WEAK ÅNGSTRÖM BANDS OF $^{13}C^{16}O$ AND $^{12}C^{18}O$ MOLECULES

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The weak Ångström bands 1–4, 1–5, 1–6 of the molecule $^{13}C^{16}O$ and 1–5, 1–6 of the molecule $^{12}C^{18}O$ were obtained and investigated. The following constants were calculated for $^{13}C^{16}O$:

$$\sigma_{14} = (18600.721 \pm 0.009)\ \text{cm}^{-1},$$
$$\sigma_{15} = (17284.06_4 \pm 0.020)\ \text{cm}^{-1},$$
$$\sigma_{16} = (15996.94 \pm 0.01)\ \text{cm}^{-1},$$
$$B_1' - B_4'' = (0.39133 \pm 0.00005)\ \text{cm}^{-1},$$
$$B_1' - B_5'' = (0.41347 \pm 0.00010)\ \text{cm}^{1},$$

and for $^{12}C^{18}O$:

$$\sigma_{15} = (17291.834 \pm 0.008)\ \text{cm}^{-1},$$
$$\sigma_{16} = (16007.63 \pm 0.02)\ \text{cm}^{-1},$$
$$B_1' - B_5'' = (0.41191 \pm 0.00012)\ \text{cm}^{-1}.$$

The band origins of the 1–6 bands are perturbed and shifted a few cm^{-1}. A perturbation was found in the $B^1\Sigma^+$ state in the region between $J = 7$ and $J = 8$ for $^{13}C^{16}O$ molecule.

1. Introduction

The weak Ångström bands 1–4, 1–5, 1–6 of the $^{13}C^{16}O$ molecule and 1–5, 1–6 of the $^{12}C^{18}O$ molecule were obtained and investigated. This publication belongs to series of our work concerned with the spectra of the isotopic CO molecules and it completes our early results of the investigation of the Ångström system for the $^{13}C^{16}O$ and $^{12}C^{18}O$ molecules [1–5].

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2. Experimental

The spectra were obtained in 4th and 5th order using the plane grating spectrograph PGS2 (VEB C. Zeiss, Jena). The dispersion ranged from 0.6 Å/mm to 1.2 Å/mm. The light source used for investigation of the $^{13}C^{16}O$ molecule spectrum was an ordinary high-voltage discharge tube filled with CO_2 containing 70 at.% of ^{13}C carbon whereas the lamp used for the $^{12}C^{18}O$ molecule had carbon electrodes and was filled with oxygen containing 90% of ^{18}O isotope. The gas pressures were about 3 mm Hg. The exposure times for ORWO WP1 plates ranged from 15 min for the 1–5 band of the $^{13}C^{16}O$ molecule to 120 min for the 1–6 band of the $^{12}C^{18}O$ molecule. The plates were measured a number of times. The Fe and Ne standard spectra from hollow cathode lamps were used.

3. Results

The rotational lines of the Ångström 1–4, 1–5, 1–6 bands of $^{13}C^{16}O$ molecule were obtained and measured, in general, up to the predissociation limit. The interpretation of the lines and their wave numbers are given in Tables I to V. The figures marked by one or two asterisks are the less reliable or unreliable wave number values, respectively. In the authors opinion, the relative errors for the remaining lines do not exceed 0.006 cm^{-1} and absolute errors — 0.01 cm^{-1}.

TABLE I

1–4 band lines of $^{13}C^{16}O$ (in cm^{-1})

J	R branch	Q branch	P branch
1		18601.502**	
2		603.076*	
3		605.416**	
4	18626.941	608.580**	18593.858*
5	634.541**	612.463	594.076
6	642.845*	617.156	595.109
7	652.033*	622.591	596.902*
8	661.967	628.888	599.459
9	672.682	635.942	602.885
10	684.171	643.765*	607.055*
11	696.442	652.368	611.977
12	18709.498	661.759	617.708
13	723.331	671.938	624.209
14	737.965	682.891	631.513
15	753.368	694.634	639.586
16	769.548	18707.159	648.453**
17	786.504	720.469	658.106
18	18804.230*	734.565	668.546
19		749.434	679.768

TABLE II

1–5 band lines of $^{13}C^{16}O$ (in cm^{-1})

J	R branch	Q branch	P branch
1			
2		17286.582**	
3		289.040*	17278.069**
4	17310.729*	292.362	277.645*
5	318.548*	296.489	278.107**
6	327.126	17301.439	279.385
7	336.635	307.183	281.501
8	346.929	313.855	284.405
9	358.017	321.299	288.225
10	369.963	329.556	292.826**
11	382.720	338.641	298.264
12	396.312	348.569	17304.504
13	17410.712**	359.322	311.593
14	425.965	370.909	319.504*
15	442.043	383.309	328.271
16	458.909	396.538	337.845
17	476.628	17410.611*	348.269
18		425.515	359.504*
19		441.245	371.590**
20			384.507*

TABLE III

1–6 band lines of $^{13}C^{16}O$ (in cm^{-1})

J	R branch	Q branch	P branch
1		15997.904**	
2		999.843	15992.497*
3		16002.732	991.704**
4	16024.898*	006.514*	991.788**
5	033.218*	011.163	992.802*
6	042.355	016.663	994.636*
7	052.427	022.968*	997.299
8	063.291	030.211	16000.765
9	074.982	038.234	005.161*
10	087.513**	047.101	010.363
11	16100.894	056.815	016.416
12	115.122	067.377*	023.309
13	130.198	078.799	031.070
14	146.139	091.076	039.682
15	162.952*	16104.220	049.167
16	180.585	118.231	059.532**
17	199.246*	133.212	070.894
18	16218.443*	148.790	082.777
19		165.400	095.745
20			16109.561

TABLE IV

1–5 band lines of $^{12}C^{18}O$ (in cm—^{1})

J	R branch	Q branch	P branch
1		17292.671	
2	17305.240**	294.337	17286.911*
3	311.441*	296.769	285.852**
4	318.306*	17300.066	285.412
5	326.181*	304.177	285.852**
6	334.800	309.125	287.220**
7	344.173*	314.892	289.266
8	354.433*	321.471	292.196
9	365.468	328.900*	295.944
10	377.385	337.117	17300.506*
11	390.129**	346.174	305.937
12	17403.632*	356.063	312.159
13	417.879**	366.763	319.208
14	433.144	378.306	327.100
15	449.159**	390.656	335.785
16	465.957*	17403.848	345.317*
17	483.581**	417.879*	355.746
18		432.694	366.877**
19		448.363	378.964
20			391.820*

TABLE V

1–6 band lines of $^{12}C^{18}O$ (in cm^{-1})

J	R branch	Q branch	P branch
1		16008.547*	
2		010.406	
3		013.161	
4		016.817	
5		021.357*	16002.184
6		026.747	004.754**
7	16062.263	033.012*	007.371
8	072.963**	040.076	010.793
9	084.604*	048.019**	015.081
10	097.070	056.819	020.234
11	110.396	066.459	026.210
12	124.527	076.965	033.012*
13	139.534	088.307*	040.771
14	155.346**	16100.536	049.333**
15	172.105	113.612	058.758
16	189.688	127.562	069.078*
17	16208.180	142.404	080.276
18	227.406*	157.964	092.253*
19		174.508	16105.109
20			118.890

The analysis of the bands showed that the 1–6 bands of both molecules are strongly perturbed in origin: the resulting origin shifts amount to 3 cm^{-1}. The remaining bands are unperturbed in origins. Table VI contains the band origins for both molecules. These for bands non-perturbed in origin were obtained by means of the $g_x(J)$ function [6], and for 1–6 bands — by means of extrapolation of Q branches. The errors for unperturbed bands are the standard errors and these for 1–6 bands are estimated arbitrarily.

TABLE VI

Band origins (in cm^{-1})

Band	Molecule	
	$^{13}C^{16}O$	$^{12}C^{18}O$
1–4	18600.721 ± 0.009	—
1–5	17284.064 ± 0.020	17291.834 ± 0.008
1–6	15996.94 ± 0.01	16007.63 ± 0.02

TABLE VII

Differences $B'_1 - B''_v$ (in cm^{-1})

v''	Molecule	
	$^{13}C^{16}O$	$^{12}C^{18}O$
4	0.39133 ± 0.00005	—
5	0.41347 ± 0.00010	0.41191 ± 0.00012

The differences $B'_1 - B''_v$ evaluated only for unperturbed bands by means of $f_x(J)$ function [6] are given in Table VII. The B values resulting from these differences are slightly smaller than those evaluated from constants previously published [4] (taking into consideration the B'_1 values from the same work).

The well marked rotational perturbation in the region between $J = 7$ and $J = 8$ was found in $B^1\Sigma^+(v = 1)$ state, which was assumed to be perturbationless. The appearence of this perturbation shows that the rotational constant of the perturbing state is higher than the rotational constant of perturbed $B^1\Sigma^+$ state.

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