

Calculating The Absorption Population And Maximum Quantum Number Of Electronic States Of Isotopic H^1F^{19} And H^2F^{19} Of Hydrogen Fluoride Molecules

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Abstract: A theoretical calculation has been carried out of some of the spectroscopic properties of isotopic H^1F^{19} and H^2F^{19} Hydrogen fluoride molecules, such as the population of the absorption spectrum of electronic transitions X and B as a function of the temperature in the range from 50 to 500 K, and values of J in the range of 0 to 20. It was found that the values of calculated spectroscopic properties studied in this paper for H^2F^{19} molecule greater than that of H^1F^{19} molecules, and the population of the molecule increase as the temperature increase with increase of J reaching maximum values, the decrease reaching minimum values. Besides, a calculation is being carried out for determination of the maximum rotational quantum number of the same electronic transitions. The theoretical calculation shows that the value of J_{max} increases with the increases in temperature, and its values (J_{max}) for the electronic state X greater than that of B as the of the temperature increases.

Keywords: absorption population, electronic transition, excited electronic state, ground electronic state, Hydrogen fluoride molecules, maximum J quantum number, temperature.

1. Introduction

The importance of diatomic molecules is due to their existence in nature and chemical processes, including combustions, reactions and atmospheric studies. Mehler [1] found that the small amount of correlation recovered by BN molecule is caused by the bonding and lone pair geminals, whereas, Engvoild [2] Studied the strongest absorption lines of boron of BH molecule in the far ultraviolet and infrared solar spectrum, whereas, Blint and Goddard [3] studied the electronic wavefunctions for the ground state and low-lying of the excited state of BH molecules such as potential curve of the excited state in the zero rotational level, while Oh et al., [4] Studied the polymeric boron hydride, which was more stable than that of polyethylene-type geometry, whereas Zhou et al [5] used density functional theory to improve the hydrogen storage properties of polarizable substrates of BH molecule. Many investigators had been studied experimentally Nitric Oxide NO [6-9]. Boltzmann distribution has been carried out by many investigators such as Kvaran and Wang [10] whom calculated HCl and DCl molecules, whereas, Houfek et al [11] studied HCl, HBr and HI molecules, while Camden et al [12] studied HCL molecule. Al-Amiedy [13] studied the absorption of CO molecule as a function of variation of temperature. It was found that the most rotational populated level of the isotopes $^{12}C^{16}O$, $^{12}C^{18}O$, and $^{14}C^{16}O$ increases as temperature increases. While Al-Amiedy et al [14] a calculation have been carried out for the determination of a maximum rotational quantum number J_{max} of LiH, AgCl, HI and BrF molecules and the intensity of the absorption spectrum of LiH molecules as a function of the variation of the temperature ranging from 10 to 1000 K. This study shows that the maximum rotational quantum number and hence intensity increased as the temperature increased. Also, the values of J_{max} of rotational quantum number energy level versus different values of temperature show that the value of electronic state A is greater than for electronic states X and B

as value the of the temperature increases. This because the rotational energy is inversely proportional to the reduced mass, then its value is larger for the molecules with smaller reduced mass such as BrF molecule have higher intensity than the other molecules such as AgCl molecule. Whereas, Al-Amiedy et al [15]. 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. Also, Al-Amiedy et al [16] carried out a calculation for some spectroscopic properties of Na_2 molecule such as absorption spectra of electronic transition X, A and B as a function of the temperature in the range of 10 to 1000 K. the study shows that the population and maximum rotational quantum number increases as the temperature increases of the same electronic transition. Whereas, Al-Amiedy et al [17] carried out for theoretical calculation of some of the spectroscopic properties of CN free radical, such as the intensity of the absorption spectrum of electronic transitions X, A and B as a function of the temperature in the range from 10 to 1000 K. The most Boltzmann populated rotational level of CN free radical for electronic state A is greater than for X, B electronic states as the value of the temperature increases. The values of J_{max} of rotational quantum number energy level versus different values of temperature show that the value of electronic state A is greater than for electronic states X and B as value the of the temperature increases. This because the rotational energy is inversely proportional to the reduced mass, then its value is larger for the molecules with smaller reduced mass. Al-Amiedy et al [18] carried out theoretical spectroscopic properties of $^{12}C^{16}O$ molecule, has been carried out such as the absorption intensity spectrum of electronic transitions X, A and B as a function of the temperature in the range from 50 to 500 K. This study shows that the intensity of the molecule increases as the temperature increases. Beside, a calculation is being carried out for determination of

maximum rotational quantum number of the same electronic transitions. It was found that the most Boltzmann populated rotational level of $^{12}\text{C}^{16}\text{O}$ molecule for electronic state A is greater than for X and B electronic states as the of the temperature increases

2. Theoretical Boltzmann distribution aspect

The rotational energy level (in SI unit, i.e. In Joule unit) of diatomic molecules resulting from solving the Shrodinger equation is given by the following relation [19]:

$$(1) \quad \varepsilon_J = E_J / hc = J(J + 1)B$$

Where the B is rotation constant Generally, the selection rule of diatomic molecule raised from state J to state J+1 is given by [20]

$$(2) \quad \Delta\varepsilon = \varepsilon_{J+1} - \varepsilon_J$$

Boltzmann distribution is the factor governing the population of the rotational levels of the molecules. If N_0 represents the n=umber of molecules in $J = 0$ and N_J is the number of molecules in the other J state, this distribution is given by [19]:

$$(3) \quad N_J / N_0 = \exp(-E_J / kT)$$

The population of the rotational level depends on the rotational energy, on the temperature and on the degeneracy $2J+1$ as the following relation

$$(4) \text{ Population} \propto (2J + 1) \exp(-E_J / kT)$$

Since the population is proportional to the population, it is proportional to the above quantities in the same manner.

2.1 - Maximum quantum number

Assuming, for the moment, that (4) Indeed a good representation of the true spectrum, the transition with maximum population could be treated by this equation as a continuous distribution. Thus, differentiating with respect to the J, we obtain

$$(5) \quad \frac{dN_J}{dJ} = \left\{ 2 - \frac{Bhc}{kT} (2J + 1)^2 \right\} \exp[-BhcJ(J + 1)/kT]$$

The maximum is found from $dN_J/dJ = 0$. Hence

$$(6) \quad J_{\max} = \sqrt{\frac{kT}{2Bhc}} - \frac{1}{2}$$

Where h is Planck constant, c is the velocity of light. Since J_{\max} must be an integer, one takes the nearest integer obtained from (6) As the maximum.

3. Computational calculations

The Dunham constants [20,21] were taken to two electronic states. A calculation has been carried out to find the absorption population of H^1F^{19} and H^2F^{19} molecules using (1) Listed in Table.1a and 1.b.

Table 1a: Spectral constants (cm^{-1}) used as input data for calculation for isotopic molecule H^1F^{19} [20,21].

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} [20,21].

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)	9.16e-09	2.09e-08

A computational programs similar to that carried out by Al-Amiedy [13] using (4) For a H^1F^{19} and H^2F^{19} molecule with the bond lengths of 0.917\AA (X state), 2.0\AA (B state) for measured in (amu) unit, by substituting the values of the rotational quantum number (J) ranging from 0 to 20 and the temperature ranging from 50 to 500 K from the electronic transitions X and B. Also, a computer program similar to that carried out by Al-Amiedy et al [13] has been carried out using (6) For H^1F^{19} and H^2F^{19} molecules and for the same electronic transitions.

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 [22].

5. Results and discussion

Figures 1 and 2 show the Boltzmann population of the rotational energy level of the X and B electronic states of H^1F^{19} molecules versus the rotational quantum number J at different temperature. When the temperature at of 0 K, the most populated is ground rotational level $J=0$, while at 100 K the most populated is for rotational level $J=1$ for X (population=1.64) and $J=2$ for B (population=3.53). However, at room temperature the most populated rotational level at $J=2$ for X (population=2.74) and $J=5$ for B (population=6.16).

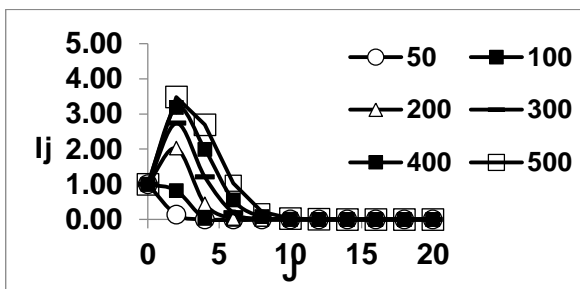


Figure 1: Boltzmann population of the rotational energy level versus the rotational quantum number J at different temperatures of the ground state $X^1\Sigma^+$ of H^1F^{19} molecule.

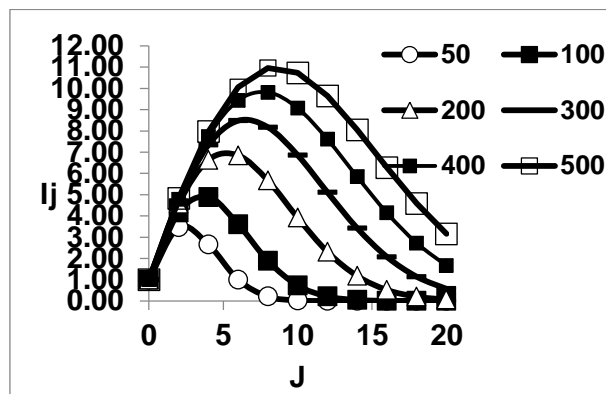


Figure 4: Boltzmann population of the rotational energy level versus the rotational quantum number J at different temperature of the excited state $B^1\Sigma^+$ of H^2F^{19} molecule.

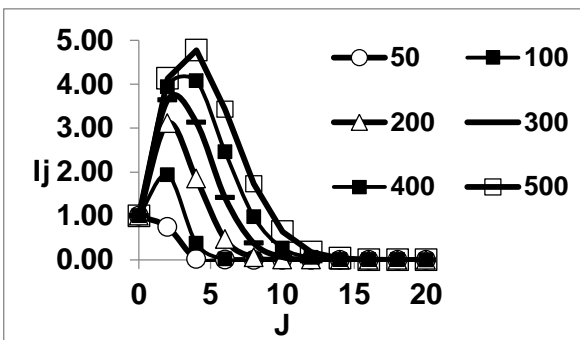


Figure 2: Boltzmann population of the rotational energy level versus the rotational quantum number J at different temperatures of the ground state $X^1\Sigma^+$ of H^2F^{19} molecule.

Figures 5 and 6 shows the Boltzmann population of the rotational energy level versus the rotational quantum number J at room temperature of the ground state $X^1\Sigma^+$ and excited state $B^1\Sigma^+$ of H^1F^{19} and H^2F^{19} molecules. It's clear from the figures that the population of H^2F^{19} greater than that of H^1F^{19} molecules, beside that the population of excited state $B^1\Sigma^+$ greater than that of ground state $X^1\Sigma^+$.

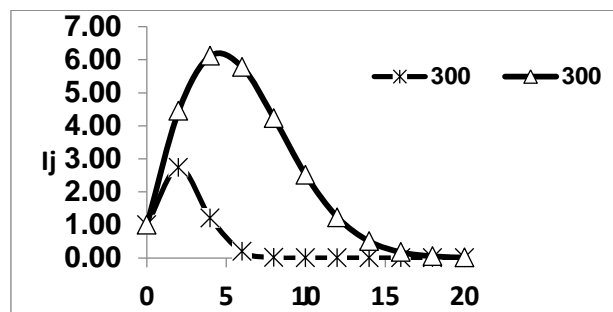


Figure 5: Boltzmann population of the rotational energy level versus the rotational quantum number J at 300K temperature of the ground $X^1\Sigma^+$ and excited state $B^1\Sigma^+$ of H^1F^{19} molecules

Figures 3 and 4 show the Boltzmann population of the rotational energy level of the X and B electronic states of H^2F^{19} molecules versus the rotational quantum number J at different temperature. When the temperature at of 0 K, the most populated is ground rotational level $J=0$, while at 100 K the most populated is for rotational level $J=1$ for X (population=2.19) and $J=4$ for B (population=4.89). However, at room temperature the most populated rotational level at $J=3$ for X (population=3.71) and $J=7$ for B (population=8.49).

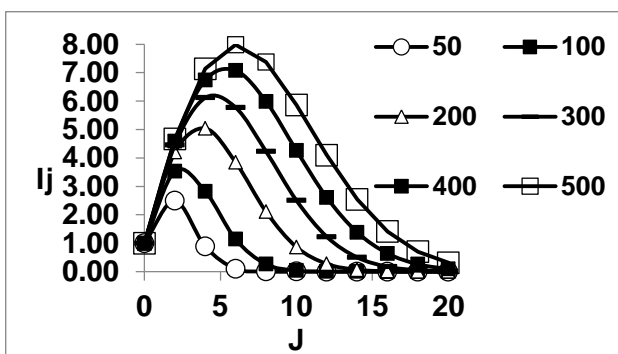


Figure 3: Boltzmann population of the rotational energy level versus the rotational quantum number J at different temperature of the excited state $B^1\Sigma^+$ of H^1F^{19} molecule.

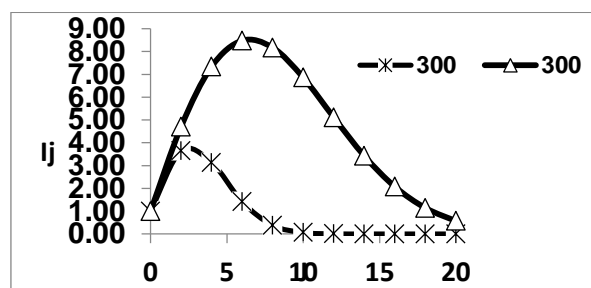


Figure 6: Boltzmann population of the rotational energy level versus the rotational quantum number J at 300K temperature of the ground $X^1\Sigma^+$ and excited state $B^1\Sigma^+$ of H^2F^{19} molecules.

Figures 7 and 8 shows the values of maximum rotational quantum number J_{max} of the absorption spectrum of the electronic state X and B for H^1F^{19} and H^2F^{19} molecules against the variation of the temperature. When the temperature increased the J_{max} increased. It's obvious that its values for H^2F^{19} molecule greater than that of H^1F^{19}

molecule. It's due to the fact that the reduced mass H^2F^{19} of higher than that of H^1F^{19} molecule.

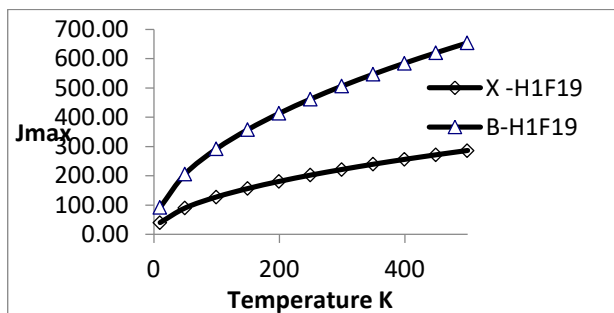


Figure 7: Maximum rotational quantum number J_{max} versus rotational energy level versus the rotational quantum number J at different temperature of the electronic transitions X and B for H^1F^{19} molecule.

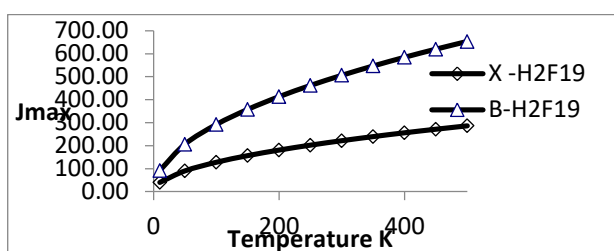


Figure 8: Maximum rotational quantum number J_{max} versus rotational energy level versus the rotational quantum number J at different temperature of the electronic transitions X and B for H^2F^{19} molecule.

5. Conclusions

In general, the values of calculated spectroscopic properties studied in this paper for H^2F^{19} molecule greater than that of H^1F^{19} molecule. The most Boltzmann populated rotational level of the electronic state X greater than B electronic states as the of the temperature increases, while the population increased until reaching maximum values the decreased reaching zero values when the rotational quantum number J increased. The values of J_{max} of rotational quantum number energy level versus different values of temperature shows that the value of J_{max} increases with the increases in temperature, and its values (J_{max}) for the electronic state X greater than that of B as the of the temperature increases. This because the rotational energy inversely proportional to the reduced mass, then the molecules with smaller reduce mass.

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