Measurements of The Spectroscopic Properties of Hydrogen Iodide Molecules

Zeyad Adnan Saleh*

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Abstract

A calculation have been carried out for determination some of the spectroscopic properties of Hydrogen Iodide HI molecules such as, the intensity of the absorption spectrum as a function of the variation of the temperature ranging from 10 to 1000 K. This study shows that the populations and hence intensity of the molecule increased as the temperature increased. Another determination of the maximum rotational quantum number J_{max} of N_2 , CO , BrF AgCl and HI molecules has been carried out.

1. Introduction:

Boltzmann distribution has been carried out by many investigators such as Kvaran and Wang [1] whom calculated HCl and DCl molecules, whereas, Houfek et al [2] studied HCl, HBr and HI molecules, while Al-Amiedy [3] studied the abosorption intensity of CO molecule, and Camden et al [4] studied HCl molecule.

The maximum rotational quantum number of LiH, AgCl, HI and Brf molecules has been carried out by Al-Amiedy et al [5].

2. Theoretical aspect:

2.1 Botzmann distribution:

The rotational energy (in Joule unit) level of diatomic molecules resulting from solving Shrodinger equation is given by the following relation [6]:

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

where $B=h/(8\pi^2 Ic)$ (2)

Generally, the selection rule of diatomic molecule raised from state J to state J+1 given by [7]:

$$\Delta\varepsilon = \varepsilon_{J+1} - \varepsilon_J \qquad (3)$$

Boltzman distribution is the factor governed the population of the rotational levels of the molecules, if N_o represents the number of molecules in J=0 and N_J is the number of molecules in the other J state. This distribution is given by [8]:

$$N_J / N_0 = \exp (-E_J / kT) \qquad (4)$$

The population of the rotational level is proportional to the rotational energy and temperature and the degenercy (2J+1) as the following relation :

$$\text{Population} \propto (2J+1) \exp (-E_J / kT) \qquad (5)$$

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

2.2 Maximum quantum number:

Assuming, for the moment,that Eq. (4) is indeed a good representation of the true spectrum, we can find the tran sition with maxim um intensity by treating this equa - tion as a continuous distribution and differentiating with respect to J.

$$\frac{dN_J}{dJ} = e^{(-BJ(J+1)/kT}\left\{2 - \frac{B}{kT}(2J+1)^2\right\} \qquad (6)$$

for maximum $(\frac{dN_J}{dJ} = 0)$ and hence we obtain

$$J_{max} = \sqrt{\frac{kT}{2Bhc}} - \frac{1}{2} \qquad (7)$$

since J_{max} must be an integer, one takes the nearest value obtained from Eq. (7) as the maximum.

3. Computational calcula tions:

A computational programs [3] has been carried out using equations (4) and (5) for ^1H ^{127}I and ^2H ^{127}I molecules with bond length of 2.666 A and the masses measured in (amu) unit,

* **Physics Department, College of Science , Al-Mustansriyah University , Baghdad-Iraq.**

by substituting the values of the rotational quantum number ranging from 1-45 and the temperature ranging from 10 -1000 K.Also, a computational program simialr to that carried out by Al-Amiedy et al [5] has been carried out using Eq. (6) for N_2 ,CO, BrF AgCl and HI by substituting the values of the temperature ranging from 10 to 1000 K.

4. Results and Discussion

Figure (1) shows the normalized of the above calculated absorption spectrum for $^{1}H\ ^{127}I$ molecule against J values.While Figure (2) represent the normalized values of the above calculated absorption spectrum against 2B(J+1) values. When the temperature at of 0 K , the most populated is ground rotational level (J=0), while at 10 K the most populated is first excited rotational level (J=1).However, at room temperature the most populated rotational level at (J=6).

Spectrum of the other isotopic substituted of HI molecule shows the same tendency of the above $^{1}H\ ^{127}I$ molecule.

Figure (3) shows the values of J_{max} of the absorption spectrum against the variation of the temperature.When the temperature increased the J_{max} increased. The spectrum of the other molecules investigated in this work such as N_2 shows the same tendency of the above HI molecule.

5. Concusions:

It was found from the theoretical results that :

– The most populated rotational level is increased as the of the temperature increases.

– The values of Boltzmann and relative intensity of 2 isotopes $^{1}H\ ^{127}I$ and $^{2}H\ ^{127}I$ have the same trend because the bond length is the same in spite the change in the mass number.

– The isotope $^{2}H\ ^{127}I$ has more massive than $^{1}H\ ^{127}I$ since the rotational energy inversely proportional with reduced mass of the molecule tend to proportional to populated lower rotational level than that of $^{1}H\ ^{127}I$.

– The values of Boltzmann population of the J_{max} of rotational quantum number energy level versus different values of temperature shows that its values increased with the increased of the temperature. And because the rotational energy inversely proportional with the reduced mass, then the molecules with smaller reduce mass such as N_2 molecule have high intensity than the other molecules such as HI molecule.

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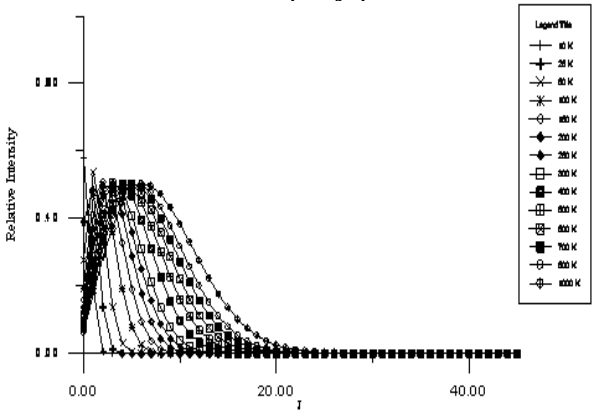

Figure (1): Boltzmann population of the rotational energy level versus the rotational quantum number J at different temperature of $^{1}H\ ^{127}I$ molecules.

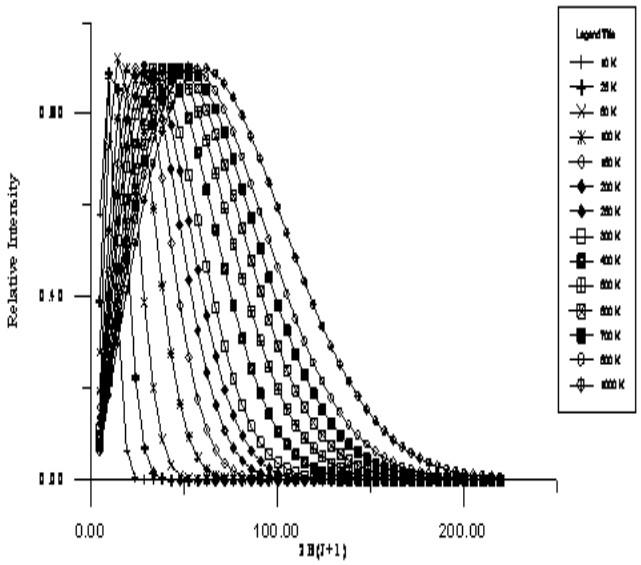

Figure (2): Boltzmann population of the rotational energy level versus the rotational energy level vs 2B(J+1) at different temperature of $^{1}H^{127}I$ molecules.

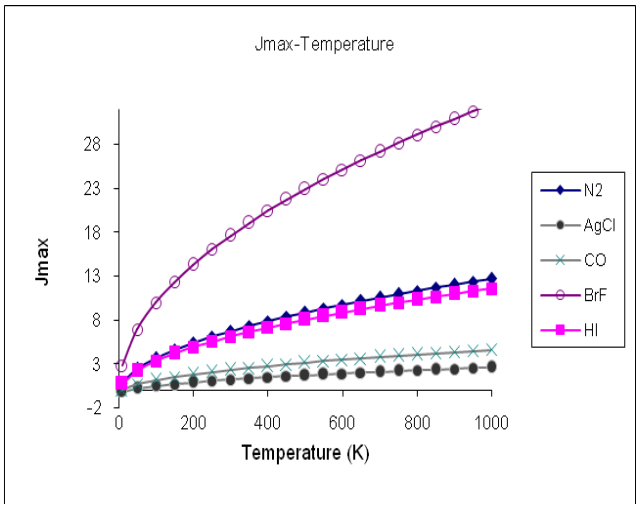

Figure (3). Maximum rotational quantum number J_{max} versus the temperature .

قياس الخواص الطيفية لجزيئة ايوديد الهايدروجين

*الدكتور زياد عدنان صالح**

**قسم الفيزياء – كلية العلوم – الجامعة المستنصرية*

الخلاصة:

لقد تم قياس بعض الخواص الطيفية لجزيئة ايوديد الهايدروجين مثل شدة طيف الامتصاص كدالة لدرجة الحرارة لمدى يتراوح بين 10 الى 1000 كلفن وتبين من الدراسة ان الشدة تتناسب طرديا مع درجة الحرارة. كما تم حساب اعظم قيمة للعدد الكمي الدوراني J_{max} لجزيئات N_2 , CO , BrF AgCl HI