

Vibrational Spectroscopy

Elixir Vib. Spec. 90 (2016) 37531-37533

Elixir
ISSN: 2229-712X

Potential Energy Curves for (HCl) Molecule by using Two Different Functions

Adil N.Ayyash¹, Ahmed N. Ayyash² and Ilham K.Onees³

¹Department of Physics, College of Science, University of Anbar, Anbar, Iraq.

²Department of Chemistry, Ministry of Science and Technology, Baghdad, Iraq.

³Department of Communication, Hawler Institute of Technology, Hawler, Iraq.

ARTICLE INFO

Article history:

Received: 3 December 2015;

Received in revised form:

2 January 2016;

Accepted: 7 January 2016;

Keywords

HCl Molecule,

Potential Energy Function.

ABSTRACT

This study has been carried out of calculating potential energy curves (Deng-Fan potential and Varshni potential) of ground state of diatomic molecule (HCl). Potential energy curves depended on spectroscopic Parameters (ω_e , $\omega_e x_e$, r_e , α , μ , β , D_e) and our results have been compared with experimental results.

© 2016 Elixir All rights reserved.

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 curves are necessary. The empirical potential energy functions like Varshni [2] and Deng-Fan potential [3] are usually applied and the potential energy curves 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.

Theory

Potential Energy Functions

The height of an asymptote of a potential energy curve, above the lowest vibrational level, is equal to the work that must be done in order to dissociate that molecule, and is known as the heat of dissociation or dissociation energy D_0 . Another constant D_e is also the dissociation energy but it is taken as a height of an asymptote from x-axis or measured from minima of the potential energy curve. The relation between D_0 and D_e is here [12]

$$D_e = D_0 + G(0) \quad (1)$$

where

$$G(0) = \omega_e/2 - \omega_e x_e/4 + \omega_e y_e/8 + \dots \quad (2)$$

$$D_e = \Delta G_{\max}(v) \quad (3)$$

The relation in defining the dissociation energy D_e in terms of molecular constants is

$$D_e = \omega_e^2 / 4 \omega_e x_e \quad (4)$$

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 [13]:

$$U(x) = D_e \left(1 - \frac{r}{r_e} e^{-\beta x} \right)^2 \quad (5)$$

$$x = r - r_e$$

$$\beta = \left[\frac{8\pi^2 \mu (\omega_e x_e) c}{h} \right]^{1/2} \quad (6)$$

where β , r_e and D_e have the same physical significant as in the Morse potential function and $\omega_e x_e$: the anharmonicity constant, μ : reduced mass, c : speed of light and h : plank constant.

On the other hand, another function of potential called Deng-Fan potential function has the form [3]:

$$U_{Deng-Fan}(r) = P_1 + \frac{P_2}{e^{\alpha r} - 1} + \frac{P_3}{(e^{\alpha r} - 1)^2} \quad (7)$$

$$P_1 = D_e$$

$$P_2 = -2D_e (e^{\alpha r_e} - 1)$$

$$P_3 = D_e (e^{\alpha r_e} - 1)^2$$

α : spectroscopic parameter.

Results and discussion

In the present work, the spectroscopic parameters for diatomic molecule (HCl) are summarized in table 1 [14,15], dissociation energy is obtained using (eq.4) compared with another energy. And potential energy curves for two functions began with Varshni potential function for ground state (eq. 13) and other function "Deng-Fan potential function" for ground state (eq. 14).

The D_e value of HCl molecule is found to be (37349.23 cm^{-1}) for ground state, that dissociation due to approaching the bond length (r) from infinity values, where this is one of three conditions of potential curve. This result is in good agreement with the experimental value [16] as in table below.

Tele:

E-mail addresses: adil_nameh78@yahoo.com

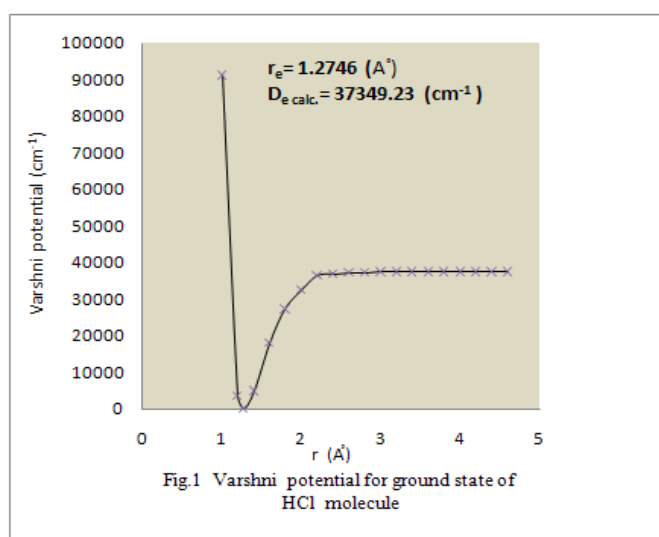
Table 1. Spectroscopic parameters of ground state of HCl molecule measured in (cm^{-1}) and r_e in (Å°) [14,15]

| Parameter | Value |
|---------------------------------|---------|
| ω_e | 3131.35 |
| $\omega_e x_e$ | 65.61 |
| r_e | 1.2746 |
| B_e | 10.95 |
| α | 2.3805 |
| $\mu(\text{g}) \times 10^{-23}$ | 0.9808 |

Table 2. Dissociation energy of ground state of HCl molecules measured in (cm^{-1})

| Result | Value |
|------------|----------|
| calc. | 37349.23 |
| expt. [16] | 36300.00 |

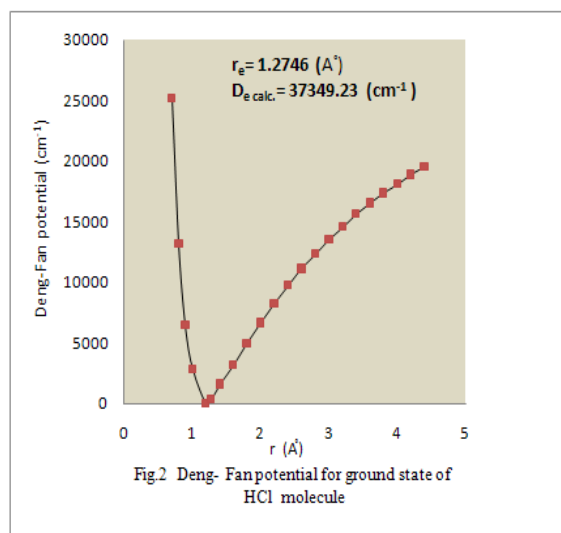
This theoretical value are agreement with experimental result. In calculating Varshni potential for this molecule (eq. 5) is used for the ground state, and here are the results as figure (1).



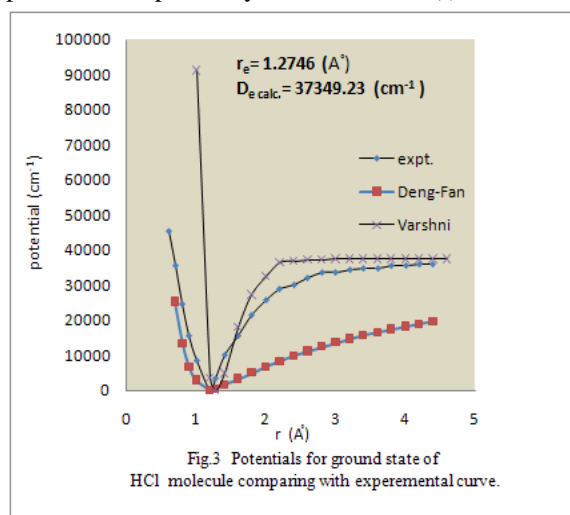
The calculations of HCl molecule appeared the maximum value of varshni potential is at ($r = 1 \text{ Å}$) that mean the minimum value of bond length give us maximum potential in ground state of this molecule. At bond length ($r = 1.2746 \text{ Å}$), the potential equal (zero), then the potential increase 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.

To calculate Deng-Fan potential for HCl molecule eq. (7) is used for the ground state by depending on dissociation energy, bond length, spectroscopic constants in table 1, and here are the results of Deng-Fan potential for this molecule in figure (2).

The calculations of HCl molecule appeared the maximum value of Deng-Fan potential is at ($r = 0.7 \text{ Å}$) that mean there are difference in the behavior of this curve comparing with Varshni potential for this molecule at small value of (r). At bond length ($r = r_e$), the potential equal (zero), the dissociation happen after that because the diatomic molecule dissociate when the value of (r) increase to determinate limit.



Behavior of potential curve of HCl molecule is different rather than behavior of curve in Varshni potential that is due to form and parameters of each suggested function. At the end all results for two functions compared with experimental result [16] as shown in figure (3), and behavior of curve in Varshni potential was close to experimental curve than Deng-Fan potential except in very small values of (r).



Conclusions

The potential of HCl molecule by using Varshni function for ground state is agreement with experimental results which is best than Deng-Fan potential curve and the important notice that bond length (r) with spectroscopic constants have an effect upon values of the potential. In general all values of potentials in beginning be high and decrease with increasing bond length and after ($r=r_e$) be increasing in the values with increasing values of (r). Dissociation energies for this molecule for ground state very convergence with experimental dissociation energies.

References

- [1] G. Herzberg, Spectra of diatomic molecules, Van National Reinhold Company. New York, (1950).
- [2] T. Cheng L J. Serb. Chem. Soc.V. 74, No.12, P.1423–1428, (2009).
- [3] Z. H., Deng Y P Fan, Shandong Univ. J. 7 (1957) 162.
- [4] L.Ian Cooper and S. Alan Dickinson, Journal of Chemical Physics, 13120. (2009).
- [5] C.Housecroft and A.G. Sharpe "Inorganic Chemistry" (Pearson Prentice Hall, 2nd ed., p. 170. (2005).

- [6] S. Mclain,;C. Benmore, J. Urquidi,. *Ang. Chem., Int. Edition* 43 (15), 52–55, (2004).
- [7] W. Heitler,; London, *F. Z. Phys.*, 44, 455. (1927).
- [8] Y. Varshni, *Rev. Mod. Phys.* 29, 664 (1957); 31.839 (1959).
- [9] G.VanHooydonk, *Z. Naturforsch. Z. Naturforsch.* 37a, 710 (1982).
- [10] F. J Zeng, R F Linghu and M J. Yang Kaili University 27 28. (2009).
- [11] P. Usha proc. Indian natn. Sci. Acad., 47, A, No. 2, , pp. 248-252. (1981).
- [12]A.Schadee, *J. Quan. Spectrosc.Radiat.Transf.*, 5, pp.233-239, (1978).
- [13]L. Teik-Cheng, *J. Serb. Chem. Soc.V.* 74, No.12, P.1423–1428, (2009).
- [14]Z-Niu, S-Heng,, Z-Ping, Z-L`ue and S-Feng, *Chin. Phys. B* Vol. 19, No. 5 (2010).
- [15]I. Nasser, Abdelmonem MS, Bahlouli H, Alhaidari AD. *J Phys B*;40:4245. (2007).
- [16] G. Barrow, *Introduction to molecular spectroscopy*, McGraw-Hill, book company, Inc. New York, (1962).