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Spectroscopic Investigation for Diatomic Molecule (AlBr) by Using Different Functions

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Abstract: ***The present work concerns by study of spectroscopic properties for AlBr. Dissociation energy had been calculated theoretically for ground state $X^1\Sigma^+$ of AlBr molecule by Herzberg relation and by depending on spectroscopic constants for this molecule. Our results are compared with experimental results and appear good convergence, also showed an important effect for bond length (r) for occur the dissociation. The potential of this molecule is studied in this work by using more of potential function as (Varshni potential function) and (Extended Rydberg potential function), the results appear that potential curve of AlBr molecule for ground state $X^1\Sigma^+$convergeswith experimental results, and the dissociation happen when (r) approach from (∞).***

Keyword: dissociation energy, ground state of AlBr molecule

1. Introduction

A potential energy curve is a graphical representation of the change in potential energy of the molecule as a function of the distortion of the bond of the molecule from its equilibrium distance. The knowledge of potential energy curves is of prime importance in the study of diatomic molecular spectra [1]. In the calculations of Franck Condon factor, dissociation energy and thermodynamic quantities etc, the studies of potential energy carves are necessary. The empirical potential energy functions like Varshni [2] and extended Rydberg [3,4] are usually applied and the potential energy carves are drawn. Naturally to compute the turning points of various vibrational levels the accurate spectroscopic constants are required. The empirical potential energy functions also require these molecular constants.

2. Theoretical Part

The empirical equation for the diatomic molecule, which in many cases is quite accurate, was proposed by Morse and D_e is again the dissociation energy from the potential minimum. Note that for $r\text{-}r_e = \infty, V_m = D_e$. This dissociation energy differs from the measured dissociation energy of a molecule; however the quantity D_e is the energy that would be necessary to dissociate the molecule if it could be at the minimum of the potential energy curve. Because of the zero point energy, this is impossible, and therefore [5]:

$$D_e=D_0+1/2 \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (1)$$

D_0 is the measured dissociation energy and $1/2\ v_0$ is the zero point energy measured in cm^{-1} unit and the values of D_e and D_0 have the same units.

Another relation for dissociation energy is called Gaydon relation [6]:

$$D_e = \frac{\omega_e^{\ 2}}{(5\omega_e\chi_e - 2B)} \ldots\ldots\ldots\ldots\ldots\ldots (2)$$

Another relation for dissociation energy is called Herzberg relation [5]:

$$D_e = \frac{\omega_e^{\ 2}}{4\,\omega_e\chi_e} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (3)$$

One of functions of potential is Varshni function which is different from Morse function by term(r/r_e) so the function had written as [2]:

$$U_{(x)} = D_e\left(1-\frac{r}{r_e}e^{-\beta x}\right)^2 \ldots\ldots\ldots\ldots\ldots\ldots (4)$$

x=r-re

$$\beta = \left[\frac{8\pi^2\mu(\omega_e\chi_e)c}{h}\right]^{1/2} \ldots\ldots\ldots\ldots\ldots\ldots\ldots (5)$$

On the other hand, another function of potential called Extended Rydbergpotential function has the form[3,4]:

$$U_{ext} = D_e - D_e\{1 + a_1\rho + a_2\rho^2 + a_3\rho^3\}e^{-a_1\rho} \ldots\ldots (6)$$

Where $\rho = r\text{-}r_e$, a_1,a_2 and a_3 are the constants defined through following discussions. The constant $a_1$is determined from the solution of the following quadratic equation:

$$D_e a_1^{\ 4} - 6f_2a_1^2 - 4f_3a_1 - f_4 = 0 \ \ldots\ldots\ldots\ldots (7)$$

The parameters f_2,f_3 and f_4 are called force field parameters and are defined as:

$$f_{2=4\pi^2\mu\omega_e{}^2c^2} \ ,$$

$$f_3 = -\left(\frac{3f2}{r_e}\right)\left[1+\left(\frac{\alpha_e\omega_e}{6B_e}\right)^2\right] ,$$

$$f_4 = -\left(\frac{f3}{r_e}\right)^2\{15\left[1+\left(\frac{\alpha_e\omega_e}{6B_e{}^2}\right)\right] - \left(\frac{8\omega_e x_e}{B_e}\right)\}$$

Usually the largest positive root of equation (7) is selected as a_1. The other parameters calculated from:

$$a_2 = \left(\tfrac{1}{2}\right)[a_1^2 - (f_2/D_e)] \qquad a_3 = [a_1a_2 - (a_1^3/3) - (f_3/6D_e)]$$

3. Results and Discussion

Spectroscopic properties of AlBr molecule are studied such as potential curves for two functions began with potential Varshni function for ground $X^1\Sigma^+$ state (eq. 4) compared with other function "Extended Rydberg potential function" for ground $X^1\Sigma^+$ state (eq. 6) then dissociation energy is obtained using (eq.3) compared with another energy.

Table 1: The spectroscopic constants for AlBr **molecule measured (cm^{-1})[7,8,9].**

Spectroscopic constant	$X^1\Sigma^+$
T_e	0
ω_e	378.10
$\omega_e x_e$	1.307
B_e	0.1591

Where T_e: electronic energy above ground state (cm^{-1}) ,ω_e: the fundamental vibration frequency (cm^{-1})$\omega_e x_e$: the anharmonicity constant (cm^{-1}), B_e: the rotational constant at equilibrium bond length (cm^{-1})

Result of Dissociation Energy

In order to obtained dissociation energy, the relation are used (eq. 3), and here are the results in table (2). The D_e values are found to be (27344.9 cm^{-1}) for $X^1\Sigma^+$, that dissociation due to approaching the bond length (r) from infinity values, where this is one of three conditions of potential curve. These results are in good agreement with the experimental values.

Table (2): Dissociation energy obtained (cm^{-1})

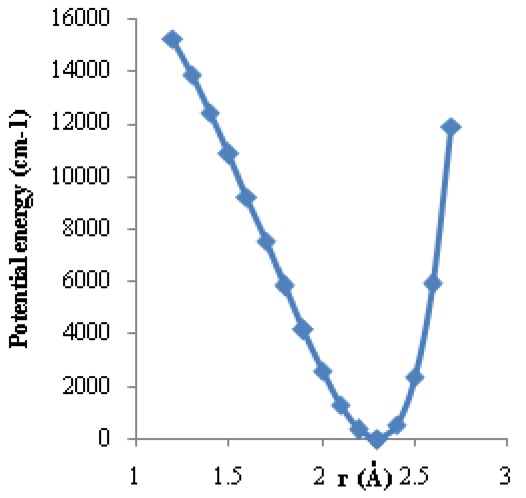
State	D_e (cm^{-1})	D_e(cm^{-1})
$X^1\Sigma^+$	27344.9	27337 [1]

Result of Varshni Potential Function:

To calculate Varshni potential for AlBr molecule (eq. 4) is used for the ground state $X^1\Sigma^+$, and here are the results in table (3) and figure (1). The calculations appear the maximum value of varshni potential is at (r = 1.2 $\mathring{A}$) that mean the minimum value of bond length give us maximum potential in ground state of AlBr molecule. At bond length (r_e = 2.29 $\mathring{A}$), the potential equal (0), then the potential increase by increasing bond length until reach at the point which happen in it the dissociation because that the diatomic molecules dissociate when the value of (r) increase to determinate limit.

Table 3: Varshnipotential for ground state

r ($\mathring{A}$)	$X^1\Sigma^+$ $U_{Varsh}(x)$ cm^{-1}
1.2	15222.55
1.3	13765.8
1.4	12420.33
1.5	10732.56
1.6	9150.66
1.7	7432.77
1.8	5714.34
1.9	4150.22
2	2498.12
2.1	1176.35
2.2	3517
2.29	0
2.3	1.1722
2.4	530.43
2.5	2322.32
2.6	5811.51
2.7	11811.54



Fifure 1: Calculated Varshni Potential Curves for ground state X¹Σ of AlBr molecule

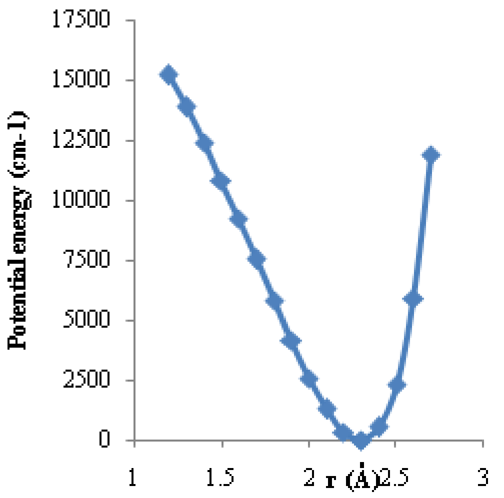
Results of Extended Rydberg Potential Function:

To calculate Extended Rydberg potential for AlBrmolecule eq. (6) is used for the ground state $X^1\Sigma^+$by depending on dissociation energy, bond length, spectroscopic constants, and here are the results of Extended Rydberg potential for this molecule for the ground state $X^1\Sigma^+$ in table (4) and figure (2).

The calculations appear the maximum value of Extended Rydberg potential is (15143.35 cm^{-1}) in ground state at (r = 1.2 $\mathring{A}$) which is the minimum value of bond length. At bond length (r_e = 2.29A°), the potential equal (0) , then the potential increase by increasing bondlength until reach at the point which happen in it the dissociation because that the diatomic molecules dissociate when the value of (r) increase to determinate limit. That behavior of potential is similar to behavior the excited state of this molecule.

Table 4: Extended Rydberg potential function for ground state

r ($\mathring{A}$)	$X^1\Sigma^+$ $U_{Ext\text{-}Ryd.}(x)$ cm^{-1}
1.2	15143.35
1.3	14343.8
1.4	12322.54
1.5	10655.78
1.6	9100.32
1.7	7323.82
1.8	5634.32
1.9	4111.83
2	2343.44
2.1	1155.44
2.2	3437
2.29	0
2.3	1.1632
2.4	528.44
2.5	2300.72
2.6	5800.21
2.7	11801.21



Fifure 2: Calculated Extended Rydberg Potential Curves
for ground state $X^1\Sigma$ of AlBr molecule

Table 5: Comparing Extended Rydberg function and Varshni for ground state

r (A°)	Varshni potential	Extended Rydberg potential
1.2	15222.55	15143.35
1.3	13765.8	14343.8
1.4	12420.33	12322.54
1.5	10732.56	10655.78
1.6	9150.66	9100.32
1.7	7432.77	7323.82
1.8	5714.34	5634.32
1.9	4150.22	4111.83
2	2498.12	2343.44
2.1	1176.35	1155.44
2.2	3517	3437
2.29	0	0
2.3	1.1722	1.1632
2.4	530.43	528.44
2.5	2322.32	2300.72
2.6	5811.51	5800.21
2.7	11811.54	11801.21

The Extended Rydberg potential is similar to behavior results of varshni potential with simple different.

4. Conclusions

Dissociation energies of AlBr molecule have calculated for ground $X^1\Sigma^+$ state and showed that bond length (r) has an effect upon the values of the dissociation energies, where the dissociation happen when (r) approach from infinity values, that meaning near from experimental values. The potentials of AlBr molecule by using Varshni function and Extended Rydberg function for ground $X^1\Sigma^+$ state are in good agreement with experimental results and the important notice that bond length (r) with spectroscopic constants have an effect upon values of the potential.

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