

WEAK ÅNGSTRÖM BANDS OF $^{12}\text{C}^{16}\text{O}$ MOLECULE

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Weak $1-v''$ progression bands in the Ångström system of the $^{12}\text{C}^{16}\text{O}$ molecule were obtained and discussed. The wave numbers were determined and rotational analysis was performed of the hitherto unmeasured bands 1-4, 1-5 and 1-6 obtained with dispersions of $0.7 \frac{\text{Å}}{\text{mm}}$, $0.5 \frac{\text{Å}}{\text{mm}}$ and $1 \frac{\text{Å}}{\text{mm}}$, respectively.

Perturbation shifts of the band origins were found. These were for the 1-4 band: $(0.5 \pm \pm 0.2) \text{ cm}^{-1}$ and for the 1-6 band: $(0.22 \pm 0.02) \text{ cm}^{-1}$. The origin of the 1-5 band shows no shift. Rotational constants of the upper level $B^1\Sigma^+$ were calculated and compared with previous results.

Introduction

In the course of a systematic investigation of the CO molecule, an attempt was made to analyse the so far unmeasured weaker bands of the Ångström system. In the study of this system undertaken by many authors, unfortunately the higher bands of the $1-v''$ progression were always omitted. In this work the authors analysed the bands 1-4, 1-5 and 1-6 of the $^{12}\text{C}^{16}\text{O}$ molecule, obtained with as high a dispersion as possible and also aimed at a high precision of measurements and especially at accurate wave length gauging.

Experimental

Emission bands spectra were obtained in a common discharge tube filled with $^{12}\text{C}^{16}\text{O}_2$ of 6-8 mm Hg pressure. The discharge of current density 0.3 A/cm^2 was photographed in the fourth and fifth row of a two-metre flat-grid spectrograph PGS-2 (VEB Carl Zeiss, Jena). The exposures ranged from 30 min. to 1 hour. The photograph of the 1-4 band was obtained in dispersion $0.7 \frac{\text{Å}}{\text{mm}}$, the 1-5 band in dispersion $0.5 \frac{\text{Å}}{\text{mm}}$, and the 1-6 band in dispersion $1 \frac{\text{Å}}{\text{mm}}$. For wavelength gauging, standard Ne and Fe lines obtained in a hollow-cathode-type lamp were used. The plates were measured a number of times in both directions using an Abbe type comparator.

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TABLE I

1-4 band lines (in cm^{-1})

<i>J</i>	<i>R</i> branch	<i>Q</i> branch	<i>P</i> branch
1		18533.105**	
2		534.276**	
3		536.381*	
4		539.717	18524.461**
5		543.919**	524.796**
6	18575.889**	548.908	525.917**
7	585.545*	554.725**	527.905
8	596.031**	561.354	530.696
9	607.263	568.819	534.292**
10	619.356	577.065*	538.707*
11	632.267	586.151	543.919**
12	645.981**	596.106*	549.998
13	660.506	606.756	556.875*
14	675.860**	618.227	564.555
15	692.090*	630.619	573.147**
16	708.979*	643.771	582.418*
17		657.754	592.563*
18			603.548**

TABLE II

1-5 band lines (in cm^{-1})

<i>J</i>	<i>R</i> branch	<i>Q</i> branch	<i>P</i> branch
1		17191.937	
2			
3	17209.918**	194.545	17183.142
4	217.235**	198.021	182.639
5	225.416	202.355*	183.142
6	234.464*	207.567	184.508
7	244.374	213.641	186.754**
8	255.160	220.589	189.860
9	266.805	228.402	193.838
10	279.345**	237.085	198.681
11	292.688**	246.640	204.412
12	307.053*	257.050*	210.996
13	322.099**	268.354	218.486*
14	338.085	280.517	226.814
15	354.832	293.554	235.917
16	372.662	307.455	246.086
17		322.236*	257.050**
18			268.845*

TABLE III

1-6 band lines (in cm^{-1})

J	R branch	Q branch	P branch
1	15889.850**	15882.619**	15878.326**
2	896.037	884.494	876.796**
3	902.605*	887.290	875.721**
4	910.207	891.024	875.646**
5	918.733*	895.707*	876.474
6	928.286*	901.399	878.326
7	939.207*	908.436	881.515*
8	948.841	914.323*	883.536
9	961.497	923.214	888.526
10	974.876	932.995	894.246
11	989.313*	939.805 945.482	901.011
12	16005.116	953.723*	909.147
13	007.823 023.352	967.500*	904.224** 919.729
14	029.397	972.620 984.131	918.127
15	049.515*	989.074*	930.588
16	068.866	16001.736 007.144	942.289
17		019.388	954.583
18			967.345**

TABLE IV

Wave numbers of band origins (in cm^{-1})

Band	Band origin		Perturbational shift
	calculated	observed	
1-4	18532.06	18531.6 \pm 0.2	$-(0.5 \pm 0.2)$
1-5	17189.32	17189.34 \pm 0.02	—
1-6	15881.46	15881.67 \pm 0.02	$-(0.22 \pm 0.02)$

Results

Wave numbers of the rotational lines in the bands 1-4, 1-5 and 1-6 were obtained for the $^{12}\text{C}^{16}\text{O}$ molecule. In the authors opinion, the relative error of the measured wave numbers lies within the range (0.003-0.006) cm^{-1} and the absolute error values are (0.005-0.008) cm^{-1} . The numbers listed with one asterisk are for various reasons, slightly less accurate, whereas the ones accompanied by two asterisks are much less accurate.

The analysis of the 1-6 band gave values $\Delta_2 F_c$ and $\Delta_2 F_d$ (both components of the Δ doubling) in the A'' , corresponding, in principle, to the values obtained by Onaka from the analysis of the 6-13 band in the IV positive system [3]. The real positions of the wave origins were determined (Table IV) and compared with positions calculated on the basis of the oscillation constants given by Rytel [4]. In this way the perturbation shifts were founded.

The shift of the 1-4 band agrees within measurement error with the shift of the 0-4 band, whereas the 1-5 band shows no shift, contrary to earlier expectations [2], [4].

Using the least-square method the rotational constant were found for the B state, namely:

$$B_1 = (1.9219 \pm 0.0002) \text{ cm}^{-1}$$

$$D_1 = (7.7 \pm 0.7) \text{ cm}^{-1}$$

in agreement with our earlier results [2], [4].

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