Rotation Effect in Morse Potential For K_2 Molecule

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Abstract:

The rotation effect upon Morse potential had been studied and the values of the effective potential in potential curves had been calculated for electronic states ($X^2\Sigma^+_g$, B Π_u) K_2 molecule. The calculation had been computed for rotational quantum number (J = 5). Also, drawing potential curves for these systems had been done using Herzberg and Gaydon equations .It was found that the values of the dissociation energy which resulting from using Herzberg equation greater than that of Gaydon equation. Besides, it was found that the rotation effect for (X and B) electronic states in Morse potential is very small and in this case may negligible.

Key words: Morse Potential, Dissociation energy.

Introduction:

 The absorption or emission of electromagnetic radiation in visible and UV regions resulted from the transition between the electronic energy levels of the molecules. The spectra of diatomic molecules contain a large numbers of spectral lines. This complexity in the spectrum is due to containing fine structures of vibrational and rotational transitions [1-2].

Various investigations have been performed to study the "diffuse bands "in the visible alkali spectra [3]. In the case of potassium they occur in low power discharges, in optically excited vapors, in absorption measurements and in potassium rare gas mixtures [4]. Similar results are established with sodium as well. Recently a measurement of the diffuse bands for sodium and potassium with a lifetime analysis of the excited state has been given [5-6]. In all emission experiments the peak of the potassium diffuse band is located at about 572.5 nm [7-8]. It is well separated from other features of the visible spectrum, lying in between the B-X and the C-X molecular band systems [9]. The emission of the diffuse band has been identified to stem from the $2^3\Pi_g$ to $1^3\Sigma^+_u$ transition. This has been further substantiated in recent potential calculations by Konowalow and co-workers [10]. Their results have been used to calculate the absorption profile of the K_2 diffuse band, showing good agreement with the experiment.

Theory

The total energy for molecule is[1]:

$$E_T = E_e + E_{vib} + E_{rot} \qquad (1)$$

where E_e is the electronic energy, E_{vib} is the vibrational energy, E_{rot} is the rotational energy.

$$E_e > E_{vib} > E_{rot}$$

The value of energy for the electronic state depending upon the upon the internuclear distance (r) (bond length), because the potential is a function of the distance between two atoms of this

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molecule according to a different electronic transitions. The Morse potential functions V_m, which almost verify an experimental potential curve used in work [11]:

$$V_m(r) = D_e\left[1 - e^{-\beta(r-re)}\right]^2 \qquad (2)$$

where r is the distance between the atom, r_e is the equilibrium bond distance defined by the following relation:

$$r_e = \sqrt{\frac{h}{8\pi^2 B\mu c}} \qquad (3)$$

μ is reduced mass of molecule, c is the velocity of light in vacuum and h is Planck constant.

$$\mu = \frac{m1\,m2}{m1+m2} \cdot \frac{1}{Av} \qquad$$

where Av is Avogadro number, ß is a constant for each electronic state of molecule under investigation, and it represents the value of bending profile of potential curve

$$\beta = \left[\frac{8\pi^2 \mu(\omega e\chi e)c}{h}\right]^{\frac{1}{2}} \qquad (4)$$

where D_e is a spectral dissociation energy of diatomic molecule, a brief account for procedure being used for the calculation of dissociation energy of diatomic molecule which given by the following relation [1]:

$$D_e = \frac{\omega e^2}{4\,\omega e\chi e} \qquad (5)$$

where ωe is the harmonicity constant and $\omega e\chi e$ is the anharmonicity constant.

The relation is to be compared with the dissociation energy given Gaydon[11]:

$$D_e = \frac{\omega e^2}{5\omega e\chi e - 2B} \qquad (6)$$

where B is the rotation constant of each electronic state of the molecule.

Rotation effect

As a result for a failure of Born-Oppenhiemer approximation [1] in the excited states (such as in vibronic transition), so the rotational transitions magnitudes through the electronic transition will effect upon the potential (eq. 2) and will be:

$$V_{effective} = V_m + V_{rot} \qquad (7)$$

$$V_{rot} = \frac{h}{8\pi^2 \mu r^2 c} J(J+1) \qquad (8)$$

where J is the rotational quantum number.

In the present work, the spectroscopic constants are listed in Table 1:

Table (1) Spectral constants used for calculation [12].

Spectroscopic constant	$K_2 X \Sigma^+_g$	$K_2 B \Pi_u$
T_e	0	15378
ω_e (cm^{-1})	92.64	75
$\omega_e \chi_e$ (cm^{-1})	0.354	0.3876
r_e (cm)	3.923 x 10^{-8}	4.235 x 10^{-8}
B (cm^{-1})	0.05622	0.04824

Results and Discussion:

Figures (1) and (2) show the results of Herzberg and Gaydon equations calculations for Morse potential function and for the ground state $X \Sigma^+_g$ and the excited state $B \Pi_u$ of K_2 molecule. It was found that the values of the dissociation energy which resulting from using Herzberg equation greater than that of Gaydon equation because the bond length of the excited state greater than of the ground state .

Figure (3) and (4) show the results of Herzberg and Gaydon equations calculations in Morse potential and the rotational effect upon this potential by using (eq. 7) the values of D_e for the ground state of $X \Sigma^+_g$ and the excited state $B \Pi_u$ of K_2 molecule (J = 5). It

was found that the rotation effect for (X and B) electronic states upon Morse potential is very small and in this case may negligible.

Figure (5) and (6) show the results of the effective potential (eq. 7) by using the values of D_e of electronic state (X and B) of K_2 molecule with quantum number (J = 5). It was found that the effect potential by using the values of D_e of the ground state greater than the effective potential of the excited state of K_2 molecule with quantum number (J = 5).
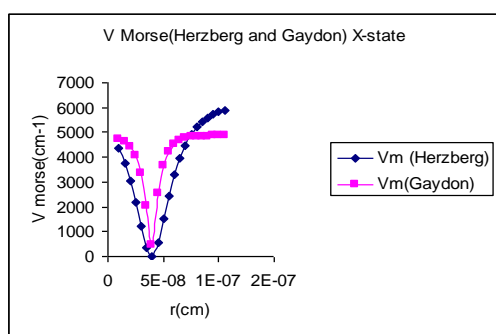

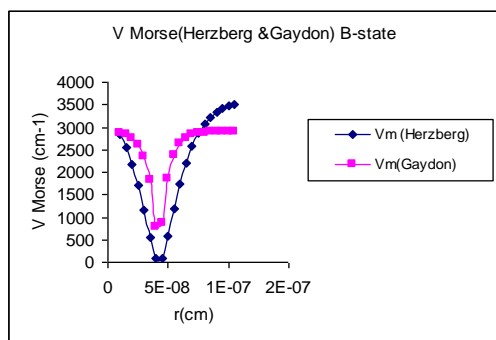**Fig (1) Morse potential in the ground state X Σ^+_g of K2 molecule**

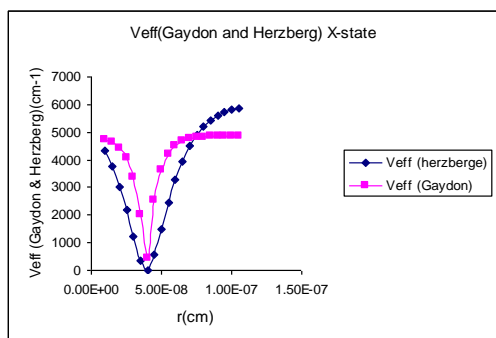**Fig (2) Morse potential in the excited state BΠ$_u$ of K2 molecule**

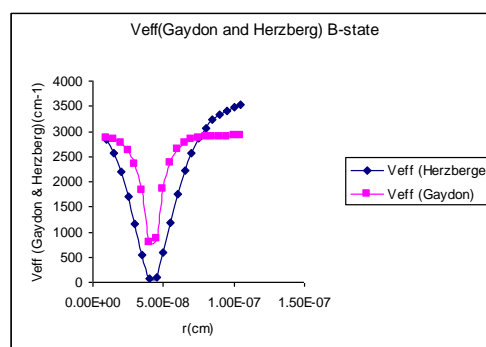**Fig (3) Effective potential in the ground state XΣ^+_g of K2 molecule (J=5)**

Fig (4) Effective potential in the excited state BΠ$_u$ of K2 molecule (J=5)
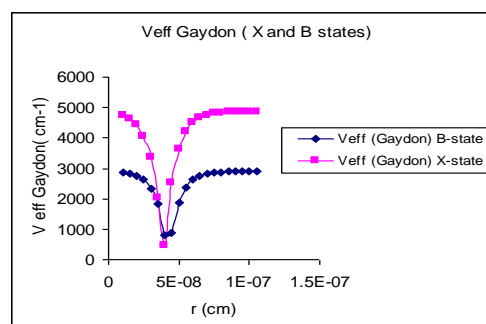

Fig (5) Effective potential using Herzberg equation in X and B states of K2 molecule (J=5)
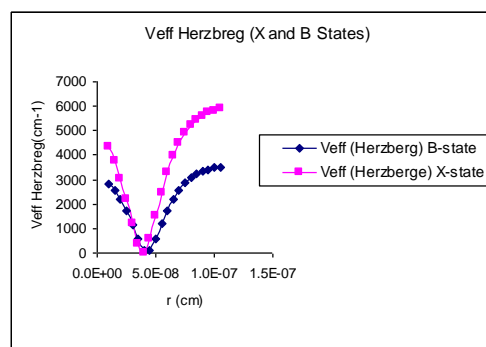

Fig (6) Effective potential using Gaydon equation in X and B states of K2 molecule (J=5)

References:

1. Graybeal J.D., 1988, Molecular Spectroscopy, McGraw–Hill Book Company.
2. John M. Brown and Alan Carringtion, 2003, Rotational spectroscopy of diatomic molecules, Cambridge University press, UK.
3. Jose J. Torrent and Barron V., 2003, the visible diffuse reflectance

spectrum in relation to the color and crystal properties of hematite, Clay and Clay minerals, 51(3): 309-317.

4. Ligare M., Schaefer S., Huennekens J. and Happer W., 1983, Infrared spectroscopy of dense potassium vapor jet, Oat .Commun. 48 :39 – 43.

5. Klyavinsh P. and Janson M.L, 1982, observation and interpretation of the Li_2 diffuse band in the region of 420 nm, Opt. Spectry . 52: 630.

6. Kopystynska A. and Kowalczyk P., 1978, Detated temporal behavior of laser – excited sodium tracer in nitrogen and application to nitrogen number density measurement at low densities, Opt. Commun 25: 351.

7. Shvegzhda Zh.D., Papernov S.M. and Janson M.L., 1983, Fluorescence studies of the K_2 diffuse band at 572.5 nm, Chem. Phys. Letters 101: 187.

8. Ban T., Aumiler D., Beuc R and Pichler G., 2004, Rb_2 diffuse band emission excited by diode lasers, Eur. Phys. J.D.30(1): 57 – 64 .

9. Radzewicz Cz. Kowalczyk P. and Krasinski J., 1983, Continue in the visible absorption spectrum of K_2, Opt. Commun. 44: 139.

10. Konowalow D.D. and Fish J. L., 1984, double – minimum $2^1\Sigma_u^+$ state of Na_2, Chem. Phys, and 84: 463.

11. Wiley J. in New York, 2009, Dissociation energies and spectra of diatomic molecules, by Gaydon A. G., Bibliography, pp.: 220 – 229.

12. Sarvepreet kaur and Gahajan C.,2002, universal relation between spectroscopic constants, pramana-J. phys., 59(3):479-486.

دراسة التأثيرات الدورانية في جهد مورس لجزيئة K_2

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الخلاصة:

لقد تمت دراسة بعض الخواص الطيفية لجزيئة K_2 مثل التأثيرات الدورانية في جهد مورس بوصفها دالة لطول الآصرة وحساب قيمة الجهد المؤثر وللمستويات الالكترونية ($X^2\Sigma_g^+$, B Π_u) للعدد الكمي الدوراني ($J = 5$) , وكذلك حساب طاقة التفكك باستعمال معادلتي Herzberg و Gaydon واظهرت النتائج ان قيمتها باستعمال معادلة Herzberg اكبر من طاقة التفكك باستعمال معادلة Gaydon. لقد وجد ان تأثير الدوران للحالات الالكترونية (X و B) في دالة جهد مورس قليلة جدا بحيث يمكن اهمالها.