PREDICTIONS OF SEVERAL OH Λ DOUBLING TRANSITIONS SUITABLE FOR RADIO ASTRONOMY*

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Intensity anomalies have been observed in the 18-cm OH interstellar radio lines.[1] Optical pumping with a cascade decay mechanism has been proposed as one possible explanation of these results.[2-4] Another mechanism proposes that the OH radicals are formed in excited states.[5] With either of these mechanisms, there are several low-lying rotational states which may have a population which is large enough to be observed. Zuckerman, Palmer, and Penfield[6] searched for one of these transitions, the $^2\Pi_{1/2}$, $J=\frac{1}{2}$ lambda doublet, on the basis of some order of magnitude estimates of the relative lifetimes. They calculated the transition frequencies from the lambda-doubling results of Dousmanis, Sanders, and Townes[7] (DST) and the magnetic hyperfine coupling constants which were obtained by Radford.[8] A very similar but somewhat less accurate estimate of these transition frequencies was reported by Barrett.[9] Zuckerman, Palmer, and Penfield,[6] using the 140-ft Green Bank radio telescope, searched for but did not detect these lines. They concluded that the line intensities had an upper limit of between 1 and 2 % of the intensities of the 18-cm OH lines.

In this paper, new experimental results are reported which more precisely define the microwave spectrum of the OH free radical. More accurate line frequencies have been determined incidental to Stark-effect analysis of several transitions.[10] Molecular parameters have been determined which are considerably more reliable than those which have been available in the literature. Because the low-frequency limit of our spectrometer is 8.2 GHz, we have not been able to measure directly any of the lambda-doubling transitions below this frequency limit. However, enough higher frequency transitions have been observed that, if the $J=\frac{3}{2}$, $^2\Pi_{3/2}$ transition as observed by Radford[11] is included, a fairly complete analysis of the microwave spectrum can be obtained.

The transition frequencies were measured with a Stark modulation spectrometer employing a precision, flat, parallel-plate absorption cell and a modulation frequency of 100 kHz. The OH radicals are generated by the fast chemical reaction of hydrogen atoms with NO_2.

The absorption cell is constructed such that the reactant gases enter through separate nozzles located on the sides of the parallel plates forming the wave guide. Three nozzles are used to inject hydrogen atoms, which are generated by an H_2 discharge in quartz tubes passing through three separate 2450-MHz tuned cavities, each excited by its own magnetron driving oscillator. The second reactant gas, NO_2, is injected exactly opposite these nozzles. The parallel plates forming the wave-guide absorption cell consist of two precision-ground, type-304, stainless-steel slabs 48 in.$\times$5 in.$\times\frac{3}{4}$ in., spaced 0.5 cm apart. These plates are coated with a Teflon-spray-type coating. The waste-product gases are discharged through the open slit between the plates. The entire wave-guide system is enclosed in a 14-in.-i.d. stainless-steel vacuum chamber, and exhausted by a 250-liter/sec pump. Typical absorption-cell dynamic pressures were adjusted to about 20-30 mTorr. Observed line half-widths were 100 kHz. Both scope and recorder detection were used. Very slow recorder scans employed phase-locked klystron signal generators with small digital sweep increments. Signal-to-noise ratios of 3000/1 were obtained with scan speeds of 1 min and time constants of 0.1 sec. The measured spectrometer sensitivity is $\approx 10^{-9}$ cm^{-1}. Strong lines could be measured to an accuracy of ± 0.01 MHz, while weak lines were about a factor of 2 worse. The reference frequency standard was directly compared with the National Bureau of Standards standard, and was estimated to be accurate to three parts in 10^{10}.

Very low residual magnetic fields (less than 0.05 G) were maintained in the region of the absorption-cell plates. Thus, no Zeeman splittings were observed from this cause. Such splittings have been noted by Powell and Lide.[12] DST reported line half-widths of 800 kHz and operating pressures of 100 mTorr. They used Zeeman modulation, so that residual magnetic fields

Table I. Predicted frequencies for OH transitions potentially useful for radio astronomy. Frequencies are in MHz. The Einstein A coefficients, $A(F,FP) = A_{FF'}$, are given in sec^{-1}. Values given for the $^2\Pi_{3/2}$, $J=\frac{3}{2}$ state are for comparison to transitions observed by radio astronomy.†

J	FF	FI	PI(1/2)	A(F,FP)*	PI(3/2)	A(F,FP)*
0.5	0.0	1.0	4660.457	1.03E-09		
0.5	1.0	1.0	4750.390	7.64E-10		
0.5	1.0	0.0	4764.990	3.86E-10		
1.5	1.0	2.0	7749.235	1.87E-10	1611.844	1.29E-11
1.5	1.0	1.0	7761.329	9.37E-10	1665.403	7.11E-11
1.5	2.0	2.0	7819.650	1.04E-09	1667.349	7.71E-11
1.5	2.0	1.0	7831.744	1.16E-10	1720.908	9.42E-12
2.5	2.0	3.0	8116.852	4.25E-11	6016.520	1.09E-10
2.5	2.0	2.0	8135.160	6.00E-10	6030.731	1.53E-09
2.5	3.0	3.0	8188.947	6.24E-10	6035.059	1.57E-09
2.5	3.0	2.0	8207.255	3.14E-11	6049.270	7.90E-11
3.5	3.0	4.0	5447.828	4.41E-12		
3.5	3.0	3.0	5472.064	1.21E-10		
3.5	4.0	4.0	5522.693	1.25E-10		
3.5	4.0	3.0	5546.929	3.62E-12		
5.5	6.0	5.0	8613.650	4.09E-12		
5.5	5.0	5.0	8581.184	2.63E-10		
5.5	6.0	6.0	8535.274	2.59E-10		
5.5	5.0	6.0	8502.808	3.33E-12		

†This table is an abbreviated version of our results. A complete lists of all predicted transitions below 40 GHz, which can be obtained from us upon request, will be published later.

*The E found in columns 5 and 7 designates 10 with an exponent of the number immediately following the E, e.g., $E-09=10^{-9}$

could produce errors in the apparent line frequency. A combination of these factors could easily account for an improvement of a factor of 100 in frequency measurements.

The calculated transition frequences were obtained by exact diagonalization of the molecular Hamiltonian which was given by DST.[7] The molecular constants which we used are those defined by DST. However, two centrifugal distortion constants are necessary to give a satisfactory fit of the experimental data. These are defined by the following two equations:

$$\langle\Sigma|BL_y|\pi\rangle = \langle\Sigma|B_0L_y|\pi\rangle[1-J(J+1)D/B_\Sigma],$$

$$\langle\Sigma|AL_y|\pi\rangle = \langle\Sigma|A_0L_y|\pi\rangle[1-J(J+1)\delta/B_\Sigma].$$

These off-diagonal matrix elements connect the Σ and Π electronic states of OH. B_Σ is the rotational constant of the Σ state. $\vec{L}$ represents the orbital electronic motion, where z is along the internuclear axis. D represents the effect of centrifugal streching on the internuclear distance, and δ represents the effect of rotation on the electronic distribution. Of the eight molecular constants required for the lambda transitions three were obtained from the optical OH studies of Dieke and Crosswhite.[13] The lambda-doubling transitons were insensitive to these three parameters. The remainder of these constants were evaluated from the microwave spectra by the application of least-squares methods. Four additional constants a, b, c, and d are required to describe the nuclear hyperfine splittings. Out of these only one, d, is sensitive to the transitions which we have fitted. Suitable values of these constants have been determined by Radford.[8]

The $\Delta F+\pm1$ hyperfine transitions also depend upon the other three constants. Since only the $\Delta F=0$ transitions were fitted with the d hyperfine constant, there are slight deviations between the experimental and calculated values of the $\Delta F=\pm1$ frequencies.

A computer program has been written to perform the exact diagonalization and frequency cal-

Table II. Molecular constants for OH assuming $c=2.997\,929\times10^{10}$ cm/sec. $D_{\text{cent. dist.}}$ is the normal centrifugal distortion constant. δ is a constant which is related to the variation of the electronic wave function with molecular rotation. λ, as derived from this work, agrees fairly well with both the optical (Ref. 13) and EPR (Ref. 8) results.

Σ state energy $=E_\Sigma-E_\Pi$	$9.797\,981\,0\times10^8$ MHz[a]
B_Σ, rotational constant for Σ state	$5.084\,780\times10^5$ MHz[a]
B_Π, rotational constant for Π state	$5.550\,66\times10^5$ MHz[a]
$A_{\text{spin-orbit}}$, spin-orbit coupling constant	$(-4.163\,508\pm0.000\,36)\times10^6$ MHz
$\langle\Sigma|BL_y|\Pi\rangle$	$(3.773\,822\pm0.000\,16)\times10^5$ MHz
$\langle\Sigma|(2B+A)L_y|\Pi\rangle$	$(-1.531\,211\pm0.000\,06)\times10^6$ MHz
$D_{\text{cent. dist.}}$	$(1.075\,99\pm0.0027)\times10^2$ MHz
δ	$(-4.4539\pm0.012)\times10^1$ MHz
$\lambda=A_{\text{SO}}/B_p$	-7.5009 ± 0.0001

[a]These constants are taken from the results of Dieke and Crosswhite (Ref. 13).

Table III. Comparison of observed and calculated frequencies (MHz) in OH. Unmarked frequencies are values measured in this work.

Electronic State	J	F → F′	ν_{calc}	ν_{obs}	$\nu_c - \nu_o$	Experimental Error Limits	Calculated Laboratory Intensity, cm^{-1}
$^2\Pi_{3/2}$	3/2	2 → 1	1611.844	1612.231*	-.387	.002*	2.01E-07
		1 → 1	1665.403	1665.401*	+.002	.002*	1.11E-06
		2 → 2	1667.349	1667.358*	-.009	.002*	1.20E-06
		1 → 2	1720.908	1720.533*	+.375	.002*	1.47E-07
$^2\Pi_{1/2}$	3/2	1 → 1	7761.329	7760.36†	+.97	1.0†	5.97E-06
		2 → 2	7819.650	7819.92†	-.27	1.0†	6.59E-06
$^2\Pi_{1/2}$	5/2	2 → 2	8135.160	8135.51†	-.35	1.0†	2.35E-06
		3 → 3	8188.947	8188.94†	+.007	1.0†	2.45E-06
$^2\Pi_{3/2}$	7/2	3 → 3	13434.605	13434.62	-.015	.01	5.45E-05
		4 → 4	13441.374	13441.36	+.014	.01	5.51E-05
$^2\Pi_{3/2}$	9/2	4 → 5	23805.451	23805.13	+.32	.01	1.66E-06
		4 → 4	23817.616	23817.64	-.024	.01	8.92E-05
		5 → 5	23826.634	23826.62	+.014	.01	8.96E-05
		5 → 4	23838.799	23838.46	+.34	.01	2.03E-06
$^2\Pi_{3/2}$	11/2	5 → 5	36983.501	36983.47	+.031	.03	9.01E-05
		6 → 6	36994.485	36994.43	+.055	.05	9.94E-05

*Frequencies observed by Radford (Ref. 11).

†Frequencies observed by DST, but we estimate their error limit to be much larger than they quote.

culations in double precision. This program has been modified to work with a least-squares program for evaluating the molecular parameters. The program includes computation of Einstein A coefficients and intensities. The accuracy of the present analysis gives considerable confidence in our predicting other low-lying lambda-doubling transition frequencies. The transitions which result from this analusis are given in Table I, along with the Einstein A coefficients for the hyperfine components.

These frequencies differ by a significant amount from other values which have been reported. The differences result from (a) more accurate frequency measurements (we find that DST's error limits should be ±1.0 MHz rather than ±0.05 MHz which they quote), (b) from least-squares fitting the new microwave constants which have been obtained using these frequencies, and (c) from the use of two centrifugal distortion constants. The nuclear hyperfine coupling constants are those given by Radford.[8] The new constants are listed in Table II. The predicted and observed line frequencies for all observed OH lambda-doubling transitions in the microwave spectrum up to 40 GHz are given in Table III.

Values of the Einstein spontaneous emission coefficients A were calculated for a dipole moment of 1.66 ± 0.1 D. The A coefficients for the $^2\Pi_{3/2}$, $J=\frac{3}{2}$ transitions agree with the value reported by Turner[14] and by Carrington and Miller.[15,16]

As can be seen from Table I, the $J=\frac{1}{2}$, $^2\Pi_{1/2}$ $\Delta F=0$ and $\Delta F=\pm 1$ hyperfine transition frequencies are about 33 and 42 MHz, respectively, from where Zuckerman, Palmer, and Penfield attempted to search. Thus, it would seem that their conclusions about the upper limits of the intensities of these transitions must be invalid. Another search would be worthwhile for these and other low-frequency OH transitions in the interstellar medium.

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SUM RULE FOR THE NUCLEON MASS

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A sum rule for the nucleon mass is derived in a theory which expresses the energy-momentum tensor in terms of currents. A rough evaluation indicates that it is not inconsistent with experiment.

It has, from time to time, been suggested that the energy momentum tensor $\theta_{\mu\nu}$ of hadrons should be introduced into the current-algebra scheme.[1] In the first place, $\theta_{\mu\nu}$ stands on the same footing as the weak and electromagnetic currents in the sense that its matrix elements are (in principle!) directly measurable. More importantly, it obviously contains real dynamics, as current commutators by themselves do not, and it might allow us to construct a complete theory directly in terms of measurable quantities. The most economical way of generating such a theory appears to be to construct $\theta_{\mu\nu}$ directly out of currents. Masses and form factors then become intertwined in a complicated way, and acceptable solutions are determined by requiring that $\theta_{\mu\nu}$ have a consistent physical interpretation. The most elegant candidate for such a theory is due to Sugawara,[2] who constructs a simple tensor having all the algebraic properties of the energy-momentum tensor of a relativistic theory out of SU(3) $\otimes$ SU(3) currents obeying the algebra of fields equal-time commutation relations (ETCR). This expression for $\theta_{\mu\nu}$ is nearly unique, sparing one the usual problem of choosing between different interactions. Rather than attack the difficult problem of trying to find a solution, we shall show that the basic equations imply a number of sum rules on measurable quantities. If they are satisfied, one would feel encouraged to exploit the full content of the theory.

Let us first set down the basic equations of the theory. We assume the existence of the SU(3) $\otimes$ SU(3) currents, which satisfy the following ETCR's (as in the algebra of fields):

$$[V_0^a(\vec{x}), V_\mu^b(\vec{y})] = [A_0^a(\vec{x}), A_\mu^b(\vec{y})] = if_{abc}V_\mu^c(\vec{x})\delta^3(\vec{x}-\vec{y}) + iC\delta_{ab}\delta_{\mu k}\partial_k\delta^3(\vec{x}-\vec{y}),$$

$$[V_0^a(\vec{x}), A_\mu^b(\vec{y})] = [A_0^a(\vec{x}), V_\mu^b(\vec{y})] = if_{abc}A_\mu^c(\vec{x})\delta^3(\vec{x}-\vec{y}),$$

$$[V_i^a(\vec{x}), V_k^b(\vec{y})] = [A_i^a(\vec{x}), A_k^b(\vec{y})] = [V_i^a(\vec{x}), A_k^b(\vec{y})] = 0, \tag{1}$$

where $\mu = 1\cdots 4$, $i,k = 1\cdots 3$, and $a,b,c, = 1\cdots 8$.

We then construct $\theta_{\mu\nu}$ out of the currents as follows[3]:

$$\theta_{\mu\nu}(x) = (2C)^{-1}\{[V_\mu^a(x), V_\nu^a(x)]_+ - g_{\mu\nu}[V_\mu^a(x)V_a^\mu(x)] + (V \leftrightarrow A)\}. \tag{2}$$