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Calculation of Lambda Doubling for $^7LiH^1$ molecule Using the System band emission for electronic transmissions

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Abstract:

The $A^2\Pi_u$-$X^1\Sigma g^+$ emission band system of $^7LiH^1$ molecule has been calculated for Lambda doubling. The relation between wave number ν_p , ν_Q , ν_R conducted the energies of the state of rotation F (J), and (J + 1) with rotational quantum number J, respectively, of $^7LiH^1$ molecule for statehood $A^2\Pi u$ using the rotation, fixed vibrational states of both the ground and raised crossovers vibrational against $v''= 0$ to $V' = 0$-4using rotational levels J = 0 to J = 20 have found.

Key word: Lambda doubling, rotational spectrum, $^7LiH^1$ molecule, vibrational states, ground states.

Introduction:

The $^7LiH^1$ molecule has been studied through different experiments. Spectroscopic data of the ground The electronic transitions involving the ground and the first excited states of the state (v= 0, 1) were also available from accurate microwave experiments for several isotopic species of the $^7LiH^1$ molecule.

It was only recently that the system $A^2\Pi$-$X^2\Sigma^+$ can be studied through high resolution Fourier transform spectroscopy. Article emission spectrum produced in Orsay Waterloo through the use of various techniques, the similarity was strong of spectra obtained enabled joint analysis [1]. Also, it was conducted a full rovibrational of $A^2\Pi$-$X^2\Sigma^+$ 0-0 and 0-1 bands, including reliance on vibratory of the fragmentation of the ground state and the turn-around in the orbit of the state $A^2\Pi$ state, It was found that the value obtained from the Lambda double p constant positive in contrast with the theoretical predictions [2]. Many researches have been carried out by a calculation of Λ- doubling constant. An experimental spectroscopic study has been on carried out by using supersonic nozzle beam for determe the spectroscopic constant and Λ-doubling of Rb_2 in B-X system [3]. Theoretical study of Λ-doubling for the asymmetry of the orbital part of the electronic wave functions in $^1\Pi$,$^2\Pi$ and $^3\Pi$ is carefully examined [4] . Hund's coupling case is used to describe the molecular states and analysis of angular distributions from two-photon ionization of Na_2 has been carried out [5]. A study for $B\Pi_u$ state of Na_2 molecule has been carried out by measuring the rotation-vibration energy levels [6]. Milošvić et al [7- 9] has studied spectrum for the transitions that are different. Kaldor [10] studies Li_2 ground and excited states by a shell in the open coupled -cluster method. Energy curves of Cs_2 was carried out using the built-effective potential (CEP), and the possibilities of the core polarization (CPP) [11]. LiLi et al [9] studied the change in hyperfine quantum number, *e/f* parity transitions and Λ-doubling component in the Na_2 $b_3\Pi_u$ state. Zaitsevskii and Skolyarov [12] studied experimentally and theoretically Π state of NaK dimer cooling liquid. The have studied experimentally the cooling liquid NaK $1^3\Delta$ case by technical disorders facilitated optical double resonance optical [13]. He had conducted a study of the important theory in the electronic states of the molecule RB2 by Park et al. Ivanov et al [14] studied the Na_2 2^3 $\Sigma g^+ \rightarrow a^3\Sigma u^+$ continua. A calculation of Λ-doubling constants for rovibronic levels of the $B^1\Pi_u$ and $D^1\Pi_u$ states of NaRb molecule have been carried out [2]. It has been found that the rotational spectrum of the ground state was irregular to a large extent. A minimum of four ladders show significant interactions to be unusual, Double lambda, with a = 1 shows the largest component of the division, and more than 2 GHz in size. The Shift = 1 transfer is also higher for the other components of the rotation frequency. In addition, the hyperfine structure differs widely between the stairs, it was observed that crossing was avoided in two transitions occurring both = 1e and 2e components. The data was analyzed with the case (c) Hamilton, effectiveness rotary, double lambda, has been identified Hyperfine constants of V35Cl. Supreme ultra-precision magnetic items that depend on parity between D 2 and D 3 were required in the analysis, derived from the theory of turbulence, in addition to the usual d parameter. Local unrest evident in these spectra indicate that there is 5:00 excited state lies in the spin manifold over the case Alardahoho far less than the expected value of 517 cm^{-1}. Λ-doubling for the $B^1\Pi_u$ state of Li_2 has been carried out [15]. Experimental and theoretical investigation of the $6^1\Sigma u^+$ and $7^1\Pi_u$ states of $^7LiH^1$ [16]. Also, Λ- doubling of the investigation with the case of the Rydberg $5^1\Pi g$ Na_2 using optical - optical double resonance spectroscopy has been done by Tsai et al [17] .

Theoretical part :

The emission of the molecule has appeared as lines that are composed of combination of rotation, vibration and electronic of spectral transitions between the electronic states, when the change in rotational quantum number is ΔJ=1, the R-branch will appear. Whereas when ΔJ=-1, P-branch will appear and when ΔJ=0, Q-branch will appear. The parent lines R(J), Q(J) and P(J) represent the emission spectrum. The values of energy for these bands can be determined using the equation (1) [4].

$$\nu = \nu_\circ + (B_V` + B_V``)m + (B_V` - B_V`` - D_V` + D_V``)m_2 - 2(D_V` + D_V``)m_3 - (D_V` - D_V``)m_4 \ldots(1)$$

For R (m=J+1) and for P (m = -J) lines.

$$\nu = \nu_\circ + (B_V` - B_V``)J(J+1) - (D_V` - D_V``)J^2(J+1)^2 \quad \ldots..(2)$$

For the Q-lines, where ν_o is the bond origin and can be determined from the equation [18]:-

$\nu_o = \Delta T_e + \Delta G_v$ ……..(3)

and

$\Delta T_e = T_{e`} - T_{e``}$

$\Delta G_v = G_{v`} - G_{v``}$ ….. (4)

$B_{v`}$, $B_{v``}$ are the rotational constants for excited and ground levels respectively.

B_v is determined from the equation (5) [19].

$B_v = B_e - \alpha_e (v+1/2)$ … (5)

Where α_e is the rotation-vibration interaction constant and it is determined by [20, 19].

$\alpha_e = 6(w_e\ \alpha_e\ \ Be^3\ )^{1/2} / w_e^2 - 6Be^2/we$ …. (6)

B_e is the rotational constant at equilibrium bond length and is determined by the equation (7) [20]

$Be = h / 8\text{Л}^2 \mu r_e^2 c$ ……… (7)

where μ is the reduced mass. and r_e is bond (Li-H) length .

D_v is the first centrifugal correction for the vibrational level v and it is determined by the equation (8) [19]

$D_v = D_e + B_e (v+1/2)$ ………….. (8)

and

$D_e = 4B_e^3/w_e^2$ ……….. (9)

B_e is the rotation –vibration interaction constant and is determined by the equation (10) [17].

$B_e = D_e(8\omega_e\chi_e/\omega_e - 5\alpha_e/B_e - \alpha_e^2\omega_e/24B_e)$ … (10)

The study of Λ-doubling is important for understanding the molecular structure. This doubling results from the split in one level which is produced from the interaction between the electronic and rotational motions [19, 18]. It increases with increasing of J. Therefore, for all rotational levels between Λ=0 degenerate doubly and the energy difference is very small for the two Λ components having the same value of J. So, the rotational levels are composed of coupling of the very close distance because of inversely on the value of J.

This small distance between Λ-components is represented by the following equation that can be used for the calculation of Λ- doubling values for the emission of P, Q and R transition [6]:-

$\Delta F_{e,f} = [F(J+1) - F(J)] - [Q(J+1) - P(J)]$…(11)

where J represents the rotational quantum number for upper level in the excited electronic state. F (J) can be calculated by the following equation [20, 21].

$F(J) = B_v [J(J+1) - \Lambda]$ … (12)

Results and Discussions:

Spectroscopic data of $^7LiH^1$ molecule is listed in Table (1).

Table 1: Spectroscopic constant of $^7LiH^1$ [22].

State/ Constant	$X\ \sum g^+$	$A\ \Pi_u$
T_e	0	26513.7cm^{-1}
ω_e	1055.12 cm^{-1}	180.711 cm^{-1}
r_e	1.595584 Å	2.59628 Å
αe	4.2338	1.6060 cm^{-1}
$\omega_e\chi_e$	13.228 cm^{-1}	13.987 cm^{-1}

1-Relation between the rotational energy levels F(J), F(J+1) with J :

It is observed from Fig 1 for (0-0) band, the distance between the rotational levels increases with increasing the values of J for all bands and this is in agreement with Graybeal [17], Banwell [19] and King [22]. The distance between rotational levels of $B^1\Pi_u$ state of $^7LiH^1$ molecule increases with increasing the value of J.

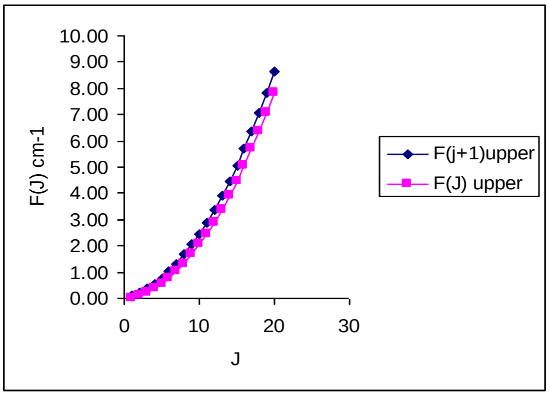

Fig (1): The relation between the rotational level energy F (J), F (J+1) determined in cm^{-1} as a function J for $^7LiH^1$

2-Relation between Λ - doubling value) with J:

It is observed from Fig 2 by applying equation (11) that **Λ** -doubling value decreases with increasing of J value and according to $\mathbf{q_\Lambda}$ values.

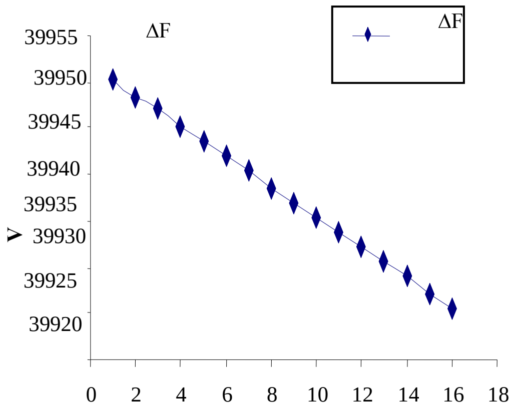

Fig (2): The relation between Λ-dubling value in cm^{-1} and J for (0-4) band of ^{7}LiH^{1} by ing equation (11)

Conclusion:

The values of $\bar{\nu}_P$, $\bar{\nu}_Q$, $\bar{\nu}_R$ are different because of the values of $B_{v''}$ and $B_{v'}$ Fig (1) shows that in the vibronic transitions, $B_{v''}$ is greater than $B_{v'}$ and the effect of terms J+1, -J and J is mentioned in equations (1) and (2) for R, P and Q bands. In Fig 2, the behavior of Λ-doubling value was parabolic manner, whereas its behavior was linear.

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حساب لمبدا دبلنغ لجزيئة $^{7}LiH^{1}$ باستخدام نظام حزم الانبعاث للانتقالات الالكترونية

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الخلاصة:

حساب لمبدا دبلنغ لجزيئة $^{7}LiH^{1}$ باستخدام نظام حزم الانبعاث للانتقالات الالكترونية $A^{2}\Pi_{u}$-$X^{1}\Sigma g^{+}$ وحساب العلاقة بين العدد الموجي ν_{p} , ν_{Q} , ν_{R} وحساب الحالات الدورانية للطاقات F(J), F(J+1) للعدد الكمي الدوراني (J) بالتتالي لجزيئة $^{7}LiH^{1}$ للحالات الارضية والمتهيجة باستخدام الثوابت الدورانية والاهتزازية للانتقالات الاهتزازية من v''=0 to v'=0- 4 باستخدام المستويات الدورانية من J=0 up to J=20 0

الكلمات المفتاحية: معامل مضاعف لمدا، الحالة الدورانية، الحالة الاهتزازية، جزيئة هايلدات الليثوم ،الحالة الارضية والحالة المتهيجة.