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LABORATORY MEASUREMENT OF ROTATIONAL SPECTRUM OF THE ^{18}OH RADICAL USING A TUNABLE FAR-INFRARED SPECTROMETER

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ABSTRACT

Far-infrared transitions between the lower rotational levels of the ^{18}OH radical in the $X^2\Pi$ state have been observed in the laboratory with a high-precision far-infrared spectrometer using a tunable radiation source. From a least-squares analysis of the observed far-infrared data together with the microwave Λ-doubling data, molecular parameters of ^{18}OH in $X^2\Pi$ have been determined to a better precision than those obtained from laser magnetic resonance data and the microwave data (Comben et al. 1986). The hyperfine structure parameters for ^{18}OH are determined for the first time.

Subject headings: line: identification — methods: laboratory — molecular data

1. INTRODUCTION

The OH radical is the first interstellar molecule detected by radio astronomy. The centimeter-wave transitions between components of Λ-doublets were detected in absorption against a number of continuum sources by Weinreb et al. (1963). Far-infrared (FIR) rotational transitions of OH were first detected in emission toward Sgr B2 and Orion KL (Storey, Watson, & Townes 1981). As for its isotopic molecule ^{18}OH, Λ-doublet transitions were first observed toward Sgr A and Sgr B2 (Gardner, McGee, & Sinclair 1970; Wilson & Barrett 1970). Recently a FIR rotational transition was detected toward Orion KL by Melnick et al. (1990). The identification of the line as the $F_1 \leftarrow F_1$, $J = 5/2^+ \leftarrow 3/2^-$ transition was based on the rotational frequencies determined from the analysis of FIR laser magnetic resonance data combined with Λ-doublet microwave transition data (Gottlieb et al. 1974; Kolbe, Zollner, & Leksovar 1981) by Comben et al. (1986). Although these FIR frequencies are accurate enough for the astronomical use at present, there still remain uncertainties of a few MHz coming from indirect determination of zero-field frequencies. It is desirable to measure more accurate FIR frequencies and to determine more precise molecular constants for further spectroscopic and astronomical uses of ^{18}OH.

In the present work frequencies of FIR transitions between the lower rotational levels of ^{18}OH in the $X^2\Pi$ state have been measured accurately in the laboratory with a spectrometer using a tunable FIR source. From the least squares analysis of these data combined with the Λ-doublet transition data, the rotational, spin-orbit, spin-rotation, Λ-type doubling, hyperfine structure parameters of ^{18}OH in $X^2\Pi$ have been determined.

2. EXPERIMENTAL

The FIR spectrometer using a tunable source has been described in detail (Evenson, Jennings, & Petersen 1984; Nolt et al. 1987). The detail of the spectrometer used in the present work has already been reported (Matsushima et al. 1994). Radiation from two stabilized CO_2 lasers and microwave radiation are mixed on a metal-insulator-metal (MIM) diode to generate tunable FIR radiation. The FIR radiation passing through a sample cell is detected by a liquid-helium–cooled silicon composite bolometer, which is operated below the lambda point of liquid helium (at 2.17 K) by reducing the vapor pressure above the liquid.

The ^{18}OH radical was generated in a dc discharge through a mixture of $H_2{}^{18}O$ and He. The partial pressure of $H_2{}^{18}O$ was 90 mtorr and that of He was 350 mtorr with a discharge current of 100 mA. The discharge product was continuously pumped out from the cell by a rotary pump or a mechanical booster pump. The discharge cell made of a Pyrex tube of 1.5 m length and 26 mm inner diameter is equipped with two stainless steel cylindrical electrodes of 0.1 mm thickness. The cathode is 20 cm long and the anode is 10 cm long and they are separated by 70 cm from each other. The windows of the cell are made of 60 μm thick polypropylene.

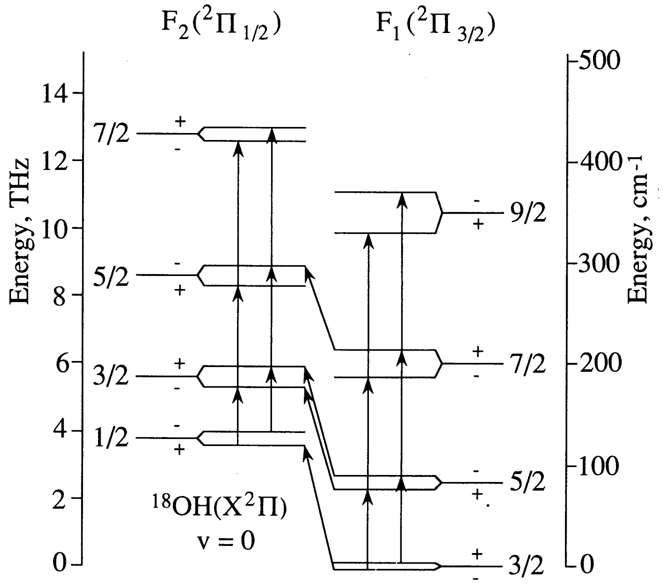

FIG. 1.—Low-lying rotational levels of ^{18}OH, showing the transitions observed in this work. The Λ-type doublet splittings are exaggerated for clarity.

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3. RESULTS AND DISCUSSION

The low-lying rotational levels and the observed transitions of ^{18}OH in the $X^2\Pi$ state are shown in Figure 1. The signal to noise ratios for the $\Delta\Omega = 0$ transitions with lower J were high, while those for $\Delta\Omega = 1$ transitions were very low. An observed signal of the $F_1 \leftarrow F_1$, $J = 5/2^+ \leftarrow 3/2^-$ transition showing resolved hyperfine structure is given in Figure 2. The observed transitions are listed in Table 1. The transition frequencies determined from laser magnetic resonance spectroscopy (Comben et al. 1986) agree with our values within a difference of a few MHz.

The observed frequencies were analyzed by employing an effective Hamiltonian written on a Hund's case (a) basis set with N^2-formalism (Brown et al. 1979). When an observed line was made up of unresolved hyperfine components, its frequency was assumed to be the average of each component with a weight of calculated relative intensity. Together with the observed frequencies, the Λ-doubling frequencies of ^{18}OH

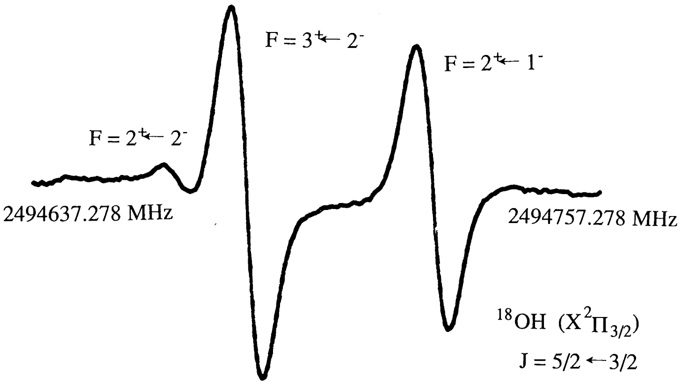

FIG. 2.—Observed spectrum of the $F_1 \leftarrow F_1$, $J = 5/2^+ \leftarrow 3/2^-$ transition of the ^{18}OH radical in its ground state, recorded with a 300 msec time constant of a lock-in amplifier. The signal is displayed as first derivative due to frequency modulation of the FIR radiation. The hyperfine structure due to the H nucleus is resolved clearly.

TABLE 1

OBSERVED AND CALCULATED FREQUENCIES OF ROTATIONAL TRANSITIONS OF THE ^{18}OH RADICAL IN THE $v = 0$ LEVEL OF THE $X^2\Pi$ STATE

TRANSITION[a]			FREQUENCY (MHz)		
$F_i'-F_i''$	$J'-J''$	$F'-F''$	Observed[b]	Calculated[c]	$O-C$
F_1-F_1......	5/2–3/2	2^+-2^-	2494668.08 (13)	2494668.19	−0.11
		3^+-2^-	2494682.550 (50)	2494682.334	0.216
		2^+-1^-	2494721.612 (58)	2494721.476	0.136
		2^--2^+	2498963.24 (11)	2498963.33	−0.09
		3^--2^+	2498981.689 (44)	2498981.799	−0.110
		2^--1^+	2499018.382 (52)	2499018.565	−0.183
	7/2–5/2	4^--3^+	3521851.821 (45)	3521851.880	−0.059
		3^--2^+	3521873.417 (50)	3521873.351	0.066
		4^+-3^-	3529150.192 (62)	3529150.173	0.019
		3^+-2^-	3529169.237 (62)	3529169.214	0.023
	9/2–7/2	5^+-4^-	4563698.96 (21)	4563699.04	−0.08
		4^+-3^-	4563712.88 (21)	4563712.90	−0.02
		5^--4^+	4573946.42 (31)	4573941.31	5.11
		4^--3^+		4573952.94	−6.52
F_2-F_2......	3/2–1/2	1^--1^+	1821925.92 (13)	1821926.11	−0.19
		2^--1^+	1821938.69 (13)	1821937.83	0.86
		1^--0^+		1821941.01	−2.32
		1^+-1^-	1824949.27 (19)	1824949.32	−0.05
		2^+-1^-	1825019.407 (41)	1825019.439	−0.032
		1^+-0^-	1825039.683 (59)	1825039.736	−0.053
	5/2–3/2	2^+-1^-	3015367.584 (59)	3015363.746	3.838
		3^+-2^-		3015369.688	−2.104
		2^--2^+	3015720.19 (34)	3015720.05	0.14
		2^--1^+	3015790.945 (45)	3015790.176	0.769
		3^--2^+		3015791.470	−0.525
	7/2–5/2	3^+-3^-	4181058.90 (21)	4181058.37	0.53
		3^+-2^-	4181131.228 (97)	4181129.786	1.442
		4^+-3^-		4181132.258	−1.030
		3^--2^+	4183704.151 (45)	4183700.892	3.259
		4^--3^+		4183706.673	−2.522
F_2-F_1......	1/2–3/2	1^+-2^-	3787796.90 (39)	3787796.66	0.24
		0^+-1^-	3787835.50 (47)	3787835.05	0.45
	3/2–5/2	2^--3^+	3115053.133 (42)	3115052.152	0.981
		1^--2^+		3115054.574	−1.441
		2^+-3^-	3116929.83 (42)	3116929.86	−0.03
	5/2–7/2	3^--4^+	2603571.07 (29)	2603571.16	−0.09

[a] The superscripts on the F quantum number denote the parity of states involved in accordance with the definition by Brown et al. 1978.

[b] The numbers in parentheses are estimated uncertainties of one standard deviation in units of the last quoted digits.

[c] Calculated frequencies were obtained using the molecular parameters listed in Table 3.

TABLE 2

Microwave Frequencies of Λ-Type Doublet Transitions of the ^{18}OH Radical in the $v = 0$ Level of the $X^2\Pi$ State

Transition[a]			Frequency (MHz)			
F_i	J	F'–F''	Observed[b]	Calculated[c]	$O-C$	Reference
F_1......	3/2	1^+-2^-	1584.274 (2)	1584.273	0.001	d
		1^+-1^-	1637.564 (2)	1637.562	0.002	d
		2^+-2^-	1639.503 (2)	1639.505	−0.002	d
		2^+-1^-	1692.795 (2)	1692.793	0.002	d
	5/2	2^--3^+	5920.505 (5)	5920.504	0.001	d
		2^--2^+	5934.644 (6)	5934.650	−0.006	d
		3^--3^+	5938.967 (5)	5938.970	−0.003	d
		3^--2^+	5953.116 (4)	5953.116	0.000	d
	15/2	7^+-7^-	69896.714 (50)	69896.690	0.024	e
		8^+-8^-	69910.546 (50)	69910.567	−0.021	e
F_2......	1/2	0^--1^+	4644.650 (6)	4644.651	−0.001	d
		1^--1^+	4735.073 (6)	4735.071	0.002	d
		1^--0^+	4749.971 (5)	4749.971	0.000	d

[a] The superscripts on the F quantum number denote the parity of states involved in accordance with the definition by Brown et al. 1978.

[b] The numbers in parentheses are estimated uncertainties of one standard deviation in units of the last quoted digits.

[c] Calculated frequencies were obtained using the molecular parameters listed in Table 3.

[d] Measured by Gottlieb et al. 1974.

[e] Measured by Kolbe et al. 1981.

TABLE 3

Molecular Parameters of the ^{18}OH Radical in the $v = 0$ Level of the $X^2\Pi$ State[a]

Parameter	This work	Comben et al.
B	552032.952 (14)[b]	552032.89 (18)
D	56.47753 (61)	56.457 (14)
H	[0.004153][c]	[0.004153]
$\tilde{A}$[d]	−4168647.59 (24)	−4168644.9 (2.1)
$\tilde{\gamma}$[d]	−3550.24 (15)	−3552.48 (72)
$\tilde{\gamma}_D$[d]	0.6828 (66)	[0.7219]
p	7007.1913 (78)	7007.1767 (58)
p_D	−1.5354 (33)	[−1.5305559]
$10^4 p_H$	[1.615]	[1.615]
q	−1144.8313 (14)	−1144.8298 (15)
q_D	0.43318 (14)	0.433337
$10^5 q_H$	[−8.022]	[−8.022]
a	86.1194 (66)	[86.1116]
b_F	−73.254 (22)	[−73.2537]
c	130.671 (46)	[130.641]
d	56.691 (18)	[56.6838]
d_D	[−0.02276]	[−0.02276]
C_I	[−0.09971]	[−0.09971]
C'_I	[0.00643]	[0.00643]

[a] Unit is MHz.

[b] The numbers in parentheses denote one standard deviation of the least-square fit in units of the last quoted digits.

[c] Parameters enclosed by square brackets were constrained at values used by Comben et al. 1986.

[d] Effective parameters. The fit was performed with parameter A_D constrained to zero.

observed by Gottlieb et al. (1974) and Kolbe et al. (1984) were included in the data set, which are shown in Table 2. The data were subject to least-squares analysis with weights given according to accuracies in the frequency measurements. The resulting molecular parameters are given in Table 3. The rotational, spin-orbit, spin-rotation, Λ-type doubling parameters have refined those given by Comben et al. (1986), which agree with ours within three standard deviations. Higher order terms of spin-rotation and Λ-type doubling parameters of ^{18}OH were determined in the first time. Hyperfine structure parameters also determined for the first time for ^{18}OH agree with those of ^{16}OH (Brown et al. 1986) within uncertainties of one standard deviations, showing no isotope effect.

An FIR transition $F_1 \leftarrow F_1$, $J = 5/2^+ \leftarrow 3/2^-$ was observed toward Orion-KL (Melnick et al. 1990). The identification of this line was based on the wavelength (120.1719 μm) for the hypothetical unsplit wavelength unperturbed by the hyperfine interaction (Comben et al. 1986). The corresponding value in the present work agrees with this wavelength value up to 7 digits, which assures the validity of the use of wavelength value mentioned above for the astronomical purpose.

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