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LABORATORY MEASUREMENTS FOR THE ASTROPHYSICAL IDENTIFICATION OF MgH[1]

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ABSTRACT

A tunable far-infrared spectrometer has been used to observe the pure rotational spectrum of MgH in a DC discharge of H_2 with magnesium. The frequencies of the hyperfine components of the $N = 1 \leftarrow 0$ transition are predicted to an estimated accuracy of ± 350 kHz, which should be sufficient for the astrophysical identification of this species.

Subject headings: infrared: spectra — interstellar: molecules — laboratory spectra

In a previous report (Leopold *et al.* 1986), we presented preliminary measurements of the pure rotational spectrum of MgH. Among our goals in that work was the reliable prediction of the frequencies for the $N = 1 \leftarrow 0$ transitions which could then serve as a basis for the astrophysical detection of this molecule (Bernath, Black, and Brault 1985). Our previous measurements, however, involved values of N ranging between 2 and 7, and only two weak lines sensitive to the magnetic hyperfine parameters were observed. In order to realize the best possible predictions for the hyperfine components of the astrophysically important $N = 1 \leftarrow 0$ transition, we have extended our measurements to lower N and, in doing so, have resolved several stronger lines which give improved values of the Fermi contact and spin dipolar hyperfine parameters. These parameters, of course, are particularly important for the present purpose since the hyperfine splittings increase with decreasing N. We have also made a direct measurement of one of these hyperfine components and, although it agrees with the predictions from our fit to within the experimental uncertainty, a rather poor signal-to-noise ratio renders the estimated accuracy of the predictions better than that of the measurement.

The experimental apparatus, in which tunable far-infrared radiation is generated from the nonlinear mixing of the radiation from two CO_2 lasers, has been described elsewhere (Evenson, Jennings, and Petersen 1984; Evenson, Jennings, and Vanek 1987). As in our previous work (Leopold *et al.* 1986), MgH was generated by running a 0.8 A DC discharge through 20 Pa of H_2 in a 1 m long, thermally insulated quartz tube in which 3–5 mm pieces of magnesium sheet were placed every 15 cm (1 Pa = 7.5 mTorr).

Table 1 lists the observed transitions and their assignments. Included in the table are our previous measurements (Leopold *et al.* 1986). The experimental uncertainties arise primarily from our ability to locate the line center and hence are directly related to the signal-to-noise ratio. The variability in the table reflects not only differences in intrinsic transition strength, but variations in the signal-to-noise ratio resulting from daily fluctuations in discharge conditions and far-IR power.

The data consist of two types of transitions: those for which $\Delta F = \Delta J = 1$, and those for which $\Delta F = \Delta J = 0$. The $\Delta F = \Delta J = 1$ transitions are the strongest and usually appear as unresolved hyperfine doublets. Only at low N do these doublets become resolvable outside the Doppler width; the highest transition for which these features can be discerned is from $N = 3 \leftarrow 2$. When resolved, however, they contribute (together with the weaker $\Delta F = \Delta J = 0$ lines measured previously) to the accurate determination of the hyperfine parameters. Measurements for the $N = 2 \leftarrow 1$ and $N = 1 \leftarrow 0$ transitions were performed with computer signal averaging. For the $N = 1 \leftarrow 0$ transition, 10 scans were averaged, but still yielded a signal-to-noise ratio too small to give less than a 2 MHz uncertainty in the frequency. Averaging for longer periods of time was not possible due to instabilities in the discharge and in the far IR power.

The data were analyzed using the Hamiltonian for a $^2\Sigma$ molecule with nuclear spin, $\boldsymbol{I}$:

$$H = B_0 N^2 - D_0 N^4 + H_0 N^6 + [\gamma_0 - \gamma_D N(N+1)] \times \boldsymbol{N} \cdot \boldsymbol{S} + b_F \boldsymbol{I} \cdot \boldsymbol{S} - t[\boldsymbol{I} \cdot \boldsymbol{S} - 3I_Z S_Z] .$$

This differs slightly from the Hamiltonian used previously (Leopold *et al.* 1986) in that the nuclear spin rotation term is omitted and the N^6 centrifugal distortion term is included. The spin rotation was omitted since it contributes negligibly to the observed frequencies, and the centrifugal distortion term is found necessary in order to simultaneously fit the data at high and low N. Note, also, that the sign of the $t[\boldsymbol{I} \cdot \boldsymbol{S} - 3I_Z S_Z]$ term has been corrected, though the value of t reported previously is consistent with the sign used above.

Fitting of the Hamiltonian to the measured frequencies was performed using a nonlinear least-squares routine in which the data were weighted by the inverse square of the experimental uncertainty. Residuals from the fitting are also given in Table 1. For the unresolved doublets, the calculated frequencies were taken as weighted averages of the individual lines using theoretical intensities as weighting factors. The table shows that the calculated frequencies all fall within the experimental uncer-

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TABLE 1

OBSERVED TRANSITIONS OF MgH

N'	J'	F'	←	N''	J''	F''	ν_{obs}[a]	$\nu_{obs} - \nu_{calc}$[a]
1	1.5	2	←	0	0.5	1	344,305.3(20)	0.2
2	1.5	2	←	1	0.5	1	687,157.17(17)	−0.06
2	1.5	1	←	1	0.5	0	687,171.00(17)	0.01
2	2.5	3	←	1	1.5	2	687,959.54(19)	0.12
2	2.5	2	←	1	1.5	1	687,972.66(17)	−0.07
3	2.5	3	←	2	2.5	3	1,028,202.5(10)	0.2
3	2.5	2	←	2	2.5	2	1,028,514.2(10)	−0.4
3	3.5	3	←	2	2.5	2	1,031,104.29(21)[b]	−1.9
3	3.5	4	←	2	2.5	3		
4	3.5	4	←	3	3.5	4	1,369,797.0(10)	−0.2
4	3.5	3	←	3	3.5	3	1,370,107.5(10)	0.5
4	3.5	3	←	3	2.5	2	1,372,700.063(98)	0.016
4	3.5	4	←	3	2.5	3		
4	4.5	4	←	3	3.5	3	1,373,485.814(55)	−0.056
4	4.5	5	←	3	3.5	4		
6	5.5	5	←	5	4.5	4	2,054,170.477(71)	−0.040
6	5.5	6	←	5	4.5	5		
6	6.5	6	←	5	5.5	5	2,054,944.054(82)	0.052
6	6.5	7	←	5	5.5	6		

[a] All values in MHz.

[b] Partially resolved, given zero weight in fit.

tainty, with the exception of the partially resolved $N = 3 \leftarrow 2$ transition. In this case, the determination of line center is particularly uncertain, and this transition was omitted from the fit.

Table 2 gives the resulting spectroscopic constants and compares them with those from our previous study. The new values are considerably more accurate and, with the exception of B_0 and D_0, agree with those of Leopold *et al.* within the quoted uncertainties. The changes in B_0 and D_0 by somewhat more than the reported uncertainties are due to the inclusion of the H_0 term in the Hamiltonian. It is noteworthy that Lemoine *et al.* (1988) have recorded the infrared spectrum of MgH and have reported constants derived from a simultaneous fit of their data with the frequencies given here. Their results are also displayed in Table 2 for comparison. As previously noted, the agreement is satisfactory except in the case of H_0 for which the infrared value (which represents more data at high N) is probably more reliable (Lemoine *et al.* 1988).

Calculated values of the hyperfine components of the $N = 1 \leftarrow 0$ transition are given in Table 3. Bernath *et al.* have calculated the Einstein coefficients for these transitions, which are repeated here for convenience. We estimate from the standard deviation in our fit that these frequencies should be accurate to $\simeq 350$ kHz which arises predominantly from uncertainties in the hyperfine parameters. The transition at 344 305.5 MHz may be somewhat more reliable (±100 kHz) since its dependence on the hyperfine parameters is particularly small. All, however, should be accurate enough for astrophysical identification of this species.

TABLE 2

SPECTROSCOPIC CONSTANTS OF MgH[a]

Constant	This Work[b]	Previous Work (Leopold *et al.*)[c]	Previous Work (Lemoine *et al.*)[d]
B_0	171,976.150(18)	171,975.25(13)	171,976.210(42)
D_0	10.62123(83)	10.5857(10)	10.6255(20)
H_0	0.000420(11)	...	0.0004804(26)
γ_0	791.107(54)	790.50(25)	791.11(12)
γ_D	0.1747(8)	0.159(10)	0.1745(16)
b_F	307.90(51)	307.2(22)	307.6(12)
t	1.05(19)	0.9[e]	0.81(45)

[a] All values in MHz.

[b] Uncertainties are one standard deviation in the fit.

[c] Values from Leopold *et al.* 1986.

[d] Values from Lemoine *et al.* 1988.

[e] Matrix ESR value of Knight and Weltner 1971.

TABLE 3

CALCULATED FREQUENCIES FOR THE HYPERFINE COMPONENTS OF THE $N = 1 \leftarrow 0$ TRANSITION OF MgH

N'	J'	F'	←	N''	J''	F''	Frequency[a]	$A \times 10^4$ (s^{-1})[b]
1	0.5	1	←	0	0.5	1	342,997.60	1.72
1	0.5	0	←	0	0.5	1	343,118.02	2.58
1	0.5	1	←	0	0.5	0	343,305.50	0.86
1	1.5	1	←	0	0.5	1	344,119.28	0.87
1	1.5	2	←	0	0.5	1	344,305.09	2.61
1	1.5	1	←	0	0.5	0	344,427.18	1.74

[a] All values in MHz.

[b] Taken from Bernath, Black, and Brault 1985.

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