Potential Energy Curves and Dissociation Energy for ($X^1\Sigma^+$- $A^1\Sigma^+$) of $Cu^{63}H^1$Molecule Using Varshni Potential and Extended Rydberg Potential Functions

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Abstract: ***The present work concerns by study of spectroscopic properties for Copper HydrideCu^{63}H^1. Dissociation energy had been calculated theoretically for ground state $X^1\Sigma^+$ and excited state $A^1\Sigma^+$ of Cu^{63}H^1 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 Cu^{63}H^1 molecule for ground state $X^1\Sigma^+$ and excited state $A^1\Sigma^+$converge with experimental results, and the dissociation happen when (r) approach from (∞).***

Keyword: Varshni and Extended Potentialfunction, dissociation energy, ($X^1\Sigma^+$ - $A^1\Sigma^+$) of Cu^{63}H^1 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 Section

Dissociation Energy

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]:

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

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]:

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

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

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

Varshni function and Extended Rydberg Potential function

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]:

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

x=r-re

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

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:

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

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

$f_2 = 4\pi^2\mu\,\omega_e^{\,2}c^2$,

$$f_3=-\left(\frac{3f_2}{r_e}\right)\left[1+\left(\frac{\alpha_e\omega_e}{6B_e}\right)^2\right]$$

$$f_4=-\left(\frac{f_3}{r_e}\right)^2\left(15\left[1+\left(\frac{\alpha_e\omega_e}{6B_e{}^2}\right)\right]-\left(\frac{8\omega_e x_e}{B_e}\right)\right)$$

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

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

3. Results and Discussion

Spectroscopic properties of $Cu^{63}H^1$ molecule are studied such as potential curves for two functions began with potential Varshni function for ground $X^1\Sigma^+$ state and excited state $A^1\Sigma^+$ (eq. 4) compared with other function "Extended Rydberg potential function" for ground $X^1\Sigma^+$ state and exited state $A^1\Sigma^+$ (eq. 6) then dissociation energy is obtained using (eq.3) compared with another energy.

Table 1: The spectroscopic constants for$Cu^{63}H^1$molecule measured (cm^{-1})[7].

Spectroscopic constant	$X^1\Sigma^+$	$A^1\Sigma^+$
T_e	0	22503
ω_e	1952	1744
$\omega_e x_e$	35	32.8
B_e	7.9	6.9

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 (27216.457 cm^{-1}) and (23182.439 cm^{-1}) for $X^1\Sigma^+$ and $A^1\Sigma^+$ respectively, 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 values ofV.M.Rao et al. [8] and C.M. Marian[9] .

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

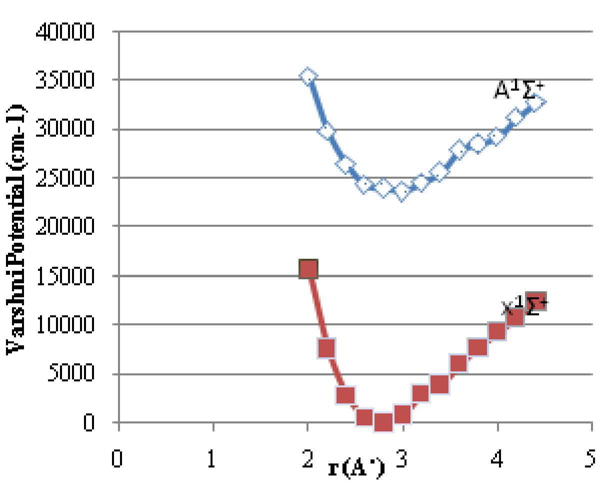
State	D_e (cm^{-1})	D_e(cm^{-1})
$X^1\Sigma^+$	27216.457	26720 [8]
$A^1\Sigma^+$	23182.439	22800 [9]

Result of Varshni Potential Function

To calculate Varshni potential for $Cu^{63}H^1$ molecule (eq. 4) is used for the ground state $X^1\Sigma^+$ and the excited state $A^1\Sigma^+$, and here are the results in table (3) and figure (1). The calculations appear the maximum value of varshni potential is at (r = 2 A°) that mean the minimum value of bond length give us maximum potential in ground state of $Cu^{63}H^1$ molecule. At bond length (r = 2.8 A°), the potential equal (34), 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. That behavior of potential is similar to behavior the excited state $A^1\Sigma^+$ ofthis molecule.

Table 3: Varshnifunction for ground state $X^1\Sigma^+$ and exited state $A^1\Sigma^+$

r (A°)	$X^1\Sigma^+$ $U_{Varsh}(x)$ cm^{-1}	$A^1\Sigma^+$ U_{Varsh} (x) cm^{-1}
2	30545	35477
2.2	15656	29865
2.4	5633	26434
2.6	1120	24333
2.8	34	24001
3	1132	23752
3.2	3622	24553
3.4	5396	25651
3.6	9133	27907
3.8	11272	28553
4	12344	29313
4.2	16222	31244
4.4	18511	32775



Fifure 1: Calculated Varshni Potential Curves for X1Σ+ and A1Σ+

Results of Extended Rydberg Potential Function

To calculate Extended Rydberg potential for $Cu^{63}H^1$ molecule eq. (6) is used for the ground state $X^1\Sigma^+$and the excited state $A^1\Sigma^+$ by depending on dissociation energy, bond length, spectroscopic constants, and here are the results of Extended Rydberg potential for $Cu^{63}H^1$molecule for the ground state $X^1\Sigma^+$and the excited state $A^1\Sigma^+$ in table (4) and figure (2).

The calculations appear the maximum value of Extended Rydberg potential is (32422 cm^{-1}) in ground state of $Cu^{63}H^1$ molecule at (r = 2 A°) which is the minimum value of bond length. At bond length (r = 2.8 A°), the potential equal (37), 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 $X^1\Sigma^+$ and exited state $A^1\Sigma^+$

r (A°)	$X^1\Sigma^+$ $U_{Ext.}$(r) cm^{-1}	$A^1\Sigma^+$ $U_{Ext.}$ (r) cm^{-1}
2	32422	36519
2.2	16754	30723
2.4	6242	27319
2.6	1923	25121
2.8	37	25303
3	1734	23991
3.2	4100	25102
3.4	6121	26277
3.6	9928	28133
3.8	12111	29367
4	13276	30012
4.2	17553	32155
4.4	19263	33721

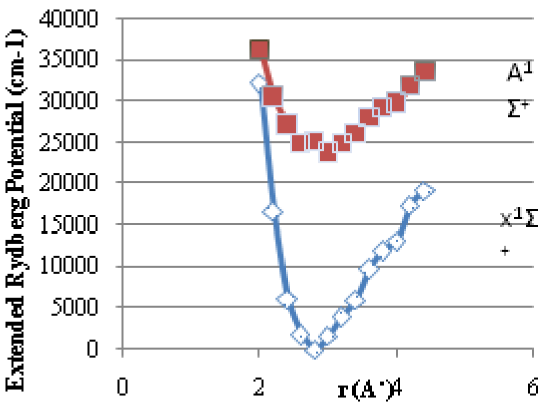
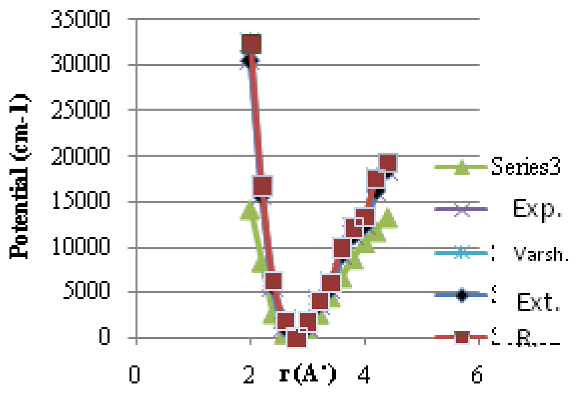


Figure 2: Calculated Extended Rydberg Potential Curves for X1Σ+ and A1Σ+

The $X^1\Sigma^+$ potential-curves from the Varshni and Extended Rydberg calculations are compared with the experimental curves as in table (5) and Fig. (3). Both of the theoretical curves are in quantitative agreement with experiment. The Varshni and Extended Rydberg potential curves for the $A^1\Sigma^+$state are compared with the corresponding experimental curve in table (6) and Fig. (4). As can be seen, the computed and experimental shape are in general agreement. Therefore behavior results of Extended Rydberg potential is similar to behavior results of varshni potential with simple different but the results are in good agreement with experimental values.

Table 5: Comparing Extended Rydberg function and Varshni and experimental for ground state $X^1\Sigma^+$

r (A°)	Varshni potential	Extended Rydberg potential	Experimental potential [9]
2	30545	32422	14228
2.2	15656	16754	8432
2.4	5633	6242	2744
2.6	1120	1923	480
2.8	34	37	162
3	1132	1734	1057
3.2	3622	4100	2660
3.4	5396	6121	4540
3.6	9133	9928	6732
3.8	11272	12111	8768
4	12344	13276	10549
4.2	16222	17553	11786
4.4	18511	19263	13339



Fifure 3: Extended Rydberg Potential and Varshni potential Curves with Experimental curve for X1Σ+

Table 6: Comparison Extended Rydberg function and Varshni and experimental forexited state $A^1\Sigma^+$

r (A°)	Varshni potential	Extended Rydberg potential	Experimental potential [9]
2	35477	36519	40765
2.2	29865	30723	38059
2.4	26434	27319	29572
2.6	24333	25121	25537
2.8	24001	25303	24018
3	23752	23991	23842
3.2	24553	25102	24484
3.4	25651	26277	25763
3.6	27907	28133	27329
3.8	28553	29367	28397
4	29313	30012	29820
4.2	31244	32155	31398
4.4	32775	33721	32385

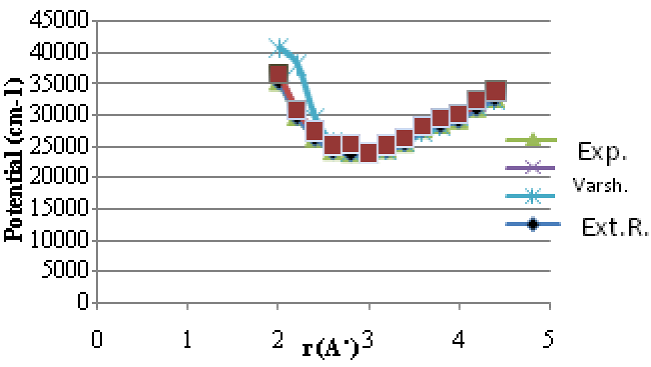


Figure 4: Extended Rydberg Potential and Varshni Potential Curves with Experimental curve for A1Σ+

4. Conclusions

Dissociation energies of $Cu^{63}H^{1}$ molecule have calculated for ground $X^{1}\Sigma^{+}$ state and exited state $A^{1}\Sigma^{+}$ 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 $Cu^{63}H^{1}$ molecule by using Varshni function and Extended Rydberg function for ground $X^{1}\Sigma^{+}$ state and exited state $A^{1}\Sigma^{+}$ 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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