Fourier Transform Emission Spectroscopy of the $A'^{3}\Phi - X^{3}\Phi$ System of CoH

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The emission spectrum of CoH has been investigated in the red and infrared regions using a Fourier transform spectrometer. The bands observed in the 1 μ m-800 nm spectral region have been classified into ${}^{3}\Phi_{3}-{}^{3}\Phi_{3}$ and ${}^{3}\Phi_{4}-{}^{3}\Phi_{4}$ subbands of a new electronic transition $A'{}^{3}\Phi-X{}^{3}\Phi$. The rotational analysis of the 0–1 and 0–0 bands of the ${}^{3}\Phi_{4}-{}^{3}\Phi_{4}$ subband and the 0–0 band of the ${}^{3}\Phi_{3}-{}^{3}\Phi_{3}$ subband has been obtained and the spectroscopic constants have been determined. The effective principal equilibrium constants for the lowest energy spin component, $X{}^{3}\Phi_{4}$, obtained from this work are $\Delta G(1/2) = 1858.7932(32) \text{ cm}^{-1}$, $B_{e} = 7.255382(74) \text{ cm}^{-1}$, $\alpha_{e} = 0.212444(93) \text{ cm}^{-1}$, and $r_{e} = 1.531291(8)$ Å. © 1996 Academic Press, Inc.

INTRODUCTION

There is continued interest in transition metal hydrides due to their importance in astrophysics, organometallic chemistry, and surface science (1-5). Transition metal hydrides provide simple models for the bonding of hydrogen atoms to transition metals and also test the quality of wavefunctions of *ab initio* calculations. Because of the high cosmic abundances of the first row transition metals, their hydrides are expected to be present in various stars and nebulae, and the interstellar medium. Several of these molecules, for example, NiH (6) and CrH (7), have been observed in the spectra of sunspots and FeH (8, 9) and TiH (10) have been identified in the spectra of M-type stars. CoH is also expected to be present in the spectra of sunspots.

The electronic spectra of CoH molecules have been known since 1937 when Heimer (11) observed two bands in the visible region at 420.3 and 449.2 nm in a King furnace. From the rotational analysis he assigned these two bands as the 1–0 and 0–0 bands of a ${}^{3}\Phi_{4}-{}^{3}\Phi_{4}$ transition. Since then there have been additional studies of CoH (12, 13) and CoD (14–16) in emission as well as in absorption, confirming the ground state as $X^{3}\Phi_{1}$. Only the $X^{3}\Phi_{4}$ and $X^{3}\Phi_{3}$ spin components of the ground state have been identified despite several attempts to locate the $X^{3}\Phi_{2}$ component. Recently Varberg *et al.* (13) observed six new bands in the red region by laser excitation spectroscopy. Most of the bands obeyed the selection rule $\Delta\Omega = 0$ with $\Omega'' = 4$ but Varberg *et al.* also observed resolved fluorescence from an excited $\Omega = 3$ spin component which enabled them to measure the spin–orbit splitting between the $\Omega'' = 4$ and $\Omega'' = 3$ spin components of the ground state. This study found that the $X^3\Phi_3$ spin component is located at $728(\pm 3)$ cm⁻¹ above the lowest energy $X^3\Phi_4$ spin component.

Like the spectra of other first row transition metal hydrides, the electronic spectra of CoH are expected to be very complex. The open *d*-shells of the transition metals give rise to a large number of low-lying electronic states with large spin and orbital angular momenta. The different spin components are split by large spin–orbit interactions. There are extensive perturbations between the spin components of the close-lying states. For these reasons there are problems in predicting the spectroscopic properties as well as in the analysis of the observed spectra. CoH is a typical example since almost all of the excited states observed so far are involved in perturbations.

The ground state of CoH has been investigated by midinfrared laser magnetic resonance (17) as well as by farinfrared laser magnetic resonance (18, 19). The ground state fine and hyperfine molecular parameters have been determined with high precision from these measurements. The photoelectron spectra of CoH⁻ have been studied by Miller *et al.* (20) Their observations provided evidence for another electronic state located about 0.8 eV above the ground state.

There have been several theoretical studies of the spectroscopic properties of CoH. Chong *et al.* (21) have predicted some spectroscopic properties of the ground state of CoH using the modified coupled pair functional (MCPF) method. Anglada *et al.* (22) have determined the ionization potential of the ground state of CoH in addition to the spectroscopic properties of the low-lying electronic states of CoH⁺. More recently, Freindorf *et al.* (23) have performed a detailed study of the spectroscopic properties of the ground and low-

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lying excited states of CoH. The spectroscopic constants $(T_{\rm e}, \omega_{\rm e}, D_{\rm e}, r_{\rm e})$ of about 30 electronic states (with excitation energies below 4 eV) of singlet, triplet, and quintet multiplicity have been obtained.

Guided by the theoretical predictions of Freindorf *et al.* (23), we have recently investigated the red and infrared spectra of CoH and its isovalent molecule CoF. For CoF we have identified a new ${}^{3}\Phi_{-}{}^{3}\Phi$ transition in the near-infrared region with the ${}^{3}\Phi_{3}-X^{3}\Phi_{3}$ subband at 10 289 cm⁻¹ (24). In the present paper we report the observation of the two subbands, ${}^{3}\Phi_{4}-{}^{3}\Phi_{4}$ and ${}^{3}\Phi_{3}-{}^{3}\Phi_{3}$, of the analogous $A'{}^{3}\Phi_{-}X^{3}\Phi$ transition of CoH. The rotational structures of the 0–1 and 0–0 bands of the ${}^{3}\Phi_{4}-{}^{3}\Phi_{4}$ subband and the 0–0 band of the ${}^{3}\Phi_{3}-{}^{3}\Phi_{3}$ subband have been analyzed and the analysis is reported in this paper.

The $A'^{3}\Phi_{4}-X^{3}\Phi_{4}$ subband has also been observed by Barnes *et al.* (25), who observed three vibrational bands of this subband using a pulsed supersonic molecular beam source and concluded that these bands, as well as the bands observed by Varberg *et al.* (13), fit into a single transition with the 0–0 band at 12 407 cm⁻¹. These authors also studied the hyperfine structure associated with the ⁵⁹Co nucleus and extracted the hyperfine parameters in addition to the rotational constants. From this study they concluded that the $A'^{3}\Phi$ state arises from a $(7\sigma)^{1} (3d\delta)^{3} (3d\pi)^{3} (8\sigma)^{1}$ configuration.

EXPERIMENTAL

The red and near-infrared spectra of CoH molecules were excited in a commercial carbon tube furnace by melting Co metal at a temperature of about 2200°C in the presence of 130 Torr of H_2 . The spectra observed in this experiment were very rich with strong vibration–rotation bands of HF as well as vibration–rotation bands of CO.

The emission from the furnace was observed with the 1m Fourier transform spectrometer associated with the McMath–Pierce solar telescope of the National Solar Observatory at Kitt Peak. The spectrometer was operated with a CaF₂ beam splitter, RG 850 red pass filters, and Si photodiode detectors. A total of 5 scans were coadded in 23 min of integration at a resolution of 0.026 cm⁻¹.

The spectral line positions were extracted from the observed spectra using a data reduction program called PC-DECOMP, developed by J. Brault. The peak positions were determined by fitting a Voigt lineshape function to each spectral feature. ⁵⁹Co has 100% natural abundance and it has a large nuclear spin ($I = \frac{7}{2}$) and a large nuclear magnetic moment of 4.627 nuclear magnetons. The lower J lines of the different bands were broadened by partially resolved hyperfine structure. The width of the individual lines in the different bands varied from 0.070 to 0.190 cm⁻¹. In the absence of any other precisely known atomic or molecular transitions in the spectral region under investigation, we decided to calibrate the CoH bands using the measurements of the vibration–rotation transitions of HF by LeBlanc *et al.* (26) For this purpose we determined the calibration factor using the HF vibration–rotation lines in the 3500–4400 cm⁻¹ region in another scan. The calibration was transferred to the spectrum near 12 000 cm⁻¹ using some lines common to both spectra near 9000 cm⁻¹. The precision of measurements is not expected to be constant over the entire region due to the varying width of the individual rotational lines as well as the changing signal-to-noise ratio. Sharp and unblended lines are expected to be accurate to ± 0.002 cm⁻¹ but the uncertainty of the broader lines is estimated to increase to at least ± 0.005 cm⁻¹.

OBSERVATION AND ANALYSIS

We have observed several new bands of CoH in the 3.3 μ m-800 nm spectral region, but the structure of the bands at longer wavelengths below 1 μ m is very complex, most probably due to extensive perturbations. The bands observed in the 1 μ m-800 nm region are also perturbed but they are relatively free from overlapping by other bands and more suitable for rotational analysis. In this paper we focus on the analysis of the bands in the region 800 nm-1 μ m. The analysis of the near-infrared bands is still continuing.

There are three prominent bands with *R* heads at 10 552, 12 027, and 12 407 cm⁻¹. The bands at 10 552 and 12 407 cm⁻¹ have been assigned as the 0–1 and 0–0 bands of the ${}^{3}\Phi_{4}-X^{3}\Phi_{4}$ subband while the band at 12 027 cm⁻¹ has been assigned as the ${}^{3}\Phi_{3}-X^{3}\Phi_{3}$ subband of a new $A'{}^{3}\Phi-X^{3}\Phi$ transition. The assignment of the $A'{}^{3}\Phi_{4}-X^{3}\Phi_{4}$ subband is consistent with the assignment of Barnes *et al.* (25). The $A'{}^{3}\Phi_{3}-X^{3}\Phi_{3}$ subband was not observed by these authors.

The structure of the bands of the ${}^{3}\Phi_{4}-X^{3}\Phi_{4}$ subband consists of two P, two Q, and two R branches. The P branches are stronger than the R and O branches. The first lines have been clearly observed in all of the branches of the 0-1 and 0-0 band of this transition, confirming our Ω assignments. The intensity of the Q branches falls rapidly with increasing J, consistent with the $\Delta \Omega = 0$ assignment. The low J lines in different branches are relatively much broader due to partial hyperfine splitting. There are strong perturbations in the excited state v = 0 vibrational level. The *e* and *f* parity levels are affected by strong perturbations in different J regions. All of the *e* parity levels of the excited state are perturbed at $J \ge 7$ while all the f parity levels of the $A'^3 \Phi_4$ spin component are perturbed at $J \ge 11$. A part of the spectrum of the 0–0 band of the ${}^{3}\Phi_{4} - X^{3}\Phi_{4}$ subband near the band origin is provided in Fig. 1. Once the lower J lines were assigned, the assignment of the perturbed lines was achieved with the help of the predicted high-J combination differences for the unperturbed $\Omega'' = 4$ spin component. The lines affected by perturbations were not included directly in the fit but the combination differences corresponding to all

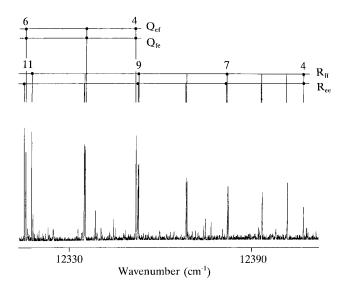


FIG. 1. A portion of the 0-0 band of the $A^{t3}\Phi_4 - X^3\Phi_4$ system of CoH near the band origin. A large perturbation at R(11) is clearly evident.

the observed lines (up to J'' = 32) were included. The combination differences are expected to be accurate to ± 0.007 cm⁻¹, so that improved molecular constants can be derived from the higher J'' data. For example, the high-J combination differences indicated the presence of a small Ω -doubling in the ground state $\Omega'' = 4$ spin component. Small differences between $\Delta_2 F_e(J)$ and $\Delta_2 F_f(J)$ are present for J'' > 13 and increase rapidly to a value of 2.165 cm⁻¹ at J'' = 25. Even though the observed minus calculated differences for the line positions are large for perturbed lines, the corresponding ground state corresponding combination differences fit within the experimental error of ± 0.007 cm⁻¹.

The band with an *R* head at 12 027 cm⁻¹ has been assigned as the 0–0 band of the $A'^3\Phi_3 - X^3\Phi_3$ subband. This subband is weaker in intensity than the $A'^{3}\Phi_{4}-X^{3}\Phi_{4}$ subband and the Q branches are not as strong as in the $A'^{3}\Phi_{4} - X^{3}\Phi_{4}$ subband. The analysis of this subband provides combination differences between a P and an R branch similar to those obtained for the $\Omega'' = 3$ spin component by Klynning and Kronekvist (15). We have arbitrarily chosen to denote these branches as R_{ee} and P_{ee} in this paper. These branches are affected by local perturbations in the excited state at several J values, most notably at J' = 17, 19, and 23. The other Ω -doubling component could only be seen in the *P* branch for $J'' \leq 14$. The corresponding R-branch lines pile up in a head and cannot be clearly picked out. We did not observe any bands with $\Delta v \neq 0$ in this subband. We also did not find evidence for the $A'^{3}\Phi_{2}-X^{3}\Phi_{2}$ subband. The rotational lines of the $A'^{3}\Phi_{4} - X^{3}\Phi_{4}$ and $A'^{3}\Phi_{3} - X^{3}\Phi_{3}$ subbands are provided in Tables 1 and 2, respectively.

Recently we have also found the analogous transition of the isovalent CoF molecule in the same general spectral region as the $A'^{3}\Phi - X^{3}\Phi$ transition of CoH. The rotational structure of this transition is similar for CoF and CoH except that a Q branch was not observed for CoF in any of the bands and the Ω -doubling was not resolved for $\Omega'' = 4$. For CoF, we also located the third ${}^{3}\Phi_{2}-X^{3}\Phi_{2}$ subband.

Since the molecular constants of the $X^3\Phi_4$ and $X^3\Phi_3$ spin components are quite different, we chose to determine the constants for the different spin components from an independent fit of the individual subbands. The observed lines of the different subbands were fitted with the following Hund's case (*c*) expression:

$$F_{v}(J) = T_{v} + B_{v}J(J+1) - D_{v}[J(J+1)]^{2} + H_{v}[J(J+1)]^{3} + L_{v}[J(J+1)]^{4} \pm \frac{1}{2} \{qJ(J+1) + q_{D}[J(J+1)]^{2} + q_{H}[J(J+1)]^{3} + q_{L}[J(J+1)]^{4} \}.$$
[1]

In addition to *B*, *D*, *H*, and *L*, the Ω -doubling constants q_H and q_L were also required in the v = 0 vibrational level of the $X^3\Phi_4$ spin component. For the v = 0 vibrational level of the excited ${}^3\Phi_4$ state the rotational constants *B*, *D*, *H*, q_H , and q_L were required to obtain a satisfactory fit. The sign of the Ω -doubling constants was arbitrarily determined by placing *e* above *f* for the two spin components of $X^3\Phi$. For the 0-0 band of the $A'{}^3\Phi_3 - X^3\Phi_3$ subband only one Ω -doubling component was fitted and the Ω -doubling constant was set to zero. The spectroscopic constants from the fit of $A'{}^3\Phi_4 - X^{}^3\Phi_4$ and $A'{}^3\Phi_3 - X^{}^3\Phi_3$ subbands are provided in Tables 3 and 4.

DISCUSSION

The recent theoretical calculation by Freindorf *et al.* (23) predicts many low-lying singlet, triplet, and quintet states giving rise to many red and infrared transitions. This calculation predicts two groups of triplet states below 1.7 eV, each composed of ${}^{3}\Phi$, ${}^{3}\Delta$, ${}^{3}\Pi$, and ${}^{3}\Sigma^{-}$ states. The first group correlates with the ground state dissociation limit $\text{Co}[{}^{4}\text{F}_{g}(d^{7}s^{2})] + \text{H}[{}^{2}\text{S}]$ while the second group dissociates to the first excited atomic limit $\text{Co}[{}^{4}\text{F}_{g}(d^{8}s^{1})] + \text{H}[{}^{2}\text{S}]$. The ground state of CoH is of ${}^{3}\Phi$ symmetry and is derived from the electronic configuration $6\sigma^{2}7\sigma^{2}d\pi^{3}d\delta^{3}$. According to this calculation the next higher excited states are ${}^{3}\Sigma^{-}$, ${}^{3}\Pi$, and ${}^{3}\Delta$ states. Allowed transitions from the ${}^{3}\Delta$ and ${}^{3}\Phi$ state are expected to be present at 10 600 and 13 100 cm⁻¹, respectively.

For both CoH and CoF we have observed several bands in the red and infrared regions of the spectrum. The analysis of a ${}^{3}\Phi - {}^{3}\Phi$ transition of CoF with the excited state ${}^{3}\Phi_{3}$ spin component at 10 300 cm⁻¹ has been completed recently (24). The CoH bands discussed in this paper belong to the analogous ${}^{3}\Phi - {}^{3}\Phi$ transition. The analysis of these bands indicates

TABLE 1 Observed Wavenumbers (in cm $^{-1}$) of the ${\cal A}'^3\Phi_4$ – $X^3\Phi_4$ Subband of CoH

	0-0 Band								
J	Ree	Pee	Rff		Pff		Qef		Qfe
4	12406.663		12406.663				12351.816		12351.816
5	12401.335	12280.531	12401.335		12280.531		12335.355		12335.355
6	12392.996 *	12249.917	12393.081		12249.917		12315.890		12315.890
7	12381.800 *	12216.350	12382.085		12216.350		12293.446	*	12293.523
8	12368.264 *	12179.882 *	12368.518		12179.971		12268.229	*	12268.511
9	12352.453 *	12140.706 *	12352.680		12140.987		12240.742	*	12240.990
10	12334.904 *	12099.354 *	12335.032	*	12099.605		12211.060	*	12211.302
11	12315.338 *	12055.905 *	12317.810	*	12056.131				
12	12291.242 *	12010.915 *	12292.468	*	12011.054	*			
13	12261.775 *	11964.143 *	12276.353	*	11966.621	*			
14	12224.868 *	11913.072 *	12263.453	*	11914.285	*			
15	12186.398 *	11856.866 *	12166.064	*	11871.481	*			
16	12148.071 *	11793.518 *	12135.740	*	11832.147	*			
17	12109.623 *	11728.895 *	12102.099	*	11708.628	*			
18	12050.221 *	11664.731 *	12066.705	*	11652.505	*			
19	12007.163 *	11600.776 *	12024.892	*	11593.420	*			
20	11962.516 *	11516.210 *	11986.180	*	11532.951	*			
21	11916.074 *	11448.360 *	11949.816	*	11466.482	*			
22	11867.160 *	11379.298 *	11907.572	*	11403.556	*			
23	11817.690 *	11308.852 *	11867.923	*	11343.384	*			
24	11764.849 *	11236.341 *	11832.142	*	11277.893	*			
25	11710.318 *	11163.715 *			11215.555	*			
26	11654.147 *	11088.170 *			11157.628	*			
27	11598.072 *	11011.394 *							
28	11534.600 *	10933.446 *							
29	11473.752 *	10856.119 *							
30	11411.122 *	10771.883 *							
31		10690.799 *							
32		10608.468 *							

J	Ree		Pee		Rff		Pff		Qef		Qfe
4	10552.116				10552.116				10497.266		10497.266
5	10548.919		10428.099		10548.919		10428.099		10482.938		10482.938
6	10543.118	*	10400.040		10543.218		10400.040		10466.016		10466.016
7	10534.898	*	10369.447		10535.177		10369.447		10446.547	*	10446.639
8	10524.743	*	10336.363	*	10525.008		10336.481		10424.698	*	10425.009
9	10512.752	*	10301.016	*	10512.985		10301.298		10401.033	*	10401.300
10	10499.455 '	*	10263.906	*	10499.567	*	10264.160				
11	10484.557	*	10225.099	*	10486.999	*	10225.351				
12	10465.485 '	*	10185.232	*	10466.765	*	10185.308	*			
13	10441.588 '	*	10143.955	*	10389.445	*	10146.355	*			
14	10410.616 '	*	10098.728	*	10377.106	*	10100.038	*			
15	10378.498 '	*	10048.975	*	10357.988	*	9996.774	*			
16	10346.952 '	*	9992.402	*	10334.369	*	9958.820	*			
17	10315.700 '	*	9934.976	*	10307.846	*	9914.397	*			
18	10263.908 '	*	9878.436	*	10279.967	*	9865.790	*			
19	10228.897	*	9822.517	*	10246.085	*	9814.629	*			
20	10192.705	*	9746.417	*	10215.703	*	9762.481	*			
21	10155.154 *	*	9687.444	*	10188.079	*	9704.739	*			
22	10115.530 *	*	9627.684	*	10154.977	*	9650.931	*			
23	10075.753 *	*	9566.950	*	10124.879	*	9600.370	*			
24	10033.069 *	*	9504.574	*			9544.831	*			
25	9989.083	*	9442.484	*			9492.884	*			
26	9943.857 *	*	9377.890	*							
27			9312.439	*							
28			9246.210	*							

* Perturbed (see text for details).

 TABLE 2

 Observed Wavenumbers (in cm⁻¹) of

 the $A'^3\Phi_3 - X^3\Phi_3$ Subband of CoH

		0-	0 Band		
J	Ree		Pee		Pff
4	12022.630	*	11908.757	*	
5	12025.663	*	11886.920	*	
6	12026.699		11863.034	*	11863.281
7	12025.459		11837.450	*	11837.745
8	12021.959		11809.869		11810.281
9	12016.179		11780.275		11780.907
10	12008.060		11748.636		11749.691
11	11997.517		11714.934		11716.871
12	11984.622		11679.151		11682.908
13	11969.343		11641.298		11650.565
14	11951.675		11601.376		11622.216
15	11931.641		11559.385		
16	11908.598	*	11515.379		
17	11884.599		11469.377		
18	11857.456	*	11420.821	*	
19	11828.708		11371.743		
20	11797.309	*	11319.964	*	
21	11763.653		11267.162		
22	11726.873		11212.210	*	
23			11155.576		
24			11096.370		

* Perturbed (see text for details).

that the excited state $\Omega' = 3$ and $\Omega' = 4$ spin components are involved in strong perturbations. We are unable to comment at this time about the nature of the perturbing states involved but, as predicted by Freindorf *et al.* (23), there should be a number of suitable triplet and quintet states present in this energy range.

The present analysis provides spectroscopic constants for the v = 0 and 1 vibrational levels of the ground state $X^3 \Phi_4$ spin component (Table 3) which have been used to obtain the ground state $\Delta G(1/2)$ interval and the equilibrium rotational constants provided in Table 5. The ground state equilibrium

TABLE 3Spectroscopic Constants (in cm⁻¹) from the $A'^3\Phi_4 - \lambda^3\Phi_4$ Subband of CoH

	Х ³ Ф.	4	$A'^3\Phi_4$		
Constants	v=0	v=1	v=0		
T _v	0.0	1858.7932(32)	12385.3049(69)		
$\mathbf{B}_{\mathbf{v}}$	7.149160(57)	6.936716(73)	5.45515(39)		
$10^4 \times D_v$	3.9913(23)	3.9767(41)	-5.684(63)		
$10^7 \times H_v$	0.0424(38)	0.1019(88)	3.80(31)		
$10^{11} \times L_{\nu}$	-1.026(23)	-1.627(61)			
$10^6 \times q_{Dv}$		2.47(31)			
$10^7 imes q_{H\nu}$	-0.0498(20)	-0.2772(95)	1.17(11)		
$10^9 \times q_{\scriptscriptstyle L\nu}$	0.02489(25)	0.04616(79)	-2.695(95)		

TABLE 4Spectroscopic Constants (in cm⁻¹) from the $A'^3 \Phi_3 - X^3 \Phi_3$ Subband of CoH

	$X^{3}\Phi_{3}$	$A'^3\Phi_3$	
Constants ^a	v=0	v=0	
T _v	728.0 ^b	12705.884(19)	
\mathbf{B}_{v}	7.28610(18)	6.37541(48)	
$0^3 \times D_v$	0.51136(62)	1.0391(33)	
$0^7 \times H_v$	-0.1419(62)	9.363(88)	
$0^{10} \times L_v$		-6.071(82)	

*Constants have been determined using only the $R_{\rm ee}$ and $P_{\rm ee}$ branches. See text for details.

^bFixed to the value of ref. 13.

constant $B_e = 7.255382(74) \text{ cm}^{-1}$ provides the equilibrium bond length of 1.531291(8) Å. Our $\Delta G(1/2)$ value of 1858.7932(32) cm⁻¹ is slightly different from the value of Lipus *et al.* (17) because they fitted the $X^3\Phi_3$ and $X^3\Phi_4$ spin components together.

An extensive search for the bands involving the remaining $X^3\Phi_2$ spin component of CoH has been unsuccessful. However, there are a large number of unassigned lines present throughout the spectrum. Most of these lines show hyperfine broadening as expected for transitions involving the Co atom. While many atomic lines are present, there are also many lines which seem to be molecular on the basis of their lineshape and intensity. There are no unassigned bandheads in this region and no obvious branch structure is present.

In the analogous transition of CoF (24) we observed the $X^3\Phi_2$ spin component of the ground state in addition to the $X^3\Phi_3$ and $X^3\Phi_4$ spin components. Interestingly the $X^3\Phi_2$ spin component of CoF was found to be perturbed. A similar situation is possible for CoH but in this case the perturbation may be much stronger. This may result in transitions with no obvious branch pattern. If this is the case, some of the numerous unassigned lines in our spectra could be due to transitions involving the $X^3\Phi_2$ spin component.

CONCLUSION

We have investigated the electronic spectra of CoH in the red and infrared using a Fourier transform spectrometer. The

TABLE 5Equilibrium Constants (in cm $^{-1}$) for the $\chi^3 \Phi_4$ Spin Component of CoH				
Constants	$X^{3}\Phi_{4}$			
B _e	7.255382(74)			
$lpha_{ m e}$	0.212444(93)			
r _e (Å)	1.531291(8)			
ΔG(1/2)	1858.7932(32)			

observed bands in the 1- μ m region have been classified into two subbands, ${}^{3}\Phi_{3}-X^{3}\Phi_{3}$ and ${}^{3}\Phi_{4}-X^{3}\Phi_{4}$, of a new electronic transition $A'{}^{3}\Phi-X^{3}\Phi$. The analysis of the 0-1 and 0-0 bands of the $A'{}^{3}\Phi_{4}-X^{3}\Phi_{4}$ subband and the 0-0 band of the $A'{}^{3}\Phi_{3}-X^{3}\Phi_{3}$ subband has been obtained and the spectroscopic constants for the different spin components have been determined. Our work is consistent with recent theoretical predictions by Freindorf *et al.* (23) and recent experimental work on the isovalent CoF molecule (24).

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