STUDYING OF THE POTENTIAL CURVES OF GROUND STATE OF DIATOMIC MOLECULE USING TWO FUNCTIONS

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Abstract:

Diatomic molecules have been studied theoretically for ground state $X^2\Pi$ of (CH,CO,LuF,HBr) free radicals . It had been constructed dissociation energy using potential curves for the ground state by using Morse and Varshini functions to calculate potential curve for each molecule; compared between the results and experimental values had obtained. The results have good agreement with experimental results. Finding that Varshini function approximate with experimental values more than Morse function does.

Keyword: *Diatomic, Morse function, Varshini function, potential curve.*

Introduction:

A free radical is a molecule with a high degree of chemical reactivity due to the presence of an unpaired electron [Dasch] (2002). Most radicals are so reactive that they normally only exist in extremely dilute solutions. However, the presence and nature of even these reactive radicals can frequently be detected by the magnetic properties due to the odd electron [Pryor] (1966). Molecules are most stable in the ground state. A free radical is easily formed when a covalent bond between entities is broken and one electron remains with each newly formed atom [Karlsson] (1997). Free radicals have a very short half-life, which makes them very hard to measure in the laboratory. Multiple methods of measurement are available today, each with their own benefits and limits. Radicals can be measured using electron spin resonance (ESR) and spin trapping methods [Karlsson] (1997). Once activated it generates molecules known as free radicals, which destroy the unwanted tissue and leave the surrounding tissue undamaged [Bijlefeld & Burke] (2003). It is well known that the Morse potential model describes very well the vibrations of diatomic molecules. This is because such systems can be modeled by two positive charges (the two atomic nuclei) that produce the Coulomb potential in which the electronic cloud moves. The Morse potential is an element in the class of potentials for which an analytic solution of the Schrodinger equation exists for zero angular momentum [Nasser] (2008). The important of studying potential curves is to know the values of energy can the molecule stand before it dissociate.

Theoretical Part

Potential functions:

There are many functions for potential curve of diatomic molecules such as:

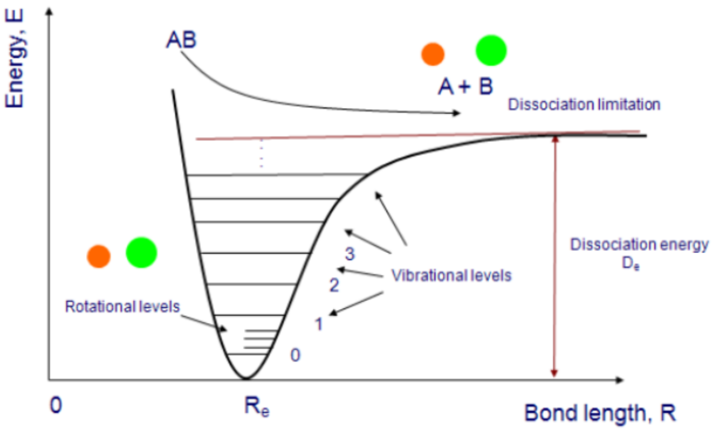

Fig. (1): Shows the Potential energy [P.E.] surface for a diatomic molecule [Long] (2010). * When (R=r)

1-Morse function:

Morse function is a simple form of a potential, which represents the potential energy of a diatomic molecule more realistically for larger interatomic separations, is due to Morse and is given by [Kumrarn & Rajamanickam] (2002):

$$U(x) = D_e(1 - e^{-\beta x})^2 \quad (1)$$

For small deviations x= r-r_e(where r is the bond length) from the equilibrium intermolecular distance is a popular choice of a simple analytic form for the potential [Passarinho & da Silva] (2006).

D_e is the dissociation energy; it's the energy that would be necessary to dissociate the molecule if it could be at the minimum of the potential curve [Herzberg] (1950).

r_e is the equilibrium bond constant. For instance, r_e is determined from the rotational constant and given in equation (2) [Hayes et al,] (1998):

$$r_e = \sqrt{\frac{h}{8\pi^2 B_e \mu c}} \quad (2)$$

When:

h is Planck's constant.

B_e is the rotation constant equilibrium bond constant.

μ is the reduced mass of the two nuclei.

C is the speed of light.

β is empirically chosen constant for the molecule in equation, it represents the value of bending of potential curve for each electronic state of molecule under investigation, and is given by the following relation [Hanna] (1969):

$$\beta = \left[\frac{8\pi^2 \mu(\omega_e \chi_e)c}{h}\right]^{1/2} \quad (3)$$

Where

$\omega_e\chi_e$ is a harmonic constant.

h is Planck's constant.

C is the speed of light.

μ is the reduced mass of the two nuclei.

2-Varshini function:

The other function of potential is Varshini function. It differs from Morse function by term r/re so the function had written as [Saleh] (2013):

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

Where β is given in equation (3)

Results and Discussions:

Potential curves are studied for diatomic that molecules have ground state of twoMorse potentialfunction and Varshni potential function graphic and calculate by using Microsoft office excel.

The spectroscopic constants for the molecules is given by table (1)

Table (1): The spectroscopic constants:

Spectroscopic constant(cm^{-1})	CH (15)	CO (15)	LuF (14)	HBr (15)
$Y_{10} \approx \omega_e$	2860.7508	2170.21	1904.03	2649.67
$Y_{20} \approx -w_e x_e$	-64.4387	13.461	13.97	45.21
$Y_{01} \approx B_e$	14.45988	1.9314	1.7046	8.473
r_e (Å)	1.12336	1.20558	1.188	1.4188

- *Y_{10} ,Y_{20} ,Y_{01} are representing to Dunham coefficients.*

To calculate Morse potential gives in equation (1) and Varshni potential gives in equation(3) for CH molecule are calculated and the results given in table (2):

Table (2): Morse and Varshni functions potential for ground stat $X^2\Pi$ of CH Free radical molecule:

r (cm)	Morse Potential (cm^{-1})	Varshni Potential (cm^{-1})
6.00E-09	1.10E+05	7.32E+03
8.00E-09	2.95E+04	4.01E+03
8.88E-09	1.40E+04	2.40E+03
9.73E-09	5.55E+03	1.15E+03
1.01E-08	3.09E+03	7.00E+02
1.20E-08	1.75E+02	5.44E+01
1.40E-08	4.21E+03	1.71E+03
1.60E-08	1.01E+04	5.01E+03
1.80E-08	1.56E+04	9.07E+03
2.00E-08	2.00E+04	1.32E+04
2.20E-08	2.34E+04	1.70E+04
2.40E-08	2.59E+04	2.03E+04
2.60E-08	2.77E+04	2.30E+04
2.80E-08	2.89E+04	2.51E+04
3.00E-08	2.98E+04	2.68E+04
3.20E-08	3.04E+04	2.81E+04
3.40E-08	3.08E+04	2.90E+04
3.60E-08	3.11E+04	2.98E+04
3.80E-08	3.13E+04	3.03E+04
4.00E-08	3.14E+04	3.07E+04

Figure (2) shows Morse and Varshni potential curve in ground state X $^2\Pi$ of CH radical

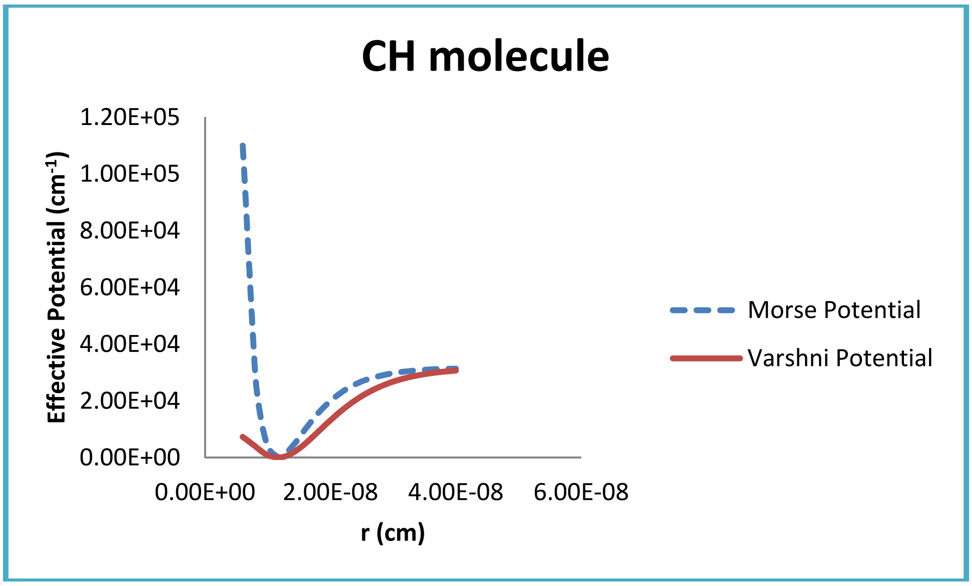

Fig.(2): Morse and Varshni potential curve in ground state X $^2\Pi$ of CH radical.

To calculate Morse potential gives in equation (1) and Varshni potential gives in equation (3) of CO molecule are calculated and the results given in table (3):

Table (3): Morse and Varshni functions potential for ground stats of CO Free radical molecule:

r(cm)	Morse Potential (cm^{-1})	Varshni Potential (cm^{-1})
6.00E-09	6.69E+05	5.06E+04
8.00E-09	1.79E+05	2.32E+04
8.88E-09	8.83E+04	1.31E+04
9.73E-09	3.85E+04	5.98E+03
1.01E-08	2.36E+04	3.54E+03
1.20E-08	1.32E+01	2.51E+02
1.40E-08	1.05E+04	7.22E+03
1.60E-08	2.93E+04	1.97E+04
1.80E-08	4.63E+04	3.35E+04
2.00E-08	5.95E+04	4.62E+04
2.20E-08	6.88E+04	5.68E+04
2.40E-08	7.51E+04	6.52E+04
2.60E-08	7.94E+04	7.15E+04
2.80E-08	8.22E+04	7.62E+04
3.00E-08	8.41E+04	7.96E+04
3.20E-08	8.53E+04	8.20E+04
3.40E-08	8.60E+04	8.37E+04
3.60E-08	8.65E+04	8.49E+04
3.80E-08	8.69E+04	8.57E+04
4.00E-08	8.71E+04	8.63E+04

Figure (3) Shows Morse and Varshni potential curve in ground state X $^2\Pi$ CO radical:

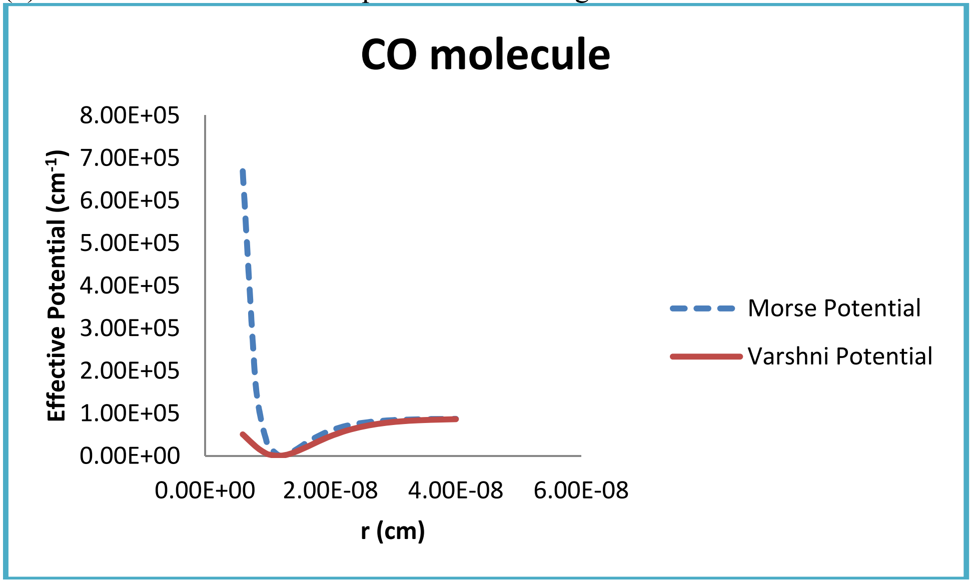

Fig.(3): Morse and Varshni potential curve in ground state X $^2\Pi$ CO radical.

To calculate Morse potential gives in equation (1) and Varshni potential gives in equation (3) of LuF molecule are calculated and the results given in table (4):

Tabel(4): Morse and Varshni functions potential for ground stats of LuF Free radical molecule :

r (cm)	Morse Potential (cm^{-1})	Varshni Potential (cm^{-1})
6.00E-09	6.34E+05	6.37E+04
8.00E-09	1.55E+05	2.65E+04
8.88E-09	7.30E+04	1.45E+04
9.73E-09	2.99E+04	6.39E+03
1.01E-08	1.75E+04	3.74E+03
1.20E-08	5.20E+01	2.50E+02
1.40E-08	1.04E+04	6.82E+03
1.60E-08	2.57E+04	1.77E+04
1.80E-08	3.86E+04	2.90E+04
2.00E-08	4.78E+04	3.87E+04
2.20E-08	5.40E+04	4.64E+04
2.40E-08	5.81E+04	5.21E+04
2.60E-08	6.06E+04	5.62E+04
2.80E-08	6.22E+04	5.90E+04
3.00E-08	6.32E+04	6.10E+04
3.20E-08	6.39E+04	6.23E+04
3.40E-08	6.42E+04	6.32E+04
3.60E-08	6.45E+04	6.38E+04
3.80E-08	6.46E+04	6.41E+04
4.00E-08	6.47E+04	6.44E+04

Figure (4) Shows Morse and Varshni potential curve in ground state X $^2\Pi$ LuF radical:

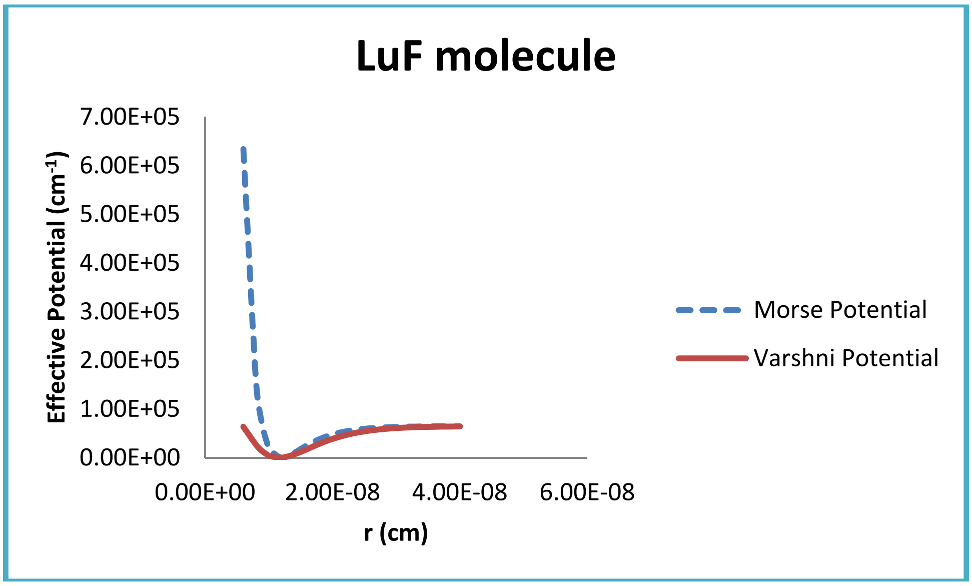

Fig.(4): Morse and Varshni potential curve in ground state X $^2\Pi$ LuF radical.

To calculate Morse potential gives in equation (1) and Varshni potential gives in equation (3) of HBr molecule are calculated and the results given in table (5):

Table (5): Morse and Varshni functions potential for ground stats of HBr Free radical molecule:

r (cm)	Morse Potential (cm^{-1})	Varshni Potential (cm^{-1})
6.00E-09	8.56E+04	7.78E+03
8.00E-09	2.45E+04	4.08E+03
8.88E-09	1.19E+04	2.41E+03
9.73E-09	4.85E+03	1.14E+03
1.01E-08	2.73E+03	6.91E+02
1.20E-08	1.62E+02	5.26E+01
1.42E-08	4.62E+03	1.86E+03
1.60E-08	1.02E+04	4.67E+03
1.80E-08	1.63E+04	8.34E+03
2.00E-08	2.16E+04	1.20E+04
2.20E-08	2.59E+04	1.53E+04
2.40E-08	2.92E+04	1.81E+04
2.60E-08	3.17E+04	2.03E+04
2.80E-08	3.36E+04	2.21E+04
3.00E-08	3.50E+04	2.34E+04
3.20E-08	3.61E+04	2.45E+04
3.40E-08	3.68E+04	2.52E+04
3.60E-08	3.74E+04	2.58E+04
3.80E-08	3.78E+04	2.62E+04
4.00E-08	3.81E+04	2.65E+04

Figure (5) Shows Morse and Varshni potential curve in ground stateX $^2\Pi$ HBr radical:

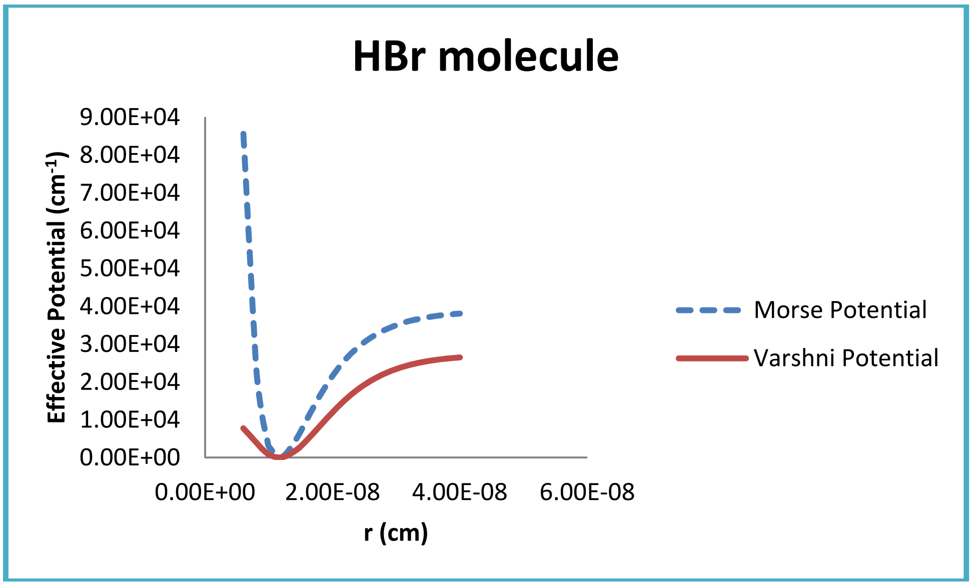

Fig.(5): Morse and Varshni potential curve in ground state X $^2\Pi$ HBr radical.

Dissociation energy:

The dissociation energy calculated graphically from potential figures compared with experimental values.

Table (6): comparing between the results from graphs with the experimental value.

D_e (cm^{-1})	CH	CO	LuF	HBr
Morse	$3.14*10^4$	$8.71*10^4$	$6.47*10^4$	$3.81*10^4$
Varshni	$3.07*10^4$	$8.63*10^4$	$6.49*10^4$	$2.65*10^4$
Exp. [M. H. Stans]	$2.792*10^4$	$8.945*10^4$	$4.76*10^4$	$2.96*10^4$

Conclusion:

The potentials of these molecules by using Morse and Varshni functions are in agreement with experimental results and the useful of Varshni function is as approximated value. The curves calculated by Varshni function have accurate values more than curves calculated by Morse function because of the term (r/r_e) that added to the function at both results of Potential curve and dissociation energy.

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کورتی:

هەردوو تەنولکێن گەڕدیلەیی هاتنە شلۆڤەکرن ب شێوەکی تیوری دشێوێ ئاستێ ووزا بنچینەی دابو تەنولکێن (x^2 π) بنچینەی یێن سەربەست (CH, Co, LuF, HBr). هەروەکی مە هژمارتی ووزا ژێکڤەبوونێ ب رێکا وێنەکرنا شیانێن ئەلکترونا د ئاستێ بنچینەی دا ب رێکا کارئینانا هەردوو نەخشەیێن مورس و فارشنی بۆ شیانان، ئەنجام نێزیك بوون دگەڵ ئەنجامێن پڕاکتیکی، و بەراوردکرنا دناڤبەرا هەردوو نەخشان دا و دگەڵ ئەنجامێن هژمارتی یێن بەرێ هنگێ بۆمە دەرکەفتین دیارکر نەخشێ فارشنی پتر نێزیکی ئەنجامێن پڕاکتیکی بو ژ یێ مورسی.

الخلاصة:

تمت دراسة منحنى الجهد نظريا لجزيئات ثنائية الذرة للحالة$X^2\Pi$ الارضيةللجزيئات (**CH**, **CO**, **LuF**, **HBr**) جذور حرة . حيث تم حساب طاقة التفكك من خلال منحنيات الجهد للحالة الالكترونية الارضية باستخدام دالتي مورس وفارشني للجهد. وكانت النتائج قريبة من النتائج العملية. وبالمقارنة بين الدالتين والنتائج المحسوبة سابقا وجد ان دالة فارشني تقارب النتائج العملية اكثر من دالة مورس .