Bull. Astr. Soc. India (1996) **24**, 31–38

Some vibrational bands of A-X system of BO molecule in the umbral spectrum of Sun

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Received 20 March 1995; accepted 12 June 1995

Abstract. Vibrational transition probabilities, namely Franck - condon factors and $\bar{r}$ - centroids, have been evaluated using an approximate analytical method for the A-X system of BO molecule. Morse potential energy curves for $x^2\Sigma$ (v = 0–50) and $A^2\pi_i$ (v = 0–50) states of BO have been constructed using the latest spectroscopic data. The value of $\bar{r}$ - centroids for the band have been found to increase with the corresponding wavelengths. The sequence differences $\Delta\bar{r}$ - remain approximately constant for the $\bar{r}$ - centroids. We show results for some others bands of BO in the umbral spectrum of Sun.

Key words : BO molecule—vibrational bands—umbral spectrum of Sun

1. Introduction

When one tries to estimate the physical conditions (i.e., temperature, pressure, density, and abundance) of the emitter from the relative intensities of the bands of a molecule, one must have a theoretical knowledge of the corresponding potential energy curves, $\bar{r}$ – centroids, and the vibrational transition probabilities (FCF_S) for the respective bandheads in a band system. The largest observational problem with the spectra is blending of the BO lines with other stronger lines. We guess that transition probabilities is related to problems with blending in the solar spectrum. The (0,0), (0,1) and (0,2) bands and lines of A-X system of the BO had questionable presence and may be observed in the umbral spectrum (Engvold 1970' Sotirovski 1971; Wöhl 1971) and in M-type stellar spectra, such as those of Betelgeuse, β Pegasi and R Leonis listed by Straughan & Walker (1976). The FCF_S and $\bar{r}$ - centroids of D-B system of BO have been listed by Huber & Herzberg (1979).

We analyse here Vibrational $\bar{r}$ - centroids and Morse potential energy curves of $x^2\Sigma$ (v = 0 – 50) and $A^2\pi_i$ (v = 0 – 50) states of the BO molecule using the experimental data available in literature (Pearse & Gaydon 1963).

2. Calculations

2.1. Franck-condon factors

The relative intensities of the vibrational bands within a band system of a diatomic molecule are controlled mainly by the population distribution over the vibrational levels and by the Franck-Condon factor ($q_{v',v''}$) defined as

$$q_{v',v''} = |{}^*\Psi_{v'}\ \Psi_{v''}|^2 ,$$

Where v′ and v″ are the vibrational quantum numbers of the upper and lower electronic states respectively; $\Psi_{v'}$ and $\Psi_{v''}$ are the vibrational eigenfunctions; and r is the internuclear distance. The derived molecular constants, $\propto_{cal}$, $\propto$, K and ς have been calculated by using molecular constants μ, T_e, w_e, $w_e x_e$, B_e, r_e and $\propto_e$ of Huber & Herzberg (1979) and equations given by Fraser & Jarmain (1953). These results are listed in table 4. FCF_S have been calculated for a Morse (1929) model by using Fraser & Jarmain (1953) method and experimental data of Pearse & Gaydon (1963) table 5.

2.2. $\bar{r}$ - Centroids

The $\bar{r}$ - centroids, $\bar{r}v', v''$ representing the characteristic internuclear separation corresponding to (v′, v″) transition in a diatomic molecular band system have been defined by Nicholls & Jarmain (1956) by the relation

$$\bar{r}v', v'' = \int \Psi_{v'}\, r\, \Psi_{v''}\, dr \,/ \int \Psi_{v'}\ \Psi_{v''}\, dr,$$

where r is the internuclear separation.

The $\bar{r}$ - centroids have been computed by the quadratic equation method of Nicholls & Jarmain (1956), since $r_e = |r_{e1} - r_{e2}| > 0.05$Å, the graphical method has not been used to evaluate $\bar{r}$-centroids.

These values are listed in table 5. The value $|\propto_1 - \propto_2| / |\propto_1 + \propto_2| < 0.05$ for this system, the r_e shift correction has not been applied.

2.3. Potential energy curves

The construction of accurate potential energy curves is of importance in physical problems arising in astrophysics, gas kinetic and molecular spectroscopy. The quantities r_{min} and r_{max} are computed by solving the Morse potential function.

Tables 1 and 2 list the various quantities.

Table 1. Values of energy levels, turning points, centres, and half-widths for the $A^2\pi_i$ state of BO molecule using Morse potential function.

Vibrational quantum number	Energy level U + Te (cm^{-1})	r_{min} (Å)	r_{max} (Å)	Centre (Å)	Half-width (Å)
0	24586.3208	1.305968	1.400633	1.353301	0.047333
1	25824.707	1.279268	1.444465	1.361867	0.082599
2	27040.779	1.263140	1.478037	1.370589	0.107449
3	28234.537	1.251351	1.507592	1.379472	0.128121
4	29405.981	1.242101	1.534940	1.388521	0.146420
5	30555.111	1.234573	1.560910	1.397742	0.163169
6	31681.927	1.228314	1.585964	1.407139	0.178825
7	32786.429	1.223042	1.610395	1.416719	0.193677
8	33868.616	1.218570	1.634403	1.426487	0.207917
9	34928.49	1.214763	1.658129	1.436446	0.221683
10	35966.05	1.211524	1.681685	1.446605	0.235081
11	36981.3	1.208778	1.705155	1.456967	0.248189
12	37974.23	1.206465	1.728610	1.467538	0.261073
13	38944.85	1.204537	1.752106	1.478322	0.273785
14	39893.15	1.202959	1.775693	1.489326	0.286367
15	40819.14	1.201697	1.799413	1.500555	0.298858
16	41722.82	1.200724	1.823303	1.512014	0.311290
17	42604.18	1.200018	1.847398	1.523708	0.323690
18	43463.23	1.199560	1.871726	1.535643	0.336083
19	44299.96	1.199332	1.896317	1.547825	0.348493
20	45114.38	1.199319	1.921194	1.560257	0.360938
21	45906.49	1.199509	1.946383	1.572946	0.373437
22	46676.28	1.199889	1.971906	1.585898	0.386009
23	47423.76	1.200448	1.997783	1.599116	0.398668
24	48148.92	1.201178	2.024036	1.612607	0.411429
25	48851.77	1.202068	2.050683	1.626376	0.424308
26	49532.3	1.203112	2.077744	1.640428	0.437316
27	50190.53	1.204302	2.105236	1.654769	0.450467
28	50826.44	1.205630	2.133177	1.669404	0.463774
29	51440.03	1.207091	2.161585	1.684338	0.477247
30	52031.31	1.208678	2.190475	1.699577	0.490899
31	52600.27	1.210385	2.219865	1.715125	0.504740
32	53146.93	1.212207	2.249770	1.730989	0.518782
33	53671.27	1.214139	2.280206	1.747173	0.533034
34	54173.29	1.216176	2.311190	1.763683	0.547507
35	54653.0	1.218312	2.342736	1.780524	0.562212
36	55110.4	1.220543	2.374859	1.797701	0.577158
37	55545.48	1.222865	2.407576	1.815221	0.592356

Table 1. Continued

Vibrational quantum number	Energy level U + Te (cm^{-1})	r_{min} (Å)	r_{max} (Å)	Centre (Å)	Half-width (Å)
38	55958.25	1.225274	2.440900	1.833087	0.607813
39	56348.7	1.227764	2.474848	1.851306	0.623542
40	56716.84	1.230332	2.509433	1.869883	0.639551
41	57062.67	1.232974	2.544671	1.888823	0.655849
42	57386.18	1.235686	2.580576	1.908131	0.672445
43	57687.38	1.238463	2.617162	1.927813	0.689350
44	57966.26	1.241301	2.654445	1.947873	0.706572
45	58222.83	1.244198	2.692439	1.968319	0.724121
46	58457.09	1.247148	2.731159	1.989154	0.742006
47	58669.03	1.250148	2.770618	2.010383	0.760235
48	58858.65	1.253195	2.810832	2.032014	0.778819
49	59025.97	1.256284	2.851814	2.054049	0.797765
50	59170.97	1.259411	2.893581	2.076496	0.817085

Table 2. Values of energy levels, turning points, centres, and half-widths for the $x^2\Sigma$ state of BO molecule using Morse potential function

Vibrational quantum number	Energy level U + Te (cm^{-1})	r_{min} (Å)	r_{max} (Å)	Centre (Å)	Half-width (Å)
0	939.8925	1.160912	1.248088	1.204500	0.043588
1	2401.963	1.134501	1.286294	1.210398	0.075897
2	4640.412	1.117865	1.314877	1.216371	0.098506
3	6455.242	1.105236	1.339605	1.222421	0.117185
4	8246.452	1.094949	1.362150	1.228550	0.133601
5	10014.04	1.086241	1.383277	1.234759	0.148518
6	11758.01	1.078692	1.403411	1.241052	0.162360
7	13478.36	1.072040	1.422817	1.247429	0.175389
8	15175.09	1.066108	1.441675	1.253892	0.187784
9	16848.2	1.060771	1.460113	1.260442	0.199671
10	18497.69	1.055937	1.478229	1.267083	0.211146
11	20123.56	1.051536	1.496097	1.273817	0.222281
12	21725.81	1.047512	1.513774	1.280643	0.233131
13	23304.44	1.043820	1.531310	1.287565	0.243745
14	24859.45	1.040425	1.548774	1.294600	0.254175
15	26390.84	1.037297	1.566109	1.301703	0.264406
16	27898.61	1.034410	1.583435	1.308923	0.274513
17	29382.76	1.031743	1.600746	1.316245	0.284502
18	30843.29	1.029279	1.618064	1.323672	0.294393

Table 2. Continued

Vibrational quantum number	Energy level U + Te (cm^{-1})	r_{min} (Å)	r_{max} (Å)	Centre (Å)	Half-width (Å)
19	32280.2	1.027000	1.635410	1.331205	0.304205
20	33693.49	1.024894	1.652800	1.338847	0.313953
21	35083.16	1.022947	1.670251	1.346599	0.323652
22	36449.21	1.021150	1.687776	1.354463	0.333313
23	37791.64	1.019492	1.705390	1.362441	0.342949
24	39110.45	1.017965	1.723105	1.370535	0.352570
25	40405.64	1.016561	1.740931	1.378746	0.362185
26	41677.21	1.015272	1.758881	1.387077	0.371805
27	42925.16	1.014093	1.776963	1.395528	0.381435
28	44149.49	1.013018	1.795189	1.404104	0.391086
29	45350.2	1.012040	1.813566	1.412803	0.400763
30	46527.29	1.011155	1.832104	1.421630	0.410475
31	47680.76	1.010358	1.850811	1.430585	0.420227
32	48810.61	1.009646	1.869695	1.439671	0.430025
33	49916.84	1.009012	1.888764	1.448888	0.439876
34	50999.46	1.008455	1.908025	1.458240	0.449785
35	52058.44	1.007970	1.927486	1.467728	0.459758
36	53093.81	1.007553	1.947154	1.477354	0.469801
37	54105.57	1.007202	1.967035	1.487119	0.479917
38	55093.69	1.006914	1.987137	1.497026	0.490112
39	56058.2	1.006685	2.007466	1.507076	0.500391
40	56999.1	1.006512	2.028028	1.517270	0.510758
41	57916.36	1.006394	2.048831	1.527613	0.521219
42	58810.01	1.006327	2.069880	1.538104	0.531777
43	59680.05	1.006309	2.091181	1.548745	0.542436
44	60526.45	1.006337	2.112741	1.559539	0.553202
45	61349.24	1.006409	2.134565	1.570487	0.564078
46	62148.41	1.006523	2.156661	1.581592	0.575069
47	62923.96	1.006677	2.179032	1.592855	0.586178
48	63675.9	1.006868	2.201686	1.604277	0.597409
49	64404.2	1.007094	2.224627	1.615861	0.608767
50	65108.89	1.007354	2.247863	1.627609	0.620255

3. Discussion

The calculated and observed values of α_e are shown in tables 3 and 4. These values are in agreement with the Pekeris (1934) relation, more so in the case of $x^2\Sigma$ than $A^2\pi_i$ states.

Since $\bar{r}_{0,0}$ is lower than $(r_{e1} + r_{e2})/2$, the potentials are anharmonic. Further we note that the internuclear separation for the transition is not negligible. As a result the primary Condon locus is therefore not narrow and $q_{0,0}$ has the lower value.

Table 3. Basic molecular constants for the A-X system of BO molecule; $\mu = 6.52094009$.

	From Huber and Herzberg (1979)					
State	T_e $(cm)^{-1}$	w_e $(cm)^{-1}$	w_ex_e $(cm)^{-1}$	B_e $(cm)^{-1}$	r_e (Å)	α_e $(cm)^{-1}$
$A^2\pi_i$	23958.76	1260.70	11.157	1.4018	1.3533	0.0196
$x^2\Sigma$	0	1885.69	11.81	1.7820	1.2045	0.0166

Table 4. Derived molecular constants for the A-X system of BO molecule; $\mu = 6.52094009$

	From Pekeris (1934), Fraser and Jarmain (1953)			
State	α_{cal} (cm^{-1})	α $(Å^{-1})$	K	ζ
$A^2\pi_i$	0.017032	2.077248355	112.9963252	1.046580632
$x^2\Sigma$	0.015908	2.137172887	159.6689246	0.957389057

In the present case $\bar{r}_{v'+1,\, v''+1} - \bar{r}_{v',v''}$ for a sequence is less than 0.01Å, showing that the two potentials involved in the transition are not very wide.

Since $r_{e1} > r_{e2}$, $\bar{r}_{v',v''}$ increases with the increase in wavelength which is expected in the red degraded band systems. It may be remarked that the value of $\bar{r}$-centroids for any band is found to increase with the corresponding wavelength.

Our results presented in last column of table 5 with question marked indicate that laboratory bandheads of A-X system of BO could also be present in the umbral spectrum of Sun, since the corresponding transition probabilities are appreciable.

Table 5. Frank-Condon factors, $\bar{r}$–centroids, wavelengths, $\Delta\bar{r}$–value for (0,0) sequence, and band origin for A-X system of BO molecule

Wavelengths with visual estimates of intensity (Å)	Band	Frank–Condon factors	$\bar{r}$-centroids (Å)	Band origin (cm^{-1})	$\Delta\bar{r}$ – Value for (0,0) sequence (Å)	Indentification*
6165.4(5)	(0,4) Q1	0.3248	1.388929	16339.8683	—	?
6159.7(5)	(0,4) R1	0.3248	1.388929	16339.8683	—	?
5551.5(8)	(0,3) Q1	0.5197	1.359331	18131.0783	—	?
5547.5(7)	(0,3) R1	0.4547	1.359331	18131.0783	—	?
5513.0(5)	(0,3) R2	0.3248	1.359331	18131.0783	—	?
5043.5(6)	(0,2) Q1	0.3898	1.330597	19945.9083	—	✔
5040.1(9)?	(0,2) R1	0.5847	1.330597	19945.9083	—	✔
5011.6(4)	(0,2) R2	0.2599	1.330597	19945.9083	—	✔
4746.9(8)	(1,2) Q1	0.5197	1.311640	21184.2943	—	?
4744.0(8)	(1,2) R1	0.5197	1.311640	21184.2943	—	?
4718.7(5)	(1,2) R2	0.3248	1.311640	21184.2943	—	?
4715.5(5)	(1,2) R21	0.3248	1.311640	21184.2943	—	?
4615.4(10)	(0,1) Q1	0.6496	1.302630	21784.3583	—	✔
4612.7(10)	(0,1) R1	0.6496	1.302630	21784.3583	—	✔
4588.8(8)	(0,1) R2	0.5197	1.302630	21784.3583	—	✔
4585.7(7)	(0,1) R21	0.4547	1.302630	21784.3583	—	✔
4365.9(8)	(1,1) Q1	0.5197	1.284374	23022.7443	0.009031	?
4363.4(10)	(1,1) R1	0.6496	1.284374	23022.7443	0.009031	?
4341.9(8)	(1,1) R2	0.5197	1.284374	23022.7443	0.009031	?
4339.4(8)	(1,1) R21	0.5197	1.284374	23022.7443	0.009031	?
4250.4(5)	(0,0) Q1	0.3248	1.275343	23646.4283	—	✔
4247.9(4)	(0,0) R1	0.2599	1.275343	23646.4283	—	✔
4227.5(4)	(0,0) R2	0.2599	1.275343	23646.4283	—	✔
4145.5(7)	(2,1) Q1	0.4547	1.266863	24238.8163	—	?
4143.4(6)	(2,1) R1	0.3898	1.266863	24238.8163	—	?
4124.1(4)	(2,1) R2	0.2599	1.266863	24238.8163	—	—
4037.4(8)	(1,0) Q1	0.5197	1.257717	24884.8143	—	?
4035.5(7)	(1,0) R1	0.4547	1.257717	24884.8143	—	?
4017.1(6)	(1,0) R2	0.3898	1.257717	24884.8143	—	?
4015.0(5)	(1,0) R21	0.3248	1.257717	24884.8143	—	?
3950.5(4)	(3,1) Q1	0.2599	1.250044	25432.5743	—	—
3848.7(10)	(2,0) Q1	0.6496	1.240778	26100.8863	—	?
3847.0(9)	(2,0) R1	0.5847	1.240778	26100.8863	—	?
3829.9(8)	(2,0) R2	0.5197	1.240778	26100.8863	—	?
3828.0(6)	(2,0) R21	0.3898	1.240778	26100.8863	—	?
3679.1(10)	(3,0) Q1	0.6496	1.224480	27294.6443	—	?
3677.8(8)	(3,0) R1	0.5197	1.224480	27294.6443	—	?

Table 5. Continued

Wavelengths with visual estimates of intensity (Å)	Band	Frank–Condon factors	$\bar{r}$-centroids (Å)	Band origin (cm^{-1})	$\Delta\bar{r}$ – Value for (0,0) sequence (Å)	Indentification*
3662.3(6)	(3,0) R1	0.3898	1.224480	27294.6443	—	?
3660.6(5)	(3,0) R21	0.3248	1.224480	27294.6443	—	?
3526.8(7)	(4,0) Q1	0.4547	1.208779	28466.0883	—	?
3525.5(7)	(4,0) R1	0.4547	1.208779	28466.0883	—	?
3511.3(6)	(4,0) R2	0.3898	1.208779	28466.0883	—	?
3510.0(5)	(4,0) R21	0.3248	1.208779	28466.0883	—	?
3389.1(5)	(5,0) Q1	0.3248	1.193640	29615.2183	—	?
3387.6(7)	(5,0) R1	0.4547	1.193640	29615.2183	—	?
3374.7(5)	(5,0) R2	0.3248	1.193640	29615.2183	—	?

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* ✔ identified in the umbral spectrum of Sun.

? expected to be present in the umbral spectrum of Sun

Acknowledgements

We are thankful to Dr. M. Jauhari, Director General of National Test House for patronage and providing necessary facilities to complete this work. The authors thankfully acknowledge the useful comments and suggestions given by the anonymous referee.

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