

# High Frequency Transitions in the Rotational Spectrum of SO<sub>2</sub>

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A large number of rotational transitions of <sup>32</sup>S<sup>16</sup>O<sub>2</sub>, <sup>34</sup>S<sup>16</sup>O<sub>2</sub>, and <sup>32</sup>S<sup>18</sup>O<sup>16</sup>O have been measured in the mm-, submm-, and terahertz (~1 THz) spectral regions. These data sets have been combined with all previously measured SO<sub>2</sub> microwave and selected far infrared data to obtain a highly precise set of ground state rotational constants for these isotopomers. The rotational constants for the three isotopomers are in MHz as follows:

Parameter	<sup>32</sup> S <sup>16</sup> O <sub>2</sub>	<sup>34</sup> S <sup>16</sup> O <sub>2</sub>	<sup>32</sup> S <sup>18</sup> O <sup>16</sup> O
A	60778.54977 (44)	58991.18295 (51)	59101.1690 (27)
B	10318.07348 (7)	10318.50993 (9)	9724.64284 (56)
C	8799.703399 (70)	8761.302481 (97)	8331.56018 (51)

Centrifugal distortion constants up to  $P^{10}$  are included in the fit. A frequency listing of all the data used in the frequency range between about 7 GHz and 1 THz is included. © 1998 Academic Press

## I. INTRODUCTION

The sulfur dioxide molecule is a simple near-prolate asymmetric rotor. The rotational spectrum consists of *b*-type transitions and, as a result, covers a large range of rotational quantum numbers. Therefore, the spectrum of its various isotopic species, both in the ground and vibrational states, has long been used to test Hamiltonian models involving centrifugal distortion (*J*). For some years its spectrum has been used to calibrate spectrometers in both the microwave and infrared region. From a practical standpoint, it is one of the more significant pollutant molecules in the Earth's atmosphere, since it is produced in combustion processes and is the most important contributor to acid rain. It also plays an important role in the chemistry of Venus' atmosphere (2), and since its original detection in the interstellar medium by Snyder *et al.* (3), it has proved to be an ubiquitous and abundant constituent of star-forming regions.

In this paper, we report the measurement of a large number of high frequency (200–1050 GHz) transitions of the <sup>32</sup>S<sup>16</sup>O<sub>2</sub>, <sup>34</sup>S<sup>16</sup>O<sub>2</sub>, and <sup>32</sup>S<sup>18</sup>O<sup>16</sup>O isotopomers in the vibrational ground state. This new data when combined with all known previously measured transitions, especially the recent very high precision measurements of Alekseev *et al.* (4) and Mehrotra *et al.* (5), resulted in a complete set of highly precise rotational constants for these isotopomers. Since the spectrum of this molecule has proven to be of use in so many studies, we include here a complete listing of all the data used in this study.

## II. EXPERIMENTAL

The newly supplied experimental data sets consist of two parts collected in two different frequency regions by two laboratories. With the Cologne terahertz spectrometer the frequency region between 500 and 1000 GHz was scanned, whereas the RAD spectrometer of the Institute of Applied Physics provided new data in the lower frequency region, i.e., 180–380 GHz. The other data are taken from the literature.

The new SO<sub>2</sub> data taken with the Cologne terahertz spectrometer were recorded in response to high-frequency interstellar spectral line surveys in high-mass star-forming regions. In the Caltech line survey of the Orion A region in the 325–360 GHz frequency band it was found that the total integrated line intensity for all SO<sub>2</sub> lines dominates the emission (6). Figure 1 displays a comparison between a laboratory and astronomical recording of the  $\nu_6$  branch head at 663 GHz presented on the same frequency scale (7). The astronomical measurements are taken from the Caltech 607–725 GHz spectral line survey (8). Figure 2 shows the band-head region of the laboratory spectrum in higher frequency resolution to substantiate the *J* assignment. The Cologne terahertz spectrometer has been described in various publications, e.g., (14, 15). Most recently a detailed evaluation of the sensitivity and measurement accuracy of the spectrometer has been presented (16). Near 1 THz, lines with an absorption coefficient of  $\sim 10^{-8}$  cm<sup>-1</sup> are clearly detectable ( $\geq 5\sigma$ ). With the spectrometer operated in the Doppler-limited mode, the achieved frequency accuracy for isolated, strong lines is estimated to be around  $\pm 5$  kHz. In

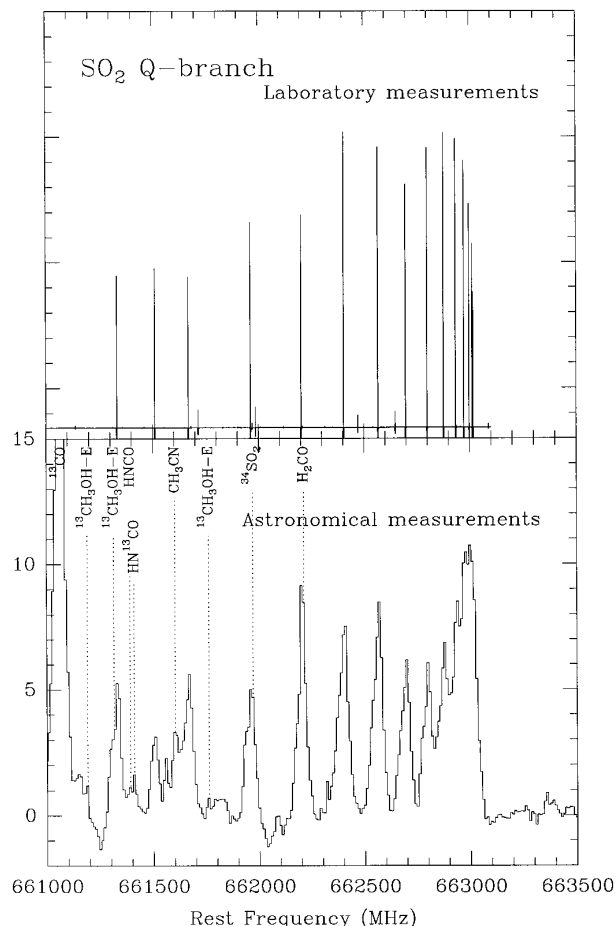


FIG. 1. A comparison between laboratory and interstellar spectrum of the  $K_a = 6$   $'Q_6$  band head of  $\text{SO}_2$ .

case the spectrometer is operated in the sub-Doppler mode, line positions are routinely determined to better than 1 kHz. The sample pressure for the  $\text{SO}_2$  measurements was kept below about 3 Pa (30  $\mu\text{bar}$ ), and all spectra were recorded in the Doppler resolution mode. In addition to the spectra of the three isotopomers of  $\text{SO}_2$  discussed in this study, we have measured the  $^{33}\text{SO}_2$  isotopomeric species, and, in consequence, we have detected several emission lines of the  $^{33}\text{S}$ -isotopomer in the Orion A interstellar molecular cloud (17).

In the range 180–380 GHz the spectral lines were measured using a RAD spectrometer with a submillimeter frequency synthesizer (13). The measurements were made at room temperature. The gas pressure in the cell ranged from 30 to 60 Pa, corresponding to linewidths from 4 to 8 MHz. The measurements were carried out by frequency modulating the microwave radiation. The spectral lines were observed as the first derivative of the line profile. The frequency of the radiation was automatically tuned to the zero point of the response-determinator and this frequency position was measured which corresponds to the absorption maximum in the line. Predominantly isolated lines have been measured; however, in some cases small systematic errors up to 100 kHz may be caused by the influence of wings of neighboring lines, an effect that has not been taken into account in the measurements. Experimental estimates are based on systematic errors that occurred due to possible interference of the submillimeter radiation in the cell and in the microwave waveguide system elements, contributing to base-line problems. In the worst cases they cause an error up

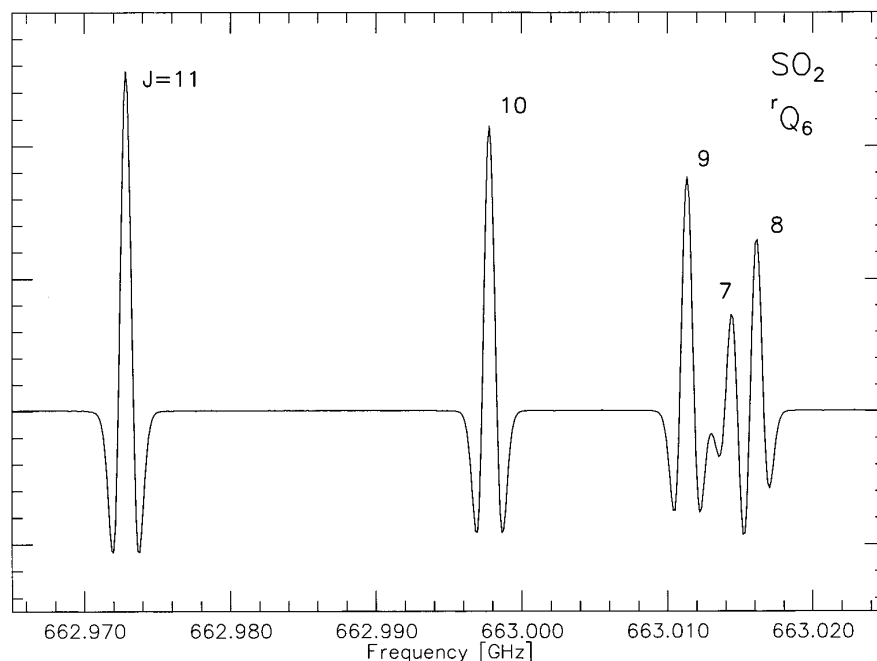


FIG. 2. Laboratory recording and  $J$  assignment of the  $'Q_6$  band head. The line shape is of second derivative.

TABLE 1  
Observed Pure Rotational Transitions of <sup>32</sup>SO<sub>2</sub>

Transition	Frequency (MHz)	Obs. - Calc. (kHz)	Exp. Unc. (kHz)	Ref.	Transition	Frequency (MHz)	Obs. - Calc. (kHz)	Exp. Unc. (kHz)	Ref.
1 1 1 0 0 0	69575.9271	-1	2	a	12 3 9 12 2 10	237068.8700	33	150	
2 1 1 2 0 2	53528.8651	2	2	a	12 3 9 13 2 12	20335.4053	0	1	b
3 1 3 2 0 2	104029.4183	0	2	a	14 1 13 13 2 12	182705.8900	-158	100	
4 1 3 4 0 4	59224.8714	1	2	a	15 3 13 15 2 14	275240.1500	-38	300	d
5 1 5 4 0 4	135696.0200	3	80		16 3 13 16 2 14	214689.3800	-19	150	
6 1 5 6 0 6	68972.1587	0	2	a	17 3 15 17 2 16	285743.5500	-43	200	
9 1 9 8 0 8	193609.4900	63	100		18 1 17 17 2 16	288519.9600	-40	200	
8 1 7 8 0 8	83688.0930	1	2	a	20 3 17 20 2 18	197142.1800	113	100	
11 1 11 10 0 10	221965.2100	-12	150		21 3 19 21 2 20	316099.0100	127	200	
10 1 9 10 0 10	104239.2952	-2	2	a	22 3 19 22 2 20	195320.7000	276	100	
12 1 11 12 0 12	131014.8600	19	80		24 3 21 24 2 22	200287.5300	102	150	
15 1 15 14 0 14	281762.6000	-4	200		26 3 23 26 2 24	213068.4000	-33	150	
16 1 15 16 0 16	200809.1800	-142	150		29 3 27 28 2 26	616472.4100	128	100	c
15 3 13 16 0 16	239832.7540	-68	60	d	28 3 25 29 2 28	31089.9200	-7	100	
17 3 15 18 0 18	238166.3180	-70	90	d	30 3 27 31 2 30	72437.2871	0	2	a
20 1 19 20 0 20	282292.8000	-10	200		32 3 29 33 2 32	119483.0800	3	80	
21 3 19 22 0 22	253753.3150	-138	150	d	33 5 29 34 2 32	285768.2700	77	200	
27 3 25 28 0 28	314922.4280	-289	300	d	37 3 35 36 2 34	709510.6770	-47	100	c
35 1 35 34 0 34	624344.4890	-101	100	c	38 3 35 39 2 38	275375.8900	204	450	d
38 1 37 38 0 38	624108.1380	19	100	c	41 3 39 40 2 38	771258.2960	139	100	c
47 1 47 46 0 46	834688.6280	-77	100	c	41 5 37 42 2 40	288117.0860	27	120	d
46 1 45 46 0 46	766701.5200	116	100	c	44 3 41 44 2 42	574210.3780	12	50	e
2 2 0 1 1 1	192651.0200	78	300		45 3 43 45 2 44	684929.0690	252	100	c
3 2 2 2 1 1	208700.3200	-15	150		46 3 43 46 2 44	616525.7320	-54	100	c
2 2 0 2 1 1	151378.6300	-32	80		47 5 43 48 2 46	354083.9660	-211	120	d
2 2 0 3 1 3	100878.1053	-1	2	a	4 4 0 4 3 1	358038.0800	195	200	
4 0 4 3 1 3	29321.3300	0	4		5 4 2 5 3 3	358013.0900	-61	200	
3 2 2 3 1 3	158199.7400	-40	80		6 4 2 6 3 3	357925.9600	113	200	
3 2 2 4 1 3	69653.5788	0	2	a	7 4 4 8 3 5	204384.3000	110	100	
4 2 2 4 1 3	146605.5200	1	80		8 4 4 9 3 7	185278.6000	262	100	
6 0 6 5 1 5	72758.2434	1	2	a	9 4 6 9 3 7	357671.7800	-41	200	
4 2 2 5 1 5	70134.3728	0	2	a	10 4 6 11 3 9	146550.0800	36	80	
6 2 4 5 1 5	282036.5800	13	200		11 4 8 11 3 9	357387.5700	-11	200	
6 2 4 6 1 5	140306.1700	4	80		11 4 8 12 3 9	124864.7400	-16	80	
5 2 4 6 1 5	23414.2493	0	1	b	13 4 10 13 3 11	357165.3600	-34	200	
6 2 4 7 1 7	44052.8600	-12	20		12 4 8 13 3 11	107843.4701	0	2	a
8 0 8 7 1 7	116980.4400	-9	80		14 2 12 13 3 11	47913.4200	-6	20	
8 2 6 8 1 7	134004.8600	47	80		15 2 14 14 3 11	7169.6130	0	1	b
8 2 6 9 1 9	24083.4781	0	1	b	13 4 10 14 3 11	82951.9380	1	2	a
10 0 10 9 1 9	160827.8800	39	80		14 4 10 15 3 13	69464.0777	1	2	a
10 2 8 10 1 9	129514.8100	10	80		15 4 12 15 3 13	357241.1900	-8	200	
11 2 10 11 1 11	205300.5700	30	100		16 2 14 15 3 13	104033.5817	0	2	a
12 0 12 11 1 11	203391.5500	66	100		17 2 16 16 3 13	28858.0370	17	20	
10 2 8 11 1 11	11788.8410	-34	20		15 4 12 16 3 13	38518.2250	7	20	
12 2 10 12 1 11	128605.1300	18	80		17 4 14 17 3 15	357962.8900	-22	200	
12 2 10 13 1 13	8420.2800	5	40		16 4 12 17 3 15	31922.2100	-61	30	
14 2 12 14 1 13	132744.8600	26	80		19 2 18 18 3 15	43016.2800	3	100	
14 2 12 15 1 15	14587.6970	-64	20		21 2 20 20 3 17	48120.4400	8	30	
16 0 16 15 1 15	283464.6000	-172	200	b	22 2 20 21 3 19	286416.3200	45	200	
16 2 14 16 1 15	143057.1100	28	80		23 2 22 22 3 19	43178.1400	-28	100	
17 4 14 16 1 15	1030310.9730	-34	50	e	24 4 20 24 3 21	296535.4900	57	200	
17 2 16 17 1 17	273752.8220	-144	90	d	25 2 24 24 3 21	27932.2000	-211	200	
16 2 14 17 1 17	30205.5200	-26	100		26 4 22 26 3 23	280807.2800	24	200	
18 2 16 18 1 17	160342.9900	16	80		32 2 30 31 3 29	571532.5510	-1	50	e
18 2 16 19 1 19	54633.5933	2	2	a	36 4 32 36 3 33	281688.9800	47	200	
20 0 20 19 1 19	358215.6400	0	200		40 4 36 41 3 39	54138.8000	-272	300	
20 2 18 20 1 19	184969.8000	-26	100		41 6 36 42 3 39	308232.6850	57	120	d
20 2 18 21 1 21	86828.9381	-1	2	a	42 4 38 43 3 41	108915.4234	0	2	a
22 2 20 23 1 23	125427.1300	-120	80		48 4 44 48 3 45	530380.6950	-21	100	c
26 2 24 26 1 25	296168.7100	28	200		50 4 46 50 3 47	580132.5010	130	100	c
26 2 24 27 1 27	215094.5400	25	150		55 6 50 56 3 53	334273.7220	-360	150	d
31 2 30 30 1 29	576042.0560	-22	100	c	8 5 3 9 4 6	287485.4400	-65	200	
32 0 32 31 1 31	571553.3180	-7	150	e	13 5 9 12 4 8	708392.5420	77	100	c
31 4 28 32 1 31	276254.6230	40	180	d	12 5 7 13 4 10	209936.0500	8	140	
35 2 34 35 1 35	571383.1230	44	100	c	13 5 9 14 4 10	190148.6500	51	100	
37 2 36 37 1 37	606896.4460	-67	100	c	15 5 11 16 4 12	150381.1000	28	80	
40 0 40 39 1 39	712010.5540	78	100	c	18 3 15 17 4 14	9403.2420	7	12	b
40 2 38 40 1 39	590076.6690	37	100	c	16 5 11 17 4 14	131274.9300	68	80	
54 0 54 53 1 53	957178.8660	67	450	e	17 5 13 18 4 14	109757.5851	0	2	a
4 3 1 5 2 4	160543.0600	36	80		20 3 17 19 4 16	61636.1885	0	2	a
5 3 3 6 2 4	139355.0600	30	80		18 5 13 19 4 16	91550.4392	-1	2	a
8 1 7 7 2 6	25392.8195	0	1	b	19 5 15 20 4 16	67848.6332	1	2	a
6 3 3 7 2 6	123057.6900	3	80		21 3 19 20 4 16	37351.8000	-10	100	
7 3 5 8 2 6	97702.3335	0	2	a	22 3 19 21 4 18	118577.4300	2	2	a
10 1 9 9 2 8	76412.1651	0	2	a	20 5 15 21 4 18	51736.5900	-67	30	
8 3 5 9 2 8	86639.0877	-1	2	a	23 3 21 22 4 18	66724.8768	0	2	a
9 3 7 10 2 8	53015.2374	0	2	a	21 5 17 22 4 18	24039.6410	11	20	
12 1 11 11 2 10	129105.8300	44	80		22 5 17 23 4 20	12132.4000	-63	200	
10 3 7 11 2 10	52051.7100	-50	30		25 3 23 24 4 20	90548.1474	0	2	a
11 3 9 12 2 10	4546.0180	6	20		27 3 25 26 4 22	107060.2085	-3	2	a

<sup>a</sup> Alekseev *et al.*<sup>b</sup> Merotra *et al.*<sup>c</sup> Helminger and deLucia.<sup>d</sup> Measurements taken at Nizhni Novgorod.<sup>e</sup> Measurements taken at Cologne.

All other frequencies are from the compilation of Lovas.

TABLE 1—Continued

Transition					Frequency (MHZ)	Obs. - Calc. (kHz)	Exp. Unc. (kHz)	Ref.	Transition					Frequency (MHZ)	Obs. - Calc. (kHz)	Exp. Unc. (kHz)	Ref.	
29	3	27	28	4	24	114565.3704	0	2	a	31	8	24	32	7	25	143357.8000	-22	80
31	3	29	30	4	26	111755.0214	0	2	a	32	8	24	33	7	27	123194.7000	4	80
33	3	31	32	4	28	97994.0891	0	2	a	33	8	26	34	7	27	102690.0611	-2	2 a
35	3	33	34	4	30	73430.4271	2	2	a	35	6	30	34	7	27	25049.4513	0	1 b
37	3	35	36	4	32	38909.7000	0	100	c	36	6	30	35	7	29	51185.2200	-23	60
41	5	37	41	4	38	517100.0990	15	100	c	35	8	28	36	7	29	61489.8551	1	2 a
49	5	45	49	4	46	619796.1810	52	100	c	37	6	32	36	7	29	67011.2900	22	40
50	5	45	51	4	48	32829.9300	29	100	c	36	8	28	37	7	31	41177.5000	43	100
52	5	47	52	4	48	464664.6440	39	100	c	38	6	32	37	7	31	97466.3665	-1	2 a
54	5	49	54	4	50	515421.6590	-19	100	c	37	8	30	38	7	31	19637.0642	0	1 b
56	5	51	56	4	52	568464.5950	-43	100	c	39	6	34	38	7	31	108955.9153	1	2 a
58	5	53	58	4	54	621617.9680	79	100	c	40	6	34	39	7	33	146393.7200	14	80
6	6	0	5	5	1	676484.3980	-26	100	c	41	6	36	40	7	33	150486.9200	-11	80
8	6	2	7	5	3	714779.5830	36	100	c	42	6	36	41	7	35	198847.8600	26	100
11	6	6	10	5	5	772188.2500	143	100	c	43	6	38	42	7	35	191020.8900	-41	100
11	6	6	12	5	7	331580.2440	45	90	d	49	6	44	48	7	41	297256.7670	-245	90 d
14	6	8	13	5	9	829477.9530	25	100	c	48	8	40	48	7	41	718681.0460	68	100 c
13	6	8	14	5	9	292882.6970	115	60	d	50	6	44	49	7	43	461410.2010	-11	100 c
17	6	12	18	5	13	214728.3300	48	150	c	55	6	50	54	7	47	350110.3710	35	450 d
18	6	12	19	5	15	195080.4400	152	100	c	9	9	1	9	8	2	864511.7740	-4	50 e
20	6	14	19	5	15	943211.5370	-126	100	c	10	9	1	10	8	2	864531.6090	-7	50 e
20	6	14	21	5	17	155389.6200	-7	80	c	11	9	3	11	8	4	864549.0520	-12	50 e
21	6	16	22	5	17	134943.3000	8	80	c	10	9	1	11	8	4	653928.0550	29	30 e
24	4	20	23	5	19	22482.5595	0	1	b	12	9	3	12	8	4	864562.8660	-8	60 e
23	6	18	23	5	19	556959.9090	1	140	c	13	9	5	13	8	6	864571.6120	-76	70 e
22	6	16	23	5	19	115317.5566	0	2	a	15	9	7	15	8	8	864568.3010	-16	60 e
23	6	18	24	5	19	94064.6950	0	2	a	16	9	7	16	8	8	864552.8320	-14	60 e
25	4	22	24	5	19	26776.5740	-15	20	c	17	9	9	17	8	10	864525.7850	-21	50 e
24	6	18	25	5	21	74866.5109	1	2	a	20	9	11	21	8	14	461875.9050	11	100 c
26	4	22	25	5	21	72668.0566	-1	2	a	29	9	21	30	8	22	286651.4600	80	200
27	4	24	26	5	21	64277.1759	0	2	a	33	9	25	34	8	26	207421.3800	-83	150
25	6	20	26	5	21	52188.4800	-4	60	c	34	9	25	35	8	28	187446.7500	17	100
26	6	20	27	5	23	34097.7200	-26	30	c	36	9	27	37	8	30	147239.2800	-14	80
28	4	24	27	5	23	127428.2300	30	80	c	37	9	29	38	8	30	126962.4600	-53	80
27	6	22	28	5	23	8911.1660	53	103	b	40	7	33	39	8	32	23034.8144	0	1 b
29	4	26	28	5	23	99392.5129	0	2	a	38	9	29	39	8	32	106674.8279	-1	2 a
30	4	26	29	5	25	187370.3300	121	100	c	41	7	35	40	8	32	42680.0900	23	100
31	4	28	30	5	25	130859.4000	-26	80	c	39	9	31	40	8	32	86153.7638	0	2 a
32	4	28	31	5	27	252563.7490	-143	150	d	42	7	35	41	8	34	66761.1093	0	2 a
43	4	40	42	5	37	153677.1400	-16	80	c	40	9	31	41	8	34	65714.0922	-1	2 a
45	4	42	44	5	39	120023.4000	-82	80	c	43	7	37	42	8	34	85246.9990	1	2 a
45	6	40	45	5	41	565066.2300	-53	100	c	41	9	33	42	8	34	44875.8600	-37	30
46	4	42	45	5	41	768497.9210	76	100	c	42	9	33	43	8	36	24319.6578	0	1 b
47	4	44	46	5	41	76539.9912	-4	2	a	44	7	37	43	8	36	111875.5411	0	2 a
49	4	46	48	5	43	24915.7487	0	1	b	45	7	39	44	8	36	128103.8100	-23	80
9	7	3	8	6	2	835294.8380	-90	100	c	46	7	39	45	8	38	158845.0800	10	80
11	7	5	10	6	4	873600.7260	127	100	c	48	7	41	47	8	40	208302.8000	-9	150
12	7	5	11	6	6	892745.9050	-394	100	c	49	7	43	48	8	40	213703.0000	-18	150
18	7	11	19	6	14	297782.5700	-18	200	c	57	7	51	56	8	48	368330.6690	-267	90 d
19	7	13	20	6	14	278250.9700	2	200	c	10	10	0	10	9	1	964551.5430	9	50 e
25	7	19	26	6	20	159447.9600	22	80	c	11	10	2	11	9	3	964580.9600	-59	100 e
26	7	19	27	6	22	139474.5400	37	80	c	12	10	2	12	9	3	964609.4740	3	60 e
27	7	21	28	6	22	118994.2360	3	2	a	13	10	4	13	9	5	964635.9770	57	80 e
28	7	21	29	6	24	98976.2940	0	2	a	14	10	4	14	9	5	964659.3200	0	50 e
30	5	25	29	6	24	36338.0500	-57	30	c	15	10	6	15	9	7	964678.5440	-1	50 e
29	7	23	30	6	24	77926.7070	-1	2	a	16	10	6	16	9	7	964692.3890	0	80 e
31	5	27	30	6	24	47660.6000	-21	50	c	17	10	8	18	9	9	619888.4240	44	100 c
30	7	23	31	6	26	58042.4100	-229	200	c	19	10	10	19	9	11	964688.3580	-14	80 e
31	7	25	32	6	26	36065.2300	-48	30	c	20	10	10	20	9	11	964667.0150	-13	40 e
33	5	29	32	6	26	87926.2739	0	2	a	21	10	12	21	9	13	964633.0160	-51	80 e
34	5	29	33	6	28	135963.0000	-25	80	c	22	10	12	22	9	13	964584.7990	0	100 e
32	7	25	33	6	28	16681.0300	8	100	c	25	10	16	25	9	17	964335.9680	-21	50
35	5	31	34	6	28	126980.7000	-1	80	c	26	10	16	26	9	17	964211.8700	-34	50 e
36	5	31	35	6	30	192236.1800	23	100	c	27	10	18	27	9	19	964063.7520	-37	50 e
42	7	35	42	6	36	614113.6820	86	100	c	28	10	18	28	9	19	963889.3900	-35	50 e
48	7	41	48	6	42	555750.3340	43	100	c	29	10	20	29	9	21	963686.4940	-36	50 e
50	7	43	50	6	44	529606.8820	-21	100	c	30	10	20	30	9	21	963452.6120	-48	50 e
53	5	49	52	6	46	209874.3700	-11	150	c	31	10	22	31	9	23	963185.3650	-32	50 e
51	9	43	52	6	46	1020137.0930	-17	100	e	32	10	22	32	9	23	962881.9580	-33	80 e
54	7	47	54	6	48	476625.5430	12	100	c	33	10	24	33	9	25	962539.9630	-29	140 e
56	7	49	56	6	50	455093.0980	-65	100	c	33	10	24	34	9	25	310017.1960	-17	120 d
57	5	53	56	6	50	115904.9387	0	2	a	34	10	24	34	9	25	962156.0980	-24	230 e
57	7	51	57	6	52	667419.8370	-154	100	c	34	10	24	35	9	27	290338.5420	-67	120 d
59	5	55	58	6	52	56572.0000	-161	50	c	35	10	26	35	9	27	961728.1900	-24	380 e
9	8	2	10	7	3	572554.2690	31	40	e	36	10	26	36	9	27	961251.8830	-20	630 e
14	8	6	15	7	9	476621.5470	18	100	c	36	10	26	37	9	29	250816.7080	-85	120 d
24	8	16	25	7	19	282636.2400	26	200	c	38	10	28	39	9	31	211053.1000	-13	150
27	8	20	28	7	21	223434.4700	-26	150	c	39	10	30	40	9	31	191067.2300	78	100
28	8	20	29	7	23	203570.1500	47	100	c	40	10	30	40	9	31	958804.9540	-4	60 e
29	8	22	30	7	23	183582.7100	-25	100	c	41	10	32	41	9	33	958045.4380	0	60 e

TABLE 1—Continued

Transition	Frequency (MHz)	Obs. - Calc. (kHz)	Exp. Unc. (kHz)	Ref.	Transition	Frequency (MHz)	Obs. - Calc. (kHz)	Exp. Unc. (kHz)	Ref.
41 10 32 42 9 33	150878.8100	-7	80		55 10 46 54 11 43	9240.7370	37	40	b
42 10 32 42 9 33	957203.8310	0	50	e	56 10 46 55 11 45	30218.8400	96	100	
42 10 32 43 9 35	130680.0100	27	80		54 12 42 55 11 45	97177.2731	0	2	a
43 10 34 43 9 35	956308.7530	5	50	e	57 10 48 56 11 45	51086.1000	-100	100	
45 8 38 44 9 35	17539.9400	0	100		55 12 44 56 11 45	76860.5500	-14	50	
43 10 34 44 9 35	110363.8000	-40	80		56 12 44 57 11 47	56481.3007	0	2	a
44 10 34 44 9 35	955306.2220	6	50	e	58 10 48 57 11 47	72383.6912	0	2	a
45 10 36 45 9 37	954265.6690	9	50		59 10 50 58 11 47	93372.9528	0	2	a
46 8 38 45 9 37	39446.9900	-16	100		57 12 46 58 11 47	36003.5400	-6	100	
44 10 34 45 9 37	90005.1263	-2	2	a	60 10 50 59 11 49	115090.7045	-4	2	a
46 10 36 46 9 37	953072.6190	8	80		58 12 46 59 11 49	15470.4000	-30	100	
45 10 36 46 9 37	69480.4355	0	2	a	69 10 60 68 11 57	311975.7870	218	270	d
47 8 40 46 9 37	59883.5317	1	2	a	35 13 23 36 12 24	571775.1540	-43	100	c
46 10 36 47 9 39	48958.1800	-39	30		37 13 25 38 12 26	533208.7860	-49	100	c
47 10 38 47 9 39	951882.3790	8	60		40 13 27 41 12 30	475196.4760	-11	100	c
48 10 38 48 9 39	950456.6180	6	60		41 13 29 42 12 30	455809.9620	-56	100	c
47 10 38 48 9 39	28179.2000	-115	50		53 13 41 54 12 42	220597.1400	122	150	
49 8 42 48 9 39	102707.2523	2	2	a	57 13 45 58 12 46	140800.1600	-1	80	
48 10 38 49 9 41	7503.4400	1	1	b	60 11 49 59 12 48	5189.2450	0	1	b
50 8 42 49 9 41	127081.9600	-3	80		59 13 47 60 12 48	100563.0067	2	2	a
51 8 44 50 9 41	145970.2900	35	80		61 11 51 60 12 48	25883.6000	-4	200	
53 8 46 52 9 43	189575.3000	-220	100		62 11 51 61 12 50	46752.9000	-7	200	
54 8 46 53 9 45	220102.6800	56	150		61 13 49 62 12 50	60072.5800	-48	50	
55 8 48 54 9 45	233345.4300	-59	120	d	62 13 49 63 12 52	39730.0000	-107	200	
57 8 50 56 9 47	276992.8400	-60	200		63 13 51 64 12 52	19306.2000	-14	200	
61 8 54 60 9 51	362022.9670	-112	150	d	65 11 55 64 12 52	109740.4069	6	2	a
15 11 5 15 10 6	1064205.9960	0	150	e	15 14 2 16 13 3	1052274.1380	16	90	e
16 11 5 16 10 6	1064241.1400	2	150	e	16 14 2 17 13 5	1033183.1890	22	50	e
17 11 7 17 10 8	1064272.2890	-637	150	e	17 14 4 18 13 5	1014093.8480	117	150	e
18 11 7 18 10 8	1064300.3540	-4	150	e	18 14 4 19 13 7	995005.3280	16	100	e
19 11 9 19 10 10	1064322.3580	-11	50	e	33 14 20 34 13 21	708381.1450	-45	100	c
20 11 9 20 10 10	1064337.8360	-2	80	e	35 14 22 36 13 23	670047.1990	61	100	c
23 11 13 23 10 14	1064333.4250	529	300	e	40 14 26 41 13 29	573977.5280	103	100	c
24 11 13 24 10 14	1064309.7810	-22	50	e	42 14 28 43 13 31	535433.8770	79	100	c
26 11 15 26 10 16	1064223.0250	-15	150	e	43 14 30 44 13 31	516132.7280	-1	100	c
30 11 19 31 10 22	469422.3430	-11	100	c	45 14 32 46 13 33	477466.1790	25	100	c
34 11 23 34 10 24	1063097.5450	-9	50	e	46 14 32 47 13 35	458098.1930	11	100	c
35 11 25 35 10 26	1062839.3820	-3	60	e	51 14 38 52 13 39	360859.1960	-27	150	d
36 11 25 36 10 26	1062548.3730	22	50	e	66 12 54 65 13 53	21761.4000	52	200	
37 11 27 37 10 28	1062222.2880	3	50	e	64 14 50 65 13 53	103807.6172	-1	2	a
38 11 27 38 10 28	1061858.7830	7	50	e	67 12 56 66 13 53	42397.7000	100	200	
37 11 27 38 10 28	333043.3430	-108	180	d	67 14 54 68 13 55	43321.7000	-8	200	
39 11 29 39 10 30	1061455.6230	10	90	e	68 14 54 69 13 57	23041.1000	-47	200	
39 11 29 40 10 30	293717.6990	-105	120	d	70 12 58 69 13 57	104915.5817	-2	2	a
40 11 29 40 10 30	1061010.0250	14	150	e	20 15 5 21 14 8	1053599.8820	5	80	e
40 11 30 41 10 31	273982.6070	216	90	d	21 15 7 22 14 8	1034528.1280	6	50	e
41 11 31 41 10 32	1060519.9160	18	240	e	43 15 29 44 14 30	614155.8150	112	100	c
42 11 31 42 10 32	1059981.8100	25	390	e	57 15 43 58 14 44	343476.7110	25	90	d
42 11 31 43 10 34	234353.0140	-5	150	d	71 13 59 70 14 56	17719.1500	301	100	
43 11 33 43 10 34	1059394.2300	19	610	e	72 15 57 73 14 60	46786.9000	-266	200	
44 11 33 44 10 34	1058752.2310	29	957	e	73 15 59 74 14 60	26644.5000	-143	200	
43 11 33 44 10 34	214451.8900	54	150		25 16 10 26 15 11	1054291.5550	-15	80	e
44 11 33 45 10 36	194491.7500	78	100		26 16 10 27 15 13	1035242.7450	-11	50	e
46 11 35 46 10 36	1057297.5160	25	50	e	27 16 12 28 15 13	1016194.6570	-2	70	e
47 11 37 47 10 38	1056481.1610	25	50	e	30 16 14 31 15 17	959049.9840	-11	70	e
46 11 35 47 10 38	154373.3400	1	80		33 16 18 34 15 19	901894.2820	3	80	e
47 11 37 48 10 38	134203.8200	-20	80		45 16 30 46 15 31	672850.7520	68	100	c
49 11 39 49 10 40	1054643.4680	17	80	e	55 16 40 56 15 41	480838.3050	229	100	c
50 9 41 49 10 40	13599.5000	-99	100		56 16 40 57 15 43	461546.3560	163	100	c
48 11 37 49 10 40	113970.8732	-3	2	a	57 16 42 58 15 43	442234.4750	247	100	c
51 9 43 50 10 40	34393.5500	-12	100		30 17 13 31 16 16	1054347.5720	-30	80	e
50 11 39 51 10 42	73255.2170	1	2	a	31 17 15 32 16 16	1035326.6470	-11	50	e
52 9 43 51 10 42	55932.0000	-220	100		32 17 15 33 16 18	1016306.4350	0	80	e
53 9 45 52 10 42	76762.2882	5	2	a	45 17 29 46 16 30	768898.3130	4	100	c
51 11 41 52 10 42	52744.0000	-127	100		35 18 18 36 17 19	1053771.5790	-26	80	e
54 9 45 53 10 44	98917.8393	0	2	a	36 18 18 37 17 21	1034784.3430	11	50	e
52 11 41 53 10 44	32195.4500	-15	100		37 18 20 38 17 21	1015798.1420	131	150	e
53 11 43 54 10 44	11472.3380	7	2	a	43 18 26 44 17 27	901877.9040	240	100	e
56 9 47 55 10 46	142690.1800	13	80		40 19 21 41 18 24	1052570.8420	-7	90	e
59 9 51 58 10 48	206786.9920	50	60	d	41 19 23 42 18 24	1033623.7010	54	50	e
63 9 55 62 10 52	295433.0760	-257	150	d	42 19 23 43 18 26	1014678.0950	269	200	e
65 9 57 64 10 54	339890.9380	-26	90	d	44 20 24 45 19 27	1069657.6350	-91	50	e
22 12 10 23 11 13	722704.8710	-23	100	c	45 20 26 46 19 27	1050755.1140	18	100	e
30 12 18 31 11 21	569102.7840	127	100	c	46 20 26 47 19 29	1031854.8740	127	100	e
35 12 24 36 11 25	472520.7820	117	100	c	47 20 28 48 19 29	1012956.6130	239	200	e
41 12 30 42 11 31	355705.4930	-16	90	d	49 21 29 50 20 30	1067185.1060	-172	50	e
45 12 34 46 11 35	277085.9600	22	200		50 21 29 51 20 32	1048335.8080	8	150	e
49 12 38 50 11 39	197709.4500	69	100		51 21 31 52 20 32	1029489.4850	188	150	e
52 12 40 53 11 43	137585.0500	85	80		52 21 31 53 20 34	1010645.8810	384	250	e
53 12 42 54 11 43	117412.6120	-3	2	a	56 22 34 57 21 37	1026540.1510	191	100	e

procedure and were subsequently discarded. In the fittings, about 0.25% of the high frequency line deviations were 4.5 times or greater than the estimated experimental uncer-

tainty. This was probably due to overlapping with hot band or isotopic species. Since the deviations were not systematic, these lines were not included in the final fittings.

TABLE 2  
Observed Pure Rotational Transitions of  $^{34}\text{SO}_2$

Transition						Frequency (MHz)	Obs. - Calc. (kHz)	Exp. Unc. (kHz)	Ref.	Transition						Frequency (MHz)	Obs. - Calc. (kHz)	Exp. Unc. (kHz)	Ref.
1	1	1	0	0	0	67750.2980	0	2	a	17	2	16	16	3	13	33212.8100	3	50	
3	1	3	2	0	2	102031.8784	-2	1000		16	4	12	16	3	13	332836.2250	-14	100	
1	1	1	2	0	2	10547.8630	0	1	f	15	4	12	16	3	13	25171.0400	21	50	
2	1	1	2	0	2	51822.0900	215	100		17	4	14	17	3	15	345929.3490	53	100	
5	1	5	4	0	4	133471.4700	39	100		16	4	12	17	3	15	20548.1900	21	50	
4	1	3	4	0	4	57687.5330	-7	2	a	19	2	18	18	3	15	45079.6800	-53	100	
6	1	5	6	0	6	67768.7795	-1	2	a	21	2	20	20	3	17	47293.1100	-59	100	
9	1	9	8	0	8	191013.3900	78	100		21	4	18	21	3	19	352082.9210	18	100	
8	1	7	8	0	8	83043.8240	2	2	a	23	2	22	22	3	19	39024.1000	-136	100	
10	1	9	10	0	10	104391.7061	0	2	a	25	2	24	24	3	21	20260.8000	-10	100	
12	1	11	12	0	12	132114.0400	-12	100		25	4	22	25	3	23	367369.2990	40	100	
13	1	13	12	0	12	248698.6040	-96	100	d	27	4	24	27	3	25	379498.6180	16	100	
16	1	15	16	0	16	203504.2690	51	100	d	30	4	26	30	3	27	249099.3520	138	100	d
18	1	17	18	0	18	243936.0520	87	100	d	38	4	34	38	3	35	315193.2590	48	100	d
18	3	15	18	0	18	599550.5840	7	100		44	4	40	44	3	41	447981.1980	31	100	c
25	1	25	24	0	24	447275.2490	-9	100	c	46	4	42	46	3	43	498409.9990	18	100	c
30	1	29	30	0	30	479152.2730	69	100	c	48	4	44	48	3	45	548333.6130	-21	100	c
34	1	33	34	0	34	551699.8710	104	100	c	55	4	52	54	3	51	1025770.0150	38	50	e
37	1	37	36	0	36	656549.4960	-130	100	c	6	5	1	5	4	2	558717.5490	16	100	c
40	1	39	40	0	40	658797.5170	125	100	c	9	5	5	8	4	4	615985.5290	128	100	c
3	2	2	2	1	1	203225.1400	78	100		7	5	3	8	4	4	291146.2270	242	100	d
4	0	4	3	1	3	31011.1800	32	50		11	5	7	10	4	6	654069.8810	-64	100	c
2	2	0	3	1	3	95810.4135	0	2	a	14	5	9	13	4	10	711021.0600	140	100	c
4	2	2	4	1	3	141158.7600	-181	100		17	5	13	16	4	12	766772.8350	-51	100	c
6	0	6	5	1	5	74404.5793	1	2	a	18	3	15	17	4	14	23732.9900	-1	50	
5	2	4	6	1	5	17970.4200	165	100		16	5	11	17	4	14	115744.6662	0	2	a
6	2	4	6	1	5	134826.1200	-129	100		19	3	17	18	4	14	14754.7000	-46	50	
8	2	6	7	1	7	330191.1030	-56	100		17	5	13	18	4	14	93852.0657	0	2	a
8	0	8	7	1	7	118478.5480	2	2	a	20	3	17	19	4	16	77231.3753	1	2	a
6	2	4	7	1	7	39819.2000	52	100		18	5	13	19	4	16	76031.2305	1	2	a
8	2	6	9	1	9	20699.2600	-42	50		21	3	19	20	4	16	47002.3400	-31	59	
10	2	8	11	1	11	9650.6300	-156	50		22	3	19	21	4	18	135566.2800	-5	200	
11	2	10	11	1	11	201376.4170	-70	100	d	20	5	15	21	4	18	36294.5400	-4	50	
14	2	12	14	1	13	129803.3600	-34	100		23	3	21	22	4	18	74698.1706	1	2	a
15	2	14	15	1	15	245178.5870	-143	100	d	24	3	21	23	4	20	198348.5400	23	100	
14	2	12	15	1	15	15994.1000	-41	100		25	3	23	24	4	20	96075.2978	-1	2	a
16	2	14	16	1	15	141653.1600	-246	100		26	3	23	25	4	22	264682.7600	-138	100	d
16	2	14	17	1	17	33672.1000	-136	100		27	3	25	26	4	22	109260.5100	1	2	a
21	2	20	21	1	21	330667.5650	-202	100		29	3	27	28	4	24	112577.8993	0	2	a
20	2	18	21	1	21	94250.8406	0	2	a	31	3	29	30	4	26	104914.6988	0	2	a
24	2	22	23	1	23	1054659.4890	-8	80	e	38	5	33	38	4	34	310375.9900	89	100	d
23	2	22	23	1	23	362834.0860	-91	100		44	5	39	44	4	40	330519.2370	150	100	
24	2	22	24	1	23	260326.9970	45	100	d	6	6	0	5	5	1	656900.7130	-3	100	c
28	0	28	27	1	27	498995.0360	42	100	c	6	6	0	6	5	1	542302.2310	-59	60	e
28	2	26	28	1	27	347483.1240	104	100		7	6	2	7	5	3	542291.7170	-63	50	e
31	2	30	30	1	29	572591.3100	-88	300	e	9	6	4	8	5	3	714223.7010	-93	100	c
34	0	34	33	1	33	604080.0040	-9	100	c	8	6	2	8	5	3	542270.0660	-59	50	e
35	2	34	35	1	35	570537.9420	29	300	e	8	6	2	9	5	5	370280.0080	133	100	
37	2	36	37	1	37	605924.4030	-104	100	c	9	6	4	9	5	5	542233.4830	-61	80	e
7	3	5	7	2	6	248364.7630	-7	100	d	10	6	4	10	5	5	542177.3740	-63	220	e
6	3	3	7	2	6	114574.4390	3	2	a	11	6	6	11	5	7	542097.6450	-52	589	e
8	1	7	7	2	6	30975.4500	36	50		13	6	8	14	5	9	273930.1000	117	100	d
8	3	5	9	2	8	78397.0175	0	2	a	21	6	16	22	5	17	115722.1453	-3	2	a
10	1	9	9	2	8	82124.3470	0	2	a	22	6	16	23	5	19	96193.8592	2	2	a
9	3	7	9	2	8	250358.4930	107	100	d	24	4	20	23	5	19	40652.4200	16	50	
9	3	7	10	2	8	43619.9100	-34	100		25	4	22	24	5	19	41540.9000	4	50	
10	3	7	11	2	10	44226.2400	17	100		23	6	18	24	5	19	74580.7642	2	2	a
12	1	11	11	2	10	134873.8400	42	100		26	4	22	25	5	21	92428.8728	1	2	a
12	3	9	13	2	12	13207.9000	-105	100		25	6	20	26	5	21	32272.3400	-59	50	
14	3	11	14	2	12	215999.6550	-80	100	d	26	6	20	27	5	23	14850.4000	-37	100	
17	3	15	17	2	16	279075.1980	-66	100	d	29	4	26	28	5	23	111902.7923	-2	2	a
18	3	15	17	2	16	648737.5970	46	100	c	34	4	30	33	5	29	350619.3300	-154	100	
18	3	15	18	2	16	194812.0600	23	100		36	6	30	36	5	31	480055.4370	41	100	c
20	3	17	20	2	18	189123.8900	133	100		37	4	34	36	5	31	184532.8070	-139	100	d
22	3	19	22	2	20	189392.4560	106	100	d	38	4	34	37	5	33	501920.1460	40	100	c
25	3	23	24	2	22	573527.2090	-98	300		38	6	32	38	5	33	459535.9110	41	100	c
24	3	21	24	2	22	197044.3000	190	100		37	8	30	38	5	33	1060418.9610	-30	250	e
25	3	23	25	2	24	356222.2500	-136	100		42	4	38	41	5	37	652745.7910	202	100	
30	3	27	30	2	28	270229.5550	-124	100	d	42	4	38	41	5	37	652745.5610	-27	50	c
32	3	29	32	2	30	309816.0170	52	100	d	43	6	38	43	5	39	542257.6730	-101	100	c
38	3	35	38	2	36	448811.0480	57	100	c	45	6	40	45	5	41	553329.1380	-56	100	c
40	3	37	40	2	38	495286.9690	-36	100	c	46	6	40	46	5	41	374322.5310	-91	100	
5	4	2	4	3	1	441174.0320	-3	100	c	48	6	42	48	5	43	365141.1440	262	100	
11	4	8	12	3	9	112532.3159	-2	2	a	7	7	1	6	6	0	773885.7200	-82	100	c
12	4	8	13	3	11	95922.8159	0	2	a	9	7	3	10	6	4	449079.3570	51	100	c
14	2	12	13	3	11	58552.7177	0	2	a	15	7	9	16	6	10	333683.9180	24	100	
14	4	10	13	3	11	613338.1480	0	100	c	22	7	15	23	6	18	196854.5610	101	100	d
15	2	14	14	3	11	13184.8000	-53	100		28	5	23	27	6	22	11695.0500	-28	100	
16	4	12	15	3	13	652652.8650	50												

TABLE 2—Continued

Transition										Frequency (MHZ)	Obs. - Calc. (kHz)	Exp. Unc. (kHz)	Ref.	Transition										Frequency (MHZ)	Obs. - Calc. (kHz)	Exp. Unc. (kHz)	Ref.																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
28	7	21	29	6	24	76220.1176	3	2	a	44	8	36	43	9	35	27657.1500	-54	50																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														

### III. DERIVATION OF ROTATIONAL CONSTANTS

The high-frequency data measured in this work were combined with all known previous measurements of SO<sub>2</sub>. Data reported before 1985 have been taken from the compilation of Lovas (10). In addition to this data, there have been a number of additional studies including mm-region measurements of Helminger and DeLucia (11) and the very high precision measurements mentioned above (4, 5) that have also been

included in the data set. In order to fix more precisely the higher order distortion terms, we have also included the high  $K_a$  transitions measured in the far infrared region by Carlotti *et al.* (9). Several low  $J$  transitions have also been recorded on the FT microwave instrument at National Institute of Standards and Technology and were included in the fitting. For the <sup>32</sup>SO<sub>2</sub> molecule, the microwave data consisted of 480 transitions including states with  $J$  ranging as high as 74 with  $K_a$  up to 22.

TABLE 3  
Observed Pure Rotational Transitions of  $^{32}\text{S}^{18}\text{O}^{16}\text{O}$

Transition						Frequency (MHz)	Obs. - Calc. (kHz)	Exp. Unc. (kHz)	Ref.	Transition						Frequency (MHz)	Obs. - Calc. (kHz)	Exp. Unc. (kHz)	Ref.
1	1	1	0	0	0	67430.6000	68	200		14	4	11	15	3	12	70670.7500	48	200	
1	1	0	1	0	1	50767.4000	69	200		15	4	12	16	3	13	49699.0000	-123	200	
1	1	1	2	0	2	13291.1955	0	1 f		15	4	11	16	3	14	59503.5000	-108	200	
2	1	1	2	0	2	52189.8000	33	200		17	2	16	16	3	13	22326.7000	-79	200	
3	1	2	3	0	3	54377.6200	86	200		18	2	17	17	3	14	30962.7000	-192	200	
4	1	3	4	0	4	57394.6000	76	200		16	4	12	17	3	15	41768.9000	-73	200	
6	1	6	5	0	5	144375.4200	-254	200		16	4	13	17	3	14	27983.7000	-47	200	
5	1	4	5	0	5	61323.0000	-429	200		18	2	16	17	3	15	141890.3100	223	200	
6	1	5	6	0	6	66262.2200	34	200		17	4	13	18	3	16	24344.3000	-106	200	
7	1	6	7	0	7	72318.1200	94	200		19	2	18	18	3	15	37783.9000	-20	200	
8	1	7	8	0	8	79599.0600	270	200		20	2	19	19	3	16	42615.2000	-202	200	
9	1	8	9	0	9	88201.6600	-76	200		21	2	20	20	3	17	45307.3000	173	200	
13	1	12	13	0	13	136749.3100	-81	200		22	2	21	21	3	18	45742.0000	164	200	
37	1	36	37	0	37	571832.7270	-158	200	e	23	2	22	22	3	19	43841.4000	16	200	
4	0	4	3	1	3	25913.0500	-72	200		24	2	23	23	3	20	39569.5000	-32	200	
4	2	2	4	1	3	143714.9200	207	200		25	2	24	24	3	21	32931.5200	107	200	
5	0	5	4	1	4	46232.4000	2	200		26	2	25	25	3	22	23970.3000	-86	200	
6	0	6	5	1	5	66887.5100	110	200		32	4	28	31	3	29	1059904.2910	-113	150	e
4	2	2	5	1	5	70966.6400	123	200		40	4	36	41	3	39	23320.2500	-102	200	
4	2	3	5	1	4	49650.0000	35	200		6	5	1	5	4	2	558166.1240	-70	120	e
5	2	3	5	1	4	140880.1900	218	200		7	5	2	6	4	3	576240.6300	-145	190	e
5	2	3	6	1	6	57827.7000	-27	200		8	5	3	7	4	4	594309.1600	-394	690	e
6	2	4	6	1	5	137821.4700	111	200		9	5	4	8	4	5	612368.6990	-58	100	e
7	0	7	6	1	6	87752.9200	246	200		9	5	5	8	4	4	612366.6380	-53	80	e
5	2	4	6	1	5	27599.8000	-10	200		10	5	6	9	4	5	630408.7160	-31	100	e
7	2	5	7	1	6	134717.7300	-192	200		10	5	5	9	4	6	630414.1100	-17	100	e
6	2	4	7	1	7	45881.4000	-99	200		19	3	16	18	4	15	18095.3000	-122	200	
7	2	5	8	1	8	35297.0000	42	200		20	3	18	19	4	15	9167.5000	-6	200	
8	2	6	8	1	7	131766.9100	-77	200		20	3	17	19	4	16	42631.4000	-96	200	
9	2	7	10	1	10	18925.2000	-109	200		21	3	19	20	4	16	25012.4000	47	200	
10	2	8	11	1	11	13477.7500	-10	200		21	3	18	20	4	17	68240.3200	-97	200	
11	2	9	12	1	12	10047.0000	10	200		22	3	19	21	4	18	94940.1800	-321	200	
12	2	10	13	1	13	8735.2500	-103	200		22	3	20	21	4	17	40061.4000	74	200	
13	2	11	14	1	14	9605.8000	-30	200		21	5	16	22	4	19	45736.6000	-94	200	
15	2	13	15	1	14	131783.6400	260	200		23	3	21	22	4	18	54153.1000	-99	200	
14	2	12	15	1	15	12681.6500	24	200		21	5	17	22	4	18	39724.4000	-64	200	
15	2	13	16	1	16	17949.1000	-45	200		22	5	17	23	4	20	27018.7000	-40	200	
16	2	14	16	1	15	136657.5500	307	200		23	5	18	24	4	21	8412.2000	-113	200	
17	2	15	17	1	16	143096.2900	78	200		32	5	27	31	4	28	1040831.0110	-23	100	e
16	2	14	17	1	17	25362.7000	-15	200		37	3	35	36	4	32	56467.5000	-69	200	
17	2	15	18	1	18	34849.6000	39	200		38	3	36	37	4	33	39337.8000	-155	200	
19	2	17	19	1	18	160926.6700	45	200		39	3	37	38	4	34	20205.4000	-158	200	
18	2	16	19	1	19	46314.0000	-41	200		51	5	46	52	4	49	16970.2500	-183	200	
34	0	34	33	1	33	574425.0980	-154	300	e	54	3	51	53	4	50	952370.2520	-32	100	e
38	2	37	37	1	36	658754.6780	-100	100	e	52	5	47	53	4	50	45284.1500	-128	200	
60	2	59	59	1	58	1022314.9200	-66	200	e	55	5	51	54	4	50	1030990.0550	2	150	e
8	1	7	7	2	6	18261.7000	-40	200		56	5	52	55	4	51	1041089.8350	-9	150	e
9	1	8	8	2	7	41999.0000	-135	200		6	6	0	6	5	1	549156.2650	-105	100	e
10	1	9	9	2	8	66210.2600	39	200		7	6	2	7	5	3	549151.0180	-107	100	e
11	1	10	10	2	9	90833.5500	-102	200		8	6	2	8	5	3	549137.4140	-101	80	e
9	3	7	10	2	8	59454.6700	21	200		9	6	4	9	5	5	549112.4100	-125	80	e
10	3	8	11	2	9	37345.2000	-264	200		10	6	4	10	5	5	549072.5730	-43	120	e
10	3	7	11	2	10	57098.7000	-164	200		11	6	6	11	5	7	549014.0890	-252	319	e
11	3	8	12	2	11	41461.4000	58	200		12	6	7	12	5	8	548933.0320	-169	200	e
11	3	9	12	2	10	14330.0500	-107	200		12	6	6	12	5	7	548932.4080	-24	200	e
13	1	12	12	2	11	141009.7900	-9	200		13	6	8	13	5	9	548824.7110	-106	100	e
12	3	9	13	2	12	26567.2000	-135	200		13	6	7	13	5	8	548822.9580	-135	100	e
13	3	10	14	2	13	12568.0000	-76	200		14	6	9	14	5	10	548684.3100	-59	100	e
16	3	13	15	2	14	566549.9030	51	100	e	14	6	8	14	5	9	548680.6790	-67	100	e
16	3	13	16	2	14	212789.9500	35	200		16	6	11	16	5	12	548286.5710	-72	120	e
26	3	24	25	2	23	573923.2960	146	300	e	16	6	10	16	5	11	548272.8570	-96	80	e
28	3	26	27	2	25	586826.1430	106	150	e	18	6	12	18	5	13	547653.1520	-49	100	e
29	3	27	28	2	26	593928.4380	104	120	e	18	6	13	18	5	14	547696.9580	-50	80	e
28	3	25	29	2	28	15940.3000	-33	200		20	6	14	20	5	15	546749.1330	-38	100	e
31	3	29	30	2	28	609989.3710	70	100	e	20	6	15	20	5	16	546872.2070	-25	100	e
29	3	26	30	2	29	33156.1000	52	200		22	6	17	21	5	16	944886.8710	-16	100	e
32	3	30	31	2	29	619100.4240	60	100	e	22	6	16	22	5	17	545463.3590	-17	100	e
30	3	27	31	2	30	52061.6000	148	200		24	6	18	24	5	19	543659.8020	-1	120	e
33	1	32	32	2	31	571870.1750	-86	300	e	25	4	21	24	5	20	25701.3500	-80	200	
39	5	34	39	2	37	1039698.4270	100	100	e	25	4	22	24	5	19	10019.8000	-85	200	
44	3	42	44	2	43	627800.4340	34	300	e	24	6	19	24	5	20	544379.3470	-8	120	e
60	1	59	59	2	58	1022310.1860	-40	250	e	26	4	22	25	5	21	49091.7500	-81	200	
12	4	8	11	3	9	566790.7410	26	80	e	26	4	23	25	5	20	28202.6000	7	200	
12	4	9	11	3	8	565621.2110	19	100	e	26	6	20	26	5	21	541145.2150	19	120	e
13	2	11	12	3	10	9610.0000	-47	200		26	6	21	26	5	22	542688.6420	1	120	e
13	4	10	12	3	9	582955.1970	37	80	e	26	6	21	27	5	22	49312.7000	-44	200	
13	4	9	12	3	10	584902.2120	26	60	e	26	6	20	27	5	23	51717.0000	-245	200	
14	2	12	13	3	11	34462.2000	-171	200		28	6	22	28	5	23	537645.9250	36	150	e
13	4																		



TABLE 3—Continued

Transition					Frequency (MHZ)	Obs. - Calc. (kHz)	Exp. Unc. (kHz)	Transition					Frequency (MHZ)	Obs. - Calc. (kHz)	Exp. Unc. (kHz)	Ref.		
29	4	26	28	5	23	80292.7200	-36	200	42	7	36	41	8	33	32735.1000	3	200	
28	6	23	29	5	24	8360.6000	-5	200	43	7	36	42	8	35	55238.4000	15	200	
28	6	22	29	5	25	13120.1000	-96	200	43	7	37	42	8	34	52749.2000	18	200	
30	6	24	30	5	25	532784.9380	57	100	e	42	9	33	43	8	36	53622.5000	129	200
30	6	25	30	5	26	538642.6660	24	150	e	43	9	34	44	8	37	34071.9500	-136	200
32	6	27	32	5	28	536552.0100	43	200	e	43	9	35	44	8	36	33830.1000	-28	200
35	6	30	35	5	31	533993.6510	52	100	e	44	9	35	45	8	38	14416.9000	3	200
41	6	36	41	5	37	535499.5750	-21	120	e	44	9	36	45	8	37	14075.2000	152	200
50	4	47	49	5	44	36251.2000	-107	200	10	10	0	10	9	1	943256.0860	174	250	
51	4	48	50	5	45	10290.5100	75	200	11	10	2	11	9	3	943284.6350	182	200	
59	4	55	58	5	54	1039962.9990	80	100	e	12	10	3	12	9	4	943312.5450	156	179
12	7	6	12	6	7	648215.1700	-84	150	e	13	10	4	13	9	5	943338.9090	21	200
13	7	6	13	6	7	648168.9830	-71	80	e	14	10	5	14	9	6	943363.2060	159	120
15	7	9	15	6	10	648020.2740	-125	110	e	15	10	6	15	9	7	943384.0560	158	80
16	7	9	16	6	10	647911.1730	49	239	e	18	10	9	18	9	10	943416.0270	159	120
17	7	11	17	6	12	647774.1340	-288	479	e	21	10	12	21	9	13	943376.6760	138	120
18	7	11	18	6	12	647604.7240	-49	100	e	22	10	12	22	9	13	943341.4720	187	150
18	7	12	18	6	13	647605.7220	-17	100	e	23	10	13	23	9	14	943292.5900	112	200
19	7	13	19	6	14	647401.2340	8	100	e	24	10	14	24	9	15	943228.1160	-401	400
19	7	12	19	6	13	647399.3330	-44	100	e	25	10	15	25	9	16	943147.9400	202	300
20	7	14	20	6	15	647156.5320	-42	100	e	26	10	17	26	9	18	943048.4480	55	300
20	7	13	20	6	14	647153.1140	-49	120	e	27	10	18	27	9	19	942928.7740	109	300
21	7	15	21	6	16	646867.2230	-52	100	e	28	10	19	28	9	20	942786.7570	98	150
21	7	14	21	6	15	646861.1300	-45	100	e	29	10	20	29	9	21	942620.5930	191	300
22	7	16	21	6	15	1045254.0880	-29	80	e	47	8	39	46	9	38	25883.6000	-101	200
22	7	15	21	6	16	1045260.4620	-127	80	e	47	8	40	46	9	37	25218.9500	-42	200
22	7	16	22	6	17	646528.5880	-41	100	e	46	10	36	47	9	39	80287.5400	1	200
23	7	16	23	6	17	646117.8090	-37	100	e	48	8	41	47	9	38	45202.9000	54	200
23	7	17	23	6	18	646135.7440	-40	100	e	48	8	40	47	9	39	46118.0500	-137	200
26	7	19	26	6	20	644506.4270	-32	120	e	48	10	38	49	9	41	41452.5500	73	200
27	7	20	27	6	21	643805.2160	-6	100	e	48	10	39	49	9	40	41368.2000	-14	200
27	7	21	27	6	22	643923.1280	-8	100	e	49	10	40	50	9	41	21775.2000	-19	200
28	7	21	28	6	22	643005.4670	-17	100	e	49	10	39	50	9	42	21894.8000	39	200
28	7	22	28	6	23	643185.5470	23	100	e	11	11	1	11	10	2	1040624.6890	-107	100
27	7	21	28	6	22	135306.9600	271	200	12	11	2	12	10	3	1040662.6290	-112	100	
29	7	23	29	6	24	642365.4770	-10	100	e	13	11	3	13	10	4	1040700.9280	-143	100
29	7	22	29	6	23	642095.0400	-51	100	e	14	11	4	14	10	5	1040738.9050	-218	100
30	5	25	29	6	24	12763.2000	20	200	15	11	5	15	10	6	1040776.0710	-112	70	
30	7	24	30	6	25	641459.7120	-11	100	e	16	11	6	16	10	7	1040811.2580	-228	100
31	5	26	30	6	25	34421.9000	-66	200	17	11	6	17	10	7	1040844.1140	-102	60	
31	5	27	30	6	24	25503.9500	-58	200	20	11	10	20	10	11	1040917.9240	-146	100	
30	7	23	30	6	24	641059.9680	92	120	e	21	11	11	21	10	12	1040931.8770	519	100
32	5	28	31	6	25	44731.5000	-257	200	22	11	11	22	10	12	1040937.3440	100	100	
31	7	25	31	6	26	640465.8970	0	100	e	23	11	13	23	10	14	1040934.6900	79	100
30	7	23	31	6	26	77973.3800	42	200	24	11	13	24	10	14	1040922.2530	-39	100	
31	7	24	31	6	25	639883.2230	11	100	e	25	11	14	25	10	15	1040898.6790	-389	609
32	5	27	31	6	26	56706.1000	-214	200	26	11	16	26	10	17	1040863.6140	-53	70	
32	7	25	32	6	26	638545.5040	0	100	e	25	11	15	26	10	16	570320.5910	-69	300
32	7	26	32	6	27	639382.9400	-9	100	e	27	11	17	27	10	18	1040814.8020	33	100
31	7	24	32	6	27	58599.2000	-287	200	28	11	18	28	10	19	1040750.9270	-67	60	
32	7	26	33	6	27	37826.5000	-324	200	29	11	18	29	10	19	1040670.8530	-64	60	
32	7	25	33	6	28	39127.4000	-142	200	30	11	20	30	10	21	1040572.9980	-55	100	
33	7	27	33	6	28	638211.4310	-10	100	e	31	11	21	31	10	22	1040456.2370	372	100
33	7	26	33	6	27	637023.6100	2	100	e	32	11	22	32	10	23	1040317.7100	-46	100
33	7	27	34	6	28	17727.7500	-3	200	33	11	22	33	10	23	1040157.0400	-35	100	
33	7	26	34	6	29	19561.9000	-181	200	34	11	24	34	10	25	1039972.1060	-8	100	
34	7	28	34	6	29	636953.9490	8	150	e	35	11	25	35	10	26	1039761.0330	-66	100
34	7	27	34	6	28	635290.1580	-20	80	e	36	11	26	36	10	27	1039522.1630	-33	70
35	7	28	35	6	29	633312.9930	6	100	e	37	11	27	37	10	28	1039253.4810	-26	70
35	7	29	35	6	30	635615.4010	-33	120	e	38	11	27	38	10	28	1038953.2630	220	150
62	5	58	61	6	55	18589.5500	-65	200	39	11	28	39	10	29	1038619.1270	324	200	
11	8	4	10	7	3	945944.1050	31	100	e	40	11	30	40	10	31	1038248.7580	16	120
15	8	8	14	7	7	1018318.9930	38	150	e	41	11	30	41	10	31	1037840.4880	46	150
16	8	9	15	7	8	1036398.7660	29	60	e	42	11	32	42	10	33	1037391.9490	-120	200
17	8	10	16	7	9	1054469.4880	27	60	e	43	11	33	43	10	34	1036900.7340	-178	319
36	6	30	35	7	29	23337.2000	-118	200	47	11	37	47	10	38	1034460.0560	126	150	
36	6	31	35	7	28	19813.3000	-97	200	47	11	36	47	10	37	1034457.9860	-124	150	
37	6	31	36	7	30	44398.8000	-204	200	48	11	37	48	10	38	1033714.4870	-133	150	
37	6	32	36	7	29	39594.4000	99	200	48	11	38	48	10	39	1033717.4530	96	150	
38	6	33	37	7	30	59408.7000	-93	200	50	11	40	50	10	41	1032053.4910	-40	150	
37	8	30	38	7	31	45832.1000	-55	200	50	11	39	50	10	40	1032047.4330	-74	150	
37	8	29	38	7	32	46309.0000	-142	200	52	9	44	51	10	41	17520.1500	12	200	
38	8	30	39	7	33	26706.9000	-31	200	52	9	43	51	10	42	17755.1000	36	200	
38	8	31	39	7	32	26029.9000	0	200	53	9	45	52	10	42	37384.4000	81	200	
9	9	1	8	8	0	1008087.4440	284	200	e	53	9	44	52	10	43	37709.9500	35	200
10	9	1	9	8	2	1026196.1080	138	50	e	54	9	45	53	10	44	57805.0000	2	200
11	9	3	10	8	2	1044306.2650	110	100	e	54	9	46	53	10	43	57357.2000	171	200
12	9	4	11	8	3	1062417.1030	150	50	e	53	11	42	54	10	45	48765.0000	184	200
41	7	34	40	8	33	14140.5000	-92	200	53	11	43	54	10	44	48736.2000	92	200	
41	7	35	40	8														

TABLE 3—Continued

Transition	Frequency (MHZ)	Obs. - Calc. (kHz)	Exp. Unc. (kHz)	Ref.	Transition	Frequency (MHZ)	Obs. - Calc. (kHz)	Exp. Unc. (kHz)	Ref.
55 11 45 56 10 46	9732.6000	-26	200		64 11 54 63 12 51	41425.2000	-1	200	
57 10 48 56 11 45	9831.0800	464	200		64 13 52 65 12 53	43860.6000	35	200	
57 10 47 56 11 46	9912.0000	461	200		64 13 51 65 12 54	43865.0000	-61	200	
58 10 49 57 11 46	29545.5000	-46	200		65 13 53 66 12 54	24595.6000	-8	200	
58 10 48 57 11 47	29658.3000	46	200		65 13 52 66 12 55	24601.9500	-40	200	
59 12 48 60 11 49	36637.4000	56	200		68 12 57 67 13 54	14129.1500	-93	200	
59 12 47 60 11 50	36651.1000	77	200		69 12 58 68 13 55	33602.8000	-118	200	
60 12 49 61 11 50	17233.5000	154	200		69 12 57 68 13 56	33620.5000	-9	200	
60 12 48 61 11 51	17252.9000	179	200		70 14 56 71 13 59	31825.6000	-99	200	
63 11 52 62 12 51	21820.0000	-224	200		70 14 57 71 13 58	31823.5500	-84	200	
64 11 53 63 12 52	41478.1000	-49	200		19 15 5 20 14 6	1062390.2570	259	250	e

For the  $^{34}\text{SO}_2$  and the  $^{32}\text{S}^{18}\text{O}^{16}\text{O}$  isotopic species, 298 and 342 transitions were fit. In the fitting, each datum was assigned a weight equal to the square of the reciprocal of its estimated experimental uncertainty. The weights cover a large dynamic range, starting with 0.028 for the far infrared data reaching  $10^6$  for the most precise FTMW measurements.

In the data analysis, a standard Watson Hamiltonian (12) was used in the  $I'$  representation. Since levels with high values of the rotational quantum numbers were included in the fittings, it was necessary to include higher-order diago-

nal terms through  $P^{10}$ . These terms were added one-by-one until the data fit to within the estimated experimental uncertainty. These very high-order terms should be regarded as empirical fitting parameters with very little physical significance. Since the data is more limited for the  $^{34}\text{SO}_2$  and  $^{32}\text{S}^{18}\text{O}^{16}\text{O}$  isotopic species, a number of the higher-order terms could not be obtained in the fittings, and these were fixed at the values derived for the most abundant isotopics species. The microwave data used in these fittings are given in Tables 1–3, and the spectroscopic constants obtained are

TABLE 4  
Ground State Rotational Constants of Several Isotopic Species of Sulfur Dioxide in MHz

	$^{32}\text{S}^{16}\text{O}_2$	$^{34}\text{S}^{16}\text{O}_2$	$^{32}\text{S}^{18}\text{O}^{16}\text{O}$
A	60778.5497700(4400)	58991.1829500(5101)	59101.1689600(26823)
B	10318.0734800(764)	10318.5099300(899)	9724.6428400(5571)
C	8799.7033990(699)	8761.3024810(972)	8331.5601810(5109)
$\Delta_J \times 10^{-3}$	6.611475(128)	6.568494(162)	5.903075(378)
$\Delta_{JK} \times 10^{-1}$	-1.1696161(206)	-1.1166602(267)	-1.0835815(429)
$\Delta_K$	2.59034044(745)	2.44020246(1024)	2.44293678(6249)
$\delta_J \times 10^{-3}$	1.7010282(106)	1.7222182(261)	1.4878101(941)
$\delta_K \times 10^{-2}$	2.536981(118)	2.461910(153)	2.312804(1606)
$H_J \times 10^{-8}$	1.10634(378)	1.10715(375)	0.90292(626)
$H_{JK} \times 10^{-8}$	2.358(170)	1.252(199)	0.724(1863)
$H_{KJ} \times 10^{-5}$	-1.945017(713)	-1.809302(957)	-1.680719(6988)
$H_K \times 10^{-4}$	3.710988(566)	3.393985(709)	3.273802(5153)
$h_J \times 10^{-9}$	5.40214(644)	5.41571(1271)	4.48579(1559)
$h_{JK} \times 10^{-9}$	-1.143(969)	-1.143 <sup>a</sup>	-1.143 <sup>a</sup>
$h_K \times 10^{-5}$	1.66358(610)	1.53908(654)	1.32775(8790)
$L_J \times 10^{-15}$	-9.74(277)	-9.74 <sup>a</sup>	-9.74 <sup>a</sup>
$L_{JK} \times 10^{-13}$	-2.062(905)	-2.062 <sup>a</sup>	-2.062 <sup>a</sup>
$L_{KJ} \times 10^{-11}$	2.042(193)	2.181(227)	-4.227(1233)
$L_{KKJ} \times 10^{-9}$	4.4668(282)	4.3159(465)	1.74341930)
$L_K \times 10^{-8}$	-7.9119(209)	-7.1818(272)	-1.6366(1235)
$P_{KKKJJ} \times 10^{-14}$	3.991(356)	3.991 <sup>a</sup>	3.991 <sup>a</sup>
$P_{KKKJ} \times 10^{-12}$	-1.5212(561)	-2.0704(628)	-1.5212 <sup>a</sup>
$P_K \times 10^{-11}$	1.8650(314)	1.9609(368)	1.8650 <sup>a</sup>

<sup>a</sup> Fixed at value of  $^{32}\text{S}^{16}\text{O}_2$  isotopic species.

presented in Table 4. The uncertainties in the constants are one standard deviation.

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