

# The Vibration Intensity Of Electronic States Of Isotopic Of Hydrogen Fluoride $H^1f^{19}$ And $H^2f^{19}$ Molecule

Dhia Hamdi Al-Amiedy

University of Baghdad, Baghdad, College of Science for Women, Physics Department  
Iraq. +09647902701188  
amiedy48@gmail.com

**Abstract:** A calculation has been carried out for the calculation of some of the spectroscopic properties of isotopes of Hydrogen fluoride  $H^1F^{19}$  and  $H^2F^{19}$  molecules such as, the population of the vibration spectrum of electronic transition of ground state X, and excited states B as a function temperature ranging from 0 to 1000 K. This study shows that the populations and hence the intensity of the molecule decreased exponentially as the temperature increased. It was found that the population of the vibration spectrum of electronic transition of ground state X, greater than that of the excited states B

**Keywords:** electronic transition, excited states, ground state, vibration spectrum.

## 1. Introduction

Boltzmann distribution has been carried out by many investigators such as Liu, Jian Li et al [1] studied the vibrational state distribution of  $Na_2^+$  Ions in ultracold collisions, whereas Kvaran and Wang [2] whom calculated HCl and DCl molecules, whereas. Houfek et al [3] studied HCl, HBr and HI molecule, The experiments concerning NaRb were performed by Jastrzebski et al [4] and by Docenko et al [5-7] whereas Pashov et al [8] studies Na and Rb molecules, whereas Camden et al [9] studied HCL molecule, and Al-Amiedy et al [10] studied the calculation has been carried out for calculation of some the spectroscopic properties of  $Na_2$  molecules, such as the intensity of the vibration spectrum of electronic states X, A and B as a function of temperature in the range from 100 to 1000 K. This study shows that the population and hence intensity of the molecule increases as the temperature increases. It was shown that the population of B state is greater than that of A state which is greater than that of X state. While Al-Amiedy and Saadi [11] carried out for studying some of the spectroscopic properties of Copper Hydride  $CuH$  molecules, such as the intensity of the vibration spectrum of electronic transition of ground state X and excited states A and B as a function of temperature in the range from 100 to 600 K. This study shows that the populations and hence intensity of the molecule decreases exponentially as the temperature increases. The population of the vibration energy level decreases with the increase of vibrational quantum number, and inversely decreases with the increase of the temperature. It was shown that the population of B state is greater than the population of A state, which is greater than that of X state. Whereas Al-Amiedy [12] carried out for calculation of some of the spectroscopic properties of isotopes of Lithium Hydride  $Li^7H^1$  and  $Li^7H^2$  molecules such as, the population of the vibration spectrum of electronic transition of ground state X, and excited states A as a function temperature ranging from 0 to 1000 K. This study shows that the populations and hence intensity of the molecule decreased exponential as the temperature increased. It was found that the population of the vibration spectrum of electronic transition of ground state X, greater than that of the excited states A. The population of the vibration energy level decreases with increase of

vibrational quantum number  $v$ , and inversely decreases with the increase of the temperature. The Boltzmann populated is decreased with increase the values of vibrational quantum number, and population of A state greater than the population of X state.

## 2. Theoretical aspect

### 2.1 Boltzmann distribution:

The vibrational energy (in Joule unit) level of diatomic molecules resulting from solving Shrodinger equation for a Morse oscillator is given by the following relation [13]:

$$E_v = \Delta G(v) \quad (1)$$

Generally, the selection rule of diatomic molecule raised from state  $v$  to state  $v+1$  given by [13]:

$$\Delta \varepsilon_v = \varepsilon_{v+1} - \varepsilon_v \quad (2)$$

Where  $E_v$  and  $G(v)$  denotes the vibrational energy in the joule unit, and  $G(v)$  is given by the following relation:

$$G(v) = \omega_e \left( v + \frac{1}{2} \right) - \omega_e x_e \left( v + \frac{1}{2} \right)^2 \quad (3)$$

Where  $v$  is the vibrational quantum number,  $\omega_e$  is the harmonic constant,  $\omega_e x_e$  is the anharmonicity. Generally, the vibrational energy change when the diatomic molecule raised from level  $v$  to level  $v+1$  is given by [13]:

$$\Delta G = \{G(v+1) - G(v)\} \quad (4)$$

Boltzmann distribution is the factor governing the population of the vibrational levels of the molecules. If  $N_0$  represents the number of molecules in  $v=0$  levels and  $N_v$  is the number of molecules in the  $v$  level, this distribution is given by [13]:

$$\frac{N_v}{N_0} = \exp\left(-\frac{E_v}{kT}\right) \quad (5)$$

$$\frac{N_v}{N_0} = \exp\left[-\frac{hc\{G(v) - G(0)\}}{kT}\right] \quad (6)$$

Where k is the temperature of the molecule and h is the Planck's constant.

### 3. COMPUTATIONAL CALCULATIONS

The Dunham constants [13] were taken from three states. A calculation has been carried out to find the population of the vibrational energy level of H<sup>1</sup>F<sup>19</sup> and H<sup>2</sup>F<sup>19</sup> molecules using (6) Listed in Table 1a and 1b. A computational programs has been elaborated similar to that carried out by substituting the values of the vibrational quantum number (v) ranging from 1 to 26 and the temperature ranging from 100 to 600 K for the electronic transitions X and B using (5) in Ref. [12], for H<sup>1</sup>F<sup>19</sup> and H<sup>2</sup>F<sup>19</sup> molecule with the bond lengths of 0.917Å (X state), 2.0 Å (A state) and the masses measured in (amu) units, The Dunham constants [12] were taken from two electronic states were listed in Table 1a and 1b.

**Table 1a.** Spectral constants (cm<sup>-1</sup>) used as input data for calculation for isotopic molecule H<sup>1</sup>F<sup>19</sup> [14,15].

Spectroscopic constant (cm <sup>-1</sup> )	H <sup>1</sup> F <sup>19</sup> X <sup>1</sup> Σ <sup>+</sup>	H <sup>1</sup> F <sup>19</sup> B <sup>1</sup> Σ <sup>+</sup>
T <sub>e</sub>	0	84776.7
Y <sub>10</sub> = ω <sub>e</sub>	4138.32	1159.18
Y <sub>20</sub> = ω <sub>e</sub> χ <sub>e</sub>	89.88	18.005
r <sub>e</sub> (cm)	9.17E-09	2.09E-08

**Table 1b.** Spectral constants (cm<sup>-1</sup>) used as input data for calculation for isotopic molecule H<sup>2</sup>F<sup>19</sup> [14,15].

Spectroscopic constant (cm <sup>-1</sup> )	H <sup>2</sup> F <sup>19</sup> X <sup>1</sup> Σ <sup>+</sup>	H <sup>2</sup> F <sup>19</sup> B <sup>1</sup> Σ <sup>+</sup>
T <sub>e</sub>	0	84824
Y <sub>10</sub> = ω <sub>e</sub>	2998.19	839.4
Y <sub>20</sub> = ω <sub>e</sub> χ <sub>e</sub>	45.761	8.9
r <sub>e</sub> (cm)	9.17E-09	2.09E-08

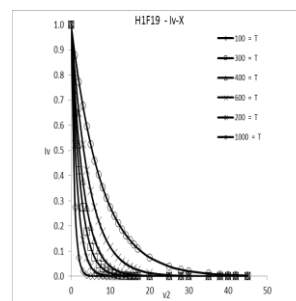
### 4. ISOTOPIC MOLECULES EFFECT

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 [16].

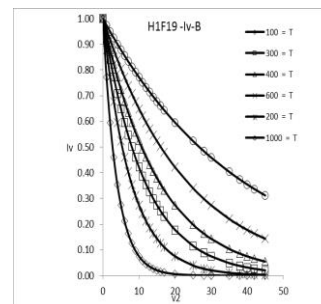
### 5. RESULTS AND DISCUSSION

The Boltzmann population of the vibrational energy level of H<sup>1</sup>F<sup>19</sup> molecule versus the vibrational quantum number v, from v =0 to v =45. When the temperature at of 0 K, the most populated is ground vibrational level v =0, when the temperature increased the populated vibrational level decreased inversely as shown in Figure 1 for the ground state X<sup>1</sup>Σ<sup>+</sup> while Figure 2 shows are exciting state B<sup>1</sup>Σ<sup>+</sup> molecule. Figures 3 and 4 shows the Boltzmann population of the vibrational energy level versus the vibrational quantum number v at different temperature of the electronic transitions X for H<sup>1</sup>F<sup>19</sup> and H<sup>2</sup>F<sup>19</sup>. The Boltzmann population of the vibration energy level decreased with the increase of the values of vibrational quantum number, and the values of

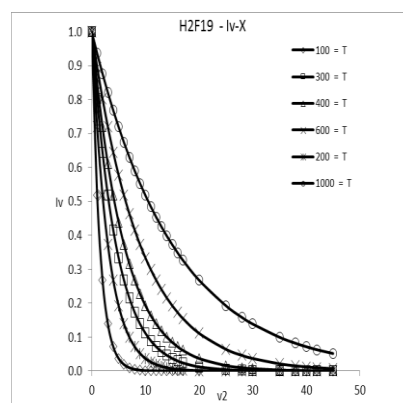
X for H<sup>2</sup>F<sup>19</sup> higher than that of H<sup>1</sup>F<sup>19</sup> due to the values of spectroscopic constants of H<sup>2</sup>F<sup>19</sup> higher than that of H<sup>1</sup>F<sup>19</sup>. The Boltzmann population of the vibrational energy level of H<sup>2</sup>F<sup>19</sup> molecule versus the vibrational quantum number v, from v =0 to v =45. When the temperature at of 0 K, the most populated is ground vibrational level v =0, when the temperature increased the populated vibrational level decreased inversely as shown in Fig. 5 for the ground state X<sup>1</sup>Σ<sup>+</sup> while Figure 6 shows excited state B<sup>1</sup>Σ<sup>+</sup> molecule.



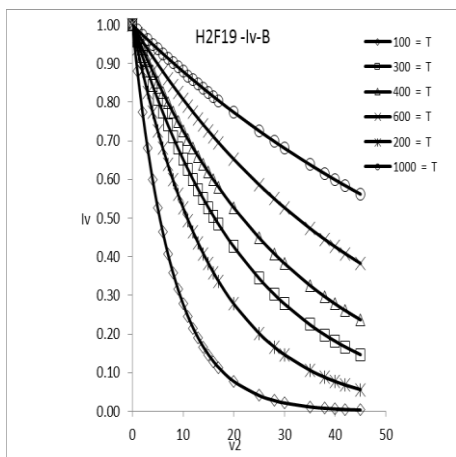
**Figure 1:** Boltzmann population of the vibration energy level versus the vibrational quantum number v at different temperature of the ground state X<sup>1</sup>Σ<sup>+</sup> of H<sup>1</sup>F<sup>19</sup> molecule.



**Figure 2:** Boltzmann population of the vibration energy level versus the vibrational quantum number v at different temperature of the excited state B<sup>1</sup>Σ<sup>+</sup> of H<sup>1</sup>F<sup>19</sup> molecule.



**Figure 5:** Boltzmann population of the vibration energy level versus the vibrational quantum number v at different temperature of the electronic transitions X<sup>1</sup>Σ<sup>+</sup> of H<sup>2</sup>F<sup>19</sup> molecule.



**Figure 6:** Boltzmann population of the vibration energy level versus the vibrational quantum number  $v$  at different temperature of the ground state  $B^1\Sigma^+$  of  $H^2F^{19}$  molecule.

## 6. CONCLUSIONS

The population of the vibration energy level decreases with increase of vibrational quantum number  $v$ , and inversely decreases with the increase of the temperature. The Boltzmann populated is decreased with increase the values of vibrational quantum number, and population of B state greater than the population of X state.

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## Author Profile



### DHIA HAMDY AL-AMIEDY

Received the B.S. in Physics from College of Education-University-University of Baghdad - Iraq, and Ph.D. degrees in Molecular Physics in 1979 from University of keele. U.K.. During 1980-2013, he stayed in Physics Department-College of Science for Women-University of Baghdad-Iraq. He retired in 2014 and until now He is Professor Emeritus in College of Science for Women-University of Baghdad-Baghdad-Iraq.