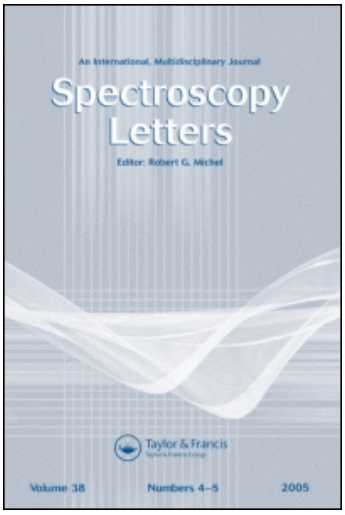

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ROTATION ANALYSIS OF THE B-X 0-1 BANDS OF GaO

Key words: Electronic bands, gallium oxide, isotope effect

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ABSTRACT

The 0-1 band of the $B^2\Sigma^+$-$X^2\Sigma^+$ system of $^{69}Ga^{16}O$ and $^{71}Ga^{16}O$ has been measured and rotationally assigned. Principal molecular constants (T_{01}, B_0', B_1'', B_e'', D_0', D_1'',α_e'') have been obtained.

INTRODUCTION

The electronic spectrum of isotopic $Ga^{16}O$ molecules lying between 300 and 500 nm, has been the subject of investigation for a long time (for previous references see Pearse and Gaydon[1], Hubert and Herzberg[2] and Glushko[3]). At the present time, the indetification and the analysis of doublet band system have resulted in assignment of two doublet electronic states ($B^2\Sigma^+$ and $X^2\Sigma^+$) involved in transition. The last addition to this knowledge was advanced in 1979

by Yadav et al.[4]. The authors reinvestigated the electronic spectrum in the region 360-420 nm, earlier analyzed by Raziunas et al.[5]. Using higher resolution, Yadav and coworkers have obtained new data for the 0-0 and 1-0 bands of the $B^2\Sigma^+$-$X^2\Sigma^+$ system. In the course of our study of the emission spectrum of isotopic $Ga^{18}O$, we have recorded also the spectrum of isotopic $Ga^{16}O$ molecules[6] with rather well resolved 0-1 band. The data from this band may contribute to the reliability of the upper state constants, and we have considered it worthwhile to analyse it; this analysis forms the subject of the present paper.

EXPERIMENTAL

The spectrum of $Ga^{16}O$ was produced in a low-pressure arc of the type described by Bojović[7]. The gallium metal was placed in the copper electrode (cathode) cup, and arced in the atmosphere of oxygen, using a copper rod as anode. The favorable conditions for obtaining GaO bands were at pressure of 130 Torr, and d.c. current of 1.5 A. The 0-1 band was photographed in the 7th order of a 600 grooves/mm grating blazed at 2.7 μm on a Czerny-Turner spectrograph (disp. 0.02 nm/mm), using Ilford HP5 film, and 25μm slit width. The exposure times up to 2 hrs were used. The lines were measured on Abbe comparator against Th hollow-cathode reference lines whose wavelenghts were taken from Zalubas's Tables[8]. The positions were reduced to wavenumbers in the usual way. The accuracy of the measurements was 0.05cm^{-1} for unblended lines.

RESULTS AND DISCUSSION

The $B^2\Sigma^+$-$X^2\Sigma^+$ system of GaO is a transition between two states which belong to Hunds's case (b). The rotational structure of the bands consist of two series of lines corresponding to $\Delta N = \pm 1$. The R and P branches consist of $R_1, R_2, {}^RQ_{21}$ and P_1, P_2, ${}^PQ_{12}$ sub-branches, respectively. Two satellite branches, ${}^RQ_{21}$ and ${}^PQ_{12}$, are very weak and usualy are not observed.

In our spectrograms the heads of the 0-1 band of both isotopic molecules, $^{69}Ga^{16}O$ and $^{71}Ga^{16}O$, are well resolved; their positions in cm^{-1} are: $R_1=24950.35$, $R_2=24949.86$ for $^{69}Ga^{16}O$ and $R_1=24952.31$, $R_2=24951.77$ cm^{-1} for $^{71}Ga^{16}O$. The structure of the corresponding branches was well resolved after $N>25$.

The rotational assignments for analyzed band of both isotopic $Ga^{16}O$ molecule were made following the analysis of Yadav's and collaborators[4] as well as the analysis of isotopic $Ga^{18}O$ molecules from our previous work[6]. The line measurements and rotational assignments together with the residuals "obs-calc" are listed in Table 1.

The correct relative numbering was verified by the combination differences obtained for the 0-0[4] and 0-1 bands (Table 2). The agreement of the upper state combination differences for common upper state of two bands, confirm the correctness of the analysis.

The standard nonlinear least-squares program was modified for the $^2\Sigma^+$-$^2\Sigma^+$ transition by introducing of the series of levels of the $^2\Sigma$ states treated as independents and written in the form:

$$F_1(N)= B_v N (N+1) - D_v N^2 (N+1)^2 + \ldots + \tfrac{1}{2} \gamma N$$
$$F_2(N)= B_v N (N+1) - D_v N^2 (N+1)^2 + \ldots - \tfrac{1}{2} \gamma (N+1)$$

were $F_1(N)$ refers to the components having $J=N+\frac{1}{2}$ and $F_2(N)$ to those with $J=N-\frac{1}{2}$. B_v and D_v are the effective rotational constants and γ is the sin-splitting constant.

The spectrum was treated by the direct fitting method, each line having the same weight.

The molecular constants resulting from analysis are given in Table 3. The constant B_o' agrees well with that obtained by Yadav et al.[4]. The both upper and lower B_v constants follow the isotope relation [with $\rho= (\mu^{69}Ga^{16}O/\mu^{71}Ga^{16}O)^{1/2}$ $=0.99734$]. The values for spin-splitting constants ($\gamma'=0.019$ and $\gamma''=0.0012$) reported by Yadav[4] and Raziunas[5] were accepted in this work.

TABLE 1. Wavenumbers of the rotational lines of the B-X 0-1 band of $^{69}Ga^{16}O$ and $^{71}Ga^{16}O$ (cm^{-1})

	$^{69}Ga^{16}O$				$^{71}Ga^{16}O$			
N	R_1	P_1	R_2	P_2	R_1	P_1	R_2	P_2
24		24909.51(-15)				24911.89(0)		24911.56(5)
25		907.61(-19)				910.06(0)		909.51(-15)
26		906.08(-17)				908.10(-7)		907.61(-16)
27		903.78(-18)				906.08(-16)		905.63(-20)
28		901.62(-35)				904.33(4)		903.78(-8)
29		899.90(-4)				902.49(21)		901.62(-22)
30		897.77(-11)				900.31(7)		899.45(-34)
31		895.58(-18)				898.25(10)		897.77(8)
32	24946.85(9)	893.43(-18)		24893.00(-9)		896.10(8)		895.58(4)
33	946.14(-15)	891.19(23)		890.81(-7)		893.93(8)		893.43(6)
34	945.70(12)	889.46(27)		888.65(2)		891.74(10)		891.19(5)
35	944.96(3)	886.76(-11)		886.42(9)		889.46(7)		888.65(-23)
36	944.14(10)	884.63(4)		883.73(-26)		887.16(7)		886.42(-15)
37	943.72(21)			881.58(-3)		884.84(8)		884.20(-3)
38		879.96(14)		879.44(25)		882.40(3)		881.86(2)
39	941.57(-30)	877.58(21)				879.96(0)		879.44(3)
40	940.71(-29)	874.99(11)	24940.39(10)	874.43(22)		877.58(8)		877.15(21)
41	939.99(-11)	872.47(12)	939.41(4)	871.63(4)		874.99(0)		874.43(0)
42	939.42(26)	869.86(8)	938.40(0)	868.95(-12)		872.47(2)		871.63(-25)
43	938.40(24)	867.41(25)	937.42(3)	866.49(5)	24940.71(21)	869.86(0)	24939.41(34)	868.95(-33)
44	937.42(26)	869.86(25)	936.46(12)	863.53(23)	939.42(-5)	867.41(17)	938.79(-7)	866.49(-16)
45	936.45(30)	861.95(15)	935.35(10)	860.73(-32)	938.40(-2)	864.72(15)	937.42(-38)	863.98(1)
46	934.98(5)	859.14(8)	934.07(-4)	857.97(-32)	937.42(9)	861.95(9)	936.45(-25)	24860.73(-32)
47	933.62(-14)	856.23(-4)	932.85(-8)	855.70(-20)	936.00(-18)	859.14(3)	935.35(-20)	
48	932.41(-14)	853.34(-10)	932.05(34)	852.36(-28)	934.98(-2)	856.23(-8)	934.47(11)	
49	930.84(-46)	850.52(-5)	930.11(-33)	849.60(-14)	933.82(3)	853.34(-13)	932.85(-28)	
50	929.63(-38)	847.47(-18)	929.01(-12)	846.86(4)	932.41(-10)	850.42(-17)	931.41(25)	
51	928.59(-29)	844.56(-14)		843.56(-28)	931.41(20)	847.47(-20)	930.11(33)	
52	927.63(33)	841.60(-10)	926.52(14)	840.99(15)	929.63(-22)	844.56(-16)	929.01(-18)	
53	926.08(20)	838.58(-8)	925.10(12)	837.41(-37)	928.59(12)	841.60(-11)	927.63(-16)	
54	24924.51(9)	24835.48(-10)	24923.57(11)	24834.49(-19)	24926.08(-28)	24838.58(-9)	24927.63(-16)	

55	24923.09(18)	24832.44(-2)	24922.14(20)	24831.20(-34)	24925.61(5)	24835.48(10)	24924.51(-35)
56	921.55(19)	829.26(-3)	920.47(10)	828.21(-13)	924.02(-1)	832.44(-2)	923.09(25)
57	920.12(35)	826.16(7)	918.92(16)	825.14(0)	922.58(11)	829.26(-3)	921.55(-22)
58	918.19(6)	822.63(-20)	917.26(16)	822.09(23)	921.00(13)	826.16(7)	920.12(-4)
59	916.55(10)	819.53(-11)	915.74(30)	818.86(31)	919.40(18)	822.63(-19)	918.19(-32)
60	914.58(-14)	816.63(32)	913.72(6)	815.61(39)	917.67(14)	819.53(0)	916.55(26)
61	912.90(-36)	813.04(21)	912.19(31)	811.40(-30)	915.74(-4)	816.33(13)	914.58(-30)
62	911.46(31)	809.49(8)	910.59(34)		913.72(-29)	813.07(25)	912.44(-26)
63	909.51(21)	806.06(12)	908.62(44)	804.61(-27)	912.19(0)	809.49(9)	911.04(-40)
64	907.18(-21)	802.44(0)	906.48(21)	801.25(-11)	910.06(26)	805.60(-33)	909.09(31)
65	905.52(6)	798.90(2)	904.33(2)		908.10(32)		907.18(-32)
66	903.23(-24)	794.99(-30)	902.49(18)	794.30(12)	906.48(0)		905.02(33)
67	901.20(-24)	*	900.32(6)	*	904.61(12)	794.99(-30)	903.23(-20)
68	899.45(7)	*	898.25(8)	*	902.49(3)		901.20(-33)
69	897.19(-6)	*	896.10(6)	*	900.32(-5)		899.08(-37)
70	894.94(-15)	780.73(23)	893.93(6)	779.52(20)	898.25(0)		896.54(31)
71	892.56(-33)	776.58(-10)	891.74(9)	775.54(5)	896.10(0)	780.73(20)	894.94(-23)
72	890.39(-25)	773.01(16)	889.46(8)	771.52(-9)	893.93(4)	776.58(-14)	892.56(30)
73	888.65(28)	769.05(10)	887.16(8)	767.45(-27)	891.74(10)	773.00(12)	890.19(-22)
74	885.84(-18)	764.89(-12)	884.84(11)		889.46(11)	769.25(25)	887.95(-27)
75	883.58(-6)	761.08(4)	882.40(7)	759.61(-16)	886.76(-25)	764.89(-18)	885.39(-30)
76	881.23(0)	757.28(26)	879.96(7)	755.78(5)	884.63(0)	761.08(-2)	883.38(-33)
77	878.85(8)	753.43(48)	877.15(-26)	24751.86(21)	882.40(19)	24757.28(-18)	880.90(-29)
78	876.23(-2)	748.65(-19)	874.99(11)		879.96(21)		878.37(27)
79	873.91(21)		872.47(16)		877.15(-8)		875.77(30)
80	870.91(-19)	739.92(-38)	869.86(16)		874.43(-25)		873.18(-32)
81	868.17(-28)	735.93(-33)					24870.63(-18)
82	865.42(-35)	731.84(-14)	864.31(-3)				
83	863.11(6)	727.75(-14)	861.47(-12)		866.92(16)		
84	860.30(3)	723.15(-8)	858.60(-20)		863.98(-5)		
85	857.44(0)	24719.28(39)	855.69(-27)		861.47(20)		
86	24854.52(-6)		24853.34(26)		24858.60(15)		

(continued)

TABLE 1. Continued

	$^{69}Ga^{16}O$				$^{71}Ga^{16}O$			
N	R_1	P_1	R_2	P_2	R_1	P_1	R_2	P_2
87	24851.79(11)	24709.89(-4)	24850.42(26)		24855.70(11)			
88	848.92(19)	705.61(21)	846.86(-33)		852.36(-32)			
89	845.94(21)	700.64(-17)	844.08(-10)		24849.60(-14)			
90	842.98(29)	696.31(12)						
91	839.78(18)	691.16(-35)	838.00(-1)					
92	835.94(-32)	686.89(8)	834.94(7)					
93	833.28(-1)	682.05(0)	831.88(21)					
94	829.81(-25)	676.71(-32)	828.21(-23)					
95	826.66(-14)		825.14(-1)					
96	823.38(-11)	667.81(29)	821.67(-16)					
97		24662.87(28)	817.96(-30)					
98	816.33(-40)		814.71(-33)					
99	813.60(30)		811.40(-18)					
100	809.84(4)		808.00(-7)					
101	806.49(22)		804.61(9)					
102	803.07(38)		801.25(33)					
103	799.84(28)		797.68(40)					
104	*		*					
105	*		*					
106	*		*					
107	*		*					
108	780.06(-17)		778.53(20)					
109	776.10(-24)		773.94(-53)					
110	772.53(13)		770.20(30)					
111	768.17(-23)		766.53(3)					
112	764.57(20)		762.56(12)					
113	760.08(-20)		758.12(-22)					
114	756.18(27)		754.29(9)					
115	24751.86(-11)		24749.54(-47)					

* *overlaped by Ga line at 403.298 nm*

Numbers in parentheses indicate obs.-calc. wavenambers in units of 10^{-2} cm^{-1}

TABLE 2. Combination differences $\Delta_2F'(N)$ from the 0-0 and 0-1 bands of $^{69}Ga^{16}O$

	0-0*		0-1	
N	$R_1(N)-P_1(N)$	$R_2(N)-P_2(N)$	$R_1(N)-P_1(N)$	$R_2(N)-P_2(N)$
39	64.51	64.51	63.99	
40	66.13	66.04	65.72	
41	67.79	67.71	67.52	
42	69.39	69.35	69.56	
43	71.02	71.09	70.99	
44	72.62	72.70	72.70	
45	74.30	74.21	74.50	74.62
46	75.94	75.87	75.84	76.10
47	77.59	77.52	77.39	77.15
48	79.14	79.01	79.07	79.69
49	80.80	80.82	80.32	80.51
50	82.48	82.44	82.16	82.15
51	84.11	83.92	84.03	
52	85.76	85.77	86.03	85.53
53	87.43	87.48	87.50	87.69
54	89.06	89.03	89.03	89.08
55	90.78	90.65	90.65	90.94
56	92.35	92.27	92.29	92.26
57	94.03	94.00	93.96	93.78
58	95.66	95.60	95.56	95.17
59	97.31	97.18	97.02	96.88
60	98.99	98.89	98.25	98.11
61	100.67	100.49	100.15	100.79
62	102.35	102.26	101.97	
63	103.99	103.82	103.45	104.01
64	105.65	105.40	104.96	105.23
65	107.16	107.04	106.62	
66	108.77	108.65	108.24	108.19

* *Datafrom Ref. 4*

TABLE 3. Molecular constants of $Ga^{16}O$ for B-X system

	This work		Yadav et al.[a]	
Constants	$^{69}Ga^{16}O$	$^{71}Ga^{16}O$	$^{69}Ga^{16}O$	$^{71}Ga^{16}O$
$T_{0,1}$	24941.70(4)	24943.63(2)		
B_0'	0.4089(3)	0.4068(3)	0.40912	0.40692
B_1''	0.4299(4)	0.4068(3)		
$D_0''x10^7$	2.6(3)	2.7(4)	3.30	3.28
$D_1''x10^7$	2.4(3)	2.5(4)	3.03	3.02
B_e'			0.40988	0.4076
B_e''	0.43663	0.4336		
$\alpha_e'x10^3$			1.53	1.52
$\alpha_e'x10^3$	4.3 4.02[b]	4.0 3.96[b]		

Standard deviations in parentheses refer to the last digits.

[a] *Ref.4*

[b] *calculated from Pekeris relation and the data from Ref.9*

The constants determined from the fit are a minimum set of parameters that reproduce the experimental transition wavenumbers. The parameters are well determined and no trends are observed in the residuals. On this we can conclude that there are no major frequency perturbation affecting these transitions.

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