
LiH	234.34	306.75	195.74	243.24	257.79	30.90	16.47	3.80	10.01
AlH	288.69	284.90	184.96	211.61	335.89	1.31	35.93	26.70	16.35
MgH	192.46	096.91	025.56	002.61	112.42	49.65	86.72	98.64	41.59
NaH	196.65	205.47	142.87	175.30	244.71	4.48	27.35	10.86	24.44
Average						40.45	64.65	62.23	42.47

Table III. Electron affinities of halogen atoms from different sources (KJmole^{-1})

Source	F	Cl	Br	I
Schmidt - Bocking and Bethger(23)	327.06	353.13	195.22	309.70
Berry and Reimann(19)	322.67	348.50	342.47	295.53
Cubicciotti(20)	332.58	357.67	336.73	307.59
Pandey(18)	350.62	388.73	367.12	336.63
Börn -Mayer(5)	356.32	392.7	377.94	340.02
	±20.26	±15.43	±18.33	±10.62
Rittner(2)	338.76	365.15	343.68	313.77
	±20.26	±15.43	±18.33	±10.63
Gaussian(23)	370.80	374.37	358.64	323.72
Modified Gaussian(23)	350.63	388.65	367.73	336.65
L_5-Model (present study)	350.10	331.54	312.63	301.95
Woodcock (present study)	348.93	364.71	340.48	308.16

Table IV. Electron affinities of Hydrogen atom from different sources (KJmole^{-1})

Sources	Electron affinity
Glocker	73.33
Bates$^{(16)}$	71.40
Pritchard$^{(17)}$	70.43
Varshni& Srivastava	68.31
Varshni& Srivastava	58.66
Quantum mechanical calculation by Henrich$^{(26)}$	72.06
Pandey$^{(18)}$	83.07 ±20.26
Born -Mayer$^{(5)}$	116.36 ±20.26
Rittner$^{(2)}$	87.42 ±20.26
Varshni - Shukla I	88.32
Varshni - Shukla H	137.59
L_5 Model (Present study)	72.55
Woodcock (Present study)	90.27

Therefore, we have selected the logarithmic(7) potential model (L_5) and Woodcock(4) potential, which yield better results for these molecules. The computed values of binding energy, D_i, according to Eqs. (8) to (11) and respective percentage mean deviations with experimental values are listed in Table-l. It is evident from Table-I that the Börn-Mayer potential, which has been most widely used for various molecules, yields the poor results for the binding energy of these hydride molecules giving an average percentage deviation (APD) of 23.23% with the experimental values. The best agreement with experimental values is obtained from the logarithmic potential and the generalized pair potential (Woodcock).The logarithmic potential model (L_5) suggested by Pandey et.al(7) and Woodcock models (4) appear to be successful in predicting the binding energy of diatomic molecules. Various potential models used for the present study can be arranged in the order of superiority for these hydrides as L_5> Woodcock> Gaussian>Börn - Mayer.

For HCI, the error is the largest according to all the models. It is very interesting to note that the Börn -Mayer and Gaussian potentials give very good results for the LiH and NaH, the ionic molecules and they yield bad results for the covalent molecules and reverse in order, for the logarithmic potential, but Woodcock potential model holds good for NaH and bad for LiH. The dissociation energy of fourteen diatomic molecules (twelve different hydrides and two hydrogen halide molecules) have been computed using the different potential energy models. A comparative study has been made and it is found that the new potential model, logarithmic, yields the best results for all the fourteen diatomic molecules (LiH, BeH, BH, CH, OH, HF, NH, NaH, MgH, AIH, SiH, PH, SH and HCl). The computed values of dissociation energy, D_e, according to Eqs. (13-17) are listed in Table- II.It is evident from Table-II that Börn -Mayer (5) and Gaussian potentials (6) yield the poor results for the dissociation energy of the diatomic molecules with the average percentage deviation of 64.65 and 62.23 respectively. The best agreement with experimental values is obtained from the new logarithmic potential (L_5) and Woodcock potential.

The order of superiority can be arranged as follows on the basis of potential models used in present investigation for the determination of dissociation energy of first and second row diatomic molecules. Woodcock>L_5>Gaussian>Börn-Mayer. The Woodcock potential regenerates the comparable values for AIH, PH and NaH molecules up to the experimental scan exhibiting a percentage deviation of 1.31, 0.94 & 4.48 respectively. The electron affinity of halogen atoms and hydrogen atom from different sources, and computed in the present study are given in Table-III and IV. A comparative inference can be drawn, whichadvocates the validity of present investigation and hence proved the applicability of Woodcock potential for the determination of electron affinities of isolated atoms.

REFERENCES

1. Herzberg G., Huber K.P., 1979. "Molecular Spectra and Molecular Structure. Chapter IV. Constants of Diatomic Molecules",(Van Nostrand Heinhold Co. Inc., New York).
2. Rittner, E.S. 1951. J. Chem. Phys. 19, 1030
3. Margrave, J. L., J. Phys. Chem. Ithaca,58, 258 (1954).
4. Woodcock L.V., J. Chem. Soc. Faraday Trans.,2,1405 (1974).
5. Born M. and Mayer J.E.,Z Phys.,75,1 (1932).
6. Sandwar B.B., Sinha A.K. and Thakur L., Indian J. Pure & Appl. Phys.,20, 891 (1982).
7. Pandey J.D., Singh A.K. and Tripathi S B, J. International Academy Phys. Sci. Vol. 2, 87,(1998).
8. 08. Ross A.J., Crozet P., Incan J.D. and Effantian C., J. Phys. B19, L145 (1986).
9. 09. Amiot C., Crozer P. and Verges J., Chem. Phys. Lett, 121, 390 (1985).
10. Coxon J.A. and Wickramaaratch M.A., J. Mol.Spectros,79,380 (1980).
11. Brand J.C.D., Busieres D. and Hoy A.R., J.Mol.Spectros, 113,388 (1985).
12. Barakat B., Bacis R., Carrot F., Churassy S., Crozet P., Martin F. and Verges J., J. Chem. Phys.,102,215 (1986).
13. Verma K.K., Bhans J.T., Rajaei-RijiA.R. and Stwalley W.C., J.Chem.Phys.,78,3599 (1983).
14. Douglas A.E. and Hoy A.R., Can. J. Phys.,53,1965 (1985).
15. Dekker A.K., "Solid State Physics" Macmillan Student Ed., U.K. (1991).
16. Bates D. R., Pro R Irish Acad, 51, 151 (1947).
17. Pritchard H.O., Chem. Rev., USA, 52,529 (1953).
18. Pandey J.D., J. Chem. Soc., Section A, 5 (1969).
19. Berry R.S. and Reimann C.W., J.Chem.Phys.,38, 1540 (1963).
20. Cubicciotti D., J. Chem. Phys. 34,2189 (1961).
21. Pauling L., "The Nature of Chemical Bond and the Structure of Molecules and Crystals" 3rd Ed. (1960).
22. "Tables of Interatomic Distance and Configuration of Molecular-Ions", The Chemical Society, London, 1958.
23. Schmidt-Bocking H. and Bethge K., J. Chem. Phys., 58, 3244 (1973).
24. Henrich L.R., Astrophys J.,99,59 (1944).

****