

$^{33}\text{SO}_2$: Interstellar Identification and Laboratory Measurements

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The rotational spectrum of ^{33}S isotopically substituted sulfur dioxide, $^{33}\text{SO}_2$, has been measured up to nearly 1 THz. The combined analysis of these new data together with the published line frequencies resulted in refined molecular constants, such as the rotational ($A = 59856.4723(62)$ MHz, $B = 10318.3012(15)$ MHz, $C = 8780.1363(15)$ MHz) and centrifugal distortion constants which yielded precise frequency predictions. The carrier of six previously unidentified interstellar lines in the Caltech molecular line survey in the 325–360 GHz band could be assigned to $^{33}\text{SO}_2$. © 1997

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1. INTRODUCTION

Sulfur dioxide, SO_2 , is an ubiquitous interstellar molecule with high abundance in star forming regions such as the Orion A region. Consequently one expects to identify, in addition to the fairly intense ground state transitions, vibrationally excited lines as well as the rarer isotopomers in the dense hot cores of molecular clouds. With the Cologne terahertz spectrometer we have investigated the vibrational ground state of SO_2 and several rare isotopomers in the region of 500 up to 1100 GHz. In the present paper we report rotational spectra of $^{33}\text{SO}_2$ measured in the laboratory—as part of a larger program on the laboratory rotational spectrum of SO_2 and its isotopomers carried out by various laboratories, including Cologne (1). The first microwave measurements on $^{33}\text{SO}_2$ were reported by Bird and Townes (2) in the 20 to 30 GHz region. This $^{33}\text{SO}_2$ data set was expanded by van Riet (3, 4). The interstellar discovery of SO_2 and $^{34}\text{SO}_2$ by Snyder *et al.* (5) in the Orion Nebula molecular cloud and in Sgr B2 is now supplemented by our observations of $^{33}\text{SO}_2$ in Orion-KL. For each isotopomer, $^{33}\text{SO}_2$ and $^{34}\text{SO}_2$, six transitions in the CSO 325–360 GHz line survey of Orion-KL could be assigned on the basis of highly accurate frequency predictions. The purpose of this paper is twofold: first to present the new laboratory measurements and discuss their analysis which is somewhat more elaborate due to the electric hyperfine structure of the ^{33}S nucleus. Second, we give the astrophysical spectra which secure

the interstellar discovery of $^{33}\text{SO}_2$ and further assignments of interstellar $^{34}\text{SO}_2$.

2. EXPERIMENTAL

The Cologne terahertz spectrometer has been described in detail elsewhere (1). The accuracy of the measurements for single lines is estimated to be better than 10 kHz. However, for $^{33}\text{SO}_2$, measured in natural abundance of 0.75%, the accuracy is less due to the smaller signal-to-noise ratio. This holds particularly for lines corresponding to quantum numbers which provide absorption coefficients smaller than 10^{-6} . The effects of varying line accuracy have been weighted accordingly in the fit. Similarly the influence of the hyperfine structure has been taken into account for blended lines. The spectra were recorded at pressures between 15 and 40 μbar .

3. THEORY AND ANALYSIS

The SO_2 molecule is a near prolate asymmetric top with C_2 symmetry. Its spectrum consists of b -type transitions only. Prominent features in the frequency region between 530 and 1000 GHz are exhibited by the Q branches; e.g., the 7Q_5 branch has been completely measured from $J = 6$ up to $J = 31$. The hyperfine structure of these lines remains unresolved.

The highly reliable molecular parameters, obtained in this study, are derived from 103 new P -, Q -, and R -branch transitions. The nuclear spin $I = 3/2$ of the ^{33}S atom produces an electric nuclear hyperfine structure which has partially been resolved in the new measurements. Using Watson's A -reduced Hamiltonian (6) the rotational

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parameters A , B , and C and the centrifugal correction terms up to sixth order could be obtained. The new set of hyperfine-split transitions allowed an accurate determination of the electric quadrupole terms eQq_{aa} , eQq_{bb} , and eQq_{cc} .

The Hamiltonian \hat{H} describing the $^{33}\text{SO}_2$ rotational energy levels in the ground electronic state consists of three parts:

$$H = H_{\text{rot}} + H_{\text{cd}} + H_{\text{hfs}}. \quad [1]$$

The contributions of the rotation and the centrifugal correction terms for an A -reduced asymmetric top in the I' axis choice were developed by Watson (6). The nuclear spin $I = 3/2$ interacts with the electric field gradient of the electrons around the nonspherical distribution of the ^{33}S nuclear charge and therefore causes hyperfine splitting. Consequently, the Hamiltonian has to be expanded by an expression for the electric quadrupole hyperfine interaction. The complete Hamiltonian including the rotation, centrifugal distortion, and hyperfine structure is given in the Appendix.

4. ASTROPHYSICAL DETECTION OF $^{33}\text{SO}_2$

Hot cores are the formation sites of massive young stars. They display a multitude of strong molecular lines from many species. The study of these lines provides insights into the physical conditions of massive star forming regions and into the interactions between stars and the remnants of their parent clouds. Unbiased spectral line surveys offer the unique opportunity to investigate their complete chemical composition. The best studied site of massive star formation is the Orion hot core. It is the richest known source of molecular lines, in part due to its proximity (≈ 500 pc). Unbiased spectral line surveys also are a treasure chest for identifications of previously unknown species or transitions.

One such high sensitivity spectral line survey of the high mass star forming region Orion-KL in the 325–360 GHz frequency band was conducted at the Caltech Submillimeter Observatory on Mauna Kea, Hawaii (7). This survey found 717 resolvable features consisting of 1004 lines. After completion of the analysis, of these only 60 remain unidentified. The identified lines are weak and many of them are most likely due to isotopomers or vibrationally or torsionally excited states of known species with unknown line frequencies, but a few reach the 2–5 K level.

This is the database that was used to search for $^{33}\text{SO}_2$ lines. Six previously unidentified lines could indeed be assigned to $^{33}\text{SO}_2$ (see Fig. 1 for a plot of the lines with the corresponding $^{34}\text{SO}_2$ lines). These six lines are all lines which were expected to be detectable in this frequency band and not blended with other, stronger features. The intensity ratio of

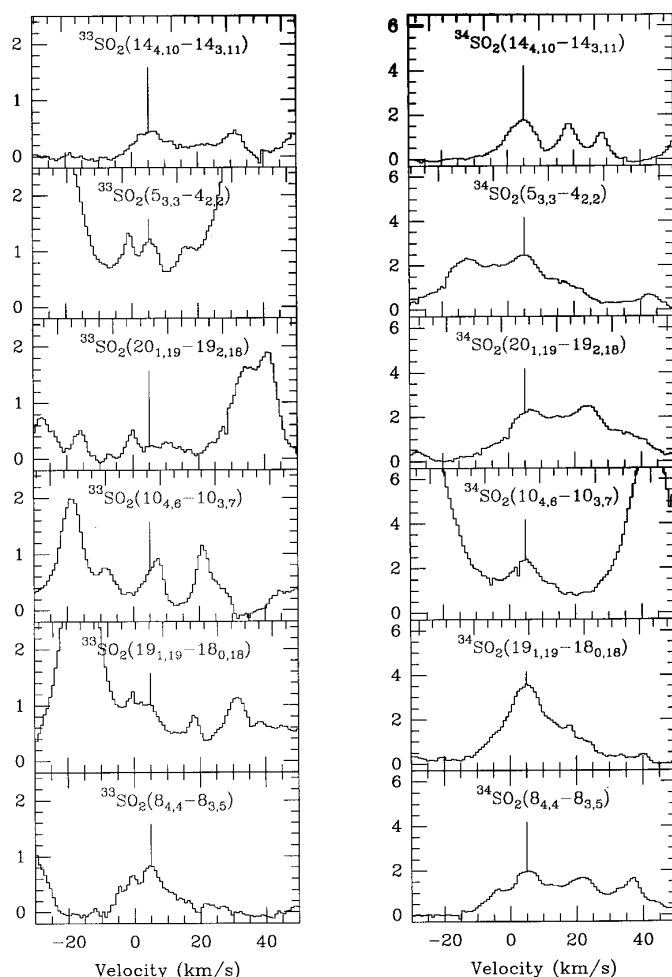


FIG. 1. Small portions of the Caltech line survey of Orion-KL (325–360 GHz) pertaining to the frequency areas of the predicted $^{33}\text{SO}_2$ and $^{34}\text{SO}_2$ line positions, which are marked. The interstellar spectra are often blended by many overlapping lines of different species, showing that the confusion limit (i.e., the point at which the identification of a line is no longer hampered by the system noise, but by the large number of weak lines) is basically reached.

the $^{34}\text{SO}_2$ to the corresponding $^{33}\text{SO}_2$ lines agree, within their uncertainties due to line blending and defining a baseline, with the expected ratio of 5.5, based on Solar System $^{34}\text{S}/^{33}\text{S}$ ratios. Although the detection of $^{33}\text{SO}_2$ contributes little to what can be learned about the physical conditions in the observed region, this detection is valuable in reducing the number of unidentified lines. Unidentified lines are potential candidates for new species, but as long as many line frequencies of isomers, isotopomers, and vibrationally or torsionally excited states of known molecules are unknown, most of the unidentified lines probably are due to these candidates. This prevents using the “true” unidentified lines to detect new species.

TABLE 1
Observed Rotational Transitions of $^{33}\text{SO}_2$ up to 950 GHz

<i>Transition</i>	<i>F</i> ← <i>F'</i>	<i>ν_{exp}^a</i>	<i>Δν_{exp}^b</i>	<i>Residuum^b</i>	<i>E^c</i>	<i>Transition</i>	<i>F</i> ← <i>F'</i>	<i>ν_{exp}^a</i>	<i>Δν_{exp}^b</i>	<i>Residuum^b</i>	<i>E^c</i>
31 _{6,26} ← 31 _{5,27}		538 420.916	100	+ 328	359.70	31 _{3,29} ← 30 _{2,28}	29.5 ← 28.5	629 314.000	50	+ 43	309.76
19 _{3,17} ← 18 _{2,16}	17.5 ← 16.5	539 785.269	300	+ 191	118.52		32.5 ← 31.5				
	20.5 ← 19.5						30.5 ← 29.5	629 316.254	50	− 88	
	18.5 ← 17.5	539 790.224	300	− 277			31.5 ← 30.5				
	19.5 ← 18.5					15 _{4,12} ← 14 _{3,11}	13.5 ← 12.5	632 646.121	70	− 48	82.38
10 _{8,2} ← 11 _{7,5}		540 034.733	100	+ 123	124.12		16.5 ← 15.5				
14 _{2,12} ← 13 _{1,13}	14.5 ← 13.5	540 198.901	200	− 459	56.99		14.5 ← 13.5	632 647.487	70	+ 122	
	13.5 ← 12.5	540 200.362	200	+ 391	56.99		15.5 ← 14.5				
	15.5 ← 14.5	540 211.931	200	+ 252	56.99	37 _{7,31} ← 37 _{6,32}		632 707.281	100	+ 344	510.74
	12.5 ← 11.5	540 213.393	200	− 183	56.99	42 _{4,38} ← 41 _{5,37}	42.5 ← 41.5	639 447.054	150	− 348	594.40
29 _{6,24} ← 29 _{5,25}		540 596.585	100	+ 254	320.48		41.5 ← 40.5				
29 _{2,28} ← 28 _{1,27}		541 456.293	150	+ 26	260.44		43.5 ← 42.5	639 450.389	150	+ 420	
10 _{4,6} ← 9 _{3,7}		542 739.523	80	− 15	43.81		40.5 ← 39.5				
37 _{3,35} ← 37 _{2,36}	37.5 ← 37.5	543 826.837	100	+ 96	442.42	36 _{0,36} ← 35 _{1,35}		640 409.269	25	− 15	378.88
	36.5 ← 36.5					31 _{7,25} ← 31 _{6,26}		641 621.128	100	+ 272	377.66
	38.5 ← 38.5	543 830.597	100	− 134		35 _{2,34} ← 34 _{1,33}		642 012.625	60	− 78	376.51
	35.5 ← 35.5					30 _{7,23} ← 30 _{6,24}		642 120.830	100	+ 237	357.78
24 _{6,18} ← 24 _{5,19}		544 728.335	100	+ 194	233.81	25 _{7,19} ← 25 _{6,20}		647 330.610	70	+ 111	267.99
25 _{6,20} ← 25 _{5,21}		544 921.621	100	+ 137	249.81	24 _{7,17} ← 24 _{6,18}		647 914.770	70	+ 94	251.98
23 _{6,18} ← 23 _{5,19}		546 737.307	100	+ 91	218.38	43 _{3,41} ← 43 _{2,42}	43.5 ← 43.5	649 673.761	70	+ 108	589.90
22 _{6,16} ← 22 _{5,17}		547 029.205	100	+ 65	203.65		42.5 ← 42.5				
21 _{6,16} ← 21 _{5,17}		548 227.172	100	− 56	189.53		44.5 ← 44.5	649 677.101	70	− 58	
20 _{6,14} ← 20 _{5,15}		548 650.931	80	+ 39	176.08		41.5 ← 41.5				
19 _{6,14} ← 19 _{5,15}		549 387.797	60	− 11	163.27	20 _{7,13} ← 20 _{6,14}		649 787.554	40	+ 39	194.39
18 _{6,12} ← 18 _{5,13}		549 782.520	60	+ 17	151.11	19 _{7,13} ← 19 _{6,14}		650 099.531	30	+ 32	181.60
17 _{6,12} ← 17 _{5,13}		550 247.277	60	+ 13	139.59	18 _{7,11} ← 18 _{6,12}		650 354.619	30	+ 24	169.45
16 _{6,10} ← 16 _{5,11}		550 555.677	45	+ 5	128.72	17 _{7,11} ← 17 _{6,12}		650 569.149	30	+ 15	157.95
15 _{6,10} ← 15 _{5,11}		550 850.014	40	− 8	118.49	18 _{3,15} ← 17 _{2,16}	18.5 ← 17.5	650 781.008	120	− 135	103.46
14 _{6,8} ← 14 _{5,9}		551 064.989	40	− 13	108.91		17.5 ← 16.5				
14 _{6,9} ← 14 _{5,10}		551 071.175	200	+ 341	108.90		19.5 ← 18.5	650 786.761	120	+ 78	
8 _{4,5} ← 9 _{1,8}	6.5 ← 7.5	551 226.933	500	+ 848	31.40		16.5 ← 15.5				
	9.5 ← 10.5					14 _{7,7} ← 14 _{6,8}		650 991.957	25	+ 2	127.29
13 _{6,8} ← 13 _{5,9}		551 246.299	30	− 44	99.96	13 _{7,7} ← 13 _{6,8}		651 075.816	10	− 2	118.35
12 _{6,6} ← 12 _{5,7}		551 381.447	25	+ 5	91.66	12 _{7,5} ← 12 _{6,6}		651 137.604	25	− 27	110.05
11 _{6,6} ← 11 _{5,7}		551 485.599	25	− 29	84.00	11 _{7,5} ← 11 _{6,6}		651 181.065	10	− 5	102.39
10 _{6,4} ← 10 _{5,5}		551 560.393	25	− 35	76.98	10 _{7,3} ← 10 _{6,4}		651 209.376	10	− 3	95.38
9 _{6,4} ← 9 _{5,5}		551 612.635	25	− 45	70.60	9 _{7,3} ← 9 _{6,4}		651 225.571	10	− 5	89.00
8 _{6,2} ← 8 _{5,3}		551 646.331	25	− 51	64.85	7 _{7,1} ← 7 _{6,2}		651 232.343	50	+ 86	78.15
7 _{6,2} ← 7 _{5,3}		551 665.880	25	− 30	59.75	33 _{3,31} ← 32 _{2,30}	31.5 ← 30.5	651 865.802	50	+ 13	349.90
6 _{6,0} ← 6 _{5,1}		551 674.884	25	+ 27	55.29		34.5 ← 33.5				
11 _{4,8} ← 10 _{3,7}		560 949.861	25	− 11	50.23		32.5 ← 31.5	651 867.538	50	− 105	
23 _{3,21} ← 22 _{2,20}	21.5 ← 20.5	567 365.275	150	+ 171	172.46		33.5 ← 32.5				
	24.5 ← 23.5					38 _{3,35} ← 37 _{4,34}	38.5 ← 37.5	655 950.346	100	− 207	476.88
	22.5 ← 21.5	567 369.832	150	− 245			37.5 ← 36.5				
	23.5 ← 22.5						39.5 ← 38.5	655 952.504	100	+ 157	
25 _{3,23} ← 24 _{2,22}	23.5 ← 22.5	580 207.778	130	+ 153	203.20		36.5 ← 35.5				
	26.5 ← 25.5					37 _{1,37} ← 36 _{0,36}		657 957.766	50	− 76	400.24
	24.5 ← 23.5	580 211.887	130	− 217		36 _{2,34} ← 35 _{3,33}		662 119.599	120	− 146	414.92
	25.5 ← 24.5					17 _{4,14} ← 16 _{3,13}	15.5 ← 14.5	665 189.528	80	+ 19	102.42
12 _{4,8} ← 11 _{3,9}	16.5 ← 15.5	580 980.969	25	− 15	57.24		18.5 ← 17.5				
16 _{3,13} ← 15 _{2,14}	15.5 ← 14.5	590 678.390	50	− 95	82.72		16.5 ← 15.5	665 191.415	80	− 120	
	17.5 ← 16.5	590 682.835	50	+ 65			17.5 ← 16.5				
	14.5 ← 13.5					38 _{0,38} ← 37 _{1,37}		675 431.622	25	− 24	422.19
27 _{3,25} ← 26 _{2,24}	25.5 ← 24.5	594 076.597	100	+ 156	236.37	12 _{5,7} ← 11 _{4,8}		681 012.743	30	− 37	68.94
	28.5 ← 27.5					39 _{1,39} ← 38 _{0,38}		692 955.782	20	− 24	444.72
	26.5 ← 25.5	594 080.136	100	− 115		19 _{4,16} ← 18 _{3,15}	17.5 ← 16.5	694 187.076	100	+ 82	125.17
	27.5 ← 26.5						20.5 ← 19.5				
36 _{3,33} ← 35 _{4,32}	36.5 ← 35.5	595 395.147	50	− 89	430.33		18.5 ← 17.5	694 189.609	100	− 149	
	35.4 ← 34.5						19.5 ← 18.5				
	37.5 ← 36.5	595 397.904	50	+ 74		13 _{5,9} ← 12 _{4,8}		699 934.556	40	− 29	76.62
	34.5 ← 33.5					38 _{2,36} ← 37 _{3,35}		702 197.513	80	− 137	460.56
13 _{4,10} ← 12 _{3,9}	11.5 ← 10.5	597 591.249	100	+ 92	64.99	37 _{3,35} ← 36 _{2,34}	35.5 ← 34.5	706 095.323	100	− 57	437.01
	14.5 ← 13.5						38.5 ← 37.5				
	12.5 ← 11.5	597 591.815	100	− 82			36.5 ← 35.5	706 095.915	100	+ 61	
	13.5 ← 12.5						37.5 ← 36.5				
34 _{0,34} ← 33 _{1,33}		605 367.499	25	− 4	337.91	12 _{4,8} ← 12 _{1,11}	10.5 ← 10.5	706 851.775	250	+ 372	53.04
14 _{4,10} ← 13 _{3,11}		619 508.714	30	− 1	73.22		13.5 ← 13.5				
16 _{2,14} ← 15 _{1,15}	16.5 ← 15.5	627 801.793	50	+ 52	74.50		11.5 ← 11.5	706 855.042	250	− 272	
	15.5 ← 14.5					39 _{2,38} ← 38 _{1,37}	12.5 ← 12.5	711 158.874	100	− 107	465.52
	17.5 ← 16.5	627 814.220	50	− 36		40 _{3,37} ← 39 _{4,36}	40.5 ← 39.5	711 730.405	100	− 233	525.85
	14.5 ← 13.5	627 815.565	50	− 29			39.5 ← 38.5				
36 _{7,29} ← 36 _{6,30}		629 000.736	250	+ 380	487.12		41.5 ← 40.5	711 732.058	100	+ 115	
							38.5 ← 37.5				

^a Frequencies given in MHz.^b Frequencies given in kHz.^c Energies *E'* given in cm^{−1}. For frequencies that are not resolved in hyperfine structure, the hyperfine quantum numbers *F* and *F'* are omitted.

TABLE 1—Continued

Transition	$F \leftarrow F'$	ν_{exp}^a	$\Delta\nu_{exp}^b$	Residuum ^b	E^c
22 _{4,18} \leftarrow 22 _{1,21}	22.5 \leftarrow 22.5 21.5 \leftarrow 21.5 23.5 \leftarrow 23.5 20.5 \leftarrow 20.5	715 318.281	100	+ 191	165.16
34 _{10,24} \leftarrow 34 _{9,25}		944 801.861	100	+ 460	515.44
32 _{10,22} \leftarrow 32 _{9,23}		945 581.125	100	+ 363	472.59
31 _{10,22} \leftarrow 31 _{9,23}		945 907.936	100	+ 307	452.13
30 _{10,20} \leftarrow 30 _{9,21}		946 196.588	100	– 266	432.31
29 _{10,20} \leftarrow 29 _{9,21}		946 449.981	100	+ 214	413.13
28 _{10,18} \leftarrow 28 _{9,19}		946 670.683	100	+ 197	394.60
27 _{10,18} \leftarrow 27 _{9,19}		946 861.206	100	– 152	376.70
26 _{10,16} \leftarrow 26 _{9,17}		947 023.896	50	+ 38	359.45
25 _{10,16} \leftarrow 25 _{9,17}		947 161.334	50	+ 103	342.84
24 _{10,14} \leftarrow 24 _{9,15}		947 275.468	50	+ 81	326.87
23 _{10,14} \leftarrow 23 _{9,15}		947 368.332	50	– 124	311.54
10 _{10,0} \leftarrow 10 _{9,1}		947 465.747	50	– 15	170.46
11 _{10,2} \leftarrow 11 _{9,3}		947 493.325	50	+ 29	177.47
21 _{10,12} \leftarrow 21 _{9,13}		947 499.407	25	+ 30	282.80
12 _{10,2} \leftarrow 12 _{9,3}		947 519.555	25	– 15	185.13
20 _{10,10} \leftarrow 20 _{9,11}		947 541.003	40	– 30	269.39
13 _{10,4} \leftarrow 13 _{9,5}		947 543.475	80	+ 74	193.43
14 _{10,4} \leftarrow 14 _{9,5}		947 563.732	25	– 27	202.36
19 _{10,10} \leftarrow 19 _{9,11}		947 569.215	25	– 10	256.62
15 _{10,6} \leftarrow 15 _{9,7}		947 579.434	80	+ 86	211.93
18 _{10,8} \leftarrow 18 _{9,9}		947 585.589	80	+ 11	244.49
16 _{10,6} \leftarrow 16 _{9,7}		947 589.169	80	– 62	222.15
17 _{10,8} \leftarrow 17 _{9,9}		947 591.794	80	+ 150	233.00

APPENDIX

The well-known Hamiltonian for asymmetric tops, employed here in the axis choice of I' , was developed by Watson:

$$\begin{aligned}
\hat{H}_{rot}^A = & \frac{1}{2}(B+C)\hat{J}^2 + \left\{ A - \frac{1}{2}(B+C) \right\} \hat{J}_z^2 - \Delta_J \hat{J}^4 \\
& - \Delta_{JK} \hat{J}^2 \hat{J}_z^2 - \Delta_K \hat{J}_z^4 + \Phi_J \hat{J}^6 + \Phi_{JK} \hat{J}^4 \hat{J}_z^2 + \Phi_{KJ} \hat{J}^2 \hat{J}_z^4 \\
& + \Phi_K \hat{J}_z^6 + \left\{ \frac{1}{4}(B-C) - \delta_J \hat{J}^2 + \Phi_J \hat{J}^4 \right\} \\
& \times (\hat{J}_+^2 + \hat{J}_-^2) + \frac{1}{2}[-\delta_K \hat{J}_z^2 + \phi_{JK} \hat{J}^2 \hat{J}_z^2 \\
& + \phi_K \hat{J}_z^4 (\hat{J}_+^2 + \hat{J}_-^2)]_+.
\end{aligned}$$

In addition the $^{33}\text{SO}_2$ rotational transitions reported here are split in hyperfine structure, partially (Table 1). The electric quadrupole hyperfine interaction requires the following expansion for the Hamiltonian:

$$\begin{aligned}
\langle J'K'F'S'I | \hat{H}_Q | JKFSI \rangle \\
= \frac{1}{2} eQ \delta_{F',F} \delta_{S',S} (-)^{I+J'+F} \\
\times \sqrt{\frac{(I+1)(2I+1)(2I+3)}{I(2I-1)}} (2J+1)(2J'+1)
\end{aligned}$$

$$\begin{aligned}
& \times \sum_{q=-2}^2 (-)^{N'-K'} \begin{Bmatrix} F & J' & I \\ 2 & I & J \end{Bmatrix} \begin{pmatrix} J' & 2 & J \\ -K' & q & K \end{pmatrix} \\
& \times \langle \gamma' | T_q^{(2)}(\nabla \mathbf{E}) | \gamma \rangle.
\end{aligned}$$

The Hfs expression above, as well as the transformation between the irreducible tensor notation and the Cartesian notation for the components $\langle T_q^{(2)}(\nabla \mathbf{E}) \rangle$, was developed by Bowater (8). Since SO_2 is a planar asymmetric top and for the $^{33}\text{SO}_2$ both, the axes of the electric quadrupole interaction and the main axes of inertia, are almost identical, the off-diagonal components for the electric field gradient become infinitely small and were not included. The asymmetry parameter η has been determined (Table 2) in accordance with the work of van Riet (3). The term η represents the position of the electric quadrupole tensor due to the bonding axes of the molecule. The value for $\eta = 1.050(17)$ determined here is in line with the value for ^{33}S -substituted deuterodisulfane

TABLE 2
Molecular Parameters of $^{33}\text{SO}_2$ in the Ground Vibrational State Determined Using an A -Reduced Hamiltonian with an I' Axis Choice

Parameter	This work	van Riet	Unit ^c
A	59 856.472 3 (62)	59 856.49	MHz
B	10 318.301 2 (15)	10 318.20	MHz
C	8 780.136 3 (15)	8 780.23	MHz
κ^a	– 0.939 769 963 (82)	– 0.939 777 5	–
Δ_J	6.591 5 (13)	6.153	kHz
Δ_{JK}	– 114.192 (10)	– 109.405	kHz
Δ_K	2.511 68 (10)	2.481827	MHz
δ_J	1.713 06 (47)	–	kHz
δ_K	25.230 (41)	–	kHz
Φ_J	11.81 (44)	–	mHz
Φ_{JK}	138 (12)	–	mHz
Φ_{KJ}	– 18.363 (51)	–	Hz
Φ_K	341.34 (54)	–	Hz
ϕ_J	5.79 (13)	–	mHz
ϕ_{JK}	36.8 ^b	–	mHz
ϕ_K	22.25 (54)	–	Hz
eQq_{aa}	– 0.60 (22)	– 1.7	MHz
eQq_{bb}	24.70 (24)	25.71	MHz
eQq_{cc}	– 24.10 (24)	– 24.01	MHz
η^a	1.050 (17)	1.14	–

^aDerived value.

^bFixed to the value obtained by $^{32}\text{SO}_2$.

($\eta = 1.528(32)$ for H^{33}SSD , $\eta = 1.595(23)$ for HS^{33}SD) and therefore states a typical attribute of ^{33}S containing species (9).

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