DISSOCIATION ENERGIES OF ScO, YO AND LaO

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Ground state dissociation energies of ScO, YO and LaO have been computed using the Lippincott potential function and a method of correlation coefficients. The results are in good agreement with the experimental values and those given by other workers.

I. INTRODUCTION

Knowledge of dissociation energies is of vital importance in astrophysics, chemical physics, thermochemistry, etc. There are many discrepancies in the available experimental and theoretical values of D.E.'s for a number of molecules. Studies in spectra of diatoms have revealed considerable information regarding molecular structure. Accurate vibrational and rotational constants of a large number of electronic states of various diatomic molecules are now available, so that the empirical potential functions can be used to infer dissociation energies. There are a number of empirical potential functions which fit to the experimentally determined Rydberg-Klein-Rees (RKR) [1] potential energy curves; amongst them are the Hulburt-Hirschfelder (H-H) [2], the Lippincott [3] and the electronegativity [4] potential functions known best. Various methods are employed for evaluating D.E.'s in which such potential functions are used.

In the present work, the three-parameter potential function proposed by Lippincott [3] and a method in which a correlation coefficient [5] is used, is applied to calculate the dissociation energies of ScO, YO and LaO molecules. These molecules are astrophysically important as their bands occur in the spectra of the M and the S type of stars [6]. The most recent ground state constants of these molecules are presented in Table 1.

II. THE POTENTIAL FUNCTIONS

The potential function suggested by Steele and Lippincott [3] is

$$U(r) = 8065.48 \, D_e \{1 - \exp[-n(r-r_e)^2/2r]\} \times$$
$$\times \{1 - a(b^2n/2r)^{\frac{1}{2}}(r-r_e) \times \exp[-(b^2nr_e/2r^2)^{\frac{1}{2}}(r-r_e)]\}, \quad (1)$$

Table 1
Constants of ground states of ScO, YO and LaO

Constant	ScO (*)	YO (+)	LaO (#)
μ_A	11.79748	13.55606	14.3433
ω_e	974.86	861.461	817.22
$\omega_e x_e$	4.23	2.867	2.206
B_e	0.5148	0.38886	0.3525
r_e	1.6661	1.788	1.8257
α_e	0.0027	0.00172	0.0014
D_e	6.96	8.023	9.384

All quantities are in cm^{-1} except r_e and D_e, which are in 10^{-10} meter units and eV respectively
* Ref [13] + Ref [14] # Ref [15]

where Δ is called the Sutherland parameter and expressed as $\Delta = (k_e r_e^2/2D_e)$; k_e is the force constant given by the expression $k_e = 5.8883 \times 10^{-2} \mu_A \omega_e^2$ (dynes.cm^{-1}). Since Δ is dimensionless D_e must be in ergs. If D_e is expressed in electronvolts (as it has been done in this paper), it should be converted into ergs by a conversion factor 1eV = 1.60199×10^{-12} ergs. The final formula for Δ is thus given by the expression

$$\Delta = (1.837808 \times 10^{10} \times \omega_e^2 \times \mu_A \times r_e^2)/D_e \, (eV), \quad (2)$$

ω_e is the harmonicity constant and r_e is the equilibrium internuclear distance. μ_A is the reduced mass. The constant n is expressed as $n = (2\Delta/r_e)$; and finally the constant a is evaluated from $a = (4/5)[1 - (1/b\Delta^{\frac{1}{2}})]$ where $b = 1.065$. Among these three parameters Δ, n and a in the potential function (1), Δ and a are dimensionless, whereas n has the units of cm^{-1}.

The Hulburt-Hirschfelder [2] (H-H) potential function is given by

$$U(r) = 8065.48 D_e[(1 - \exp(-x))^2 + (1 + bx)cx^3 \exp(-2x)], \quad (3)$$

where

$$x = [\omega_e/2(B_e D_e \times 8065.48)^{\frac{1}{2}}][(r-r_e)/r_e],$$
$$c = 1 + a_1(8065.48 D_e/a_0)^{\frac{1}{2}}, \quad (4)$$
$$b = \{2 - [(7/12) - (8065.48 D_e a_2/a_0)]/c\}. \quad (5)$$

The constants a_0, a_1 and a_2 in the above expressions are the Dunham coefficients and they are defined by the expressions

$$a_0 = (\omega_e^2/4B_e),$$
$$a_1 = -1 - (\omega_e \alpha_e/6B_e^2)$$
$$a_2 = (5/4)a_1^2 - (2/3)(\omega_e x_e/B_e). \quad (6)$$

In the above expressions, except a_0, all constants, viz. a_1, a_2, x, c and b, are dimensionless. The constant a_0 is in cm^{-1}. The spectroscopic constants $\omega_e x_e$, B_e and α_e are known as anharmonicity and rotational constants, respectively.

III. METHOD OF CORRELATION COEFFICIENTS

Once the RKR turning points corresponding to each vibrational level have been computed, they are substituted in the potential function selected and the corresponding U_{min} and U_{max} values are calculated assuming an arbitrary value of D_e. A correlation coefficient is calculated for this case and the procedure is repeated for a large number of D_e chosen systematically. Thus a variation of the correlation coefficient is obtained for different values of D_e. The particular values of D_e generating the maximum correlation coefficient is then selected as its optimum value. This method was developed by Rao et al. [7-9] who applied it to CO, AlO, Li$_2$, CN and CuH molecules. We have also applied this method to diatomic mercury halides, chromium fluoride (CrF) and boron bromide (BBr) and the results are published elsewhere [10-12].

IV. RESULTS AND DISCUSSION

The molecular constants of the ground states of ScO, YO and LaO have been taken from [13-16], respectively. Table 2 shows the results of correlation computations. In case of ScO, the Lippincott function gives the maximum correlation of 0.9999744 at D_e = 6.7eV. For YO, the Lippincott and

Table 2
Correlation coefficients for ScO, YO and LaO using Lippincott function

D_e	ScO Cor.coeff	D_e	YO Cor.coeff	D_e	LaO Cor.coeff
1	0.7397276	1	0.7215684	1	0.7718919
2	0.8885714	2	0.8752476	2	0.9038958
3	0.9535235	3	0.9460048	3	0.9583326
4	0.9822526	4	0.9784619	4	0.9825846
5	0.9946489	5	0.9929897	5	0.9936474
6	0.9992329	6	0.9987272	6	0.9983945
7	0.999018	7	0.999807	7	0.9999155
8	0.9985566	8	0.9988894	8	0.9997141
9	0.996761	9	0.9997141	9	0.9985761
10	0.9932856	10	0.9965649	10	0.9969318
6.2	0.9995991	6.3	0.9994482	6.7	0.9996889
6.3	0.9996337	6.4	0.9996139	6.8	0.9997820
6.4	0.9996545	6.5	0.9997466	6.9	0.9998564
6.5	0.9999080	6.6	0.9998498	7.0	0.9999152
6.6	0.9999534	6.7	0.9999212	7.1	0.999954
6.7	0.9999744	6.8	0.9999654	7.2	0.9999794
6.8	0.9999721	6.9	0.9999851	7.3	0.9999889
6.9	0.9999464	7.0	0.9999796	7.4	0.9999861
7	0.9999018	7.1	0.9999522	7.5	0.9999694
7.1	0.9998352	7.2	0.9999029	7.6	0.9999397
7.2	0.9997516	7.3	0.9998356	7.7	0.9998982

H-H functions are almost comparable, as the former gives a maximum correlation coefficient of 0.9999807 at 6.9eV and the latter gives the correlation coefficient of 0.9999851 at 6.9eV. It can also be seen from Table 2 that for LaO, the Lippincott function gives the a maximum correlation at D_e as 7.3eV with the correlation coefficient 0.9999889. Corresponding to this D_e, the H-H function yields an inferior correlation as the correlation coefficient is only 0.9993985. The results of the D_e values along with the values reported by different workers are presented in Table 3.

Table 3
Ground state dissociation energies of ScO, YO & LaO

Molecule	Investigator	Ref	Method	D_e (eV)
ScO	Huber & Herzberg	16	Thermochemical	6.89
	Gaydon	17	Thermochemical	6±1
	Suchard	18	Mass Spectro.	6.96±0.8
	Pedley & Marshall	19	Exptl.	6.95±0.2
	Rao etal	7	Electronegativity fun.	5.39±0.1
	Present studies		Lippincott fun.	6.8±0.1
YO	Hubert & Herzberg	16	Thermochemical	7.03
	Gaydon	17	Thermochemical	7.0±2
	Suchard	18	Mass Spectro.	7.39±0.11
	Ishwar etal	20	Lippincott fun.	6.78±0.006
	Ackerman & Rauh	21	P.E. Curves	7.29
	Present studies		Lippincott fun.	6.9±0.1
LaO	Huber & Herzberg	16	Thermochemical	8.18
	Gaydon	17	Thermochemical	7.0±2
	Ames	22	Mass Spectro.	8.25±0.11
	Behere & Sardesai	23	Electronegativity fun.	7.87
	Present studies		Lippincott fun.	7.3±0.1

The D.E.'s of ScO and YO reported in the present work are in good agreement with the values reported by other workers. For LaO, the D.E. reported differs from the thermochemical value by 10%.

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ЭНЕРГИИ ДИССОЦИАЦИИ ScO, YO И LaO

В работе даются результаты вычисления энергии диссоциации основных составляний ScO, YO и LaO. Расчеты проведены с применением потенциальной функции Липинкота и метода коэффициентов корреляции. Результаты показывают хорошее согласие с экспериментальными величинами и результатами других авторов.