

Theoretical Measurements Of Effective Potential And Dissociation Energy Of Hydrogen Fluoride H^1f^{19} And H^2f^{19} Molecule

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Abstract: The rotation effect upon Morse potential had been studied and the values of the effective potential upon potential curves had been calculated for (X, B) systems of the Silver Hydrogen fluoride H^1F^{19} and H^2F^{19} for the electronic transition $B^1\Sigma^+ - X^1\Sigma^+$ systems for the rotational quantum number ($0 \leq J \leq 150$). Drawing potential curves for these systems had been done. It was found that the values of the rotation effective potential for electronic state $X^1\Sigma^+$ had larger values than that of electronic state $B^1\Sigma^+$. It is clear that the rotation effect agrees mathematically with theory of these spectra. It was found that that the values of dissociation energies of the electronic excited state B had larger values than that of ground electronic state X.

Keywords: effective potential, electronic transition, excited states dissociation energy, ground state.

1. 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 number of spectral lines. The nature of the rotational fine structure of electronic transition is largely dependent upon the levels or states involved in the transition. If the transition had happened from an excited electronic state to ground state, the effect of rotation and vibration had been taken into account. This complexity in the spectrum is due to containing fine structures of vibrational and rotational transitions [1]. The importance of diatomic molecules is due to their existence in nature and chemical processes, including combustions, reactions and atmospheric studies. These molecules are such as the CO molecule [2], LiC molecule [3], Hydrogen Chloride HCl [4] and Nitric Oxide NO [5-7], had been studied experimentally. Al-Amiedy et al [8]. Studies the values of the rotation effect upon the Morse potential for (A-X), (B-X) and (B-X) systems of OH, HCl and NO molecules for the rotational quantum number ($0 \leq J \leq 150$). It's clear that the rotation effect agrees mathematically with the theory of these spectra. It is obvious from the calculation that the values of the effective potential for B greater than that of X and A states. This is due to the increase of the electronic energy of the state of the molecule. This effect is related to the failure of Born-Oppenheimer for any transition (i.e. rotational, vibrational and electrons transitions). This effects causes also reduction in the energy needed to dissociate from any state of the molecule. While, Al-Amiedy et al [9] calculated the rotation effect upon Morse potential was studied and the values of the effective potential upon potential curves were calculated X, A, B systems the Na_2 molecule. This calculation has computed rotational quantum number ($0 < J < 150$). Drawing potential curves for these systems are reported. It is clear that the rotation effect agrees mathematically with theory of these spectra. Also, a calculation of the maximum quantum number of J_{max} for the X, A, B systems of this molecule. It is obvious from the calculation that the values of the effective potential for B greater than that of X and A states. This is due to the increase of the electronic energy of the state of the molecule. We

must have noticed that the temperature should be low to avoid any excitation which is not desirable (rotation or vibration) in order to have excellent experimental results. Whereas, Al-Amiedy et al [10] The effective potential had been studied and the values of the curves had been calculated for the X, A, B electronic systems of the CN free radical. This calculation had been computed for rotational quantum number $0 \leq J \leq 150$. Drawing potential curves for these systems had been done. It is clear that the rotation effect agrees mathematically with theory of these spectra. Beside, a calculation of the maximum quantum number of J_{max} for the X, A, B systems of this molecule. The results of the effective potential of the electronic transitions X, A and B of CN free radical, with rotational quantum number ($J=150$) at room temperature (300 K) showed that the value of effective potential for B state is greater than that of X and A states. This is due to the increase of the electronic energy of these states of the molecule. This effect refers to a failure of Born-Oppenheimer approximation for any transition, also this effect causes a reduction in the energy needed to dissociate from any state of the molecule. We must notice that the temperature should be low to avoid any previous excitation which is not desirable in order to have excellent experimental results. Whereas, Al-Amiedy et al [11] calculated the Morse and effective potential for $A^3\Sigma_g^- - X^3\Sigma_g^-$ systems of the molecule $^{11}B_2$, for the rotational quantum number $0 \leq J \leq 150$. It has been found that the values of the rotation effective potential have larger values than that of Morse potential. A calculation of the dissociation energies has been carried out for both ground and first excited states. It was found that that the dissociation energies of the electronic excited state A have larger values than that of ground electronic state X. This effect refers to a failure of Born-Oppenheimer approximation for any transition. This effect causes also a reduction in the energy needed to dissociate any state of the molecule. It is to be noticed that the temperature should be low to avoid any previous excitation which is not desirable in order to have an excellent experimental results. We observed that the values of dissociation energy for A states are larger than those for X states. In order to know the dissociation energy of the molecules, we have to know the effect of many parameters

such as environment; chemical, atmospheric parameters upon the dissociation, for that reason, the temperature would have less effect to damaging the bond. The dissociation energy plays a role in spectroscopic studies, one of these studied measuring the potential energy of the diatomic molecules (experimentally and theoretically) [12]. Morse potential, especially for vibrational transitions with a low vibrational quantum number gives values for potential energy similar to the harmonic model [13].

2. THEORY

The electronic state of the molecule is represented by a potential curve refers to a position and values of energy for this state depending upon the internuclear distance (bond length r), where the potential is a function of the distance between two atoms of this molecule according to a different electronic transition. The Morse potential function verifying an experimental potential curve used at work given by the following relation [13]:

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

Where D_e is a spectral dissociation energy which can called Herzberg relation be calculated from the relation [13]:

$$D_e = \frac{\omega e^2}{4\omega e \chi_e} \tag{2}$$

Where ωe is the harmonicity constant and $\omega e \chi_e$ is the anharmonicity constant. This relation is to be compared with the dissociation energy given by reference [15] namely Gaydon relation:

$$D_e = \frac{\omega e^2}{(5.33\omega e \chi_e - 2B)} \tag{3}$$

β is a constant for each electronic state of the molecule under investigation, and it represents the value of the bending profile of potential curve and given by [15]:

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

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

3. Rotation effect

As a result of a failure of Born-Oppenheimer 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 (1) and will be [13]:

$$V_{\text{effective}} = V_m + V_{\text{rot}} \tag{5}$$

$$V_{\text{rot}} = \frac{h}{8\pi^2 \mu r^2 c} J(J+1) \tag{6}$$

Where r is bond length and J is the rotational quantum number. The spectroscopic constants are given in Tables 1:

Table 1a: Spectral constants (cm^{-1}) used as input data for calculation for isotopic molecule H^1F^{19} [13,14].

Spectroscopic constant (cm^{-1})	H^1F^{19} $\text{X}^1\Sigma^+$	H^1F^{19} $\text{B}^1\Sigma^+$
T_e	0	84776.7
$Y_{10} = \omega_e$	4138.32	1159.18
$Y_{20} = \omega_e \chi_e$	89.88	18.005
r_e (cm)	9.17E-09	2.09E-08

Table 1b: Spectral constants (cm^{-1}) used as input data for calculation for isotopic molecule H^2F^{19} [13,14].

Spectroscopic constant (cm^{-1})	H^2F^{19} $\text{X}^1\Sigma^+$	H^2F^{19} $\text{B}^1\Sigma^+$
T_e	0	84824
$Y_{10} = \omega_e$	2998.19	839.4
$Y_{20} = \omega_e \chi_e$	45.761	8.9
r_e (cm)	9.17E-09	2.09E-08

4. ISOTOPIC MOLECULES EFFECT

The isotopic molecules have different mass of one or both of the nuclei but not by their atomic number, whereas the reduced mass is different, and the vibrational frequency is different, their heavier molecules have a smaller frequency [3].

5. RESULTS AND DISCUSSION

5.1 The rotational effect upon the Morse potential

The rotational effect upon the Morse potential of $\text{X}^1\Sigma^+$ and excited state $\text{B}^1\Sigma$ of H^1F^{19} and H^2F^{19} molecules for rotational quantum number ($J=0-150$) for a range of temperature (100-1000 K), and electronic transitions X state (Figure 1), B state (Figure 2). It is obvious from the calculations that the value of effective potential for B state greater than that of X state. This is due to the increase of the electronic energy of these states of the molecule.

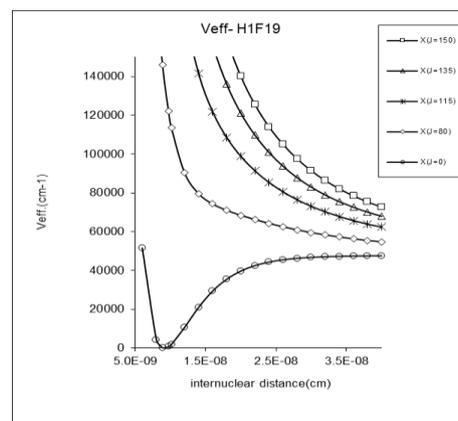


Figure 1: Effective potential in the ground state $\text{X}^1\Sigma^+$ of molecule H^1F^{19} ($J=0-150$).

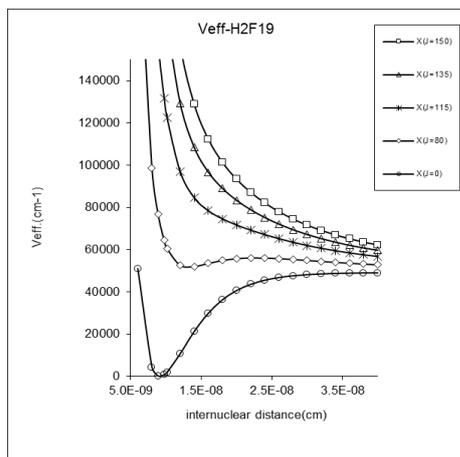


Figure 2: Effective potential in the ground state $X^1\Sigma^+$ of molecule H^2F^{19} ($J=0-150$).

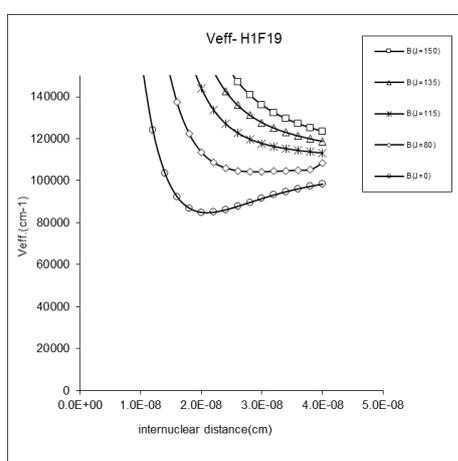


Figure 3: Effective potential in an excited state $B^1\Sigma^+$ of isotopic molecule H^1F^{19} ($J=0-150$).

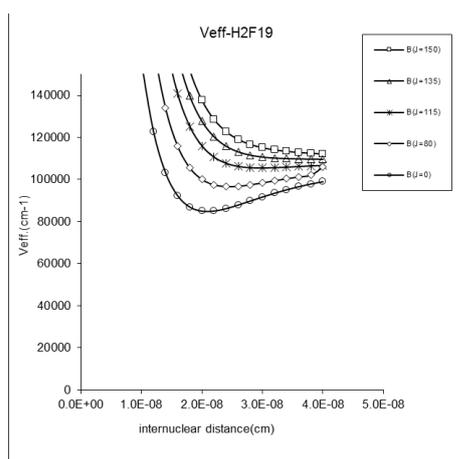


Figure 4: Effective potential in an excited state $B^1\Sigma^+$ of isotopic molecule H^2F^{19} ($J=0-150$).

Figures 3 and 4 compiles the results of the effective potential of the electronic transitions X and B of H^1F^{19} and H^2F^{19} molecules, with rotational quantum number ($J=150$) at room temperature (300 K). The calculations show clearly that the value of effective potential for B state greater than that of X state. This is due to the increase of the electronic energy of these states of the molecule. This effect refers to a failure of

Born–Oppenheimer approximation for any transition (i.e. Rotational, vibrational and electronic transition), also this effect causes a reduction in the energy needed to dissociate from any state of the molecule. We must notice that the temperature should be low to avoid any previous excitation which is not desirable (rotation or vibration) in order to have excellent experimental results.

5.2. Dissociation Energy:

Morse potential function for ground and excited states has been carried out from the experimental data by Huber and Herzberg (14). The values dissociation Energy obtained by using (2) and (3) listed in Table. 2 and Table. 3.

Table 2: Dissociation Energy (eV) of H^1F^{19} .

State	D_e (eq.2)	D_e (eq.3)
$B^1\Sigma^+$	2.312801	1.814729
$X^1\Sigma^+$	5.904929	4.607871

Table 3: Dissociation Energy (eV) of H^2F^{19} .

State	D_e (eq.2)	D_e (eq.3)
$B^1\Sigma^+$	0.007283	0.005467
$X^1\Sigma^+$	6.087689	4.940081

5. CONCLUSIONS

This effect refers to a failure of Born–Oppenheimer approximation for any transition (i.e. Rotational, vibrational and electronic transition), also this effect causes a reduction in the energy needed to dissociate from any state of the molecule. We must notice that the temperature should be low to avoid any previous excitation which is not desirable (rotation or vibration) in order to have an excellent experimental result. It was found that the value dissociation energy for X larger than that of B states for H^1F^{19} and H^2F^{19} molecules.

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