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H_2 QUADRUPOLE ROTATION-VIBRATION LINES IN INFRARED SPECTRA OF COOL STARS

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ABSTRACT

The H_2 quadrupole rotation-vibration fundamental band has been searched for in high-resolution spectra of M giants and supergiants. H_2 has been identified in the spectrum of α Her (M5 II). Upper limits to the H_2 intensities are set for α Ori (M2 Iab), α Sco (M1–2 Iab), R Leo (M8 III), W Hya (M8e), and o Cet (M4 III–M7 III).

These results are shown to be consistent with recent model-atmosphere predictions. Earlier identifications of 2–0 lines near 1 micron are reviewed, and alternative identifications for these stellar lines are presented.

Subject headings: late-type stars — line identifications — molecules — spectra, infrared

I. INTRODUCTION

The H_2 molecule is an abundant species in the atmosphere of cool giant and supergiant stars. Detection of the molecule and a corresponding estimate of its abundance would provide a valuable check on model atmospheres for these interesting stars. As is well known, H_2 does not have an electric-dipole rotation-vibration spectrum and detection has to be based upon the weak quadrupole spectrum.

Spinrad (1966) reported on stellar identifications for two lines in the 2–0 band near 1 micron. The lines were strong with equivalent widths in the range 0.1 to 1.0 cm^{-1} in M giants and supergiants from α Ori to o Ceti. Later, Spinrad and Wing (1969) noted that stronger lines of the 1–0 band near 2 microns were not present on high-resolution spectra of α Ori obtained by P. and J. Connes. An upper limit, $W_{\tilde{\nu}} \leq 0.05$ cm^{-1}, for these lines was inconsistent with the 2–0 band identifications. This significant discrepancy has remained unresolved (Spinrad 1972).

In this note, we present preliminary results of a search for lines from the stronger 1–0 band and review the results in the light of recent model-atmosphere calculations. We suggest that alternative identifications for the 2–0 lines near 1 micron can be found and that H_2 is a very minor contributor to these stellar features.

II. THE H_2 1–0 BAND

Basic information entering into the interpretation and prediction of H_2 1–0 line equivalent widths is presented in this section. This information is (i) line positions for the *S*-, *Q*-, and *O*-branches, (ii) the absorption oscillator strengths, and (iii) the thermal distribution of the H_2 molecules among rotational states.

Direct measurements of line positions are available for only seven lines (Fink, Wiggins, and Rank 1965). Small corrections for pressure shifts were applied later by Foltz, Rank, and Wiggins (1966). The measured lines are the S and *Q*-transitions with $J \leq 3$. A search of stellar spectra based only on these lines will exclude some strong lines; for example, the $Q(7)$ line is the third strongest line in the 1–0 band for a temperature $T = 3500°$ K and, more importantly, the more favorably located $S(7)$

line is the third strongest member of the *S*-branch. A calculation of line positions for the *S*-, *Q*-, and *O*-branches to $J \sim 10$ is desirable.

Molecular constants were published by Foltz *et al.* Rosen (1970) quotes their results in his recent compilation. Extrapolation to obtain higher rotational lines involves an uncertainty which increases rapidly. An extension of direct measurements of the quadrupole spectrum is likely to prove very difficult. The Lyman bands in the ultraviolet should be reobserved to extend the ultraviolet measurements to lines from higher rotational states in the lowest vibrational states $v'' = 0$ and 1. Herzberg and Howe (1959) list Lyman lines to $J'' \sim 10$ but only in bands with $v'' \geq 3$.

In this paper, the predicted rotation-vibration states (Kolos and Wolniewicz 1968) are adopted in an attempt to predict higher members of the *Q*-, *S*-, and *O*-branches. Comparison of their predictions with the observed positions for seven 1–0 lines shows an essentially constant discrepancy for all lines: $\tilde{\nu}_{\text{obs}} - \tilde{\nu}_{\text{calc}} = -0.91\ \text{cm}^{-1}$. This difference is believed to originate in the vibrational-energy calculation (Wilkinson and Pritchard 1969). This correction has been applied to the predicted line positions. The assumption has been adopted that there is no significant error in the calculation of the rotational energies.

Quadrupole line intensities may be expressed in several ways. We chose to give the absorption oscillator strength $f_{J'J''}$ for the rotational transitions. Laboratory spectroscopists prefer to give an integrated absorption strength, A, which is related to $f_{J'J''}$ by the expression

$$A = \frac{\pi e^2}{mc^2} f_{J'J''} P(J) NL = 8.85 \times 10^{-13} f_{J'J''} P(J) NL\,,$$

where A is in cm^{-1}. NL is the H_2 column density. $P(J)$ is the fraction of H_2 in the lower state of the transition. Laboratory spectroscopists use units cm^{-1} (km atm)$^{-1}$ for A. Appropriate adjustments to the above expression can be made to incorporate these units. We note that A through $P(J)$ is temperature dependent. $P(J)$ was calculated (table 2) using the partition function given by Tatum (1966).

Oscillator strengths are listed in table 1. These were calculated from quadrupole matrix elements given by Birnbaum and Poll (1969) and Dalgarno, Allison, and Browne (1969). These are based upon the electric-quadrupole moment calculations of Kolos and Wolniewicz (1965). An extrapolation of the matrix elements was necessary because the tabulations stop at $J = 4$.

TABLE 1

THE H_2 1–0 QUADRUPOLE VIBRATION-ROTATION SPECTRUM

	S-BRANCH		*Q*-BRANCH		*O*-BRANCH	
J''	ν(cm^{-1})	f	ν(cm^{-1})	f	ν(cm^{-1})	f
0.	4497.84	9.4 − 14	. . .	. . .	. . .	. . .
1.	4712.90	5.5 − 14	4155.26	3.7 − 14	. . .	. . .
2.	4917.01	4.5 − 14	4143.46	2.7 − 14	3806.76	1.8 − 14
3.	5108.41	3.8 − 14	4125.88	2.5 − 14	3568.17	2.1 − 14
4.	5285.63	3.3 − 14	4102.55	2.4 − 14	3328.97	2.2 − 14
5.	5448.38	2.7 − 14	4073.70	2.3 − 14	3091.11	2.1 − 14
6.	5593.74	2.2 − 14	4039.45	2.3 − 14	2856.37	1.9 − 14
7.	5721.04	1.7 − 14	4000.01	2.2 − 14	2626.33	1.7 − 14
8.	5831.86	1.2 − 14	3955.58	2.2 − 14	2402.29	1.5 − 14
9.	(5922)	7.6 − 15	3906.42	2.1 − 14	2185.39	1.2 − 14
10.	(5997)	4.2 − 15	3852.75	2.1 − 14	1976.47	1.0 − 14

TABLE 2

FRACTIONAL POPULATIONS $P(J)$ FOR THE GROUND VIBRATIONAL LEVEL

	Temperature (°K)						
J''	1000	1500	2000	2500	3000	3500	4000
0.......	4.26 − 2	2.79 − 2	2.02 − 2	1.54 − 2	1.21 − 2	9.80 − 3	8.08 − 3
1.......	3.23 − 1	2.24 − 1	1.67 − 1	1.29 − 1	1.03 − 1	8.40 − 2	6.96 − 2
2.......	1.28 − 1	9.93 − 2	7.82 − 2	6.28 − 2	5.12 − 2	4.24 − 2	3.55 − 2
3.......	3.24 − 1	2.98 − 1	2.55 − 1	2.15 − 1	1.82 − 1	1.54 − 1	1.31 − 1
4.......	7.13 − 2	8.18 − 2	7.84 − 2	7.07 − 2	6.23 − 2	5.46 − 2	4.77 − 2
5.......	1.15 − 1	1.73 − 1	1.90 − 1	1.87 − 1	1.74 − 1	1.58 − 1	1.42 − 1
6.......	1.71 − 2	3.58 − 2	4.62 − 2	4.99 − 2	4.95 − 2	4.72 − 2	4.40 − 2
7.......	1.95 − 2	5.90 − 2	9.17 − 2	1.11 − 1	1.18 − 1	1.19 − 1	1.15 − 1
8.......	2.12 − 3	9.72 − 3	1.86 − 2	2.54 − 2	2.95 − 2	3.15 − 2	3.19 − 2
9.......	1.81 − 3	1.31 − 2	3.14 − 2	4.93 − 2	6.27 − 2	7.14 − 2	7.60 − 2
10.......	1.51 − 4	1.79 − 3	5.51 − 3	1.00 − 2	1.41 − 2	1.72 − 2	1.93 − 2

Applications of tables 1 and 2 are made in § V. The equivalent width of a line is proportional to $P(J)f_{J'J''}$. Inspection of the tables shows that the lines from the odd-J levels are considerably stronger than adjacent lines from the even-J levels; this result arises from the nuclear-spin statistical weights.

III. A SEARCH FOR STELLAR 1–0 LINES

High-resolution infrared spectra of M giant and supergiant stars have been obtained for the interval 1.4–5.0 microns with the McDonald 107-inch (272 cm) telescope and the JPL Connes-type interferometer (Beer, Norton, and Seaman 1971). This discussion describes a search of the spectra of α Ori, α Sco, α Her, R Leo, o Cet, and W Hya for H_2 1–0 lines.

The working line list derived from table 1 is depleted seriously because many H_2 lines are either in a region of severe telluric absorption or blended with a strong stellar CO or H_2O line. The working list is reduced to $S(0)$, $S(1)$, and $S(2)$. The line $O(5)$ was searched for in stars for which spectra to 5 microns are available. Additional lines are free of blending in α Ori and α Sco.

In the search, a coincidence in the predicted and observed wavenumber of better than ± 0.1 cm^{-1} was demanded. This criterion is based on the uncertainties in the stellar radial velocity as derived from CO lines on the spectral scans and probable line position errors resulting from the finite resolution and signal-to-noise ratio. The error in the adopted line positions is negligible for those lines observed in the laboratory. Where more than one line is accessible, the relative line intensities can be used to confirm identification. In principle, the line width could also provide information; for example, at $T = 2500°$ K with a microturbulent velocity of 5 km s^{-1}, the H_2 lines will be approximately 40 percent broader than weak CO lines for the same spectral region. The width discriminant disappears as the microturbulence increases. Observations at a higher resolution and superior signal-to-noise ratio are required for application of this criterion.

Results of the search are summarized in table 3. H_2 is not detected in α Ori or α Sco. A tentative identification is proposed for α Her (fig. 1): $S(1)$ and $S(2)$ are well-resolved lines. At the Doppler shift for the time of observation, $S(2)$ is blended with a telluric H_2O line. This contributes approximately one-half the intensity of the observed lines. This estimate is based upon a comparison of the intensities of other H_2O lines with the integrated absorption coefficients listed by Benedict and Calfee (1967). $S(0)$ is a

TABLE 3

POSSIBLE IDENTIFICATIONS OF H_2 1–0 LINES

Star	Line	$W_{\bar{\nu}}$ (cm^{-1})	Remarks
α Ori..........	$S(0)$	< 0.05	Upper limit from Spinrad and Wing (1969)
	$S(1)$	< 0.05	
	$O(5)$	< 0.02	
α Sco..........	$S(0)$	< 0.003	
	$S(1)$	< 0.006	
	$S(2)$	< 0.003	
α Her..........	$S(0)$	0.005	Upper limit?
	$S(1)$	0.03	
	$S(2)$	0.02:	Blended with H_2O; see text
	$O(5)$	< 0.05	
R Leo.........	$S(0)$	0.04	Blended
	$S(1)$	0.06:	Broad blended feature
	$O(5)$	< 0.02	
W Hya........	$S(0)$	0.05	
	$S(1)$	0.05	
o Cet..........	$O(5)$	< 0.02	

very weak line. The $S(6)$ and $S(7)$ lines will be searched for when spectra at that wavelength are fully reduced. In the cooler stars, R Leo and W Hya, the $S(2)$ position is within a region of rich structure which is apparently due to stellar water vapor. The $S(2)$ line is itself masked by a strong H_2O line. Identifications for $S(0)$ and $S(1)$ can be made, but it is clear that the relative intensities are not consistent with an identification of H_2 for both lines. We prefer to interpret these measurements as upper limits for an H_2 contribution.

IV. COMPARISON WITH MODEL-ATMOSPHERE PREDICTIONS

Goon and Auman (1970) computed column densities of molecules including H_2. Their calculations are for a representative wavelength (λ = 2.22 microns) for the 1–0 band. Their integration through the model atmosphere extended to a continuum

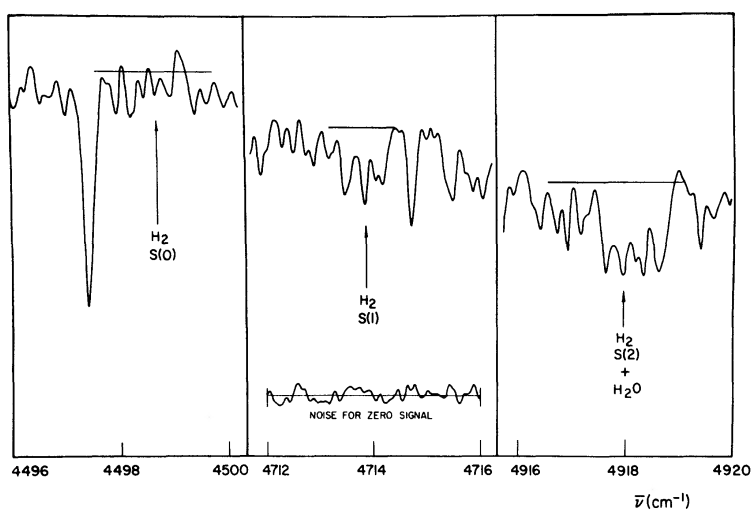

FIG. 1.—The infrared spectrum of α Her. The illustrated portions include the positions of the H_2 1–0 $S(0)$, $S(1)$, and $S(2)$ lines. The signal-to-noise ratio may be estimated from the noise level for zero signal which is shown near the bottom of the figure.

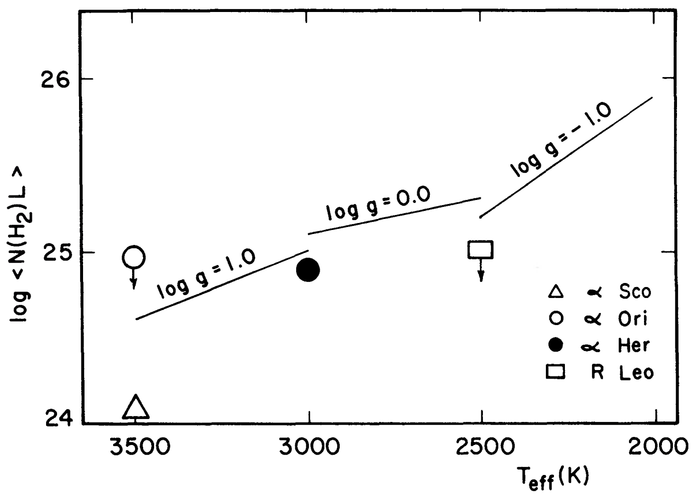

FIG. 2.—Predicted and observed column densities for H_2. The predictions (*solid lines*) from Good and Auman (1970) are the column densities above $\tau_\lambda = 0.3$ for $\lambda = 2.22$ microns. The assumed surface gravity is indicated on the figure. Observational estimates for α Ori, α Sco, α Her, and R Leo are shown. The assumed effective temperatures for these stars are nominal values. R Leo is plotted as representative of the group o Cet, W Hya, and R Leo.

optical depth $\tau_\lambda = 0.3$. The observed equivalent widths of the $S(1)$ line which is the strongest of the trio [$S(0)$, $S(1)$, and $S(2)$] are converted to a column density using the tabulated oscillator strength and a correction factor (about 10 percent) for stimulated emission. The results are compared with the model-atmosphere predictions in figure 2. The model atmospheres were calculated by Auman (1969), and the opacity contribution of the H_2O vibration-rotation transitions is taken into account in the construction of the models. Solar abundances of C and O were assumed.

The observations of H_2 are in reasonable agreement with the model atmosphere predictions. We note that Spinrad (1966) gave column densities above $\tau_\lambda = 0.1$ at 1.0 micron for earlier model atmospheres in which the H_2O opacity was not considered. These predictions, corresponding to $\log NL \geq 26.0$, are inconsistent with the observations. The inclusion of H_2O opacity reduces significantly the H_2 column densities. The CO vibration-rotation bands must also be included. Faÿ and Johnson (1973) report on models in which the line opacity from CO, H_2O, and the CN red system is included. A model corresponding to an effective temperature $T_{\rm eff} = 3500$ °K and surface gravity $\log g = 0.0$ has an H_2 column density $\log NL = 23.2$ above $\tau_\lambda = 0.50$ at $\lambda = 3.45$ microns. The column density estimate is insensitive to assumptions about the C, N, and O abundances. This result is nearly two orders of magnitude below the earlier Goon and Auman estimate, but it is consistent with the upper limit reported here for α Sco.

V. ALTERNATIVE IDENTIFICATIONS FOR THE 2–0 H_2 LINES

The results of our search for 1–0 H_2 lines are in conflict with Spinrad's (1966) identifications of 2–0 lines. Spinrad identified the $S(3)$ 2–0 lines (see below) and reported equivalent widths in a range $W_{\tilde\nu} \sim 0.3$ (α Ori) to 1.0 (o Cet) cm^{-1}. In a similar range of spectral types, we observe the $S(1)$ 1–0 line to have $W_{\tilde\nu} \lesssim 0.04$ cm^{-1}. A prediction based on this value and the relative oscillator strengths for 2–0 and 1–0 lines gives $W_{\tilde\nu} \sim 0.01$ cm^{-1} as the expected intensity for the $S(3)$ 2–0 line. The observed line is from 30 to 100 times stronger than this limit.

A variety of possible physical explanations for the appearance of strong 2–0 lines and the near absence of 1–0 lines in the same object can be entertained: time variations, a drastic wavelength variation of continuous opacity between 1 and 2 microns, departures from local thermodynamic equilibrium, etc. None of these possibilities is very attractive. The problem would be resolved if it were possible to show that the two 2–0 H_2 lines appearing in stellar spectra were satisfactorily identified with an alternative atom or molecule.

Two 2–0 lines were identified by Spinrad. They were the $S(2)$ and $S(3)$ lines. He reported attempts to observe the $S(1)$ and $S(5)$ lines and also the 3–0 $S(1)$ line. No positive detections were established, but this result was not in conflict with positive H_2 identifications in the case of stellar $S(2)$ and $S(3)$ features. Then alternative identifications have to be found for two lines.

The most accurate wavelengths for the lines are apparently obtainable from the molecular constants given by Foltz *et al.* (1966). The predictions are $\lambda_{air} = 11{,}379.29$ Å ($\tilde{\nu} = 8785.49$ cm^{-1}) for $S(2)$ and $\lambda_{air} = 11{,}171.92$ Å ($\tilde{\nu} = 8948.57$ cm^{-1}) for $S(3)$. We note that Spinrad adopted 11,379.22 and 11,171.77 Å, respectively. These differences are not significant considering the dispersion of the plates and the variable radial velocity of the stars sampled; the new wavelengths correspond to radial velocity corrections of 1.9 km s^{-1} for $S(2)$ and 4.1 km s^{-1} for $S(3)$.

The H_2 $S(3)$ line is almost coincident with the CN line $\lambda_{air} = 11{,}171.78$ Å and classified as the $Q_1(29)$ line of the 0–0 band of the red system (Davis and Phillips 1963). This line was considered and dismissed by Spinrad. However, new observations of α Ori suggest that CN provides the major contribution to the stellar line. In 1972 March, the Tull coudé scanner was used to obtain high-resolution scans for several regions within the CN 0–0 band. Preliminary reductions show that single Q-branch lines have equivalent widths in the range $W_\lambda = 0.2$–0.4 Å. The disputed line at 11,171.8 Å was not reobserved. Spinrad gave the intensity as $W_\lambda = 0.36$ Å, so the CN line does provide the major contribution.

The CN identification is not responsible for the stellar line in late M spectra where CN is weak or absent. In these spectra, we propose that stellar water vapor provides a dominant contribution. Inspection of the montage of photographic spectra (Spinrad 1966, fig. 2) for the $S(3)$ region shows that apparently all the strong terrestrial H_2O lines have stellar counterparts when the Doppler shift separates telluric and stellar H_2O lines. This effect is very clearly seen on microdensitometer tracings kindly loaned us by Professor H. Spinrad. Spinrad and Wing (1968, fig. 3) have identified stellar H_2O lines between 11,100 and 11,130 Å in the o Cet spectrum. These lines are from the same band as and of very similar excitation potential to the lines providing the complex at 11,172.0 Å which we propose is responsible for the stellar line identified previously as H_2 $S(3)$. The telluric feature is a blend of four lines (Swensson *et al.* 1970) at 11,171.70, 11,172.06, 11.172.10, 11,172.47 Å. They would be unresolved in stellar spectra. Noting that the stellar line was unusually broad for a single line, Spinrad attributed the width to a macroturbulent motion of about 20 km s^{-1}. However, the separation of the H_2O lines in the blend is 0.8 Å or 21 km s^{-1}. The intensity of the stellar line was reported to strengthen considerably near minimum light in long-period variables. This is the sense of the variation of the H_2O lines.

Our search for other identifications revealed the possibility of a contribution to the $S(3)$ 2–0 line from the TiO Φ-system ($^1\Pi$–$^1\Sigma$). The $Q(54)$ and $R(70)$ lines of the 0–0 band (Pettersson 1959) are at $\lambda_{air} = 11{,}171.92$ and 11,172.28 Å, respectively. However, stronger lines of this system are not present in the spectra of o Cet. The band head near 11,032 Å is seen in many late M spectra (see Spinrad and Wing 1969), so TiO may contribute in the coolest stars.

The identification of H_2 was also based upon the $S(2)$ 2–0 line. We note that this is almost coincident with a Cr I line at $\lambda_{air} = 11{,}379.37$ Å (Kiess 1953) which is present in the solar spectrum (Swensson *et al.* 1970). The wavelength is 0.15 Å to the red of Spinrad's assumed H_2 wavelength, but this cannot be a basis for rejection of Cr I: the associated radial-velocity difference is only 4.0 km s^{-1}. The intensity of the Cr I line can be estimated by the following argument. In a reproduction of a 4 Å mm^{-1} plate of the α Ori spectrum for the interval 10,650–11,025 Å (see Spinrad and Wing 1969, fig. 1), several Cr I lines are readily visible. They include lines at 10,667.48, 10,672.22, 10,801.32, and 10,816.96 Å. The solar intensities of these lines range from 6 to 10 on the scale used by Swensson *et al.* On this same scale, the solar line at 11,379.37 Å has an intensity between 7 and 9. The lower-state excitation potentials are comparable: the latter line is about 0.3 eV higher than the shorter-wavelength group. This argument suggests that the Cr I line provides a significant, probably major, contribution to the equivalent width, $W_\lambda = 0.12$ Å, which was measured for α Ori. Again, the H_2 component is apparently not dominant. This identification is readily tested: the 11,379.37 Å line is the weakest member of a multiplet, and the other members should appear as strong lines if the identification is valid. Since Cr I lines in this excitation potential range are present in all K and M stars, this identification probably accounts for the stellar line in all stars observed by Spinrad.

The alternative identifications which we provide for the H_2 $S(2)$, $S(3)$ 2–0 lines appear to provide a dominant contribution to the stellar lines which were previously attributed to H_2. At the present time, arguments concerning the H_2 abundance in cool stellar atmospheres cannot be based on these lines.

VI. SUMMARY

This paper has described a search for stellar H_2 quadrupole lines in the fundamental band. The identifications of H_2 in α Her and the upper limits for the other M giant and supergiant stars are consistent with model atmosphere predictions. The necessity for extending the molecular constants of the H_2 ground state has been stressed. A discrepancy between the early identifications of 2–0 H_2 lines and the 1–0 lines has been resolved by satisfactorily attributing the 2–0 lines to atomic and molecular species other than H_2. In order to exploit the H_2 1–0 lines further, spectra at a higher signal-to-noise ratio and resolution will be required. Since the available lines are so few, these observations could be made most satisfactorily with a spectrum scanner covering an interval of a few cm^{-1}.

We wish to thank Dr. Hyron Spinrad for helpful correspondence and the opportunity to inspect microphotometer tracings of his plates. We are indebted to Dr. G. Herzberg for the suggestion that the predicted H_2 energy levels be used to obtain positions for unobserved 1–0 lines.

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