

Heterodyne Frequency Measurements on OCS near 61.76 THz (2060 cm^{-1})

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Heterodyne measurements have been made on the $10^{00}\text{--}00^{00}$ and $11^{10}\text{--}01^{10}$ bands of $^{16}\text{O}^{12}\text{C}^{32}\text{S}$ and $^{16}\text{O}^{13}\text{C}^{32}\text{S}$ and the $10^{00}\text{--}00^{00}$ band of $^{16}\text{O}^{12}\text{C}^{34}\text{S}$. These measurements were combined with earlier frequency measurements and Fourier transform measurements to obtain accurate calibration frequencies for the regions 1985 to 2085 and 2550 to 2600 cm^{-1} . © 1990 Academic Press, Inc.

INTRODUCTION

We have been involved in a program to measure all the lower energy levels of carbonyl sulfide (OCS) against CO_2 laser frequency standards by means of heterodyne frequency measurement techniques. The goal of this work has been to provide accurate frequency calibration standards throughout the infrared spectrum. Until now, lack of an appropriate transfer oscillator has prevented us from making measurements above 1932 cm^{-1} . The construction of a new high-frequency CO laser has now enabled us to make heterodyne measurements up to 2085 cm^{-1} . In this paper we report heterodyne frequency measurements in the ν_1 region of OCS.³

Before this work, the most accurate measurements of the ν_1 band of OCS were those of Guelachvili (2). Guelachvili's Fourier transform spectrometer (FTS) measurements appear to have been calibrated against the CO frequencies (3), which we now believe are too high by about 11 MHz (0.00037 cm^{-1}). A much more extensive set of measurements of the absorption spectrum of OCS was made more recently by Hunt *et al.* (4). Their FTS measurements were calibrated by reference to the measurements of Guelachvili (2, 3). Even more recently Masukidi *et al.* (5) measured the laser Stark resonances of OCS in the $5\text{-}\mu\text{m}$ region but they did not indicate what band center was consistent with their analysis. None of the earlier measurements

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³ The vibrational numbering system adopted by the IAU-IUPAP joint commission on spectroscopy (1) is used throughout this paper. Some other papers use a notation that interchanges ν_1 and ν_3 .

involved zero-field frequency measurements (as distinguished from wavelength measurements) which we consider to be necessary for accurate frequency standards.

EXPERIMENTAL DETAILS

The procedure for the heterodyne frequency measurements followed here was one in which the measurements of the OCS frequencies were referred to CO_2 laser frequency standards. The technique we have developed requires the use of a liquid-nitrogen-cooled, flowing-gas carbon monoxide laser as a transfer oscillator. Each OCS frequency determination consisted of two simultaneous measurements. In one measurement, the frequency of the CO laser transfer oscillator (local oscillator) was determined relative to CO_2 laser frequency standards. In the second measurement, the frequency difference between the lasing frequency of the transfer oscillator and the frequency of a tunable diode laser (which was locked to a particular OCS transition) was determined. Details of the measurement procedure and a description of the CO laser transfer oscillator are available in Refs. (6, 7).

The synthesis scheme used for these measurements was simpler than those used for the longer wavelength measurements (6, 7) in that only a combination of CO_2 frequencies (no harmonics were required) and microwave frequencies was used. The values for the CO_2 frequencies given by Petersen *et al.* (8) and Bradley *et al.* (9) were used in these measurements.

The CO laser used for the earlier work (6, 7) was modified to work in the 4.9- μm region by the incorporation of a 240 line/mm grating and a 98% output coupler coated for operation at 4.9 μm . For operation of the $v = 2 \rightarrow 1$ transitions, it was necessary to provide a pathway for He gas to sweep the unexcited CO molecules from the regions of the laser tube which did not have gain (regions between the Brewster windows and the electrical discharge). A by-product of these measurements was a set of new frequency measurements for CO laser transitions for $v'' = 1, 2, 3,$ and 4. New and more accurate calculated CO frequencies for the low v'' region are presented elsewhere (10).

For measurements on the stronger lines, a 0.30-m-long absorption cell was used with OCS fill pressures ranging from 0.66 to 2.66 Pa (0.005 to 0.020 Torr). A 1.7-m-long absorption cell was used for some of the weaker transitions (carbon-13 OCS with a 1.1% natural abundance), and a pressure as high as 22 Pa (0.165 Torr) was recorded. We think that the pressure shift will be less than 0.1 MHz which is well within the uncertainty of the calculated values given in Tables IV and V.

ANALYSIS AND RESULTS

The observed transitions were easily assigned by referring to the list of frequencies and assigned transitions given by Hunt *et al.* (4).

As was done with our earlier heterodyne measurements on OCS (11-13), the present measurements were combined with all other frequency measurements involving the upper and lower vibrational states. In addition, some FTS measurements were included in the least-squares fit in such a way as to contribute to improving the accuracy of the rotational energy levels without affecting the accuracy of the vibrational energy levels.

For the analysis of the heterodyne measurements of the 10^00-00^00 transitions of

$^{16}\text{O}^{12}\text{C}^{34}\text{S}$, the least-squares fit included frequency measurements taken from Refs. (14-19). For the $10^0\text{-}00^0$ and $11^1\text{-}01^1$ bands of $^{16}\text{O}^{13}\text{C}^{32}\text{S}$ the fit included measurements from Refs. (14-17), and for the same bands of $^{16}\text{O}^{12}\text{C}^{32}\text{S}$ the fit included measurements from Refs. (14-19).

In addition to including the FTS measurements of Hunt *et al.* (4), we also used new FTS measurements made in our laboratory on the $11^1\text{-}00^0$ transition of $^{16}\text{O}^{12}\text{C}^{32}\text{S}$ between 2550 and 2600 cm^{-1} . The FTS measurements from Jolma *et al.* (20) and from earlier papers in this series (12, 13) were used to better define some of the rotational constants.

TABLE I
Heterodyne Frequency Measurements on Carbonyl Sulfide at 4.9 μm

Frequency Transfer		Carbonyl Sulfide		
CO Transition	$\nu_{\text{CO}} - \nu_{\text{OCS}}$	Transition	Frequency, (unc)	Obs. - Calc.
$P_v - (J'')$	MHz	$P(J'')$	MHz	MHz
$P_4(12)$	4179.0	$^3P(26)C^a$	59 693 603.1(60) ^b	1.6
$P_4(12)$	4416.0	$^3P(26)B$	59 693 840.1(60)	3.0
$P_4(11)$	1560.1	$^3P(32)A$	59 813 307.6(100)	1.7
$P_3(14)$	-4045.6	$^3P(2)A$	60 210 827.3(50)	-2.0
$P_3(14)$	1398.3	$^3R(15)B$	60 216 271.2(70)	1.8
$P_3(14)$	1647.8	$^3R(15)C$	60 216 519.6(70)	-2.2
$P_3(13)$	938.5	$^3R(8)A$	60 341 171.7(40)	1.0
$P_3(13)$	3331.3	$^3R(27)B$	60 343 564.4(40)	-1.7
$P_3(13)$	3823.0	$^3R(27)C$	60 344 056.2(40)	-0.2
$P_3(11)$	-1769.7	$P(82)A$	60 586 208.3(50)	3.6
$P_3(11)$	-1285.1	$^3R(31)A$	60 586 692.9(40)	0.1
$P_3(10)$	240.3	$P(75)A$	60 710 590.4(70)	4.9
$P_3(10)$	3515.9	$P(62)C$	60 713 866.0(50)	-1.7
$P_3(10)$	4024.3	$P(62)B$	60 714 374.4(50)	-0.8
$P_3(8)$	-3162.6	$P(61)A$	60 948 914.5(30)	-1.3
$P_3(8)$	2053.3	$P(47)C$	60 954 112.4(50)	-0.1
$P_3(8)$	2449.2	$P(47)B$	60 954 526.3(50)	1.0
$P_3(7)$	3216.1	$^4P(53)A$	61 074 639.0(40)	-1.7
$P_3(7)$	4340.8	$P(39)C$	61 075 763.7(40)	-0.8
$P_3(7)$	4708.7	$P(39)B$	61 076 131.6(50)	4.8
$P_2(13)$	3778.8	$P(36)C$	61 120 218.3(50)	-1.1
$P_2(13)$	4122.4	$P(36)B$	61 120 561.9(50)	0.2
$P_2(12)$	-344.8	$^4P(42)A$	61 241 514.1(80)	3.1
$P_2(11)$	2705.4	$P(34)A$	61 368 989.2(100)	-0.1
$P_2(10)$	1970.2	$P(9)B,C$	61 491 676.5(150)	-10.3
$P_2(9)$	3045.7	$^4P(15)A$	61 615 169.5(100)	4.4
$P_2(8)$	3024.1	$P(7)A$	61 736 557.5(50)	0.9
$P_1(13)$	-1722.0	$^4R(7)A$	61 892 945.4(70)	-1.4
$P_1(13)$	606.5	$R(25)B$	61 895 273.9(80)	4.4
$P_1(13)$	1004.9	$R(25)C$	61 895 672.3(80)	5.5
$P_1(12)$	1423.3	$R(38)B$	62 022 563.9(80)	-4.6
$P_1(12)$	1822.0	$^4R(19)A$	62 022 962.6(120)	-0.6
$P_1(12)$	2057.1	$R(38)C$	62 023 197.7(80)	-5.0
$P_1(11)$	-3936.1	$^4R(31)A$	62 142 677.4(100)	3.8
$P_1(11)$	-785.0	$R(52)B$	62 145 828.5(80)	-0.7
$P_1(10)$	-3256.7	$R(41)A$	62 267 829.9(80)	-1.7
$P_1(0)$	-1868.7	$^4R(45)A$	62 269 217.9(100)	1.4
$P_1(9)$	375.8	$R(56)A$	62 394 930.8(60)	-1.8
$P_1(9)$	1845.3	$^4R(61)A$	62 396 400.3(100)	-0.5
$P_1(8)$	1539.3	$R(73)A$	62 518 558.6(80)	-3.6

- a) The A denotes the $10^0\text{-}00^0$ band, B and C refer to the $11^1\text{-}01^1$ band. The left superscript 3 on the transition (P or R) denotes the $\text{O}^{13}\text{C}\text{S}$ isotope; a 4 indicates the $\text{O}\text{C}^{34}\text{S}$. Otherwise, the most abundant isotope is indicated.
b) The estimated uncertainty in the last digits is given in parentheses.

TABLE II
Band Centers Determined from Heterodyne Measurements on OCS

Transition	ν_0 this work (cm^{-1}) ^b	ν_0 Ref. (21, 22) (cm^{-1})	ν_0 Ref. (4) ^a (cm^{-1})
¹⁶ O ¹² C ³² S			
10 ⁰ 0-00 ⁰ 0	2062.20084(13) ^c	2062.20121(14)	2062.20123(3)
11 ¹ 0-01 ¹ 0	2054.88554(11)	2054.88563(22)	2054.88584(2)
11 ¹ 0-00 ⁰ 0	2575.30758(20)	2575.30774(22)	---
¹⁶ O ¹² C ³⁴ S			
10 ⁰ 0-00 ⁰ 0	2061.44530(16)	2061.44519(3)	2061.44564(3)
¹⁶ O ¹³ C ³² S			
10 ⁰ 0-00 ⁰ 0	2009.22818(13)	2009.22847(33)	2009.22849(3)
11 ¹ 0-01 ¹ 0	2002.42812(13)	2002.42840(95)	2002.42847(8)
11 ¹ 0-00 ⁰ 0	2507.43726(13)	2507.43754(95)	---

- a) Because of the difference in definition of the band center in Ref. (4), we give here the band centers as refit with our program.
 b) In this paper the conversion from frequency to wavenumber units used the defining value of $c=299\,792\,458$ m/s.
 c) The uncertainty (twice the standard error) in the last digits is given in parentheses. Only the uncertainties in the first column represent the true accuracy of the frequencies (see text).

In the analysis of the transitions the energy levels were given by

$$E(v, l, J) = G(v, l) + B_v J(J+1) - D_v [J(J+1) - l^2]^2 + H_v [J(J+1) - l^2]^3 \quad (1)$$

and the band centers were given by

$$\nu_0 = G(v', l') - G(v'', l'') \quad (2)$$

TABLE III
Rotational Constants (in cm^{-1}) Determined for OCS

vib. state	B_v	$D_v \times 10^8$	$H_v \times 10^{15}$
¹⁶ O ¹² C ³²			
00 ⁰ 0	0.202 856 740 6(9) ^a	4.340 54(29)	-3.442(346)
01 ¹ 0 ^b	0.203 209 831 3(32)	4.411 31(37)	-2.773(424)
10 ⁰ 0	0.201 641 530(50)	4.409 7(27)	45.3(50) ^c
11 ¹ 0 ^d	0.202 015 425(47)	4.473 71(222)	28.43(294)
¹⁶ O ¹² C ³⁴ S			
00 ⁰ 0	0.197 898 037 2(66)	4.141 50(74)	-3.057(523)
10 ⁰ 0	0.196 716 117(68)	4.214 3(36)	37.8(48)
¹⁶ O ¹³ C ³² S			
00 ⁰ 0	0.202 204 014 2(100)	4.328 74(184)	-2.994(473)
01 ¹ 0 ^e	0.202 537 160(130)	4.388 1(83)	[-3.000] ^f
10 ⁰ 0	0.201 060 532(69)	4.472 4(48)	76.5(72)
11 ¹ 0 ^g	0.201 413 034(185)	4.495 7(95)	[50.0]

- a) The uncertainty in the last digits (twice the estimated standard error) is given in parentheses.
 b) The l -type doubling constants for 01¹0 are: $q=2.121\,939\,54(92) \times 10^{-4}$, $q_J=1.433\,0(91) \times 10^{-10}$, and $q_{JJ}=7.1(38) \times 10^{-16}$.
 c) $L_v=-0.115(28) \times 10^{-17}$ also included in the fit.
 d) The l -type doubling constants for 11¹0 are: $q=2.155\,31(29) \times 10^{-4}$ and $q_J=3.764(75) \times 10^{-10}$.
 e) For ¹⁶O¹³C³²S the l -type doubling constants for 01¹0 are: $q=2.170\,782\,62(313) \times 10^{-4}$ and $q_J=1.484\,4(140) \times 10^{-10}$.
 f) Values given in square brackets were fixed.
 g) For ¹⁶O¹³C³²S the l -type doubling constants for 11¹0 are: $q=2.226\,27(87) \times 10^{-4}$ and $q_J=5.96(45) \times 10^{-10}$.

This is a slightly different definition of the band centers than was used by Hunt *et al.* When $l = 1$ the l -type doubling was taken into account by substituting for B_v in Eq. (1) the expression

$$B_v \pm 0.5[q_v - q_{vJ}(J+1) + q_{vJJ}J^2(J+1)^2],$$

where q_v was assumed to be positive. For OCS, the positive sign is needed for the f levels and the negative sign is needed for the e levels (that is, the f levels are higher in energy than the e levels).

The data were weighted by the inverse square of their estimated uncertainty. In the case of the FTS measurements, the uncertainty was based on the rms (root mean

TABLE IV
Wavenumbers (in cm^{-1}) Calculated for the $10^0\text{--}00^0$ Band of $^{16}\text{O}^{12}\text{C}^{32}\text{S}$

P-Branch	J''	R-Branch	P-branch	J''	R-Branch
---	0	2062.60412(13) ^a	2043.07934(13)	42	2077.33137(13)
2061.79513(13)	1	2063.00498(13)	2042.57232(13)	43	2077.62897(12)
2061.38698(13)	2	2063.40339(13)	2042.06290(13)	44	2077.92408(12)
2060.97641(13)	3	2063.79938(13)	2041.55109(12)	45	2078.21671(12)
2060.56342(13)	4	2064.19293(13)	2041.03689(12)	46	2078.50684(12)
2060.14799(13)	5	2064.58404(13)	2040.52029(12)	47	2078.79448(12)
2059.73014(13)	6	2064.97272(13)	2040.00130(12)	48	2079.07963(12)
2059.30987(13)	7	2065.35896(13)	2039.47991(12)	49	2079.36228(12)
2058.88717(13)	8	2065.74276(13)	2038.95613(12)	50	2079.64244(12)
2058.46205(13)	9	2066.12412(13)	2038.42997(12)	51	2079.92010(12)
2058.03451(13)	10	2066.50304(13)	2037.90141(12)	52	2080.19527(12)
2057.60454(13)	11	2066.87951(13)	2037.37046(12)	53	2080.46793(12)
2057.17216(13)	12	2067.25354(13)	2036.83713(12)	54	2080.73810(12)
2056.73736(13)	13	2067.62513(13)	2036.30141(12)	55	2081.00576(12)
2056.30014(13)	14	2067.99427(13)	2035.76330(12)	56	2081.27092(12)
2055.86050(13)	15	2068.36096(13)	2035.22281(12)	57	2081.53358(12)
2055.41845(13)	16	2068.72520(13)	2034.67993(12)	58	2081.79373(12)
2054.97398(13)	17	2069.08699(13)	2034.13467(12)	59	2082.05138(12)
2054.52709(13)	18	2069.44633(13)	2033.58702(12)	60	2082.30652(12)
2054.07779(13)	19	2069.80321(13)	2033.03700(12)	61	2082.55915(12)
2053.62608(13)	20	2070.15765(13)	2032.48459(12)	62	2082.80928(12)
2053.17196(13)	21	2070.50962(13)	2031.92980(12)	63	2083.05689(12)
2052.71542(13)	22	2070.85914(13)	2031.37264(12)	64	2083.30199(12)
2052.25648(13)	23	2071.20620(13)	2030.81309(12)	65	2083.54458(12)
2051.79512(13)	24	2071.55080(13)	2030.25117(12)	66	2083.78466(12)
2051.33135(13)	25	2071.89294(13)	2029.68688(12)	67	2084.02222(12)
2050.86518(13)	26	2072.23261(13)	2029.12021(12)	68	2084.25727(12)
2050.39659(13)	27	2072.56983(13)	2028.55117(12)	69	2084.48981(12)
2049.92560(13)	28	2072.90457(13)	2027.97975(12)	70	2084.71982(12)
2049.45220(13)	29	2073.23685(13)	2027.40597(12)	71	2084.94732(12)
2048.97640(13)	30	2073.56666(13)	2026.82982(12)	72	2085.17230(12)
2048.49819(13)	31	2073.89400(13)	2026.25129(12)	73	2085.39476(12)
2048.01758(13)	32	2074.21888(13)	2025.67041(12)	74	2085.61471(12)
2047.53456(13)	33	2074.54127(13)	2025.08715(12)	75	2085.83213(12)
2047.04914(13)	34	2074.86120(13)	2024.50153(12)	76	2086.04703(13)
2046.56131(13)	35	2075.17865(13)	2023.91355(12)	77	2086.25941(13)
2046.07109(13)	36	2075.49362(13)	2023.32321(13)	78	2086.46926(13)
2045.57846(13)	37	2075.80612(13)	2022.73051(13)	79	2086.67660(13)
2045.08343(13)	38	2076.11613(13)	2022.13545(13)	80	2086.88141(13)
2044.58601(13)	39	2076.42367(13)	2021.53803(13)	81	2087.08369(13)
2044.08618(13)	40	2076.72872(13)	2020.93826(13)	82	2087.28345(13)
2043.58396(13)	41	2077.03129(13)	2020.33613(13)	83	2087.48068(13)

a) The estimated uncertainty (twice the standard error) in the last digits is given in parentheses.

square) deviation of the measurements from the calculated transition frequency, assuming the band center is not the same as that given by the heterodyne measurements.

Table I gives the observed transition frequencies and their deviation from the calculated values given by the constants from the least-squares fit.

Table II gives the band centers as determined from the heterodyne frequency measurements. These band centers are slightly lower than those given by Guelachvili (2) and by Hunt *et al.* (4), which is in accord with the latest measurements on the CO transitions that were used to calibrate the FTS measurements (10).

The band centers are also lower than those given by Fayt *et al.* (21) and by Lahaye *et al.* (22). This might be expected to affect the Stark effect analysis of Masukidi *et al.* (5), but their value for the CO laser frequency is also too high by nearly the same amount, so the effect on the analysis is nearly canceled.

The rovibrational constants given by this analysis are shown in Table III.

TABLE V

Wavenumbers (in cm^{-1}) calculated for the $11^1_0-00^0_0$ Band of OCS

P-Branch	J''	R-Branch	P-branch	J''	R-Branch
---	0	2575.71140(19) ^a	2558.08624(19)	39	2589.96573(19)
---	1	2576.11331(19)	2557.60707(19)	40	2590.29247(19)
2574.49426(19)	2	2576.51333(19)	2557.12602(19)	41	2590.61726(19)
2574.08475(19)	3	2576.91144(19)	2556.64309(19)	42	2590.94009(19)
2573.67335(19)	4	2577.30766(19)	2556.15829(19)	43	2591.26094(19)
2573.26006(19)	5	2577.70197(19)	2555.67161(19)	44	2591.57983(19)
2572.84487(19)	6	2578.09437(19)	2555.18306(19)	45	2591.89676(19)
2572.42779(19)	7	2578.48487(19)	2554.69264(19)	46	2592.21171(19)
2572.00882(19)	8	2578.87346(19)	2554.20034(19)	47	2592.52468(19)
2571.58795(19)	9	2579.26014(19)	2553.70616(19)	48	2592.83569(19)
2571.16520(19)	10	2579.64491(19)	2553.21011(19)	49	2593.14471(19)
2570.74056(19)	11	2580.02777(19)	2552.71219(19)	50	2593.45176(19)
2570.31403(19)	12	2580.40872(19)	2552.21240(19)	51	2593.75682(19)
2569.88562(19)	13	2580.78776(19)	2551.71073(19)	52	2594.05991(19)
2569.45532(19)	14	2581.16488(19)	2551.20719(19)	53	2594.36100(19)
2569.02313(19)	15	2581.54008(19)	2550.70177(19)	54	2594.66012(19)
2568.58905(19)	16	2581.91336(19)	2550.19448(19)	55	2594.95724(19)
2568.15310(19)	17	2582.28472(19)	2549.68532(19)	56	2595.25237(19)
2567.71525(19)	18	2582.65417(19)	2549.17428(19)	57	2595.54551(19)
2567.27553(19)	19	2583.02169(19)	2548.66138(19)	58	2595.83666(19)
2566.83392(19)	20	2583.38728(19)	2548.14660(19)	59	2596.12581(19)
2566.39043(19)	21	2583.75095(19)	2547.62994(19)	60	2596.41296(19)
2565.94506(19)	22	2584.11269(19)	2547.11142(19)	61	2596.69811(19)
2565.49781(19)	23	2584.47251(19)	2546.59103(19)	62	2596.98126(19)
2565.04867(19)	24	2584.83039(19)	2546.06876(19)	63	2597.26241(19)
2564.59766(19)	25	2585.18634(19)	2545.54462(19)	64	2597.54155(19)
2564.14476(19)	26	2585.54035(19)	2545.01861(19)	65	2597.81868(19)
2563.68999(19)	27	2585.89243(19)	2544.49073(19)	66	2598.09381(19)
2563.23334(19)	28	2586.24257(19)	2543.96098(19)	67	2598.36692(19)
2562.77481(19)	29	2586.59077(19)	2543.42936(19)	68	2598.63803(19)
2562.31440(19)	30	2586.93703(19)	2542.89587(19)	69	2598.90712(20)
2561.85211(19)	31	2587.28135(19)	2542.36051(19)	70	2599.17419(20)
2561.38795(19)	32	2587.62372(19)	2541.82328(20)	71	2599.43925(20)
2560.92190(19)	33	2587.96415(19)	2541.28418(20)	72	2599.70228(20)
2560.45399(19)	34	2588.30263(19)	2540.74322(20)	73	2599.96330(21)
2559.98419(19)	35	2588.63916(19)	2540.20039(20)	74	2600.22229(21)
2559.51252(19)	36	2588.97373(19)	2539.65569(21)	75	2600.47926(22)
2559.03897(19)	37	2589.30635(19)	2539.10912(21)	76	2600.73421(23)
2558.56354(19)	38	2589.63702(19)	2538.56069(22)	77	2600.98713(24)

a) The estimated uncertainty (twice the standard error) in the last digits is given in parentheses.

We have calculated new tables of frequencies based on the results of the present measurements and analysis. Table IV gives the wavenumbers and their estimated uncertainties for the 10^00-00^00 band of $^{16}\text{O}^{12}\text{C}^{32}\text{S}$. One also could use the tables of wavenumbers given by Hunt *et al.* provided they be corrected by subtracting 0.00035 cm^{-1} .

The present measurements have also been combined with frequency measurements of the ν_2 band (01^10-00^00) to obtain calibration wavenumbers for the region 2550 to 2600 cm^{-1} by means of the transitions for the 11^10-00^00 band. Those wavenumbers are given in Table V.

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