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$\nu_1 + \nu_3$ Combination Band of SO_2

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CONTENTS

ABSTRACT

The infrared-active vibration-rotation combination band $\nu_1 + \nu_3$ of sulfur dioxide has been measured with moderately high spectral resolution. Quantum number identifications of spectral lines were made by comparison with theoretically computed spectra which include the effects of centrifugal distortion. Relative line intensities were also calculated. The band center for $\nu_1 + \nu_3$ has been determined to be 2499.60 ± 0.10 cm^{-1}.

I. INTRODUCTION

Recently we investigated the infrared-active vibration-rotation fundamental bands of sulfur dioxide at moderately high resolution.[1,2] We felt that earlier results for some combination and overtone bands obtained by Shelton, Nielsen, and Fletcher[3] could also be improved considerably, and that these bands could be analyzed by comparison with theoretically computed spectra. Consequently, as part of this program, we have obtained spectra of the $\nu_1 + \nu_3$ combination band of $^{32}S^{16}O_2$ at a resolution of about 0.15 cm^{-1}. We have assigned quantum numbers to the observed lines by using theoretical spectra which include the effects of centrifugal distortion. All transitions with $J \leq 60$ were included. Relative line intensities of these transitions were also calculated.

Experimental details of our work are given in the next Section. In Section III, the theoretical procedure is discussed briefly. In the last Section, we present our results in the form of measured spectra, and tabulated experimental and theoretical line positions. Possible applications of our results to atmospheric problems are considered.

II. EXPERIMENTAL DETAILS

The anhydrous grade $^{32}S^{16}O_2$ gas sample was obtained from Matheson Gas Products. The stated purity of the sample was 99.98% by weight; with 50, 10, and 30 p.p.m. maxima of H_2O, H_2SO_4, and non-volatiles, resp. A Perkin-Elmer Model 225 Grating Infrared Spectrophotometer, equipped with an f/5 fore monochromator for pre-dispersion of the radiation, was used to record the spectra. A 150 lines/mm grating was employed in the second order for the 2465 to 2525 cm^{-1} region measured. A servo-controlled slit program was utilized to provide constant energy to the thermopile detector. All scans were recorded on a Model 225 Auxiliary Recorder with a dispersion of 1 cm/cm^{-1} and at a speed of 0.5 cm^{-1}/min. Of the six runs taken under identical conditions, the best two with respect to reproducibility, resolution, and noise level were selected for the theoretical analysis of the band.

A 10-cm absorption cell, equipped with KCℓ windows and containing 50 torr of sulfur dioxide, was used to record the spectra. The cell was placed in the sample compartment for one hour prior to each run in order to stabilize (at approximately 315°K) the temperature increase caused by heating from the Globar radiation source. Slit widths were set at 0.22 ± 0.04 cm^{-1}. The ν_3 band of C_2D_2 was used for calibration purposes.[4]

III. THEORETICAL PROCEDURE

The theoretical approach utilized here is the same as that used by us for the analysis of the fundamental bands of this molecule. Details are given in Refs. 1 and 2. The rotational constants of the ground state, and the centrifugal distortion constants (assumed to be the same in the ground and excited states) were given in Table II of Refs. 1 and 2. The values of the excited-state rotational constants A = 2.007487, B = 0.341346, and C = 0.290987 cm^{-1}, were taken from the microwave work of Saito[5] on pure rotational transitions from $\nu_1 + \nu_3$ of sulfur dioxide.

The computer program, described in Refs. 1 and 2, takes into account the fact that in the ground state of SO_2 only symmetric levels occur because of C_{2v} symmetry and zero spin of the ^{16}O nuclei. The initial value for the $\nu_1 + \nu_3$ band center was taken from the work of Shelton et al.[3] This value was later adjusted so that the experimental and theoretical spectra would match.

IV. RESULTS AND DISCUSSION

The results of our experimental and theoretical studies of the $\nu_1 + \nu_3$ band of $^{32}S^{16}O_2$ are given in Fig. 1 and Table I. A representative portion of these results, as well as band intensity and dipole moment derivative data, are presented in Ref. 6. The spectrum, with resolution of about 0.15 cm^{-1}, extends from 2465 to 2525 cm^{-1}. In Figs. 1(a) and 1(b), the upper tracings represent measured experimental spectra, with percent absorption shown in the right-hand vertical scales. The lower tracings are calculated theoretical spectra. Their relative intensities, referred to the left-hand vertical scales, are normalized distributions of line intensities.[1,2] As can be seen in the Figure, there is good agreement between the experimental and theoretical spectra.

In Table I, the observed and calculated spectral line positions are compared. The absolute accuracy of measured line positions is $\pm$ 0.10 cm^{-1}. We estimate the relative accuracy to be $\pm$ 0.05 cm^{-1}. Only the stronger theoretical transitions corresponding to each experimental line peak have been listed in the Table. (Where there is a blank space in the column of experimental line positions, the adjacent theoretical line position corresponds to the previously tabulated experimental line.) Initial- and final-state quantum numbers, as well as theoretical relative line intensities $I^{\circ}_{n''n'}/C'$ defined by Eq.(6) in Ref. 1 [Eq.(4) in Ref. 2], are given for each theoretical transition. The quantum numbers K_{-1} and K_1 are associated with the projection of the total angular momentum (having quantum number J) on the symmetry axis in, resp., the prolate and oblate symmetric top limiting cases.[7,8]

$\nu_1 + \nu_3$, like the ν_3 fundamental, is a type A band. It has a strong central Q branch. The selection rules[9] are $\Delta J = 0, \pm 1$; $J = 0 \not\leftrightarrow 0$;

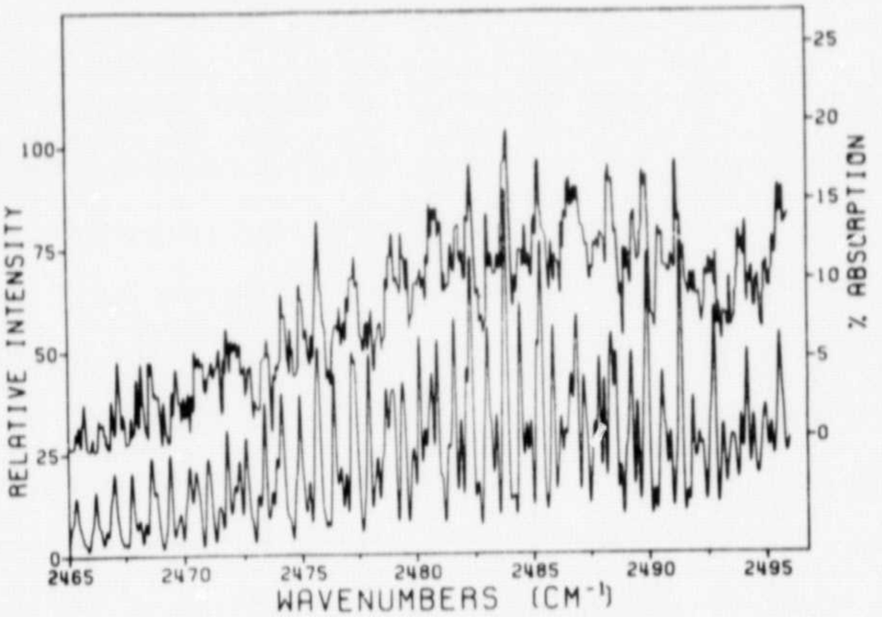

Fig. 1(a). Experimental and theoretical spectra of $\nu_1 + \nu_3$ band of $^{32}S^{16}O_2$ in range 2465 to 2495 cm^{-1}.

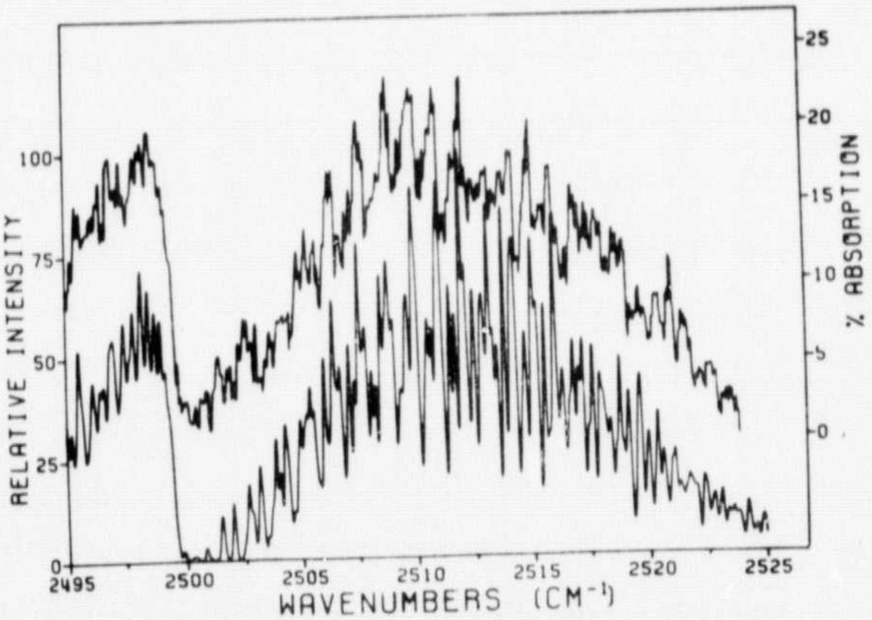

Fig. 1(b). Experimental and theoretical spectra of $\nu_1 + \nu_3$ band of $^{32}S^{16}O_2$ in range 2495 to 2525 cm^{-1}.

TABLE I

COMPARISON OF EXPERIMENTAL AND THEORETICAL SPECTRAL LINE POSITIONS, WITH QUANTUM NUMBER ASSIGNMENTS, FOR THE $\nu_1+\nu_3$ BAND OF $^{32}S^{16}O_2$ CENTERED AT 2499.60±0.10 cm^{-1}. LINE INTENSITIES [SEE EQ.(6) OF REF. 1, OR EQ.(4) OF REF. 2] ARE COMPUTED AT 300°K.

Line Position (in cm^{-1}) Exptl.	Theor.	J'	K'_{-1}	K'_1	J''	K''_{-1}	K''_1	$\frac{I^\circ_{n''n'}}{C'}$	Line Position (in cm^{-1}) Exptl.	Theor.	J'	K'_{-1}	K'_1	J''	K''_{-1}	K''_1	$\frac{I^\circ_{n''n'}}{C'}$
2465.34	2465.31	43	7	36	44	7	37	1.3624		2471.48	33	14	19	34	14	20	0.9166
	2465.33	47	0	47	48	0	48	1.6121		2471.50	31	17	14	32	17	50	0.4275
	2465.37	46	2	45	47	2	46	1.6130	2471.68	2471.69	30	18	13	31	18	14	0.3167
2465.49	2465.49	42	10	33	43	10	34	0.9843	2471.81	2471.77	36	5	32	37	5	33	3.3916
2465.74	2465.79	42	9	34	43	9	35	1.1603		2471.77	35	9	26	36	9	27	2.2546
2466.12	2466.08	40	13	28	41	13	29	0.6604		2471.80	39	0	39	40	0	40	3.7538
	2466.16	46	1	46	47	1	47	1.8353		2471.83	37	2	35	38	2	36	3.6731
2466.39	2466.36	41	10	31	42	10	32	1.0943		2471.83	38	2	37	39	2	38	3.6863
	2466.40	42	6	37	43	6	38	1.7002	2472.02	2472.04	35	8	27	36	8	28	2.6242
2466.53	2466.50	40	12	29	41	12	30	0.8233	2472.20	2472.16	35	4	31	36	4	32	3.9094
	2466.55	37	17	20	38	17	21	0.2946		2472.25	35	7	28	36	7	29	2.9973
2466.92	2466.88	40	11	30	41	11	31	1.0080	2472.35	2472.31	35	5	30	36	5	31	3.6729
	2466.89	41	5	36	42	5	37	2.0410		2472.37	33	12	21	34	12	22	1.4786
	2466.91	41	8	33	42	8	34	1.4951		2472.38	35	6	29	36	6	30	3.3566
	2466.93	39	13	26	40	13	27	0.7265	2472.53	2472.55	35	3	32	36	3	33	4.0961
2467.21	2467.20	42	4	39	43	4	40	2.0436		2472.58	38	1	38	39	1	39	4.1019
	2467.23	40	10	31	41	10	32	1.2120	2472.73	2472.69	36	3	34	37	3	35	4.0005
2467.40	2467.36	39	12	27	40	12	28	0.9067		2472.70	33	11	22	34	11	23	1.8250
	2467.39	36	17	20	37	17	21	0.3178		2472.76	32	13	20	33	13	21	1.2528
2467.78	2467.78	38	13	26	39	13	27	0.7959	2473.47	2473.43	34	5	30	35	5	31	4.0126
	2467.79	40	8	33	41	8	34	1.6583		2473.43	33	9	24	34	9	25	2.6272
2468.00	2467.98	40	7	34	41	7	35	1.8862	2473.78	2473.74	34	4	31	35	4	32	4.3558
2468.22	2468.20	38	12	27	39	12	28	0.9943	2473.93	2473.91	30	14	17	31	14	18	1.0850
	2468.22	35	17	18	36	17	19	0.3412		2473.92	33	7	26	34	7	27	3.5069
	2468.25	5	3	2	6	5	1	1.4268		2473.94	32	10	23	33	10	24	2.3675
2468.51	2468.50	36	15	22	37	15	23	0.5685	2474.12	2474.08	33	6	27	34	6	28	3.9358
2468.68	2468.64	42	2	41	43	2	42	2.5049		2474.11	33	3	30	34	3	31	4.8343
	2468.64	39	8	31	40	8	32	1.8322		2474.14	36	1	36	37	1	37	4.8469
	2468.71	39	5	34	40	5	35	2.5235		2474.16	35	1	34	36	1	35	4.7498
	2468.73	39	4	35	40	4	36	2.6688	2474.27	2474.25	32	9	24	33	9	25	2.8175
2468.81	2468.80	35	16	19	36	16	20	0.4616		2474.26	34	3	32	35	3	33	4.7111
2468.96	2468.94	38	10	29	39	10	30	1.4690	2474.50	2474.52	32	8	25	33	8	26	3.2901
2469.19	2469.24	38	9	30	39	9	31	1.7371	2474.90	2474.90	35	0	35	36	0	36	5.2408
2469.51	2469.51	40	3	38	41	3	39	2.7638		2474.90	33	2	31	34	2	32	5.1070
	2469.52	38	8	31	39	8	32	2.0165		2474.93	32	6	27	33	6	28	4.2363
2469.70	2469.71	38	7	32	39	7	33	2.2973		2474.94	34	2	33	35	2	34	5.1306
2470.05	2470.08	38	5	34	39	5	35	2.8223	2475.22	2475.18	29	13	16	30	13	17	1.4695
	2470.09	37	9	28	38	9	29	1.9026		2475.20	30	11	20	31	11	21	2.2009
2470.21	2470.21	41	0	41	42	0	42	3.1116	2475.48	2475.47	26	17	10	27	17	11	0.4801
	2470.24	40	2	39	41	2	40	3.0595		2475.51	28	14	15	29	14	16	1.1788
2470.36	2470.35	37	8	29	38	8	30	2.2104	2475.73	2475.70	31	3	28	32	3	29	5.6191
2470.50	2470.49	38	4	35	39	4	36	3.0713		2475.70	33	1	32	34	1	33	5.5245
	2470.53	37	5	32	38	5	33	3.0697		2475.74	31	6	25	32	6	26	4.5377
2470.64	2470.63	36	10	27	37	10	28	1.7519	2476.17	2476.15	30	8	23	31	8	24	3.7430
	2470.66	37	6	31	38	6	32	2.8159	2476.49	2476.47	32	2	31	33	2	32	5.9230
2470.90	2470.89	31	18	13	32	18	14	0.3057	2476.70	2476.68	29	9	20	30	9	21	3.3815
	2470.93	36	9	28	37	9	29	2.0754		2476.72	30	5	26	31	5	27	5.3483
2471.18	2471.13	34	13	22	35	13	23	1.0973	2476.90	2476.93	30	4	27	31	4	28	5.8071
	2471.20	36	8	29	37	8	30	2.4134	2477.06	2477.08	26	14	13	27	14	14	1.2458
2471.48	2471.46	35	10	25	36	10	26	1.9012	2477.21	2477.19	32	1	32	33	1	33	6.4829

TABLE I (Continued)

Line Position (in cm^{-1}) Exptl.	Theor.	J'	K'_{-1}	K'_{1}	J"	K''_{-1}	K''_{1}	$\frac{I^{\circ}_{n''n'}}{C'}$	Line Position (in cm^{-1}) Exptl.	Theor.	J'	K'_{-1}	K'_{1}	J"	K''_{-1}	K''_{1}	$\frac{I^{\circ}_{n''n'}}{C'}$
	2477.19	29	7	22	30	7	23	4.5595	2484.50	2484.48	22	1	22	23	1	23	10.2136
	2477.21	31	1	30	32	1	31	6.3317	2484.71	2484.70	19	8	11	20	8	12	5.2278
2477.36	2477.36	30	3	28	31	3	29	6.2463		2484.71	20	4	17	21	4	18	8.7312
	2477.37	29	6	23	30	6	24	5.1412	2484.89	2484.90	20	3	18	21	3	19	9.3999
2477.50	2477.48	28	9	20	29	9	21	3.5592	2485.12	2485.10	16	13	4	17	13	5	1.1068
	2477.55	26	13	14	27	13	15	1.6329		2485.15	18	9	10	19	9	11	4.2422
2477.91	2477.88	29	2	27	30	2	28	6.7047		2485.16	21	0	21	22	0	22	10.4392
	2477.94	31	0	31	32	0	32	6.9079		2485.16	19	6	13	20	6	14	7.1202
	2477.95	27	10	17	28	10	18	3.1048	2485.29	2485.28	20	2	19	21	2	20	9.9873
2478.10	2478.13	24	15	10	25	15	11	0.9366		2485.32	19	2	17	20	2	18	9.9040
2478.51	2478.52	28	4	25	29	4	26	6.5410		2485.33	19	5	14	20	5	15	8.0229
	2478.55	27	8	19	28	8	20	4.3857		2485.34	19	3	16	20	3	17	9.4804
2478.70	2478.69	30	1	30	31	1	31	7.3328	2485.85	2485.80	19	1	18	20	1	19	10.2192
	2478.69	29	1	28	30	1	29	7.1478		2485.87	20	1	20	21	1	21	10.6112
	2478.73	26	10	17	27	10	18	3.2263		2485.89	18	6	13	19	6	14	7.1157
2478.84	2478.80	27	7	20	28	7	21	5.0588	2486.06	2486.08	18	5	14	19	5	15	8.0469
	2478.89	28	3	26	29	3	27	7.0244	2486.21	2486.18	17	8	9	18	8	10	5.0655
2479.00	2478.98	27	6	21	28	6	22	5.7200		2486.22	18	4	15	19	4	16	8.8884
	2479.01	27	4	23	28	4	24	6.8560	2486.40	2486.37	18	3	16	19	3	17	9.6017
2479.18	2479.16	25	11	14	26	11	15	2.7043		2486.43	17	7	10	18	7	11	6.0576
2479.40	2479.40	23	14	9	24	14	10	1.2688	2486.55	2486.55	19	0	19	20	0	20	10.7400
	2479.43	29	0	29	30	0	30	7.7540	2486.69	2486.70	18	2	17	19	2	18	10.2017
2479.64	2479.59	26	7	20	27	7	21	5.2898	2486.82	2486.82	17	2	15	18	2	16	10.0660
	2479.67	22	15	8	23	15	9	0.8989		2486.82	17	5	12	18	5	13	8.0129
2480.19	2480.16	28	1	28	29	1	29	8.1668	2486.96	2486.94	17	4	13	18	4	14	8.8784
	2480.16	27	1	26	28	1	27	7.9441	2487.39	2487.38	16	6	11	17	6	12	6.9352
2480.37	2480.37	25	7	18	26	7	19	5.5033	2487.58	2487.56	16	5	12	17	5	13	7.9170
	2480.39	26	3	24	27	3	25	7.7682	2487.71	2487.70	16	4	13	17	4	14	8.8090
2480.51	2480.53	25	3	22	26	3	23	7.9730	2487.86	2487.83	16	3	14	17	3	15	9.5646
2480.62	2480.61	24	9	16	25	9	17	4.1414		2487.89	15	7	8	16	7	9	5.7105
2480.80	2480.78	26	6	21	27	6	22	5.9908		2487.90	17	0	17	18	0	18	10.8167
	2480.84	25	9	16	26	9	17	4.0217	2488.06	2488.06	14	9	6	15	9	7	3.4243
2481.10	2481.06	23	10	13	24	10	14	3.4886		2488.10	16	2	15	17	2	16	10.1782
	2481.14	24	7	18	25	7	19	5.6950	2488.33	2488.33	15	2	13	16	2	14	9.9654
2481.38	2481.35	24	6	19	25	6	20	6.4733		2488.35	14	8	7	15	8	8	4.4055
	2481.38	23	9	14	24	9	15	4.2382	2488.45	2488.42	15	4	11	16	4	12	8.6690
	2481.39	21	13	18	22	13	19	1.6530		2488.44	15	3	12	16	3	13	9.4307
2481.51	2481.50	24	5	20	25	5	21	7.2075	2488.63	2488.61	14	7	8	15	7	9	5.4392
2481.80	2481.83	25	2	23	26	2	24	8.2761		2488.62	16	1	16	17	1	17	10.7474
2481.96	2481.92	23	7	16	24	7	17	5.8605	2488.77	2488.78	13	9	4	14	9	5	3.0677
	2481.92	19	15	4	20	15	5	0.7283	2489.02	2489.01	14	5	10	15	5	11	7.5220
2482.15	2482.12	23	6	17	24	6	18	6.6760		2489.07	13	8	5	14	8	6	4.0473
	2482.14	23	3	20	24	3	21	8.6297	2489.15	2489.14	14	4	11	15	4	12	10.4250
	2482.15	22	9	14	23	9	15	4.3081		2489.16	12	10	3	13	10	4	1.7708
2482.34	2482.32	23	2	21	24	2	22	8.9618	2489.35	2489.33	13	7	6	14	7	7	5.0964
	2482.34	25	0	25	26	0	26	9.3131	2489.76	2489.73	13	5	8	14	5	9	7.2152
2482.58	2482.57	20	12	9	21	12	10	2.1435		2489.78	12	8	5	13	8	6	3.6190
	2482.58	21	10	11	22	10	12	3.5458	2489.92	2489.87	13	4	9	14	4	10	8.1738
2482.88	2482.89	22	6	17	23	6	18	6.8470		2489.93	13	3	10	14	3	11	8.9832
	2482.71	21	9	12	22	9	13	4.3475		2489.96	14	1	14	15	1	15	10.4250
2483.03	2483.01	23	1	22	24	1	23	9.3397		2489.96	13	1	12	14	1	13	9.8935
	2483.05	22	5	18	23	5	19	7.6532	2490.43	2490.44	12	5	8	13	5	9	6.8304
2483.20	2483.19	22	4	19	23	4	20	8.3760	2490.59	2490.56	13	0	13	14	0	14	10.1894
	2483.19	21	8	13	22	8	14	5.2070		2490.59	12	4	9	13	4	10	7.8111
2483.47	2483.44	21	7	14	22	7	15	6.0965	2490.96	2490.96	11	6	5	12	6	6	5.2780
2483.91	2483.88	21	4	17	22	4	18	8.5664	2491.15	2491.15	11	5	6	12	5	7	6.3635
	2483.95	20	8	13	21	8	14	5.2382		2491.18	10	8	3	11	8	4	2.5065
2484.24	2484.21	20	7	14	21	7	15	6.1573	2491.28	2491.29	11	4	7	12	4	8	7.3674

TABLE I (Continued)

Line Position (in cm^{-1}) Exptl.	Theor.	J'	K'_{-1}	K'_1	J''	K''_{-1}	K''_1	$\frac{I^o_{n''n'}}{C'}$
	2491.30	12	1	12	13	1	13	9.8156
2491.52	2491.49	21	20	1	21	20	2	0.6928
	2491.51	26	19	8	26	19	7	0.4835
	2491.54	30	18	13	30	18	12	0.3600
2491.81	2491.79	24	19	6	24	19	5	0.6113
	2491.80	32	17	16	32	17	15	0.3308
	2491.82	35	16	19	35	16	20	0.2570
	2491.85	10	5	6	11	5	7	5.8101
2491.99	2492.00	10	4	7	11	4	8	6.8403
2492.13	2492.11	10	3	8	11	3	9	7.7255
	2492.13	9	7	2	10	7	3	2.8850
2492.41	2492.38	19	19	0	19	9	1	1.0759
	2492.42	24	18	7	24	18	6	0.7429
2492.58	2492.54	9	5	4	10	5	5	5.1642
	2492.59	10	1	10	11	1	11	8.9121
2492.71	2492.69	9	4	5	10	4	6	6.2260
2492.86	2492.85	35	14	21	35	14	22	0.3213
	2492.87	29	16	13	29	16	14	0.5625
	2492.88	25	17	8	25	17	9	0.7855
2493.02	2493.01	19	18	1	19	18	2	1.3075
	2493.02	24	17	8	24	17	7	0.8827
	2493.04	8	6	3	9	6	4	3.2440
2493.16	2493.15	9	0	9	10	0	10	8.4390
2493.31	2493.28	22	17	6	22	17	5	1.1100
	2493.31	35	13	22	35	13	23	0.3453
	2493.32	26	16	11	26	16	10	0.8102
2493.48	2493.51	8	3	6	9	3	7	6.4742
2493.81	2493.81	17	17	0	17	17	1	1.9391
	2493.84	22	16	7	22	16	6	1.2885
	2493.85	26	15	12	26	15	11	0.9178
2493.97	2493.96	21	16	5	21	16	6	1.4424
	2493.99	25	15	10	25	15	11	1.0329
2494.12	2494.12	24	15	10	24	15	9	1.1607
	2494.15	7	1	6	8	1	7	6.9629
2494.24	2494.25	23	15	8	23	15	9	1.3025
	2494.28	18	16	3	18	16	2	2.0148
2494.39	2494.36	29	13	16	29	13	17	0.7566
	2494.38	17	16	1	17	16	2	2.2508
	2494.38	22	15	8	22	15	7	1.4598
	2494.40	6	6	1	7	6	2	1.2693
2494.63	2494.61	20	15	6	20	15	5	1.8279
	2494.63	24	14	11	24	14	10	1.2821
	2494.63	30	12	19	31	12	18	0.6973
2495.02	2495.01	16	15	2	16	15	1	2.8496
	2495.02	30	11	20	30	11	19	0.7066
2495.23	2495.22	6	1	6	7	1	7	6.2626
	2495.22	19	14	5	19	14	6	2.2570
2495.52	2495.49	27	11	16	27	11	17	1.0244
	2495.50	16	14	3	16	14	2	3.1479
	2495.51	24	12	13	24	12	12	1.4414
	2495.53	5	1	4	6	1	5	5.4105
	2495.53	5	3	2	6	3	3	3.9199
2495.71	2495.68	19	13	6	19	13	7	2.4277
	2495.73	5	0	5	6	0	6	5.6186
2496.13	2496.11	19	12	7	19	12	8	2.5385
	2496.13	14	13	2	14	13	1	4.2381
	2496.14	25	10	15	25	10	16	1.2753
2496.29	2496.28	21	11	10	21	11	11	2.0589
	2496.29	4	2	3	5	2	4	3.8820
	2496.30	17	12	5	17	12	6	3.1687
	2496.32	26	9	18	26	9	17	1.0701
2496.43	2496.40	16	12	5	16	12	4	3.5409
	2496.42	29	7	22	29	7	23	0.5750
	2496.46	25	9	16	25	9	17	1.2051
	2496.47	4	1	4	5	1	5	4.5549
2496.56	2496.56	14	12	3	14	12	2	4.4319
2496.72	2496.70	17	11	6	17	11	7	3.2144
	2496.71	12	12	1	12	12	0	5.5864
	2496.73	23	9	14	23	9	15	1.5214
	2496.75	20	10	11	20	10	10	2.2600
2496.95	2496.94	3	2	1	4	2	2	2.8155
	2496.96	14	11	4	14	11	3	4.4959
	2496.96	27	6	21	27	6	22	0.5952
	2496.97	21	9	12	21	9	13	1.9105
2497.26	2497.24	15	10	5	15	10	6	3.9420
	2497.26	21	8	13	21	8	14	1.7329
	2497.29	18	9	10	18	9	9	2.6711
2497.47	2497.46	12	10	3	12	10	2	5.5628
	2497.48	16	9	8	16	9	7	3.3356
	2497.48	19	8	11	19	8	12	2.1688
2497.61	2497.58	18	8	11	18	8	10	2.4242
	2497.59	10	10	1	10	10	0	7.1106
	2497.60	2	2	1	3	2	2	1.5866
	2497.62	22	6	17	22	6	16	1.0848
	2497.63	20	7	14	20	7	13	1.6757
	2497.64	14	9	6	14	9	5	4.1758
2498.03	2498.01	13	8	5	13	8	6	4.2522
	2498.03	16	7	10	16	7	9	2.6194
	2498.04	20	5	16	20	5	15	1.0263
2498.24	2498.20	10	8	3	10	8	2	6.1113
	2498.25	16	6	11	16	6	10	2.1371
	2498.25	18	5	14	18	5	13	1.2899
	2498.25	1	1	0	2	1	1	1.4736
	2498.26	9	8	1	9	8	2	6.9684
	2798.27	13	7	6	13	7	7	3.6799
2498.38	2498.34	12	7	6	12	7	5	4.1376
	2498.34	15	6	9	15	6	10	2.3914
	2498.40	11	7	4	11	7	5	4.6678
2498.63	2498.61	7	7	0	7	7	1	8.0630
	2498.61	14	5	10	14	5	9	2.0307
	2498.63	11	6	5	11	6	6	3.8133
2498.87	2498.87	6	6	1	6	6	0	7.7800
	2498.87	10	5	6	10	5	5	3.2825
	2498.70	12	4	9	12	4	8	1.7604
2499.11	2499.09	5	5	0	5	5	1	7.1336
	2499.09	9	4	5	9	4	6	2.5764
	2499.13	8	4	5	8	4	4	2.9642
2499.83	2499.82	21	3	18	21	3	19	0.3146
	2499.85	3	1	2	3	1	3	0.5686
2500.20	2500.22	1	0	1	0	0	0	0.9995
2500.47	2500.45	23	3	20	23	3	21	0.2355
2500.78	2500.79	2	1	2	1	1	1	1.4834
2500.99	2500.98	15	2	13	15	2	14	0.2904
2501.44	2501.42	3	2	1	2	2	0	1.5982
	2501.48	3	0	3	2	0	2	2.9713
2501.99	2501.98	4	1	4	3	1	3	3.6540

TABLE I (Continued)

Line Position (in cm^{-1}) Exptl.	Theor.	Quantum Numbers J'	K'_{-1}	K'_1	J''	K''_{-1}	K''_1	$\frac{I^\circ_{n''n'}}{C'}$
	2502.03	4	2	3	3	2	2	2.8504
2502.44	2502.44	5	4	1	4	4	0	1.5313
2502.70	2502.69	5	0	5	4	0	4	4.8434
2502.85	2502.81	5	1	4	4	1	3	4.6108
	2502.89	6	5	2	5	5	1	1.4268
2503.06	2503.04	6	4	3	5	4	2	2.7927
2503.27	2503.24	6	2	5	5	2	4	4.9292
	2503.30	7	6	1	6	6	0	1.2968
2503.47	2503.49	7	5	2	6	5	1	2.6198
2503.63	2503.64	7	4	3	6	4	2	3.8778
	2503.67	8	7	2	7	7	1	1.1520
2503.81	2503.77	7	3	4	6	3	3	4.9776
	2503.85	7	0	7	6	0	6	6.5507
2504.02	2504.01	9	8	1	8	8	0	1.0015
	2504.05	7	1	6	6	1	5	6.3590
2504.35	2504.37	8	3	6	7	3	5	5.8615
2504.50	2504.49	9	6	3	8	6	2	3.3346
2504.94	2504.97	9	0	9	8	0	8	8.0409
	2504.97	9	3	6	8	3	5	6.6500
2505.09	2505.07	10	6	5	9	6	4	4.1523
	2505.13	9	2	7	8	2	6	7.4081
	2505.13	12	10	3	11	10	2	1.3026
2505.29	2505.26	10	5	6	9	5	5	5.3248
	2505.27	9	1	8	8	1	7	7.8521
2505.71	2505.70	13	10	3	12	10	2	1.8427
	2505.75	12	8	5	11	8	4	3.2247
2506.04	2506.00	11	4	7	10	4	6	7.0748
	2506.00	12	7	6	11	7	5	4.3299
	2506.02	13	9	4	12	9	3	2.7459
	2506.05	11	0	11	10	0	10	9.2781
2506.35	2506.32	13	8	5	12	8	4	3.7659
	2506.36	11	2	9	10	2	8	8.6816
2506.52	2506.46	12	1	12	11	1	11	9.7348
	2506.57	13	7	6	12	7	5	4.8865
2506.73	2506.71	12	2	11	11	2	10	9.2244
	2506.71	12	3	10	11	3	9	8.5354
2507.10	2507.09	13	0	13	12	0	12	10.2402
	2507.14	14	7	8	13	7	7	5.3196
2507.31	2507.32	13	3	10	12	3	9	8.9964
2507.63	2507.58	13	1	12	12	1	11	9.9923
	2507.58	13	2	11	12	2	10	9.6413
	2507.70	13	7	8	14	7	7	5.6949
2507.82	2507.81	14	2	13	13	2	12	10.0477
	2507.84	14	3	12	13	3	11	9.3846
2508.10	2508.10	15	0	15	14	0	14	10.9160
	2508.12	15	5	10	14	5	9	7.8759
2508.26	2508.25	16	7	10	15	7	9	5.9974
	2508.29	15	4	11	14	4	10	8.8574
2508.49	2508.48	16	6	11	15	6	10	7.0896
	2508.49	15	3	12	14	3	11	9.6827
2508.79	2508.77	15	2	13	14	2	12	10.2802
	2508.79	18	9	10	17	9	9	4.3525
	2508.80	17	7	10	16	7	9	6.2313
2508.93	2508.88	16	2	15	15	2	14	10.5654
	2508.96	16	3	14	15	3	13	9.9208
2509.08	2509.09	17	0	17	16	0	16	11.3049
	2509.09	18	8	11	17	8	10	5.3526
2509.22	2509.18	20	11	10	19	11	9	2.8939
	2509.23	17	5	12	16	5	11	8.3407
2509.40	2509.41	17	4	13	16	4	12	9.2800
2509.91	2509.89	19	7	12	18	7	11	6.5107
	2509.92	18	2	17	17	2	16	10.7908
	2509.95	18	4	15	17	4	14	9.3853
2510.09	2510.06	19	0	19	18	0	18	11.4181
	2510.12	19	6	13	18	6	12	7.5425
2510.32	2510.32	19	5	14	18	5	13	8.5299
	2510.35	23	12	11	22	12	10	2.3716
2510.50	2510.51	20	1	20	19	1	19	11.3710
	2510.52	19	4	15	18	4	14	9.4201
2510.69	2510.69	19	1	18	18	1	17	10.9375
	2510.69	21	8	13	20	8	12	5.5863
2510.90	2510.91	22	9	14	21	9	13	4.6506
	2510.93	20	2	19	19	2	18	10.7478
	2510.95	21	7	14	20	7	13	6.5688
2511.06	2511.03	19	2	17	18	2	16	10.6336
	2511.03	20	4	17	19	4	16	9.3973
	2511.10	20	3	18	19	3	17	10.1301
	2511.10	23	10	13	22	10	12	3.7890
2511.19	2511.18	21	6	15	20	6	14	7.5445
2511.66	2511.63	21	1	20	20	1	19	10.7251
	2511.63	21	4	17	20	4	16	9.3077
	2511.71	22	6	17	21	6	16	7.4687
2511.90	2511.90	22	2	21	21	2	20	10.4689
	2511.92	22	5	18	21	5	17	8.3682
2512.09	2512.09	21	2	19	20	2	18	10.4020
	2512.09	22	4	19	21	4	18	9.1760
	2512.13	22	3	20	21	3	19	9.8632
2512.23	2512.23	23	6	17	22	6	16	7.3478
	2512.24	24	8	17	23	8	16	5.4221
2512.52	2512.51	24	7	18	23	7	17	6.3085
	2512.55	23	1	22	22	1	21	10.3083
2512.70	2512.72	23	4	19	22	4	18	8.9790
2512.84	2512.85	24	2	23	2	2	22	9.9929
	2512.86	25	0	25	24	0	24	10.3656
2513.00	2512.97	24	5	20	23	5	19	8.0171
	2513.02	25	7	18	24	7	17	6.1490
2513.22	2513.24	28	11	18	27	11	17	2.7614
	2513.25	26	8	19	25	8	18	5.1457
	2513.26	25	6	19	24	6	18	6.9898
2513.39	2513.43	25	1	24	24	1	23	9.7267
2513.52	2513.50	25	5	20	24	5	19	7.7821
	2513.52	26	7	20	25	7	19	5.9603
2513.75	2513.75	27	8	19	26	8	18	4.9730
	2513.76	27	0	27	26	0	26	9.6717
	2513.76	26	2	25	25	2	24	9.3617
2514.20	2514.14	26	4	23	25	4	22	3.1933
	2514.19	25	3	22	24	3	21	8.9968
	2514.20	28	1	28	27	1	27	9.2828
	2514.24	28	8	21	27	8	20	4.7790
2514.41	2514.43	29	9	20	28	9	19	3.8902
2514.75	2514.73	29	8	21	28	8	20	4.5693
	2514.77	28	6	23	27	6	22	6.2344
2515.03	2515.01	29	7	22	28	7	21	5.2625
	2515.02	28	3	26	27	3	25	8.0601
	2515.07	30	1	30	29	1	29	8.4488
2515.20	2515.21	30	8	23	29	8	22	4.3473

TABLE I (Continued)

Line Position (in cm^{-1}) Exptl.	Theor.	J'	K'_{-1}	K'_{1}	J''	K''_{-1}	K''_{1}	$\frac{I^{\circ}_{n''n'}}{C'}$
	2515.23	27	3	24	26	3	23	8.2831
2515.47	2515.49	31	0	31	30	0	30	8.0127
	2515.49	30	7	24	29	7	23	4.9996
2515.61	2515.58	37	13	24	36	13	23	1.0562
	2515.63	33	8	25	32	8	24	3.6409
2515.94	2515.91	32	1	32	31	1	31	7.5696
	2515.92	30	3	28	29	3	27	7.2690
	2515.97	29	4	25	28	4	24	7.1072
	2515.97	30	5	26	29	5	25	6.2364
	2515.97	31	7	24	30	7	23	4.7280
2516.19	2516.16	32	8	25	31	8	24	3.8802
	2516.23	29	3	26	28	3	25	7.4822
2516.56	2516.56	31	5	26	30	5	25	5.8759
2516.81	2516.78	32	3	30	31		29	6.4491
	2516.80	33	1	32	32	1	31	6.5295
2517.00	2517.00	32	4	29	31	4	28	5.9983
	2517.03	31	4	27	30	4	26	6.3275
2517.13	2517.14	35	0	35	34	0	34	6.2399
	2517.17	31	3	28	30	3	27	6.6385
2517.28	2517.24	35	9	26	34	9	25	2.7156
	2517.32	41	15	26	40	15	25	0.4526
2517.40	2517.38	34	7	28	33	7	27	3.8935
	2517.42	33	2	31	32	2	30	6.0759
2517.54	2517.54	36	1	36	35	1	35	5.8079
	2517.55	35	8	27	34	8	26	3.1643
	2517.56	31	5	26	30	5	25	5.8759
2517.73	2517.69	36	9	28	35	9	27	2.5180
	2517.74	42	15	28	41	15	27	0.4151
	2517.19	37	10	27	36	10	26	1.9625
2517.99	2517.99	36	2	35	35	2	34	5.2775
	2518.00	36	8	29	35	8	28	2.9312
2518.30	2518.28	39	11	28	38	11	27	1.3747
	2518.30	36	7	30	35	7	29	3.3486
	2518.33	38	1	38	37	1	37	4.9780
2518.56	2518.57	36	6	31	35	6	30	3.7534
	2518.57	38	9	30	37	9	29	2.1381
	2518.58	35	5	30	34	5	29	4.4509
2518.72	2518.71	39	0	39	38	0	38	4.5844
	2518.73	36	4	33	35	4	32	4.4814
	2518.76	38	2	37	37	2	36	4.4985
	2518.76	37	7	30	36	7	29	3.0862
2518.87	2518.88	35	3	32	34	3	31	4.9722
	2518.89	38	8	31	37	8	30	2.4844
2519.04	2519.04	35	4	31	31	4	30	4.7544
	2519.09	40	1	40	39	1	39	4.2072
2519.21	2519.21	38	7	32	37	7	31	2.8332
	2519.21	38	3	36	37	3	35	4.1085
2519.60	2519.58	37	5	32	36	5	31	3.7760
	2519.65	37	3	34	36	3	33	4.2057
	2519.65	38	5	34	37	5	33	3.4850
2519.80	2519.76	41	9	32	40	9	31	1.6229
	2519.84	42	1	42	41	1	41	3.5070
2520.08	2520.08	40	7	34	39	7	33	2.3593
2520.21	2520.20	43	0	43	42	0	42	3.1857
	2520.25	42	2	41	41	2	40	3.1342
2520.34	2520.34	40	4	37	39	4	36	3.1500
	2520.34	43	10	33	42	10	32	1.1233
	2520.35	40	6	35	39	6	34	2.6360
	2520.37	39	3	36	38	3	35	3.5074
2520.50	2520.48	40	5	36	39	5	35	2.8955
	2520.53	41	7	34	40	7	33	2.1398
2520.65	2520.61	43	1	42	42	1	41	2.8392
	2520.62	42	8	35	41	8	34	1.7014
	2520.69	42	3	40	41	3	39	2.8311
2520.79	2520.76	45	2	43	44	2	42	2.0665
	2520.77	44	7	38	43	7	37	1.5617
	2520.81	45	9	36	44	9	35	1.0642
2520.93	2520.91	45	0	45	44	0	44	2.6024
	2520.93	42	7	36	41	7	35	1.9342
	2520.94	41	6	35	40	6	34	2.3833
	2520.96	44	2	43	43	2	42	2.5632
2521.08	2521.05	41	3	38	40	3	37	2.8860
	2521.08	42	4	39	41	4	38	2.5843
	2521.08	43	2	41	42	2	40	2.5588
	2521.11	44	9	36	43	9	35	1.1894
2521.40	2521.39	44	3	42	43	3	41	2.3023
	2521.39	43	7	36	42	7	35	1.7404
	2521.45	44	8	37	43	8	36	1.3758
2521.52	2521.51	45	9	36	44	9	35	1.0642
	2521.52	41	5	36	40	5	35	2.5863
2521.65	2521.60	47	0	47	46	0	46	2.0979
	2521.65	46	2	45	45	2	44	2.0684
	2521.66	41	4	37	40	4	36	2.7355
	2521.71	43	3	40	42	3	39	2.3439
2521.78	2521.76	45	2	43	44	2	42	2.0665
	2521.77	44	7	38	43	7	37	1.5617
	2521.81	44	4	41	43	4	40	2.0909
2521.92	2521.91	46	9	38	45	9	37	0.9487
	2521.94	48	1	48	47	1	47	1.8744
	2521.94	47	10	37	46	10	36	0.7165
2522.07	2522.06	44	5	40	43	5	39	1.9117
	2522.08	46	3	44	45	3	43	1.8474
2522.25	2522.24	45	7	38	44	7	37	1.3941
	2522.27	49	0	49	48	0	48	1.6692
2522.47	2522.42	47	2	45	46	2	44	1.6470
	2522.44	43	5	38	42	5	37	2.0890
	2522.50	46	4	43	45	4	42	1.6687
2522.64	2522.61	50	1	50	49	1	49	1.4939
	2522.64	49	1	48	48	1	47	1.4750
	2522.67	47	8	39	46	8	38	0.9724
2522.79	2522.74	48	3	46	47	3	45	1.4629
	2522.78	45	6	39	44	6	38	1.5436
	2522.80	46	5	42	45	5	41	1.5202
	2522.82	46	6	41	45	6	40	1.3828
2522.97	2522.93	51	0	51	50	0	50	1.3221
	2523.97	47	3	44	46	3	43	1.4875
	2523.99	50	2	49	49	2	48	1.3058
2523.09	2523.06	49	2	47	48	2	46	1.3066
	2523.06	48	8	41	47	8	40	0.8599
	2523.08	47	7	40	46	7	39	1.0998
	2523.10	45	4	41	44	4	40	1.7529
2523.23	2523.24	52	1	52	51	1	51	1.1622
2523.40	2523.38	50	3	48	49	3	47	1.1533
	2523.38	48	7	42	47	7	41	0.9734
	2523.42	52	11	42	51	11	41	0.3175
2523.55	2523.50	48	5	44	47	5	43	1.1922

TABLE I (Continued)

Line Position (in cm^{-1}) Exptl.	Theor.	J'	K'_{-1}	K'_1	J''	K''_{-1}	K''_1	$\frac{I^*_{n''n'}}{C'}$	Line Position (in cm^{-1}) Exptl.	Theor.	J'	K'_{-1}	K'_1	J''	K''_{-1}	K''_1	$\frac{I^*_{n''n'}}{C'}$
	2523.55	53	0	53	52	0	52	1.0254	2523.71	2523.69	47	6	41	46	4	42	1.2134
	2523.58	49	3	46	48	3	45	1.1726		2523.70	51	2	49	50	2	48	1.0149
	2523.60	52	2	51	51	2	50	1.0137		2523.73	47	4	43	46	4	42	1.3754

$\Delta K_{-1} = 0, \pm 2, \cdots$; and $\Delta K_1 = \pm 1, \pm 3, \cdots$. Approximately 250 observed peaks, which are either individual or consist of a small number of closely spaced transitions, have been assigned. We have determined the band center for $\nu_1 + \nu_3$ to be 2499.60 ± 0.10 cm^{-1}. This value may be compared with 2499.55 cm^{-1} reported by Shelton et al.,[3] and 2499.0 cm^{-1} by Bailey and Cassie.[10]

Our results are potentially applicable to studies of the terrestrial atmosphere where SO_2 plays a serious role as a pollutant.[11] High-resolution infrared spectroscopy is a possible technique for the remote detection and monitoring of sulfur dioxide in situ. For example, solar spectra[12] in the 2500 cm^{-1} region may reveal SO_2 absorption features which would be susceptible to analysis. This spectral region is relatively free of absorption by H_2O and CO_2, although CH_4 and N_2O may be significant there.[7] Monochromatic laser emissions may be useful for studying terrestrial SO_2 in absorption. However, we have not yet been able to determine any relatively isolated and moderately strong lines in our laboratory spectra which fall close to observed laser oscillations,[13] even if we include the effects of air-broadening.[14]

Finally, we note that $\nu_1 + \nu_3$ of SO_2 was recently considered[15] in a determination of detectability limit of this gas in the atmosphere of the planet Mars. An upper limit of 0.0037 cm-atm was established,[15] on the basis of the ν_3 fundamental, for SO_2 in the Martian atmosphere. This value may be compared with a terrestrial atmospheric value of the order of 1 cm-atm.[16]

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