

DISSOCIATION ENERGY OF THE CuBr MOLECULE

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ABSTRACT

The experimental potential energy curves for $X^1\Sigma^+$, $A(^1\Pi)$ and $C^1\Sigma^+$ states of the cuprous bromide molecule have been constructed by the method of Lakshman and Rao. The ground state dissociation energy of the molecule has been estimated as 2.29 ± 0.02 eV by the curve fitting procedure.

INTRODUCTION

A KNOWLEDGE of the exact value of the dissociation energy of diatomic molecules is of fundamental importance for thermochemistry and it is often of interest in astrophysics. As no attempt had been made so far, to evaluate theoretically the dissociation energy of CuBr molecule, the present authors have taken up this investigation. The present paper deals with the construction of potential energy curves for $X^1\Sigma^+$, $A(^1\Pi)$ and $C^1\Sigma^+$ states of CuBr molecule using the method of Lakshman and Rao¹; and the estimation of dissociation energy for the ground state of the molecule by fitting the three-parameter Lippincott potential

function² with the experimental potential energy curve. The molecular constants required for the present study have been taken from Huber and Herzberg³ and Mishra *et al.*⁴.

POTENTIAL ENERGY CURVES

The method of Lakshman and Rao is a modified form of RKR method⁵ in which f and g terms are written in a simplified form. As the present method of Lakshman and Rao was successfully verified for several states belonging to different diatomic molecules^{3,6}, only the results of the present work are given in Tables I and II.

TABLE I

Turning points of the ground state potential energy curve of CuBr, and calculated energy values by Lippincott function at $D_0 = 18600$ cm^{-1}

v	U (cm^{-1})	$U+T_0$ (cm^{-1})	r_{min} (Å)	r_{max} (Å)	U_{min} (cm^{-1})	U_{max} (cm^{-1})
$r_0 = 2.173441$						
0	157.16	157.16	2.1204	2.2311	157.29	157.30
1	470.04	470.04	2.0842	2.2766	470.22	470.89
2	781.00	781.00	2.0606	2.3096	780.99	781.53
3	1090.04	1090.04	2.0421	2.3374	1089.01	1090.76
4	1397.16	1397.16	2.0266	2.3624	1394.56	1397.39
5	1702.97	1702.36	2.0132	2.3853	1698.21	1702.97
6	2005.60	2005.64	2.0012	2.4068	1996.41	2005.60
7	2307.00	2307.00	1.9904	2.4272	2292.97	2306.05
8	2606.44	2606.44	1.9805	2.4468	2587.39	2603.84
9	2903.96	2903.96	1.9714	2.4656	2881.06	2901.09

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TABLE II
Turning points of the potential energy curves for the upper states of CuBr

v	U (cm ⁻¹)	$U + T_e$ (cm ⁻¹)	r_{\min} (Å)	r_{\max} (Å)
<i>A</i> (¹ π) State $r_e = 2.234$				
0	147.81	20646.57	2.1799	2.2941
1	441.92	20942.70	2.1441	2.3424
2	734.01	21238.83	2.1186	2.3799
3	1024.08	21534.96	2.1035	2.4083
4	1312.13	21831.09	2.0890	2.4356
<i>C</i> ¹ Σ^+ State $r_e = 2.261$				
0	147.09	23608.25	2.2060	2.3205
1	439.67	23902.95	2.1695	2.3674
2	730.13	24197.65	2.1439	2.4015
3	1018.47	24492.35	2.1247	2.4304
4	1304.69	24787.05	2.1085	2.4562

DISSOCIATION ENERGY

An accurate evaluation of the dissociation energy of a molecule, by the method of curve fitting, requires an empirical potential function which gives the best reproduction of the experimental potential energy curve. The three parameter Lippincott potential function² has been shown to reproduce quite well the RKR curves over a wide range of energy for a number of diatomic molecules⁷⁻⁹.

The turning points of the ground state of CuBr, obtained in the present study, are used in the Lippincott function and for a particular value of D_e , the observed energy values of U are compared with the calculated energy values (U_{\min} , U_{\max}). This procedure is repeated for different values of D_e and the D_e value (18600 cm⁻¹), for which the best fit of the energy values is observed, is taken as the precise dissociation energy of the molecule.

RESULTS AND DISCUSSION

The turning points obtained for twenty vibrational levels of the three electronic states of CuBr molecule are presented in Tables I and II.

It is found that the average percentage deviations of calculated energy values for $D_e = 18200$ cm⁻¹ and 19000 cm⁻¹ are 2.30 and 1.99 respectively. Whereas the best fitting of the calculated energy values shown in Table I is achieved for $D_e = 2.31$ eV since the average percentage deviation in this case is only 0.17. Hence the dissociation energy for the ground state of CuBr is 2.31 ± 0.02 eV and the value as measured from the lowest vibrational level is $D_0 = 2.29$ eV. But this estimated value is lower than the thermochemical value (3.4 ± 0.25 eV) reported by Brewer and Lofgren¹⁰. The deviation in the present theoretical value shows the strong ionic binding in the ground state of the molecule.

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