Dissociation Energy Measurements of H_2^2 C^{12} CL_2^{35} Br^{79} I_2^{127} Molecules

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Abstract: *A calculation has been carried out of dissociation energy of the electronic transition $X^2\sum^+$ ground states of H_2^2 C^{12} CL_2^{35} Br^{79} I_2^{127} molecules.*

Keywords: Dissociation Energy , electronic state , ground state , diatomic molecules, Herzberg equation.

1. Introduction

The relative intensities of the spectroscopic transitions occurring happens between the ground and excited states could be calculated using electronic transition moment and the overlap happens between the vibrational wave functions of the states (1). Knowing the dissociation energy is useful in the investigating of radiative transitions, atmospheric, chemistry and spectroscopic studies (2).

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 play a role in spectroscopic studies, one of these study measuring the potential energy of the diatomic molecules (experimentally and theoretically) (3).

In this study, molecule with electronic band $X^2\sum^+$ has been investigated, calculating the dissociation energy for the ground state $X^2\sum^+$ by applying a fitting to the experimental potential function described by Herzberg (4), and King (5).

Saleh et al (6) carried out a calculation of dissociation energy of free radical OH. While Shenyavskaya, and Yungman (7) investigated the dissociation energy of Halides gases.

2. Theory

Dissociation Energy
In the later years, the workers (8,9) adopted spectroscopic procedure for fitting histogram for reliable values of the dissociation energy of diatomic molecules, a brief account for the procedure being used for calculation of dissociation energy of diatomic molecules which is given by the following relation (4):

$$De = \frac{\omega\,e^2}{4\omega exe} \qquad [1]$$

3. Theoretical Results

In the present work, the spectroscopic constant is listed in Table. 1

Morse potential function for ground and excited states has been carried out from the experimental data by Huber and Herzberg (11), results shown in Table (2):

Table 1: Spectral constants (cm'^{1}) used as input data for calculation for molecule (4)

Molecule	we	wexe
H_2^2	3118.4	64.09
C^{12}	1641.35	11.67
CL_2^{35}	564.9	4.0
Br^{79}	323.2	1.07
I_2^{127}	214.57	0.6127

Table 2: Dissociation Energy (Cm^{-1}) of electronic state $X^2\sum^+$ of H_2^2 C^{12} CL_2^{35} Br^{79} I_2^{127} molecules

Molecule	Theoretical values D_e [eq.1]	Experimental value D_e [4]
H_2^2	3.1617	4.553
C^{12}	3.4844	3.6
CL_2^{35}	2.6592	2.475
Br^{79}	2.0338	1.971
I_2^{127}	1.5654	1.5417

4. Conclusions

1) By applying (eq.1) It was found that Cl_2^{35} molecule has higher pissocition energy while I_2^{127} has lower dissociation energy.
2) It was found that theoretical values calculating by using (eq.1) were approximation equal to the experimental values mentioned by Herzberg.

References

[1] T. J .Zielinski and G. M. Shalhoub, Report, Copyright by Division. Chem. Edu. Inc. Amer. Chem. Soc.(1998).
[2] K. N. Prithivi and N. Rajamamickam, Rev. Mex. Fis.48, (5), 432 (2002).
[3] S.R.Laghoff,Ewine F. van Dishooeck, R. Wetmore and A. Dalgamo, J. Chem. Phys. 77,(5),1379(1982).
[4] G. Herzberg, "Molecular spectra and Molecular structure; I. Spectra of Diatomic Molecules" Van Nostrand, New York (1950).
[5] G. W. King, "Spectroscopy and Molecular Structure" Holt, Rienhart and Winston, New York (1964).
[6] SALEH, Z.A., AL-AMIEDY, D.H. and CHIAD. B.T., Franck-Condom factor and dissociation energy for OH free radical. *Atti Della Fondazione Giorgio Ronchi Anno*

Anno LXN. 3, p.439.

[7] Shenyavskaya, E.A. and Yungman, V.S., 2004. NIST-JANAF thermochemical tables. III. Diatomic hydrogen halide gases. *Journal of physical and chemical reference data,* 55(3), pp.923-958.

[8] N. Rajamanickam K. Nagarajan and V. Raja, Spectrosc. Lett., 34, 43, (2001).

[9] J.B.Baharithya and S.H.Behere, ActaPhys.Slov., 42, 274, (1992).

[10] P.HuberandG.Herzberg,"Molecular spectra and Molecular structure; IV. Constants of Diatomic Molecules", Van Nostrand, New York (1979).

[11] K. S. wadi (2011) Ratah off in Morse potential for K2 molecule, Baghdad Sci: J., 8(4) : 968-971.