High-resolution Fourier transform emission spectroscopy of YH

R. S. Ram and P. F. Bernath

Department of Chemistry, University of Arizona, Tucson, Arizona 85721 and Department of Chemistry, University of Waterloo, Waterloo, Ontario N2L 3G1, Canada

The electronic emission spectrum of YH has been investigated in the 690 nm to 3 μm spectral region using a Fourier transform spectrometer. The YH bands were excited in an yttrium hollow cathode lamp operated with neon gas and a trace of hydrogen. The observed bands have been classified into three different electronic transitions: $C\ ^1\Sigma^+ - X\ ^1\Sigma^+$, $d0^+(^3\Sigma^-) - X\ ^1\Sigma^+$, and $e\ ^3\Phi - a\ ^3\Delta$. The rotational analysis of the 0–0, 1–1, 2–2, 3–3, 0–1, 1–2, and 2–3 bands of the $C\ ^1\Sigma^+ - X\ ^1\Sigma^+$ system provided the following set of equilibrium molecular constants for the ground state: $\omega_e = 1530.456(15)$ cm^{-1}, $\omega_e x_e = 19.4369(72)$ cm^{-1}, $\omega_e y_e = 0.0361(9)$ cm^{-1}, $B_e = 4.575\,667(38)$ cm^{-1}, $\alpha_e = 0.091\,449(23)$ cm^{-1}, and $r_e = 1.922\,765(8)$ Å. Two weaker bands with origins at 14 264.7256(49) and 12 811.5753(49) cm^{-1} have been assigned as the 0–1 and 0–2 bands of a new $d0^+(^3\Sigma^-) - X\ ^1\Sigma^+$ electronic transition with $T_0 = 15\,756.4251(49)$ cm^{-1}. Three bands observed in the red region with origins at 11 377.9784(39), 11 499.3408(26), and 11 583.8294(23) cm^{-1} have been assigned as the $^3\Phi_2 - ^3\Delta_1$, $^3\Phi_3 - ^3\Delta_2$, and $^3\Phi_4 - ^3\Delta_3$ subbands of a new $e\ ^3\Phi - a\ ^3\Delta$ electronic transition. © *1994 American Institute of Physics.*

INTRODUCTION

There is considerable interest in both theoretical and experimental studies of the transition metal hydrides due to their importance in astrophysics, organometallic chemistry, and surface science.[1–5] Some transition metal hydrides are found in the spectra of cool stars. For example, TiH[6] has been identified in the spectra of M-type stars; NiH[7] and CrH[8] were seen in the spectra of sunspots.

The electronic states of the heavier transition metal hydrides are interesting because of the importance of relativistic effects such as spin–orbit coupling. Theoretical studies also provide significant insight into the nature of the metal–hydrogen bond. For these reasons *ab initio* studies of many transition metal hydrides have been carried out in recent years. Molecules for which *ab initio* studies are available include, e.g., PtH,[9] PdH,[10–12] YH,[13,14] ZrH,[15] MoH,[16] TiH,[17] and ScH.[18–20] Most of these investigations have focused on the characterization of a few low-lying electronic states and on the understanding of the metal–hydrogen bond. On the experimental side, only limited spectroscopic data are available for the transition metal hydrides obtained mainly from their electronic spectra. For example, for the II B group of metal hydrides some experimental data are available for ScH,[2,21] YH,[22,23] and LaH.[24,25]

The spectrum of YH was first observed by Bernard and Bacis[22] in 1976. In a later paper[23] these authors reported the rotational analysis of several bands of YH and YD in the 450–900 nm spectral region. Bernard and Bacis[23] classified the observed bands into five electronic transitions involving three low-lying states that they called $X\ ^3\Delta$, $A\ ^1\Pi$, and $A'\ \Sigma^+$. On the basis of some primitive *ab initio* calculations for ScH they concluded that the ground state of YH was $X\ ^3\Delta$.

Langhoff *et al.*[13] studied the low-lying states of YH and predicted a $^1\Sigma^+$ state as the ground state. More recently, Balasubramanian and Wang[14] performed complete active space self-consistent field (CASSCF) with second-order con-

figuration interaction (SOCI) and relativistic configuration interaction (RCI) calculations on 29 Ω states, taking into account both electron correlation and spin–orbit effects. Their theoretical work also contradicts the $X\ ^3\Delta$ assignment of the ground state of YH by Bernard and Bacis.[23]

Recently we have initiated a project aimed at increasing the experimental data available for transition metal oxides, nitrides, and hydrides. We have observed new transitions for NiO[26] and CoO[27] and have reported the first observation of the ScN,[28] YN,[29] and WN[30] molecules. We have also reanalyzed the $A\ ^6\Sigma^+ - X\ ^6\Sigma^+$ transition of CrH[31] and reported the first observation of HfH and HfD.[32] In this paper we report on the detailed analysis of the red and near infrared bands of YH. Our analysis is consistent with an $X\ ^1\Sigma^+$ ground state and a low-lying $a\ ^3\Delta$ state. The $A\ ^1\Pi$ state, as assigned by Bernard and Bacis,[23] has been identified as the $\Omega = 1$ component of the $a\ ^3\Delta$ state. Prior to our work, Simard *et al.*[33] recorded the laser excitation spectra of this molecule under jet-cooled conditions and demonstrated that the ground state of YH is a $^1\Sigma^+$ state. In addition to the $^1\Sigma^+ - ^1\Sigma^+$ transition previously observed by Bernard and Bacis,[23] Simard *et al.*[33] have identified several new excited electronic states in the blue and green regions of the spectrum. In this paper we will relabel all of the known states of YH in a manner consistent with the available experimental data and theoretical calculations.

EXPERIMENT

The YH molecule was made in an yttrium hollow cathode lamp. The cathode was prepared by inserting a solid rod of yttrium metal into a hole in a copper block. The central part was then bored through to provide a uniform layer of yttrium metal inside the cathode. The lamp was operated at 477 mA current and 220 V current with a slowly flowing mixture of 3 Torr of Ne and 70 mTorr of H_2.

The spectra of YH were recorded using the 1 m Fourier transform spectrometer associated with the McMath Solar

TABLE I. The correspondence between the labels for the YH transitions used by Bernard and Bacis (Ref. 23) and the labels adopted in this paper.

Bernard and Bacis	This work
$C\ ^1\Sigma^+ - A\ ^1\Pi$	$h0^+ - a\ ^3\Delta_1$
$C\ ^1\Pi - A'\ ^1\Sigma$	$D\ ^1\Pi - X\ ^1\Sigma^+$
$a\ ^3\Phi_4 - X\ ^3\Delta_3$	$g\ ^3\Phi_4 - a\ ^3\Delta_3$
$a\ ^3\Phi_3 - X\ ^3\Delta_2$	$g\ ^3\Phi_3 - a\ ^3\Delta_2$
$B'\ ^1\Sigma - A'\ ^1\Sigma$	$C\ ^1\Sigma^+ - X\ ^1\Sigma^+$
$B\ ^1\Delta - A\ ^1\Pi$	$e\ ^3\Phi_2 - a\ ^3\Delta_1$

Telescope of the National Solar Observatory. The spectra in the 3500–14 800 cm^{-1} spectral region were observed in two experiments. The 3500–9150 cm^{-1} region was recorded using InSb detectors, cold green uranium glass filters, and silicon filters with 5 scans co-added in about 40 min of integration. For the 9100–14 800 cm^{-1} region the spectrometer was operated with a red pass filter (RG715) and Si–diode detectors. A total of 3 scans were co-added in 20 min of integration. In both of these experiments the spectrometer resolution was set at 0.02 cm^{-1}.

In addition to YH bands, the observed spectra also contained Y and Ne atomic lines. The spectra were calibrated using the measurements of the Ne atomic lines made by Palmer and Engleman.[34] The absolute accuracy of the wave number scale is expected to be better than ±0.002 cm^{-1}.

OBSERVATION AND ANALYSIS

The spectral line positions were extracted from the observed spectra using a data reduction program called PC-DECOMP developed by Brault. The peak positions were determined by fitting a Voigt line shape function to each spectral feature. The branches in the different subbands were sorted using a color Loomis–Wood program running on a PC computer.

Bernard and Bacis[23] identified several electronic transitions (Table I, Fig. 1) and concluded that YH had a $^3\Delta$ ground state. In a recent theoretical work, Balasubramanian and Wang[14] have calculated the spectroscopic properties of many electronic states of YH. Their calculation predicts the ground state to be of $^1\Sigma^+$ symmetry with $^3\Pi$ and $^3\Delta$ states at 8000 and 9000 cm^{-1}, respectively, above the ground state. Langhoff et al.[13] came to similar conclusions but with the $^3\Delta$ state predicted to lie at 6900 cm^{-1} and the $^3\Pi$ state at 8100 cm^{-1}. In recent work Simard and co-workers[33] have found that the $^3\Delta$ state is the first excited state and proved that the ground state has $^1\Sigma^+$ symmetry. Our emission measurements are consistent with these results.

The main bands of YH are present in the 11 000–15 000 cm^{-1} spectral region. The observed spectrum consists of three transitions: $C\ ^1\Sigma^+ - X\ ^1\Sigma^+$, $d0^+(^3\Sigma^-) - X\ ^1\Sigma^+$, and $e\ ^3\Phi - a\ ^3\Delta$. The rotational analysis of the 0–0 and 1–1 bands of the $C\ ^1\Sigma^+ - X\ ^1\Sigma^+$ transition was published by Bernard and Bacis.[23] Our observed spectrum consists of several additional bands involving the higher vibrational levels of the ground and the excited states. We have measured the high-resolution spectra of the 2–2, 3–3, 0–1, 1–2, and 2–3
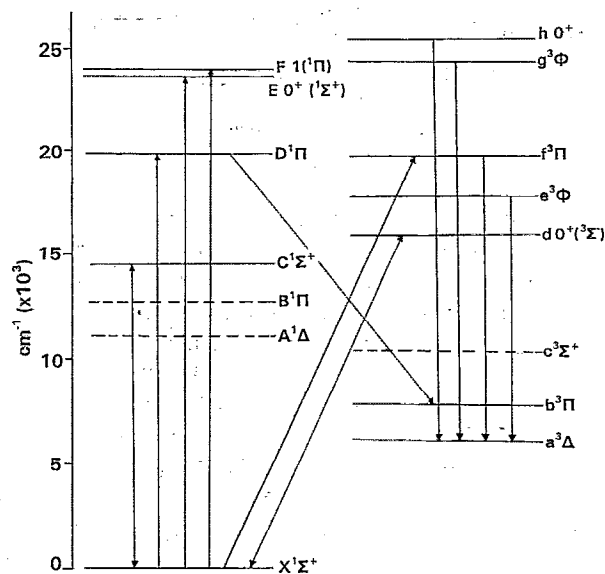

FIG. 1. A schematic energy level diagram of the electronic states of YH.

in addition to the 0–0 and 1–1 bands.[23] The analysis of these bands provides a much improved set of equilibrium constants for the ground state of YH including the first determination of the vibrational constants.

In the same spectral region as the $C\ ^1\Sigma^+ - X\ ^1\Sigma^+$ transition, we have identified two very weak bands involving the $v''=1$ and $v''=2$ levels of the $X\ ^1\Sigma^+$ state. These bands have been assigned as the 0–1 and 0–2 bands of a new transition with $T_0=15\ 756.43\ cm^{-1}$. Simard et al.[33] have recently observed a $\Delta\Omega=0$ band with an origin at 15 756.2 cm^{-1} which they tentatively assigned as the 1–0 band of the $C\ ^1\Sigma^+ - X\ ^1\Sigma^+$ system but we believe this band to be the 0–0 band of the new transition. The bands of the new transition are very weak in intensity and we assign the transition as the $d0^+(^3\Sigma^-) - X\ ^1\Sigma^+$ transition. The $v=1$ vibrational level of the $C\ ^1\Sigma^+$ state is interacting strongly with another state, probably the $v=0$ level of the d state. (Fig. 1).

In the 12 900–13 300 cm^{-1} spectral region we observe dense rotational structure with an intensity maximum at about 13 053 cm^{-1}. This structure seems to be badly perturbed and no distinct branches are obvious. The theoretical calculations of Balasubramanian and Wang[14] predict three electronic states, $^3\Sigma^+$, $^1\Delta$, and $^1\Pi$ in this region at 10 200, 11 000, and 12 700 cm^{-1}, respectively. The rotational structure may be due to the $B\ ^1\Pi - X\ ^1\Sigma^+$ electronic transition with the excited $^1\Pi$ state badly perturbed by interaction with the neighboring excited electronic states.

To even lower wave numbers we observe three bands with band origins at 11 583.83, 11 499.34, and 11 377.98 cm^{-1}. Two of these bands (at 11 583.83 and 11 377.98 cm^{-1}) were observed in the spectra of Bernard and Bacis.[23] They assigned the band at 11 377.98 cm^{-1} to a $^1\Delta - ^1\Pi$ transition while the other band remained unanalyzed. Our high-resolution work suggests that these three bands are in fact the $\Omega=4-3$, 3–2, and 2–1 subbands of an $e\ ^3\Phi - a\ ^3\Delta$ transition with the $e\ ^3\Phi$ state lying at about 17 500 cm^{-1} (Fig. 1).
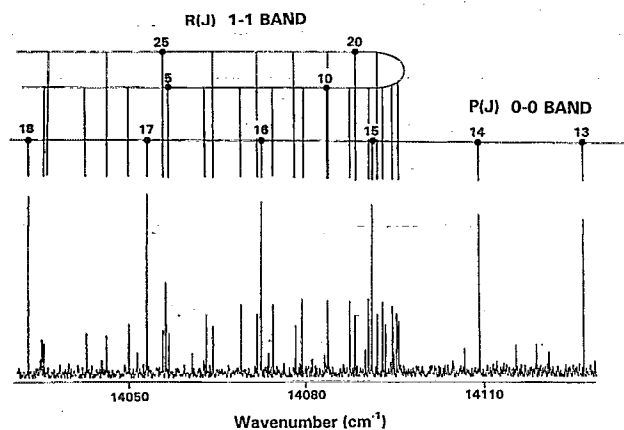
FIG. 2. A portion of the 0–0 and 1–1 bands of the $C\ ^1\Sigma^+-X\ ^1\Sigma^+$ system of YH.

While none of the *ab initio* calculations on YH has predicted a $^3\Phi$ state in this region, a more complete calculation[18] on the isovalent molecule ScH has an appropriate $^3\Phi$ state. In addition to these bands, there are some weak isolated P branches in the 11 600–12 600 cm^{-1} region but they could not be assigned with certainty because of a lack of corresponding R branches. These could be due to transitions between two excited states. A schematic energy level diagram of the known electronic states of YH is provided in Fig. 1 in which the observed electronic states are indicated by solid lines and broken lines mark those predicted by *ab initio* calculations[14] but not observed yet. The data for blue and green transitions have been taken from the work of Simard *et al.*[33] and Bernard and Bacis.[23]

The $C\,^1\Sigma^+-X\,^1\Sigma^+$ transition

In this work we have observed the 0–0, 1–1, 2–2, 3–3, 0–1, 1–2, and 2–3 bands of the $C\ ^1\Sigma^+-X\ ^1\Sigma^+$ transition. Each band of this transition has a single R and a single P branch as expected. The observation of the $R(0)$ and $P(1)$ lines confirms the assignment of these bands to a $^1\Sigma-^1\Sigma$ transition. A part of the 1–1 band near the R head is provided in Fig. 2, with a few members of the P branch of the 0–0 band also marked. The R and P branches of the 0–0 band have an anomalous intensity with the P branch being stronger than the R branch by a factor of 2.5:1. The assignment of rotational lines in the different bands of this transition was straightforward using previous work and the combination

differences of common vibrational levels. The wave numbers and assignment of rotational lines of this transition are available from PAPS[35] or by request from the authors. Two local perturbations, one at $J'=7$ and the other at $J'=24$ have been observed in the 0–0 band. The $J'=7$ perturbation can also be seen in the 0–1 band but the high J lines of this band could not be followed for $J'>22$ because of their very weak intensity.

The 1–1 band is weaker in intensity than the 0–0 band and the $v'=1$ level is involved in a strong perturbation. In the 1–1 band the lower J lines ($J'<15$) and the higher J lines can be fit separately, keeping the lower state constants fixed to the values for $v''=1$, to provide two sets of constants for the excited state. In the 1–2 band, it is difficult to follow the branches after the perturbation ($J'>15$).

In the 2–2 band, the low J ($J'<4$) and high J ($J'>21$) lines are affected by perturbations. The 3–3 band is much weaker in intensity than the 0–0, 1–1, and 2–2 bands. To identify the 3–3 band, the R and P branches were predicted with extrapolated rotational constants for the $v=3$ vibrational levels of the ground and excited states. There is a local perturbation at $J'=16$, and a few transitions near the perturbation were excluded from the fit.

The observed line positions were fit with the customary energy level expression for each vibrational level:

$$F_v(J)=T_v+B_vJ(J+1)-D_v[J(J+1)]^2$$
$$+H_v[J(J+1)]^3+L_v[J(J+1)]^4.$$

The ground-state combination differences obtained from all the observed transitions, including the perturbed ones, were used in the final fit to obtain the ground-state constants (Table II). However, the perturbed lines were excluded from the final fit to determine constants for the excited state (Table III). Note that $v'=1$, 2, and 3 of the $C\ ^1\Sigma^+$ state have both local and global perturbations.

The $d\,0^+(^3\Sigma^-)-X\,^1\Sigma^+$ transition

In addition to the relatively prominent bands of YH, we observed some isolated P branches which could not be assigned to any of the known transitions. In an attempt to determine if these branches belong to bands which connect to the ground $X\ ^1\Sigma^+$ state, we tried to fit them by fixing the ground-state constants to the known values for the different vibrational levels and changing the J assignment to minimize the standard deviation of the fit. It was found that two of these P branches fit together after fixing their lower state constants to the values for $v''=1$ and $v''=2$. The constants

TABLE II. Rotational constants (in cm^{-1}) obtained for the $X\ ^1\Sigma^+$ state of YH. The numbers in parentheses are one standard deviation in the last digit.

Constants	$v=0$	$v=1$	$v=2$	$v=3$
T_v	0.0	1491.699 5(15)	2944.849 8(21)	4359.667 4(34)
B_v	4.529 962(18)	4.438 455(19)	4.3470 69(24)	4.255 620(52)
$10^4\times D_v$	1.626 66(33)	1.616 23(49)	1.611 89(75)	1.606 14(23)
$10^9\times H_v$	4.998(21)	4.592(45)	4.677(62)	4.61(29)
$10^{14}\times L_v$	−0.202(43)	−9.40(10)	−9.40[a]	−9.40[a]

[a]Fixed to the value for $v=1$.

TABLE III. Rotational constants (in cm^{-1}) obtained for the $C\ ^1\Sigma^+$ state of YH. The numbers in parentheses are one standard deviation in the last digit.

Constants	$v=0$	$v=1$	$v=2$	$v=3$
T_v	14 295.395 6(10)	15 502.374 0(20)	16 822.452 6(32)	18 079.818 7(43)
B_v	4.195 624(17)	4.276 137(58)	4.071 726(70)	3.920 30(10)
$10^4 \times D_v$	1.701 78(34)	2.919 4(64)	2.575 2(55)	1.994 54(86)
$10^8 \times H_v$	0.540 8(22)	$-5.06(24)$	7.88(17)	3.58(27)
$10^{11} \times L_v$	$-0.031\ 51(45)$	5.24(28)	$-3.55(18)$	$-1.08(29)$

obtained from this fit are provided in Table IV. This fit places the excited-state vibrational level at $T_0 = 15\ 756.4262(55)$ cm^{-1}. In their recent work Simard et al.[33] observed a band with an origin at 15 756.2 cm^{-1} and with very similar rotational constants. They assumed that this transition was the 1-0 band of the $C\ ^1\Sigma^+ - X\ ^1\Sigma^+$ transition. This assignment is inconsistent with our analysis of the 1-1 and 1-2 bands of the $C\ ^1\Sigma^+ - X\ ^1\Sigma^+$ system which places the perturbed $v' = 1$ level of the $C\ ^1\Sigma^+$ state at 15 502.37 cm^{-1}. The solution to this problem is to assign the two weak bands in our spectra as the 0-1 and 0-2 bands of a new transition with the 0-0 band at 15 756.43 cm^{-1}, as observed by Simard et al.[33] Based on the very weak intensity compared to other bands in the same region, we assign the new transition as the $d0^+(^3\Sigma^-) - X\ ^1\Sigma^+$ transition. The spectroscopic properties of the $d\ ^3\Sigma^-$ state have not been calculated yet, but a more complete calculation[18] on ScH has an appropriate state in the correct region. As usual with molecules with Hund's case (c) tendencies, the Ω assignment of 0^+ for the d state is more certain than the $^3\Sigma^-$ parent term assignment.

The $e\ ^3\Phi - a\ ^3\Delta$ transition

In the 11 000–11 700 cm^{-1} region, there are three bands with origins at 11 377.9784(39), 11 499.3408(26), and 11 583.8294(23) cm^{-1}. Of these, the band with the origin at 11 377.9784(39) cm^{-1} was assigned earlier as a $^1\Delta - ^1\Pi$ transition by Bernard and Bacis.[23] The 11 583.8294(23) cm^{-1} band was also observed in the spectra of Bernard and Bacis[23] but they did not assign it. We assign these three transitions as $^3\Phi_2 - ^3\Delta_1$, $^3\Phi_3 - ^3\Delta_2$, and $^3\Phi_4 - ^3\Delta_3$ subbands of the $e\ ^3\Phi - a\ ^3\Delta$ transition (Fig. 1). Only the 0-0 vibrational band of this system has been observed in our spectra. Each of these subbands have P, Q, and R branches and each line is doubled at high J by Ω doubling. No satellite branches were observed.

A part of the $^3\Phi_2 - ^3\Delta_1$ subband showing some low J Q-branch lines is provided in Fig. 3. The Ω splitting in this subband is resolved from $J'' > 3$. The R and P branches of this subband are much weaker in intensity than the Q branch. Both e and f parity components of the excited state seem to be perturbed for $J' > 17$ and the perturbed transitions could

not be assigned with certainty. The splitting in the rotational lines arises mainly from the larger Ω doubling in the lower $^3\Delta_1$ state.

The subband with the origin at 11 499.3408(26) cm^{-1} has been identified as $^3\Phi_3 - ^3\Delta_2$. In this subband the intensity of the Q branch is similar to the R branch and the P branch is weak. The first member of the R branch $[R(2)]$ can be picked out easily in our spectra. A part of this band near the subband origin is illustrated in Fig 4. The Ω splitting of the $^3\Phi_3 - ^3\Delta_2$ subband is resolved for $J'' > 8$ and the doubling smaller than that in the $^3\Phi_2 - ^3\Delta_1$ subband.

The next subband to higher wave numbers with the origin at 11 583.8294(23) cm^{-1} has been assigned as the $^3\Phi_4 - ^3\Delta_3$ subband. A part of the R branch of this subband near the head is provided in Fig. 5. In this subband the R branch is stronger than the Q branch and again the P branch is the weakest. The first line in the R branch has been identified as $R(3)$ (see Fig. 5). The assignment of this subband was facilitated by the lower state combination differences obtained from the green $g\ ^3\Phi_4 - a\ ^3\Delta_3$ transition of YH previously assigned by Bernard and Bacis.[23] The analysis of this subband, in fact, provided the necessary clues for the assignment of our three subbands. Predissociation of the $g\ ^3\Phi_3$ and $g\ ^3\Phi_2$ spin components of YH allowed Bernard and Bacis to analyze only one ($g\ ^3\Phi_4 - a\ ^3\Delta_3$) of the three possible subbands.

The observed wave numbers of the different subbands were fitted separately by treating each spin component as a separate Hund's case (c) state. The term energy expression for a Hund's case (c) state is given by

TABLE IV. Rotational constants (in cm^{-1}) obtained for the $d0^+(^3\Sigma^-)$ state of YH. The numbers in parentheses are one standard deviation in the last digit.

T_0	B_0	$10^4 \times D_0$	$10^6 \times H_0$	$10^9 \times L_0$
15 756.4251(49)	4.146 81(36)	$-6.506(74)$	$-2.164(58)$	3.43(15)
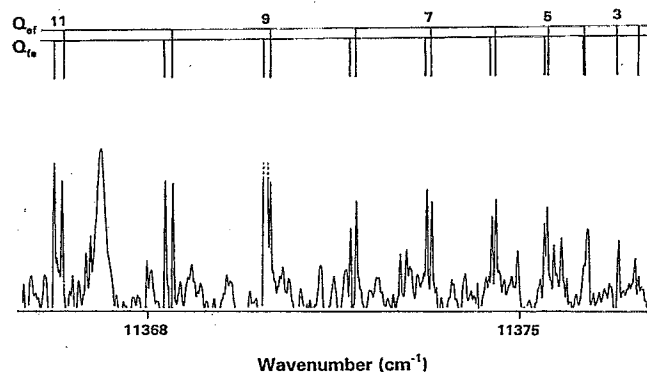
FIG. 3. A portion of the $e\ ^3\Phi_2 - a\ ^3\Delta_1$ subband of YH near the Q head.
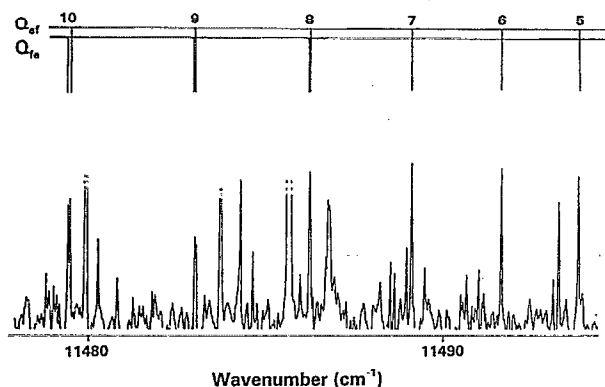
FIG. 4. A portion of the $e\ ^3\Phi_3-a\ ^3\Delta_2$ subband of YH near the Q head.

FIG. 5. A portion of the $e\ ^3\Phi_4-a\ ^3\Delta_3$ subband of YH near the R head.

$$F(J)=T_v+B_vJ(J+1)-D_v[J(J+1)]^2+H[J(J+1)]^3$$
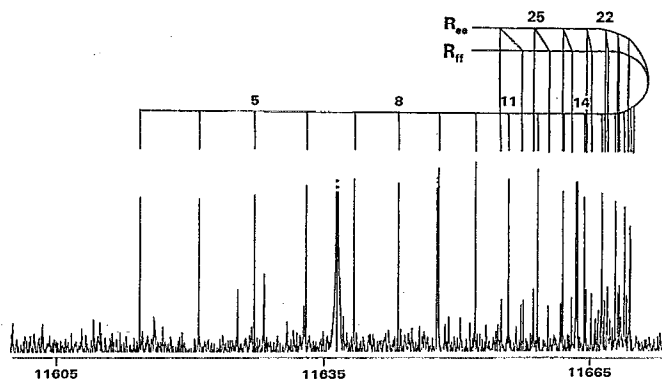$$\pm 1/2\{qJ(J+1)+q_D[J(J+1)]^2$$
$$+q_H[J(J+1)]^3\}.$$

The observed transition wave numbers of different subbands are available from PAPS[35] or from the authors. The perturbed transitions were excluded from the final fit. The rotational constants obtained from this fit for the $a\ ^3\Delta$ and $e\ ^3\Phi$ states are provided in Table V.

The e/f parity assignment is difficult. In the end we chose to put the e parity level for a given J higher in energy than the f parity level for the $^3\Delta_3$, $^3\Delta_2$, and $^3\Delta_1$ spin components. The unusual observation of Ω doubling in the $^3\Delta$ and $^3\Phi$ states is consistent with the Hund's case (c) tendencies of the excited states of YH.

DISCUSSION

The rotational constants for the different vibrational levels of the ground electronic state (Table II) have been used to evaluate the equilibrium vibrational and rotational constants which are provided in Table VI.

The rotational constants and the $\Delta G(v+1/2)$ intervals in the excited $C\ ^1\Sigma^+$ state vary in a more erratic manner than in the ground state (see Table III). The rotational constant for the $v=1$ vibrational level [4.276 137(58) cm^{-1}] is larger than that of the $v=0$ vibrational level [4.195 624(17) cm^{-1}]. Similarly the $\Delta G(3/2)$ value (1320.0786 cm^{-1}) is larger than the $\Delta G(1/2)$ value (1206.9784 cm^{-1}) in the $C\ ^1\Sigma^+$ state.

These anomalous constants are caused by the strong interaction of the $C\ ^1\Sigma^+$ state with a nearby state, probably the $d\ ^3\Sigma^-$ state. The $v=0$ level of the $d0^+(^3\Sigma^-)$ state seems to be too far away to account for the perturbations of the $v=1$ level of the $C\ ^1\Sigma^+$ state but the interaction with the $d1(^3\Sigma^-)$ state is plausible. The $d1(^3\Sigma)$ state has not been observed directly yet. The other perturbations observed in the $v'=2$ and 3 vibrational levels of the $C\ ^1\Sigma^+$ state could be caused by higher vibrational levels of the $d\ ^3\Sigma^-$ state or by other nearby states. Because of the erratic variation of $\Delta G(v+1/2)$ and B_v with v it is difficult to determine reasonable values for the equilibrium constants for the excited $C\ ^1\Sigma^+$ state.

The ab initio calculation of Balasubramanian and Wang[14] predicts that the ground $X\ ^1\Sigma^+$ state and excited $C\ ^1\Sigma^+$ state arise from mixed configurations. The ground-state electronic wave function of YH is made up of 86% of the $1\sigma^2 2\sigma^2$ configuration and 8% from the $1\sigma^2 1\pi^2$ configuration while the $C\ ^1\Sigma^+$ state has a 58% contribution from the $1\sigma^2 2\sigma 3\sigma$ configuration with the balance from several other configurations. The SOCI calculation predicts a very intense $C\ ^1\Sigma^+-X\ ^1\Sigma^+$ transition for YH. This transition is indeed found to be the strongest one in the red region of the spectrum. They also predict several dipole allowed transitions involving ground-state and low-lying singlet and triplet excited states in the region 7900–22 000 cm^{-1}. Some of these transitions have been observed by Simard et al.[33] Their calculations predict a $^1\Pi-X\ ^1\Sigma^+$ transition at 12 700 cm^{-1} and our spectrum shows the presence of dense rotational struc-

TABLE V. Rotational constants (in cm^{-1}) obtained for the $a\ ^3\Delta$ and $e\ ^3\Phi$ states of YH. The numbers in parentheses are one standard deviation in the last digit.

Constants	$a\ ^3\Delta_1$	$a\ ^3\Delta_2$	$a\ ^3\Delta_3$	$e\ ^3\Phi_2$	$e\ ^3\Phi_3$	$e\ ^3\Phi_4$
T_v	a	b	c	$a+11\ 377.978\ 4(39)$	$b+11\ 499.340\ 9(26)$	$c+11\ 583.829\ 4(23)$
B_v	4.036 73(21)	4.206 08(16)	4.301 09(12)	3.956 90(20)	4.021 77(13)	4.108 83(15)
$10^4\times D_v$	0.643(15)	1.754 8(99)	1.874 2(44)	1.425(12)	1.399 1(40)	1.820 2(41)
$10^8\times H_v$	−5.08(33)	1.61(21)	1.396(48)	4.09(23)	···	0.343(42)
$10^3\times q_v$	1.830(34)	···	···	···	···	···
$10^6\times q_{Dv}$	−3.42(16)	4.51(90)	−0.64(17)	−3.99(51)	···	1.49(15)
$10^8\times q_{Hv}$	···	−4.71(86)	0.422(82)	2.34(41)	4.38(14)	−1.053(68)
$10^{10}\times q_{Lv}$	···	1.25(20)	−0.037(10)	−0.465(82)	−1.173(53)	−0.192(72)

TABLE VI. Equilibrium constants (in cm^{-1}) for the $X\,^1\Sigma^+$ state of YH. The numbers in parentheses are one standard deviation in the last digit.

Constants	$X\,^1\Sigma^+$
ω_e	1530.456(15)
$\omega_e x_e$	19.436 9(72)
$\omega_e y_e$	0.036 1(9)
B_e	4.575 667(38)
α_e	0.091 448(23)
$10^4 \times D_e$	1.630 2(16)
$10^6 \times \beta_e$	−0.80(12)
r_e (Å)	1.922 765(8)

ture from 12 600–13 600 cm^{-1} which still remains unassigned because of perturbations in the excited state.

The equilibrium rotational constant of the ground state has been used to evaluate the ground-state equilibrium bond length. The observed equilibrium bond length for the ground state of YH is 1.922 765(8) Å. The theoretical value of 1.865 Å predicted by Balasubramanian and Wang[14] agrees only moderately well with our experimental value. The *ab initio* value[14] for ω_e of 1510 cm^{-1} compares with the experimental value of 1530.456 cm^{-1}. The calculations of Langhoff *et al.*[13] predict $r_e = 1.961$ Å and $\omega_e = 1558$ cm^{-1} for the $X\,^1\Sigma^+$ state of YH.

There is a remarkable resemblance between the energy level diagram of YH (Fig. 1) and that of ZrO.[36,37] The low-lying electronic configurations of YH and ZrO are very similar and Y and Zr are adjacent atoms in the Periodic Table. While YH and ZrO are not isoelectronic or isovalent, they are in some sense isostructural.

CONCLUSIONS

We have investigated the electronic spectra of YH in the 3000–14 800 cm^{-1} spectral region by Fourier transform emission spectroscopy. The observed spectra have been classified into three different electronic transitions, $C\,^1\Sigma^+ - X\,^1\Sigma^+$, $d0^+(^3\Sigma^-) - X\,^1\Sigma^+$, and $e\,^3\Phi - a\,^3\Delta$. The high-resolution analysis of several bands of the $C\,^1\Sigma^+ - X\,^1\Sigma^+$ transition provided spectroscopic constants for $v = 0$, 1, 2, and 3 vibrational levels in the ground state and allowed equilibrium vibrational and rotational constants to be determined for the $X\,^1\Sigma^+$ state.

ACKNOWLEDGMENTS

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