

PRESSURE-INDUCED DIPOLE LINES OF MOLECULAR HYDROGEN IN THE SPECTRA OF URANUS AND NEPTUNE*

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ABSTRACT

A moderately broad, weak absorption line centered at λ 6420 has been found on low-dispersion KPNO spectrograms of Uranus and Neptune. The probable identification for this feature is the pressure-induced dipole $S(0)$ transition of the (4, 0) rotation-vibration band of H_2 . The apparent centroid of the induced dipole lines in the Uranus spectrum seems to be considerably shifted to the violet of the H_2 quadrupole lines. The red spectrum of Uranus is illustrated, and one other unidentified line near λ 6490 is pointed out.

I. INTRODUCTION

Vibrational, rotational, and electronic dipole transitions which are strictly forbidden in an isolated homonuclear molecule such as H_2 do occur under the influence of pressure. Pressure-induced transitions arise through the temporary creation of a dipole moment due to the distortion of the electronic charge distributions of the molecules during close collisions.

Individual rotational lines in the induced bands are highly broadened because the durations of the intermolecular collisions inducing the dipole moments are very short; $\tau \approx 10^{-13}$ sec at room temperature. The lifetime of an interaction is inversely proportional to the molecular velocity, so the width of the pressure-induced lines should be directly proportional to the square root of the absolute temperature. Early laboratory experiments by Crawford, Welsh, MacDonald, and Locke (1950) and Chisholm and Welsh (1954) confirmed the predicted temperature dependence.

For planetary atmospheres our interest centers on the rotational transitions of H_2 in the far infrared for energy balance problems, and the more easily observable pressure-induced rotation-vibration bands. The fundamental (1, 0) rotation-vibration band of H_2 is at 2.4μ (Welsh, Crawford, and Locke 1949), but the weaker overtones extend down to the photographic infrared and the near red.

Herzberg (1952) was the first to show that a weak unidentified absorption feature found by Kuiper (1949) on low-dispersion spectra of Uranus and Neptune was undoubtedly the $S(0)$ line of the (3, 0) second overtone pressure-induced H_2 band. This diffuse absorption observed by Kuiper at λ 8270 was, until 1960, the only spectroscopic evidence of molecular hydrogen on the planets.

In the past three years the ultra-sharp *quadrupole* lines of H_2 in the (3, 0) and (4, 0) overtone bands have been found on high-dispersion spectra of the major planets. On Jupiter the sharp (3, 0) band lines were observed by Kiess, Corliss, and Kiess (1960) and the (4, 0) $S(1)$ line by Spinrad and Trafton (1963). The (4, 0), $S(1)$, and $S(0)$ lines were identified by Münch and Spinrad (1963) in the spectrum of Saturn and the $S(0)$ line of the (4, 0) quadrupole band has been recently found on Uranus. From the sharp quadrupole lines rough abundance estimates for molecular hydrogen in the visible atmos-

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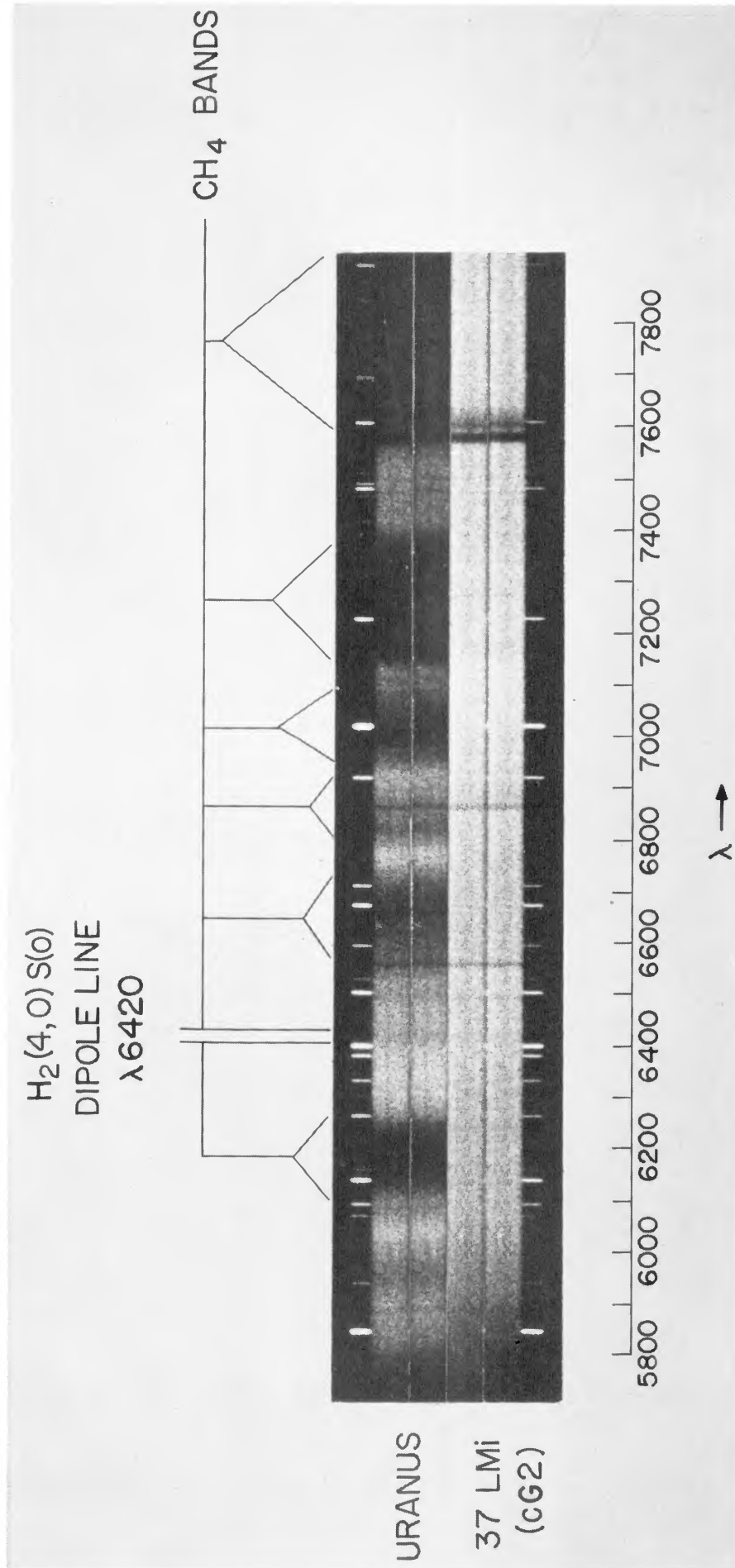


FIG. 1.—The spectrum of Uranus and 37 LMi (G-giant) over the region $\lambda\lambda$ 5800–7800. The absorptions visible in the G star are the D-lines, a weak blend at λ 6490, H α , and the telluric bands of O₂ (B at λ 6870 and A at λ 7600). The strong methane bands of Uranus are indicated; the weak, diffuse S(0) pressure-induced dipole line at λ 6420 is also indicated. Note the fuzzy absorption in Uranus at λ 6490; this feature has not yet been identified. The original dispersion was 250 Å/mm.

pheres of the major planets may be made; one needs to determine the H_2 rotational temperature and then the equivalent width of the quadrupole line. Laboratory measures of the H_2 quadrupole lines from Herzberg's spectra or the more recent work of Rank, Fink, Slomba, and Wiggins (1963) provide f -value calibration. However, the widths of the sharp quadrupole lines are unknown, and they may saturate quickly despite their very low transition probabilities. Thus curve-of-growth complications make uncertain the quoted values of the H_2 abundances. The broad pressure-induced lines probably are not troubled by saturation effects, but very limited laboratory data on their intensities are available. Theoretical calculations on the strengths of the H_2 dipole overtone bands have not yet been made.

II. THE OBSERVATIONS

Spectrograms of Uranus and Neptune were obtained with the Kitt Peak National Observatory (KPNO) 36-inch Cassegrain spectrograph in the spring of 1963. As used with a 400 1/mm Bausch and Lomb grating in the first-order red and infrared the dispersion was 250 Å/mm. The focal length of the collimator is 39.37 inches; the camera used was a Schmidt type with 3.5-inch aperture and 3.94-inch focal length. Several low-dispersion plates of Uranus, Neptune, the sky, and a G2 giant star were obtained on 103a-F, IIa-F and I-N emulsions. 37 LMi (c G2), Uranus and Neptune were trailed along the slit so that the resulting spectra are widened to 0.3 or 0.6 mm. The spectra of Uranus and 37 LMi are illustrated in Figure 1; the spectral interval covered is $\lambda\lambda$ 5800–7800.

III. DISCUSSION

The presence of a weak, diffuse absorption feature at about λ 6420 is evident on the high-contrast spectra of Uranus (see Fig. 1) and Neptune; its width of some 40 Å on Uranus is approximately the same as the line at λ 8270 found by Kuiper.

Most of the broad, strong absorptions in the Uranus spectrum are due to methane. The huge bands at $\lambda\lambda$ 6200, 6700, 7100, 7300, and 7700 strikingly alter the reflected solar continuum. Kuiper's (1950) illustrations of laboratory CH_4 bands show the methane bands observed on Uranus, but there is no obvious methane absorption over the region from $\lambda\lambda$ 6400–6500 with CH_4 path lengths up to 3.5 km at one atmosphere pressure.

We suggest the diffuse feature at about λ 6420 on Uranus and Neptune is the pressure-induced dipole rotation-vibration $S(0)$ line in the (4, 0) band. The corresponding quadrupole line wavelength measured on Saturn and Uranus is λ 6435.03, some 15 Å to the red of the dipole band center. There is little doubt that this shift is real. However, it is possible that the centroid of absorption at λ 6420 may really be the "core" of an even broader weak absorption whose profile is unknown.

Further to strengthen the hypothesis that the λ 6420 feature is a shifted induced dipole line we have tabulated the wavelengths for the H_2 induced-dipole and quadrupole lines using the data of Herzberg (1952), Spinrad and Trafton (1963), and this paper. Table 1 lists the relevant wavelengths for the two types of molecular hydrogen lines. In each case there is a significant wavelength shift between the measured center of each broad dipole line and the corresponding quadrupole line. The shifts, in the sense $\lambda_{\text{dipole}} - \lambda_{\text{quadrupole}}$, are all negative and quite large; $\Delta\lambda = -28$ Å to -15 Å; thus $\Delta\nu \approx +30$ cm^{-1} . The rough consistency of the shift supports the identification of the λ 6420 absorption as a pressure-induced H_2 dipole line in the (4, 0) band, probably the $S(0)$ transition. The $S(1)$ induced-dipole line which should be near λ 6360 has not been found on these spectrograms; it is at least twice as weak as $S(0)$, and this is to be expected since temperatures in the atmospheres of Uranus and Neptune may be as low as 50° K. For this low temperature the $S(1)$ line would only be about one-fifth as strong as the $S(0)$.

Herzberg (1952) noted that in his laboratory experiments with the (3, 0) H_2 induced band the double rotation-vibration transitions of (2, 0) + (1, 0) occur simultaneously

in the two interacting hydrogen molecules. The interactions produce new absorption lines at the sum of the two frequencies involved. Herzberg found several of the (2, 0) + (1, 0) lines of the double transition (photographic infrared) in his laboratory spectra. On the Uranus spectrograms then available none of the double transitions was strong enough to be visible against the methane-chopped continuum of the planet. We have searched for the next higher overtone double transitions; they are combinations of (3, 0) + (1, 0) falling in the red. $Q(0)$ double at about λ 6390 would be partially obscured by CH_4 , but certainly is not very strong on Uranus, $Q(1)$ double at λ 6300 is not visible, and $Q(0) + S(0)$ at about λ 6160 is covered by methane. The combination (2, 0) + (2, 0) line $Q(0)$ double is also near λ 6200 and would be obscured by the strong methane band there. No double transitions have yet been observed on Uranus, but the spectrograms have not all been ideal for the search. A reason for relatively low intensities of the double transitions in Uranus compared to the laboratory may be due to a difference in the major perturbing gas. Herzberg suggested mixtures of H_2 with He or N_2 might suppress the double transitions relative to the single transitions observed on Uranus and

TABLE 1
WAVELENGTHS FOR H_2 OVERTONE DIPOLE
AND QUADRUPOLE LINES

Band	Probable Transition	Dipole λ	Quadrupole λ	$\Delta\lambda(D-Q)$
(3, 0)	$\left\{ \begin{array}{l} Q(0) \\ Q(1) \end{array} \right\}$	8469*	8497*	-28 A
	$S(0)$	$\left\{ \begin{array}{l} 8258^* \\ (8267)^\dagger \end{array} \right\}$	8273*	-15 A
	$S(1)$	8151*
(4, 0)	$S(0)$	6420†	6435 0†	-15 A
	$S(1)$	6367.8†	.

* Observed in laboratory.

† Observed on Uranus, Saturn, or Jupiter.

Neptune, but detailed laboratory experiments with expected perturbing molecules have not been performed.

We also wish to note a weak absorption at λ 6490 on both Uranus and Neptune. This feature is much weaker in the solar spectrum and in the spectrum of 37 LMi. There is apparently no CH_4 absorption there at room temperature—but until the spectrum of cold methane is available the case should not be considered closed. No H_2 transitions fall near this wavelength; $Q(0)$ in the (4, 0) band should be near $\text{H}\alpha$ —some 70 A away and none of the double transitions are closer. This weak band is at present unidentified.

IV. DESIDERATA

Why are the H_2 overtone-induced dipole lines shifted to higher frequencies than the quadrupole lines? Or are the dipole lines observed on Uranus and in the laboratory more complex transitions than supposed?

Helium, as a perturbing gas suppresses the strength of the $S(0)$ and $S(1)$ lines relative to the Q lines in the fundamental, while H_2 and A do not (Crawford *et al.* 1950). We see the $S(0)$ line on Uranus and Neptune—the $Q(0)$ line has not been found; it must be weaker. Could this mean an underabundance of He?

Obviously more laboratory data at densities prevalent in planetary atmospheres and higher resolution spectra of Uranus and Neptune should enable us to probe the physical conditions in the envelopes of these distant planets.

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REFERENCES

- Chisholm, D. A., and Welsh, H. L. 1954, *Can. J. Physics*, **32**, 291.
Crawford, M. F., Welsh, H. L., MacDonald, J. C. F., and Locke, J. L. 1950, *Phys. Rev.*, **80**, 469.
Herzberg, G. 1952, *Ap. J.*, **115**, 337.
Kiess, C. C., Corliss, C. H., and Kiess, H. K. 1960, *Ap. J.*, **132**, 221.
Kuiper, G. P. 1949, *Ap. J.*, **109**, 540.
———. 1950, *Repts. on Progress in Phys.*, **13**, 247.
Münch, G., and Spinrad, H. 1963, *Mém. Soc. R. Sci. Liège*, Ser. 5, **7**, 541, 1963.
Rank, D. H., Fink, U., Slomba, A. F., and Wiggins, T. A. 1963, private communication.
Spinrad, H., and Trafton, L., *Icarus*, 1963 (in press).
Welsh, H. L., Crawford, M. F., and Locke, J. L. 1949, *Phys. Rev.*, **76**, 580.