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ON THE ESTIMATION OF THE DISSOCIATION ENERGY OF BS

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The true potential energy curves for the $X^2\Sigma^+$, $A^2\pi_i$ and $B^2\Sigma^+$ states of the BS molecule have been constructed by the Rydberg-Klein-Rees method as modified by Vanderslice *et al.*[5] The dissociation energy is estimated to be 5.814 ± 0.017eV from fitting the three-parameter Lippincott potential function.[6] The value recommended by Uy and Drowart[2] is 5.976eV.

Key Words : Potential Energy Curves; Lippincott Potential Function; Curve Fitting Method; Dissociation Energy

INTRODUCTION

DISSOCIATION energies of diatomic molecules are of great interest in thermochemistry, combustion physics and astrophysics. In quantitive problems of valency, statistical calculations of equilibria at high temperatures, in chemical bonding and in many other problems, the dissociation energy plays a fundamental role. Spectroscopists and chemists are concerned with the determination of reliable values of dissociation energies for the diatomic molecules.

The present study deals with the estimation of dissociation energy of BS. Many investigators[1,2,3] have determined the value of dissociation energy of BS by different methods. However, potential energy curves of BS are not available in the literature. Further, the reported values of dissociation energy of BS differ considerably.[1,2,4] The molecular constants required for the present study have been taken from Jeneouvrien and Pascat.[3]

POTENTIAL ENERGY CURVES

The RKRV method[5] is an improved form of RKR method, which makes use of Wentzel-Kramers-Brillouin (WKB) approximation from which we obtain reliable potential energy curves with the observed vibrational and rotational constants. Because the details of the method of RKRV has been described before,[5] only the results are presented in Table I for $X^2\Sigma^+$, $A^2\pi_i$ and $B^2\ \Sigma^+$ states of BS.

Note : The paper was accepted for publication on 14 March 1986.

Dissociation Energy

Accurate evaluation of dissociation energy from curve fitting requires a good empirical potential function. The three parameter Lippincott Potential function[6] has been shown to reproduce well RKRV curves over a wide range of energies and for a number of diatomic molecules.[7-11]

The turning points of the ground state of BS obtained in the present study have been used in the Lippincott function for a particular value of D_e. The observed energy values of U have then been compared with the calculated energy values (U_{min}, U_{max}). This procedure was repeated for different values of D_e. The value (46,899.12cm^{-1}) for which the best fit obtains is taken to be the dissociation energy of the molecule.

Table I

Potential energy curves for the electronic states of BS molecule

V	U (cm^{-1})	R_{min} (A°)	R_{max} (A°)
		$X^2\Sigma^+$ State	
0	588.39	1.5528	1.6712
1	1755.80	1.5152	1.7211
2	2910.71	1.4908	1.7579
3	4053.12	1.4719	1.7893
4	5183.03	1.4561	1.8177
5	6300.44	1.4424	1.8441
		$A^2\pi_i$ State	
0	375.91	1.7478	1.8959
1	1120.43	1.7019	1.9599
2	1855.23	1.6726	2.0074
3	2580.32	1.6500	2.0485
4	3895.69	1.6314	2.0858
5	4001.34	1.6155	2.1206
6	4697.27	1.6015	2.1568
7	5383.48	1.5890	2.1857
8	6059.98	1.5776	2.2167
9	6726.76	1.5673	2.2469
10	7383.82	1.5578	2.2766
11	8031.16	1.5490	2.3059
12	8668.78	1.5407	2.3348
		$B^2\Sigma^+$ State	
0	383.59	1.7317	1.8783
1	1146.21	1.6854	1.9401
2	1902.73	1.6555	1.9855
3	2653.15	1.6325	2.0242
4	3397.47	1.6134	2.0591

Results and Discussion

The turning points obtained from the RKRV method for $X^2\Sigma^+$, $A^2\pi_i$ and $B^2\Sigma^+$ states are presented in Table I. The relevant $U(r)$ values for the selected D_e values are given in Table II. The average percentage deviations for these D_e values are also listed in Table II.

Table II

Energy values from the lippincott potential function for BS

V	RKRV Å	$G(v)$	D_e=46700 cm^{-1}	D_e=46900 cm^{-1}	D_e=47100 cm^{-1}
0	1.5528	588.39	588.72	591.23	593.77
1	1.5152	1755.80	1752.59	1760.07	1767.61
2	1.4908	2910.71	2904.17	2916.56	2929.05
3	1.4719	4053.12	4043.85	4061.09	4078.49
4	1.4561	5183.03	5171.72	5193.77	5216.02
5	1.4424	6300.44	6287.86	6314.67	6441.19
0	1.6712	588.39	580.51	582.99	585.48
1	1.7211	1755.80	1739.60	1747.02	1754.50
2	1.7579	2910.71	2890.21	2902.53	2914.97
3	1.7893	4053.12	4031.79	4048.98	4066.32
4	1.8177	5183.03	5164.02	5186.04	5208.26
5	1.8441	6300.44	6286.61	6313.41	6340.46
Average % deviation			0.432	0.302	0.500

The electronegativity values of B and S are not very different and the bonding between B and S is of covalent type. The Lippincott three-parameter potential function being based on a δ-type model of binding is dispensably covalent in nature.[12] Hence, the Lippincott potential function is suited for BS molecule.

A "best" fit of energy values is achieved for 5.814eV, when the average percentage deviation in only 0.302. Thus, $D_e = 5.814 \pm 0.017$eV; the error indicates in the D_e value takes into account the error of 3 per cent inherent to Lippincott potential function and the error involved in the curve fitting.

The estimated D_e value (5.814 ± 0.017eV) agrees with the value of 5.97eV given by Uy and Drowart.[2] The estimated value of 5.814eV agrees within 5 per cent to the value (6.075eV) reported by Bell and Mclean.[1]

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