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Fourier Transform Emission Spectroscopy of the $[10.3]^3\Phi_i$–$X\,^3\Phi_i$ System of CoF

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The electronic emission spectrum of CoF was observed in the 820 nm to 3.5 μm spectral region using a Fourier transform spectrometer. The bands were excited in a carbon tube furnace by the reaction of cobalt metal vapor and CF_4 at a temperature of about 2300°C. The observed bands in the 9000–12 500 cm^{-1} region have been classified into three transitions with 0–0 bands at 10 340, 10 289, and 10 161 cm^{-1} assigned as the $^3\Phi_4$–$^3\Phi_4$, $^3\Phi_3$–$^3\Phi_3$, and $^3\Phi_2$–$^3\Phi_2$ subbands of a new $[10.3]^3\Phi_i$–$X\,^3\Phi_i$ electronic transition, respectively. The rotational analysis of 12 $^3\Phi_4$–$^3\Phi_4$ bands, 5 $^3\Phi_3$–$^3\Phi_3$ bands, and 3 $^3\Phi_2$–$^3\Phi_2$ bands has been performed, and effective equilibrium constants for each spin component have been extracted. The equilibrium vibrational and rotational constants for the lowest $X\,^3\Phi_4$ spin component are: $\omega_e = 678.1817(19)$ cm^{-1}, $\omega_e x_e = 2.73967(84)$ cm^{-1}, $B_e = 0.3894797(34)$ cm^{-1}, $\alpha_e = 0.0025984(45)$ cm^{-1}, and $r_e = 1.735698(8)$ Å.

INTRODUCTION

There has been considerable interest in the electronic spectroscopy of transition-metal-containing molecules because of their importance in high-temperature chemistry and in astrophysics. Much of the work has focused on the oxides and hydrides of transition metal elements; data for the transition metal halides are much more limited. The low-resolution work on metal halides has been summarized by Rosen (*1*) and Jones and Krishnamurty (*2*). High-resolution data are available for only a few molecules. The 3*d* transition metal fluorides for which rotational analyses are published include ScF (*3*), CrF (*4*), MnF (*5*), FeF (*6, 7*), NiF (*8, 9*), CuF (*10, 11*), and very recently CoF (*12*). The major difficulty with the study of this class of molecules is the high density of lines resulting from transitions between many electronic states with high multiplicity and high orbital angular momentum. Due to substantial spin–orbit interactions, the different spin components are far apart and frequently interact with other spin components of nearby electronic states causing perturbations. The visible spectra of these molecules are largely unclassified.

Recently we have applied high-resolution Fourier transform infrared spectroscopy to the investigation of the complex spectra of several transition metal oxides, hydrides, and nitrides. In the present work we have observed the red and near-infrared spectra of CoF using this technique. We have classified the bands observed in the 9000–12 250 cm^{-1} region into three transitions which have been assigned as the $^3\Phi_4$–$^3\Phi_4$, $^3\Phi_3$–$^3\Phi_3$, and $^3\Phi_2$–$^3\Phi_2$ subbands of a new $[10.3]^3\Phi$–$X^3\Phi$ transition. The analysis of this transition will be presented here.

There are no published theoretical calculations on the spectroscopic properties of CoF, although some are in progress (*13*). Recently Freindorf *et al.* (*14*) have performed ab initio calculations on CoH. This calculation confirms the $^3\Phi_i$ assignment of the

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ground state of CoH and predicts the presence of many low-lying electronic states below 2 eV. Since CoF should have an electronic structure similar to that of CoH, we expect that our results on CoF will be consistent with the predictions of Freindorf *et al.* (*14*). Just before we recorded the near-infrared spectra of CoF, Adam *et al.* (*12*) observed a $^3\Phi$–$^3\Phi$ transition in the visible region by laser excitation spectroscopy. Their results are also consistent with an $X^3\Phi_i$ ground state assignment for CoF.

EXPERIMENTAL DETAILS

The emission spectra of CoH and CoF in the red and near-infrared regions were observed using a carbon tube furnace (King furnace). Our first experiment was a search for CoH bands using the reaction of Co metal and H_2 at a temperature of 2300°C. On the basis of both experimental and theoretical work, several electronic transitions of CoH are expected in the red and infrared regions (*14–16*). As predicted in detail by Freindorf *et al.* (*14*), we found several transitions of CoH in the region 3000–12 250 cm^{-1} and our analysis will be published separately.

Encouraged by the theoretical work on CoH and our success in measuring the red and infrared transitions of CoH, we decided to search for the corresponding spectra of CoF. The King furnace was operated with 100 Torr of He buffer gas and several Torr of CF_4 at 2300°C to make CoF. As expected, we observed strong emission bands of CoF in the region 3000–12 250 cm^{-1}. The emitter of these bands was easily established by the spacing of the rotational lines and the vibrational intervals observed.

The emission from the furnace was observed with the 1-m Fourier transform spectrometer associated with the McMath-Pierce solar telescope of the National Solar Observatory at Kitt Peak. The spectra of CoF were recorded in two parts. For the 3000–9100 cm^{-1} region the spectrometer was operated with a CaF_2 beam splitter, silicon filters, InSb detectors, and three scans were coadded in 10 min of integration. The lower wavenumber limit was set by cold green glass (U) filters in front of the InSb detectors. For the spectral region 8500–12 500 cm^{-1} the spectrometer was operated with a RG850 red pass filter and Si-photodiode detectors. This time only two scans were sufficient to record the spectra with a good signal-to-noise ratio. In both of these experiments the spectrometer resolution was set to 0.026 cm^{-1}.

In addition to CoF the observed spectra also contained the vibration–rotation transitions of HF. The CoF spectra have been calibrated using the HF line measurements of LeBlanc *et al.* (*17*). The CoF lines have been observed with a maximum signal-to-noise ratio of 20 and have a width of 0.035 cm^{-1}. This limits the precision of our measurements of the strong and unblended molecular transitions to ± 0.001 cm^{-1}. The bands involving higher vibrational levels are much weaker in intensity and are frequently overlapped by stronger bands so that the precision of these measurements is reduced to ± 0.003 cm^{-1}.

RESULTS

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

The observed spectra of CoF consist of many bands spread from 3000 to 12 500 cm^{-1}. The present paper deals with the analysis of a strong transition observed in the region 9000–12 500 cm^{-1}, which has been assigned as the $[10.3]^3\Phi$–$X^3\Phi$ transition.

Instead of using the conventional "letter" notation for the excited state, we have chosen to label it with the band origin in square brackets (in units of 10^3 cm^{-1}) followed by the conventional term symbol. The letter notation is not suitable because there are a number of unassigned electronic states below the $[10.3]^3\Phi$ excited state. In the present case the number in the brackets corresponds to the 0–0 band origin of the middle $^3\Phi_3$ spin component. There are many relatively weak bands between 3000 and 9000 cm^{-1} which probably belong to more than one transition. The analysis of these bands will be presented in a future publication.

The observed spectrum in the region 9000–12 500 cm^{-1} has been classified into three subbands with the 0–0 bands at 10 340, 10 289, and 10 161 cm^{-1}. These bands have been assigned as the three $\Delta\Omega = 0$ subbands of a $^3\Phi-^3\Phi$ transition. A portion of the compressed spectrum of CoF, showing the 0–0 bands of the three subbands, is presented in Fig. 1. As can be observed in this figure, the $^3\Phi_4-^3\Phi_4$ subband is the strongest of the three subbands. This observation is consistent with the $X\,^3\Phi_4$ spin component lying lowest in energy, implying an inverted $X\,^3\Phi_i$ state. This conclusion has been confirmed by rotational analysis of these bands. Our analysis indicates that there is no observable Ω-doubling in the bands involving the $X\,^3\Phi_4$ spin component. The $X\,^3\Phi_3$ and $X\,^3\Phi_2$ spin components have resolved Ω-doubling, but as expected, the Ω-doubling in the $X\,^3\Phi_3$ spin component is smaller than that in the $X\,^3\Phi_2$ spin component. These observations are also consistent with data available for CoH (*16*).

We have analyzed 12 bands in the $^3\Phi_4-^3\Phi_4$ subband involving ground state vibrational levels up to $v'' = 2$ and excited state vibrational levels up to $v' = 5$. The rotational structure of each of these bands consists of a single *P* and a single *R* branch. There is no evidence of Ω-doubling in the lines of this subband. The *Q*-branch lines of a $\Delta\Omega = 0$ (with $\Omega \neq 0$) transition are expected to be relatively weak compared with the *R* and *P* branches and they were not detected. The lines in the stronger bands could be followed up to *J* values as high as 137. A part of the 1–0 band of this subband near the *R* head is presented in Fig. 2. Even though we could not observe the first lines of the *R* and *P* branches, the observation of several bands with common vibrational levels in the ground and excited states permits us to obtain an unambiguous assignment

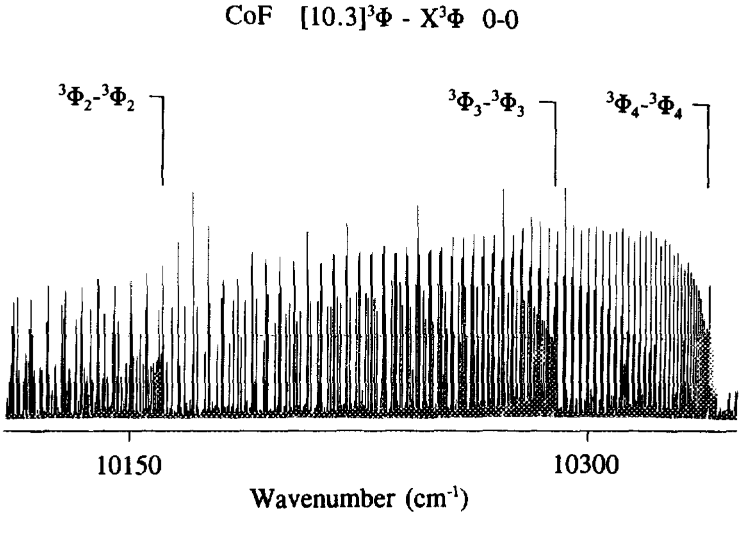

FIG. 1. A portion of the compressed spectrum of CoF showing the 0–0 bands of the three subbands.

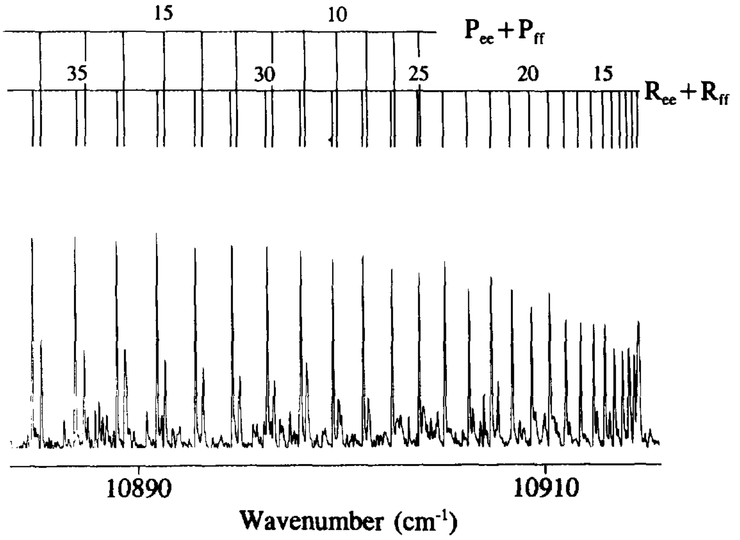

FIG. 2. A portion of the 1–0 band of the [10.3]$^3\Phi_4$–$X^3\Phi_4$ subband near the *R* head.

of the rotational lines. No rotational perturbations have been observed in any of the analyzed bands of this subband.

On the lower wavenumber side of the $^3\Phi_4$–$^3\Phi_4$ 0–0 band, a band with an *R* head at 10 289.2 cm^{-1} has been identified as the 0–0 band of the $^3\Phi_3$–$^3\Phi_3$ subband. Four more bands with *R* heads at 9621, 10 866, 10 770, and 11 439 cm^{-1} have been assigned as the 0–1, 1–0, 2–0, and 2–1 bands of this transition, respectively. The rotational analysis of all of these bands has been performed. It is expected for a $^3\Phi_3$–$^3\Phi_3$ transition that the Ω-doubling in the rotational lines, if present at all, should be observed only for high-*J* transitions. Our analysis of this subband indicates that the Ω-doubling in the 0–0 band is resolved only for *J* values larger than 61. An interesting feature of this subsystem is the observation of perturbations in the $v = 1$ vibrational level of the ground electronic state. The *f*-parity levels of the ground $^3\Phi_3$ spin component for the $v = 1$ vibrational level are affected by a perturbation at $J = 55$. Another perturbation was observed for both *e* and *f*-parity components of the $v = 0$ vibrational level of the excited $^3\Phi_3$ state at $J = 83$. The perturbed lines were not included in the final fit.

The band with an *R* head at 10 161.2 cm^{-1} has been assigned as the 0–0 band of the $^3\Phi_2$–$^3\Phi_2$ subband. This subband is the least intense of the three observed subbands and only the 0–1, 0–0, and 1–0 vibrational bands were identified. A careful inspection of the 0–0 band of this subband indicates that the Ω-doubling is resolved at the relatively low *J* value of 30. The ground $^3\Phi_2$ spin component is also perturbed. In this case the $v = 0$ vibrational level of the $X^3\Phi_2$ spin component is perturbed at $J = 36$ but the perturbation affects only the *f*-parity rotational energy levels.

The observed rotational lines in the different bands of the $^3\Phi_4$–$^3\Phi_4$, $^3\Phi_3$–$^3\Phi_3$, and $^3\Phi_2$–$^3\Phi_2$ subbands are provided in Tables I, II, and III, respectively. In the absence of the satellite branches or transitions with $\Delta\Sigma \neq 0$, we were unable to determine a single set of molecular constants by fitting the observed wavenumbers to a Hund's case (a) Hamiltonian. Rather than obtaining a combined fit for all of the subbands with assumed values for the spin–orbit (A_v) and spin–spin (λ_v) parameters, we decided to obtain an independent fit of each subband by fitting the observed line positions to the following Hund's case (c) expression:

TABLE I

Observed Wavenumbers (in cm^{-1}) of the Heads of the $[10.3]^3\Phi_4$–$X^3\Phi_4$ Subband of CoF

	0-2				0-1				0-0				1-0				2-0				2-1			
J	Ree+Rff	O-C	Pee+Pff	O-C	Ree+Rff	O-C	Pee+Pff	O-C	Ree+Rff	O-C	Pee+Pff	O-C	Ree+Rff	O-C	Pee+Pff	O-C	Ree+Rff	O-C	Pee+Pff	O-C	Ree+Rff	O-C	Pee+Pff	O-C
7											10329.224	-9			10904.045	-7								
8											10327.943	-4			10902.728	-1								
9											10326.593	5			10901.326	-1	11483.847	6	11470.679	-3				
10											10325.150	-7	10914.487	-14	10899.837	-10	11483.704	6	11469.152	-4				
11									10339.824	1	10323.648	-4	10914.344	7			11483.479	8	11467.550	6	10811.172	-4		
12					9667.442	12			10339.641	-10	10322.079	4	10914.096	1	10896.649	-4	11483.165	4	11465.851	1	10810.935	-5		
13					9667.276	12			10339.399	-6	10320.420	-5	10913.777	1	10894.931	-9	11482.770	3	11464.079	5	10810.621	-5	10791.923	-10
14			8980.162	-11	9667.037	4			10339.085	-2	10318.700	-2	10913.382	5	10893.149	2	11482.293	4	11462.199	-13	10810.234	-1	10790.145	-13
15			8978.561	-15	9666.736	2			10338.693	-2	10316.905	-2	10912.896	-4	10891.284	7	11481.736	8	11460.272	4	10809.771	5	10788.306	-1
16	9000.111	0	8976.895	-25	9666.369	2			10338.229	-1	10315.037	-1	10912.348	4	10889.323	-6	11481.090	8	11458.243	2	10809.224	4	10786.381	3
17	8999.799	-0	8975.196	-8	9665.940	5			10337.691	-1	10313.102	4	10911.712	1	10887.305	3	11480.350	-3	11456.131	1	10808.590	-6	10784.360	-12
18	8999.433	7	8973.418	-11	9665.435	0			10337.083	2	10311.085	1	10910.999	1	10885.200	2	11479.533	-7	11453.938	3	10807.915	20	10782.288	-2
19	8998.987	-6	8971.587	-6	9664.878	9			10336.396	-1	10308.996	-1	10910.210	2	10883.017	1	11478.643	-1	11451.658	0	10807.119	3	10780.126	-4
20	8998.490	-10	8969.683	-15	9664.241	7	9635.432	-1	10335.636	-3	10306.837	-1	10909.337	-1	10880.758	3	11477.678	14	11449.303	5	10806.268	9	10777.894	1
21	8997.939	-8	8967.743	-0	9663.539	5	9633.332	1	10334.806	-3	10304.609	3	10908.388	-2	10878.420	3	11476.610	11	11446.856	2	10805.316	-8	10775.587	8
22	8997.342	10	8965.732	3	9662.764	-2	9631.164	1	10333.905	-0	10302.297	-5	10907.361	-4	10876.001	0	11475.454	2	11444.329	3	10804.320	7	10773.185	-2
23	8996.673	15	8963.659	3	9661.931	-0	9628.920	-8	10332.921	-7	10299.924	-1	10906.261	1	10873.508	1	11474.221	0	11441.717	1	10803.216	-7	10770.707	-12
24	8995.931	6	8961.518	-3	9661.031	2	9626.626	-1	10331.877	-1	10297.474	-2	10905.076	-1	10870.934	-0	11472.905	-0	11439.024	1	10802.054	-3	10768.192	18
25	8995.132	3	8959.331	3	9660.063	3	9624.255	-4	10330.753	-2	10294.949	-4	10903.815	0	10868.283	-2	11471.507	1	11436.246	1	10800.815	3		
26	8994.283	9	8957.087	13	9659.019	-5	9621.821	-4	10329.555	-3	10292.358	-1	10902.476	2	10865.556	0	11470.023	-0	11433.386	0	10799.488	-2	10762.858	6
27	8993.370	12	8954.760	-1	9657.925	3	9619.325	0	10328.284	-4	10289.691	0	10901.056	1	10862.749	-1	11468.458	1	11430.442	-0	10798.091	1	10760.075	-0
28	8992.388	6	8952.386	-1	9656.751	-1	9616.755	-2	10326.944	-2	10286.948	-3	10899.558	1	10859.864	-2	11466.809	3	11427.418	2	10796.610	-3	10757.216	-7
29	8991.345	-1	8949.959	4	9655.518	4	9614.125	1	10325.524	-4	10284.137	-1	10897.979	-2	10856.906	1	11465.070	-2	11424.318	12	10795.056	-1	10754.295	2
30	8990.256	8	8947.474	13	9654.213	2	9611.426	2	10324.037	-2	10281.249	-3	10896.326	-0	10853.861	-4	11463.253	-0	11421.116	2	10793.424	-1	10751.284	-1
31	8989.099	10	8944.914	5	9652.838	-1	9608.660	2	10322.475	-1	10278.296	1	10894.592	-1	10850.745	-2	11461.351	-0	11417.842	4	10791.712	-2	10748.202	1
32	8987.878	8	8942.306	11	9651.399	-1	9605.826	0	10320.839	-0	10275.262	-2	10892.783	2	10847.561	9	11459.366	1	11414.478	-1	10789.928	1	10745.040	0
33	8986.596	5	8939.633	10	9649.893	-2	9602.927	1	10319.127	-2	10272.160	-1	10890.891	1	10844.279	0	11457.295	-0	11411.032	-5	10788.062	1	10741.810	8
34	8985.254	4	8936.894	4	9648.322	1	9599.964	2	10317.343	-3	10268.984	-2	10888.921	0	10840.928	1	11455.143	1	11407.514	2	10786.117	-0	10738.490	3
35	8983.857	8	8934.098	1	9646.681	-1	9596.932	2	10315.488	-2	10265.738	0	10886.872	-1	10837.504	6	11452.902	-2	11403.901	-3	10784.092	-4	10735.092	-4
36	8982.398	12	8931.250	6	9644.971	-4	9593.837	5	10313.557	-2	10262.415	-2	10884.746	0	10833.993	1	11450.581	-1	11400.213	0	10782.001	4	10731.624	-3
37	8980.874	11	8928.324	-6	9643.197	-3	9590.670	2	10311.553	-3	10259.022	-2	10882.540	-1	10830.408	1	11448.178	2	11396.440	2	10779.811	-10	10728.077	-5
38	8979.283	5	8925.368	10	9641.356	-3	9587.440	3	10309.476	-4	10255.557	-1	10880.257	1	10826.741	-4	11445.688	1	11392.582	1	10777.568	1	10724.458	-3
39	8977.636	3	8922.333	9	9639.449	-1	9584.149	8	10307.327	-2	10252.018	-2	10877.892	-2	10823.006	1	11443.113	-1	11388.637	-4	10775.227	-7	10720.764	3
40	8975.939	13	8919.228	-3	9637.472	-1	9580.781	3	10305.102	-3	10248.408	-1	10875.451	-1	10819.178	-9	11440.457	1	11384.616	-1	10772.822	-3	10716.999	13
41	8974.160	2	8916.074	-2	9635.432	2	9577.349	-0	10302.806	-1	10244.717	-9	10872.931	-1	10815.300	9	11437.712	-3	11380.512	1	10770.339	2	10713.143	10
42	8972.332	4	8912.864	2	9633.322	3	9573.853	-0	10300.436	-0	10240.970	-0	10870.332	-0	10811.317	-1	11434.887	-2	11376.318	-4	10767.774	2	10709.202	-2
43	8970.434	-4	8909.591	2	9631.149	8	9570.295	3	10297.992	-1	10237.143	-0	10867.654	-1	10807.267	0	11431.978	-2	11372.051	2	10765.111	-18	10705.195	-4
44	8968.483	-4	8906.257	3	9628.903	7	9566.667	3	10295.473	-2	10233.242	0	10864.896	-1	10803.135	-3	11428.985	-2	11367.692	-3	10762.400	-8	10701.115	-2
45	8966.475	2	8902.863	3	9626.591	8	9562.973	3	10292.882	-1	10229.268	-1	10862.062	-0	10798.932	1	11425.907	-2	11363.253	-3	10759.601	-8	10696.959	2
46	8964.402	3	8899.410	5	9624.207	3	9559.212	3	10290.217	-1	10225.222	-2	10859.148	-0	10794.646	-1	11422.752	5	11358.739	3	10756.734	0		
47	8962.262	-2	8895.887	-3	9621.752	-4	9555.386	3	10287.477	-2	10221.105	-1	10856.156	1	10790.286	1	11419.496	-7	11354.132	0	10753.776	-3	10688.408	-1
48	8960.065	-1	8892.316	2	9619.238	-3	9551.494	4	10284.667	-1	10216.914	-2	10853.083	0	10785.848	2	11416.173	0	11349.446	1	10750.739	-8	10684.016	-3
49	8957.805	-2	8888.662	-16	9616.657	-2	9547.536	5	10281.779	-3	10212.650	-3	10849.932	-0	10781.327	-1	11412.759	-0	11344.675	-1	10747.640	3	10679.551	-3
50	8955.480	-7	8884.975	-8	9614.008	-2	9543.508	2	10278.820	-2	10208.315	-3	10846.703	1	10776.734	1	11409.260	-2	11339.825	2	10744.447	-2	10675.008	-4

TABLE I—*Continued*

	0-2				0-1				0-0				1-0				2-0				2-1			
J	Ree+Rff	O-C	Pee+Pff	O-C	Ree+Rff	O-C	Pee+Pff	O-C	Ree+Rff	O-C	Pee+Pff	O-C	Ree+Rff	O-C	Pee+Pff	O-C	Ree+Rff	O-C	Pee+Pff	O-C	Ree+Rff	O-C	Pee+Pff	O-C
51	8953.100	-5	8881.217	-10	9611.293	0	9539.420	5	10275.784	-4	10203.910	-1	10843.393	-0	10772.062	1	11405.682	2	11334.889	0	10741.189	5	10670.391	-2
52	8950.662	0	8877.401	-10	9608.510	1	9535.257	-0	10272.691	9	10199.428	-3	10840.006	0	10767.315	4	11402.014	-0	11329.871	1	10737.842	1	10665.696	-1
53	8948.153	-4	8873.538	5	9605.669	12	9531.033	-1	10269.499	-3	10194.878	-1	10836.541	1	10762.481	-2	11398.263	-1	11324.772	2	10734.420	0	10660.925	-0
54	8945.590	0			9602.743	6	9526.746	2	10266.243	-5	10190.252	-2	10832.989	-5	10757.578	1	11394.437	6	11319.586	-0	10730.917	-4	10656.074	-2
55	8942.957	-5	8865.607	7	9599.753	2	9522.391	2	10262.918	-2	10185.553	-4	10829.370	0	10752.596	1	11390.512	-1	11314.320	-0	10727.341	-4	10651.146	-6
56	8940.268	-4	8861.538	-4	9596.696	-1	9517.973	6	10259.518	-0	10180.784	-4	10825.668	1	10747.524	-10	11386.513	2	11308.972	1	10723.686	-4	10646.143	-7
57	8937.520	-0	8857.425	1	9593.576	1	9513.480	2	10256.040	-2			10821.885	0	10742.397	1	11382.426	1	11303.539	-0	10719.961	4	10641.081	9
58	8934.701	-7	8853.249	3	9590.391	5	9508.924	-1	10252.492	-2	10171.028	-4	10818.028	4	10737.180	-1	11378.257	2	11298.026	1	10716.149	2	10635.911	-7
59	8931.837	4	8849.009	1	9587.129	0	9504.306	1	10248.868	-3	10166.052	6	10814.084	-0	10731.888	0	11373.999	-1	11292.428	-0	10712.257	-2	10630.684	-2
60	8928.895	-2	8844.709	-1	9583.806	1	9499.618	-0	10245.172	-2	10160.979	-9	10810.065	0	10726.516	-2	11369.663	1	11286.751	3	10708.304	11	10625.378	-1
61	8925.896	-3	8840.339	-12	9580.414	1	9494.866	0	10241.400	-4	10155.856	-0	10805.967	0	10721.068	-1	11365.238	-1	11280.983	-3	10704.253	3	10619.994	-2
62	8922.837	-2	8835.932	-1	9576.954	-0	9490.039	-8	10237.556	-3	10150.654	1	10801.786	-3	10715.543	-0	11360.737	4	11275.141	-0	10700.129	1	10614.532	-4
63	8919.716	-2	8831.446	-8	9573.426	-1	9485.159	-4	10233.640	-1	10145.375	-2	10797.535	1	10709.939	-1	11356.144	1	11269.215	2	10695.927	-1	10608.994	-6
64	8916.529	-5	8826.913	-2	9569.831	-1	9480.213	-0	10229.648	-1	10140.035	5	10793.200	1	10704.253	-7	11351.469	2	11263.205	1	10691.636	5	10603.392	5
65	8913.295	6	8822.320	4	9566.164	-6	9475.191	-6	10225.584	1	10134.608	-1	10788.786	1	10698.503	1	11346.712	3	11257.112	2	10687.295	-1	10597.694	-4
66	8909.978	-5	8817.662	5	9562.439	-2	9470.114	-0	10221.450	6	10129.119	2	10784.290	-1	10692.677	10	11341.868	3	11250.936	0	10682.866	4	10591.928	-5
67	8906.611	-5	8812.930	-9	9558.646	2	9464.963	-4	10217.230	-0	10123.547	-6	10779.718	-1	10686.755	1	11336.934	-4	11244.677	-1	10678.355	4	10586.089	-2
68	8903.207	21	8808.165	5	9554.781	2	9459.754	2	10212.942	-1	10117.916	-0	10775.073	4	10680.766	2	11331.929	3	11238.340	2	10673.762	-1	10580.176	2
69	8899.717	22	8803.319	-2	9550.848	2	9454.476	3	10208.576	-5	10112.206	-1	10770.339	1	10674.699	3	11326.832	2	11231.922	7	10669.093	-3	10574.184	4
70	8896.147	5	8798.420	-2	9546.845	-1	9449.126	-0	10204.144	-1	10106.426	0	10765.531	2	10668.550	-2	11321.652	1	11225.406	-4	10664.349	-2	10568.109	-1
71	8892.525	-3	8793.481	16	9542.779	2	9443.711	-3	10199.636	-0	10100.576	3	10760.645	5	10662.329	-1	11316.383	-4	11218.820	-3	10659.524	-5	10561.971	6
72	8888.851	-1	8788.441	-5	9538.644	2	9438.234	-2	10195.052	-0	10094.648	1	10755.672	-2	10656.036	5	11311.041	2	11212.152	-1	10654.627	-2	10555.741	-1
73	8885.116	2	8783.388	20	9534.431	-8	9432.689	-4	10190.397	1	10088.647	-2	10750.628	1	10649.654	-0	11305.607	-0	11205.402	2	10649.654	3	10549.443	-1
74	8881.313	-3	8778.225	-5	9530.169	0	9427.087	3	10185.662	-2	10082.577	-2	10745.501	1	10643.200	-0	11300.096	6	11198.565	0	10644.593	-2	10543.070	0
75	8877.443	-12	8773.039	5	9525.831	1	9421.405	-3	10180.854	-5	10076.437	0	10740.296	-0	10636.669	1	11294.490	-0	11191.648	-0	10639.444	-17	10536.614	-6
76			8767.778	1	9521.424	0	9415.668	1	10175.960	-20	10070.220	-3	10735.011	-1	10630.059	-1	11288.804	-1	11184.642	-7	10634.247	-3	10530.091	-3
77	8869.554	4	8762.470	9	9516.951	1	9409.861	0			10063.930	-7	10729.651	2	10623.368	-5	11283.037	1	11177.568	1	10628.961	0	10523.485	-7
78	8865.507	1	8757.097	12	9512.411	2	9403.987	-1	10166.000	1	10057.574	-4	10724.208	1	10616.611	1	11277.184	1	11170.413	10	10623.596	3	10516.808	-6
79	8861.400	0			9507.802	2	9398.051	1	10160.896	-1	10051.145	-3	10718.685	-1	10609.767	-4	11271.246	0	11163.159	2	10618.149	1	10510.060	0
80	8857.242	10	8746.154	-1	9503.126	3	9392.047	1	10155.719	-3	10044.643	-2	10713.091	5	10602.854	1	11265.226	1	11155.825	-4	10612.620	-6	10503.231	1
81	8853.014	11	8740.603	2	9498.376	-2	9385.972	-4	10150.472	-0	10038.067	-3	10707.408	2	10595.858	-1	11259.120	1	11148.420	1	10607.027	2	10496.329	4
82	8848.733	20	8734.999	11	9493.569	3	9379.840	-1	10145.148	-1	10031.420	-3	10701.644	-4	10588.788	1	11252.929	-1	11140.929	3	10601.337	-10	10489.347	3
83	8844.364	2	8729.329	14	9488.691	5	9373.642	2	10139.744	-6	10024.699	-6	10695.807	-3	10581.638	0	11246.657	1	11133.362	10	10595.592	0	10482.286	-2
84	8839.970	21	8723.584	0	9483.740	2	9367.377	4	10134.278	-0	10017.916	3	10689.893	0	10574.412	-0	11240.303	5	11125.697	2	10589.767	9	10475.164	10
85	8835.483	9	8717.799	6	9478.721	-3	9361.040	-1	10128.730	-2	10011.051	1	10683.895	-1	10567.104	-5	11233.857	2	11117.957	2	10583.846	-1	10467.941	-5
86	8830.936	-3	8711.935	-8	9473.643	2	9354.645	1	10123.113	1	10004.114	-1	10677.822	1	10559.739	10	11227.330	1	11110.133	-1	10577.857	-1	10460.670	7
87	8826.341	-1	8706.038	5	9468.495	5	9348.180	-1	10117.417	-1	9997.108	-0	10671.669	2	10552.273	0	11220.719	-0	11102.229	-2	10571.799	7	10453.306	2
88	8821.685	0	8700.059	-5	9463.278	5	9341.658	5	10111.648	-1	9990.029	-0	10665.430	-3	10544.739	1	11214.020	-4	11094.245	-1	10565.650	2	10445.870	-0
89	8816.970	5			9457.980	-7	9335.059	-0	10105.808	2	9982.881	2	10659.123	2	10537.129	1	11207.245	-1	11086.180	1	10559.416	-10	10438.366	5
90	8812.177	-8			9452.637	3	9328.404	4	10099.889	-1	9975.658	2	10652.729	0	10529.442	2	11200.386	3	11078.033	2	10553.130	3	10430.779	3
91	8807.335	-8			9447.227	13	9321.676	0	10093.897	-2	9968.361	-1	10646.259	2	10521.675	0	11193.438	2	11069.798	-2	10546.768	17	10423.113	-2
92	8802.421	-18			9441.728	2	9314.888	1	10087.828	-6	9960.994	-1	10639.704	-3	10513.835	1	11186.405	-1	11061.488	1	10540.297	-1	10415.358	-22
93	8797.474	-1			9436.177	7	9308.035	3	10081.692	-3	9953.553	-3	10633.079	1	10505.913	-2	11179.292	2	11053.092	-1	10533.770	4	10407.571	2
94	8792.452	4			9430.550	3	9301.112	-0	10075.477	-4	9946.046	0	10626.370	0	10497.919	0	11172.095	3	11044.624	7	10527.158	-0	10399.688	4

TABLE I—*Continued*

J	0-2				0-1				0-0				1-0				2-0				2-1			
	Ree+Rff	O-C	Pee+Pff	O-C	Ree+Rff	O-C	Pee+Pff	O-C	Ree+Rff	O-C	Pee+Pff	O-C	Ree+Rff	O-C	Pee+Pff	O-C	Ree+Rff	O-C	Pee+Pff	O-C	Ree+Rff	O-C	Pee+Pff	O-C
95					9424.860	3	9294.125	-2	10069.194	0	9938.461	-3	10619.581	-1	10489.847	0	11164.811	2	11036.060	1	10520.474	2	10391.722	-1
96	8782.219	7			9419.099	-1	9287.079	2	10062.829	-2	9930.808	-2	10612.716	1	10481.698	0	11157.440	-1	11027.419	-1	10513.698	-11	10383.689	1
97	8776.993	-7			9413.277	2	9279.964	1	10056.395	-1	9923.084	1	10605.770	1	10473.468	-4	11149.989	-1	11018.706	8	10506.864	-5	10375.579	1
98	8771.737	9			9407.383	1	9272.786	3	10049.880	-5	9915.287	1	10598.731	-13	10465.178	9	11142.457	2	11009.896	0	10499.959	7	10367.392	-1
99	8766.393	-1			9401.429	6	9265.536	-3	10043.297	-4	9907.414	-3	10591.639	-1	10456.796	5	11134.836	1	11001.011	0	10492.957	-1	10359.135	2
100					9395.394	-3	9258.231	1	10036.643	1	9899.477	2	10584.458	1	10448.334	0	11127.137	5	10992.044	-1	10485.885	-1	10350.799	-1
101					9389.304	1	9250.857	0	10029.909	-0	9891.463	1	10577.196	2	10439.797	-5	11119.346	2	10983.000	3	10478.734	-5	10342.383	-8
102					9383.144	2	9243.417	-1	10023.103	1	9883.378	-0	10569.853	1	10431.193	0	11111.478	4	10973.867	-1	10471.498	-16	10333.905	-3
103					9376.912	-2	9235.916	0	10016.219	-1	9875.224	2	10562.431	-1	10422.505	-1	11103.517	-1	10964.654	-3	10464.208	-4	10325.346	-5
104					9370.618	-1	9228.338	-11	10009.267	3	9866.998	4	10554.931	-1	10413.744	-0	11095.474	-5	10955.362	-4	10456.829	-5	10316.709	-11
105					9364.257	-2	9220.716	-2	10002.234	-2	9858.701	7	10547.355	2	10404.905	-1	11087.356	-0			10449.377	-3	10308.015	-1
106					9357.828	-2	9213.018	-4	9995.126	-5	9850.323	-1	10539.699	4	10395.990	-1	11079.137	-12	10936.533	-5	10441.837	-11		0
107					9351.333	-2	9205.260	-4	9987.950	-3	9841.884	3	10531.954	-4	10387.000	2	11070.866	7	10927.001	-1	10434.244	3	10290.377	-8
108					9344.773	-1	9197.432	-8	9980.696	-4	9833.369	2	10524.144	2	10377.934	3	11062.486	3	10917.383	-2	10426.549	-7	10281.460	2
109					9338.149	4	9189.561	8	9973.374	-0	9824.778	-4	10516.245	-2	10368.782	-4	11054.027	2			10418.799	2	10272.454	-4
110					9331.449	-2	9181.603	1	9965.978	5	9816.120	-5	10508.271	-1	10359.564	-2	11045.485	2			10410.963	2		
111					9324.706	15	9173.587	-2	9958.503	5	9807.395	-0	10500.218	-2	10350.270	1	11036.860	3						
112					9317.875	10	9165.516	5	9950.951	2	9798.603	7	10492.085	-2	10340.891	-4	11028.152	5						
113					9310.996	25	9157.388	18			9789.726	2	10483.876	-1	10331.440	-6	11019.356	3						
114									9935.632	4	9780.779	-3	10475.584	-2	10321.917	-4	11010.478	2						
115									9927.848	-8	9771.768	0	10467.216	-1	10312.316	-2	11001.522	7						
116									9920.013	2	9762.685	3	10458.768	-1	10302.643	2	10992.473	3						
117											9753.529	3	10450.240	-3	10292.882	-5	10983.341	-1						
118									9904.092	-5	9744.298	-1	10441.636	-1	10283.057	-1	10974.137	6						
119									9896.022	-8	9735.005	5	10432.960	7	10273.148	-4	10964.841	6						
120									9887.888	1	9725.627	-3	10424.187	-3	10263.182	12	10955.453	-3						
121											9716.179	-10	10415.358	10	10253.109	-4	10945.989	-6						
122									9871.381	0	9706.676	-1	10406.425	-2	10242.973	-7	10936.445	-4						
123									9863.009	-7	9697.090	-5	10397.427	-1	10232.774	3	10926.812	-8						
124									9854.585	7	9687.446	5	10388.341	-8	10222.494	7	10917.109	2						
125									9846.067	1	9677.710	-6	10379.196	3	10212.121	-6								
126									9837.482	2			10369.960	3	10201.693	1								
127									9828.817	-3			10360.644	0	10191.188	7								
128									9820.093	7			10351.253	2	10180.602	7								
129									9811.286	8			10341.802	22	10169.941	8								
130									9802.399	3			10332.230	0	10159.195	-1								
131													10322.590	-12	10148.398	14								
132									9784.409	-3			10312.883	-13										
133									9775.316	8			10303.105	-6										
134									9766.126	-6			10293.247	-1										
135									9756.888	6			10283.309	2										
136									9747.554	-4			10273.292	5										
137									9738.151	-9														

TABLE I—*Continued*

	2-2				3-0				3-1				4-1				4-2				5-2			
J	Ree+Rff	O-C	Pee+Pff	O-C	Ree+Rff	O-C	Pee+Pff	O-C	Ree+Rff	O-C	Pee+Pff	O-C	Ree+Rff	O-C	Pee+Pff	O-C	Ree+Rff	O-C	Pee+Pff	O-C	Ree+Rff	O-C	Pee+Pff	O-C
6							12038.907	14																
7																								
8					12047.876	5	12036.196	8					11934.062	-5										
9					12047.758	-2	12034.718	16					11933.959	-1										
10					12047.544	-16							11933.759	-4							11820.239	-12	11806.024	-12
11					12047.266	-3	12031.477	14	11374.982	7											11819.970	-14	11804.416	1
12	10144.260	-12			12046.900	9	12029.740	28	11374.673	2			11933.105	-2	11916.065	7	11266.441	1			11819.619	-11	11802.703	-7
13	10144.036	-16			12046.416	-7	12027.888	16	11374.271	-13	11355.726	-6	11932.639	-9	11914.240	4	11266.059	-14			11819.177	-14	11800.936	18
14	10143.733	-26			12045.858	-9	12025.949	6	11373.803	-10	11353.890	1	11932.103	2	11912.336	10	11265.618	-6	11245.838	-13	11818.665	-0	11799.038	-3
15	10143.384	-13			12045.211	-11	12023.915	-10	11373.246	-14	11351.961	-3	11931.454	-11	11910.323	-5	11265.085	-10	11243.949	-11	11818.047	-7	11797.069	-9
16	10142.965	2					12021.830	11	11372.620	-5	11349.958	1	11930.742	1	11908.251	8	11264.474	-11	11241.986	-1	11817.344	-12	11795.023	-6
17	10142.461	1			12043.659	-6	12019.628	4	11371.899	-8	11347.867	-0	11929.928	-1	11906.079	8	11263.782	-12	11239.933	-2	11816.568	-5	11792.895	1
18	10141.887	2			12042.753	1	12017.330	-11	11371.104	-2	11345.694	-1	11929.035	5	11903.821	10	11263.015	-6	11237.796	-6	11815.708	6	11790.677	3
19	10141.243	3			12041.756	5	12014.970	-0	11370.223	0	11343.440	-1	11928.043	-0	11901.470	6	11262.162	-6	11235.584	-4	11814.740	-6	11788.373	6
20	10140.528	4			12040.664	3	12012.505	-5	11369.251	-5	11341.103	-1	11926.960	-8	11899.036	8	11261.242	9	11233.288	-5	11813.698	-5	11785.971	-4
21	10139.744	7	10109.983	-7	12039.473	-9	12009.961	0	11368.206	-1	11338.675	-11	11925.803	-1	11896.512	6	11260.231	14			11812.576	1	11783.502	4
22	10138.893	14	10107.761	8	12038.214	-0	12007.311	-13	11367.074	-1	11336.184	-0	11924.551	-2	11893.890	-6	11259.120	1	11228.462	-0	11811.358	-1	11780.940	7
23	10137.940	-10	10105.444	-2	12036.859	2	12004.600	2	11365.856	-4	11333.601	0	11923.215	1	11891.209	10	11257.941	-0	11225.931	5	11810.060	2	11778.287	4
24	10136.953	2			12035.416	5	12001.788	4	11364.557	-5	11330.937	2			11888.407	-7	11256.684	3	11223.317	9	11808.670	0	11775.550	2
25	10135.879	-2			12033.870	-6	11998.882	0	11363.172	-10	11328.184	-3	11920.272	1	11885.541	-0	11255.327	-14	11220.611	1	11807.202	7	11772.731	4
26	10134.727	-13	10098.113	12	12032.246	-6	11995.898	7	11361.719	0	11325.355	-2	11918.673	5	11882.578	-3	11253.904	-14	11217.819	-13	11805.645	11	11769.821	2
27	10133.536	9	10095.505	-7	12030.541	2	11992.820	8	11360.167	-5	11322.453	8	11916.979	2	11879.520	-15	11252.416	3	11214.969	-3	11803.977	-9	11766.832	6
28	10132.243	0	10092.865	12	12028.738	2	11989.643	-2	11358.543	0	11319.449	-1	11915.197	-1	11876.396	-4	11250.818	-11	11212.029	-2	11802.260	8	11763.761	14
29	10130.885	-3	10090.128	5	12026.845	-0	11986.385	-3	11356.825	-6	11316.383	9	11913.330	-0	11873.180	1	11249.162	1	11209.015	5	11800.440	9	11760.586	4
30	10129.461	-2	10087.310	-12	12024.872	8	11983.047	3	11355.034	-2	11313.213	-2	11911.377	2	11869.876	6	11247.418	6	11205.905	-3	11798.528	5	11757.343	11
31			10084.455	3	12022.801	5	11979.612	1	11353.159	-0	11309.978	3	11909.333	1	11866.477	3	11245.595	12	11202.729	4	11796.536	7	11754.006	12
32	10126.411	15	10081.514	3	12020.651	14	11976.078	-12	11351.200	1	11306.652	0	11907.202	1	11862.996	6	11243.676	5	11199.448	-12	11794.453	5	11750.583	11
33	10124.770	13	10078.501	3	12018.400	11	11972.477	-4	11349.156	1	11303.248	2	11904.981	-1	11859.422	2	11241.685	8	11196.122	6	11792.282	2	11747.073	10
34	10123.059	13	10075.418	2	12016.052	-1	11968.777	-6	11347.030	2	11299.762	3	11902.675	1	11855.759	-3	11239.615	13	11192.690	0	11790.029	3	11743.471	4
35	10121.251	-12	10072.256	-7	12013.631	4	11964.997	-0	11344.819	-0	11296.202	12	11900.280	2	11852.021	5	11237.449	4	11189.185	2	11787.687	3	11739.789	3
36	10119.420	11	10069.039	-1	12011.111	-1	11961.125	1	11342.528	0	11292.537	-2	11897.795	-0	11848.181	-4	11235.204	-3	11185.606	10	11785.257	1	11736.027	7
37	10117.484	0	10065.734	-11	12008.510	1	11957.161	-0	11340.155	3	11288.807	1	11895.224	-0	11844.265	0	11232.887	0	11181.933	6	11782.743	2	11732.165	-1
38	10115.491	5	10062.404	24	12005.820	5	11953.112	2	11337.696	1	11284.986	-4	11892.563	-1	11840.261	3	11230.490	6	11178.185	7	11780.135	-4	11728.232	5
39	10113.405	-13	10058.944	-1	12003.032	-1	11948.974	1	11335.149	-4	11281.100	6	11889.818	1	11836.170	6	11228.001	1	11174.351	4	11777.451	2	11724.205	4
40	10111.281	4	10055.443	5	12000.161	-1	11944.745	-0	11332.528	-2	11277.111	-3	11886.983	2	11831.992	8			11170.436	-0	11774.676	4	11720.079	-11
41	10109.064	-1	10051.868	6	11997.195	-6	11940.424	-6	11329.826	2	11273.053	0	11884.070	13	11827.717	1	11222.788	2	11166.447	3	11771.808	-1	11715.896	3
42	10106.785	4	10048.207	-7	11994.159	8	11936.026	-1	11327.043	9	11268.911	1	11881.047	1	11823.359	-2	11220.063	8	11162.366	-4	11768.856	-3	11711.612	2
43	10104.416	-10	10044.490	-6	11991.015	2	11931.532	-4	11324.162	0	11264.681	-4	11877.947	1	11818.921	1	11217.251	7	11158.220	4	11765.817	-4	11707.240	0
44	10101.986	-13	10040.713	6	11987.787	3	11926.960	3	11321.207	1	11260.379	1	11874.764	6	11814.395	5	11214.362	13	11153.988	7	11762.691	-5	11702.781	-3
45	10099.503	3	10036.845	-2	11984.471	4	11922.286	-4	11318.170	2	11255.986	-3	11871.483	0	11809.775	0	11211.370	-3	11149.675	11	11759.484	-1	11698.243	1
46	10096.919	-10	10032.901	-16	11981.063	2	11917.533	-0	11315.048	1	11251.518	-1	11868.121	2	11805.072	1	11208.315	1	11145.258	-9	11756.171	-15	11693.603	-12
47	10094.288	2	10028.914	-2	11977.562	-4	11912.688	-2	11311.846	4	11246.966	-1	11864.667	1	11800.281	-1	11205.172	-2	11140.784	-5	11752.795	-4	11688.900	-1
48	10091.563	-8	10024.838	-6	11973.982	1	11907.759	1	11308.555	-1	11242.335	2	11861.123	-4	11795.405	0	11201.952	1	11136.228	-1	11749.328	2	11684.103	2
49	10088.780	-5	10020.701	-1	11970.312	5	11902.738	-2	11305.184	-1	11237.631	14	11857.501	3	11790.442	1	11198.635	-11	11131.582	-7	11745.762	-3	11679.222	8

TABLE I—*Continued*

	2-2				3-0				3-1				4-1				4-2				5-2			
J	Ree+Rff	O-C	Pee+Pff	O-C	Ree+Rff	O-C	Pee+Pff	O-C	Ree+Rff	O-C	Pee+Pff	O-C	Ree+Rff	O-C	Pee+Pff	O-C	Ree+Rff	O-C	Pee+Pff	O-C	Ree+Rff	O-C	Pee+Pff	O-C
50	10085.920	-7	10016.475	-13	11966.628	-3	11897.628	-3	11301.737	5	11232.819	-1	11853.782	-1	11785.390	-1	11195.253	-6	11126.864	-4	11742.111	-6	11674.240	-3
51	10082.976	-21	10012.204	-1	11962.693	1	11892.438	1	11298.197	1	11227.943	2	11849.984	6	11780.257	4	11191.786	-5	11122.071	5	11738.380	-2	11669.183	-2
52	10079.986	-8	10007.843	-7	11958.752	1	11887.155	2	11294.560	-17	11222.977	-2	11846.083	-4	11775.029	-0	11188.236	-3	11117.178	-5	11734.555	-6	11664.032	-9
53	10076.913	-6	10003.465	40	11954.722	2	11881.780	-2	11290.876	0	11217.941	4	11842.105	-1	11769.717	-2			11112.211	-8	11730.644	-7	11658.801	-10
54	10073.771	-2	9998.931	2	11950.598	-3	11876.318	-4	11287.090	-1	11212.813	1	11838.037	-1	11764.322	0	11180.894	4	11107.171	-3	11726.647	-7	11653.487	-8
55	10070.538	-17	9994.378	16	11946.393	2	11870.781	5	11283.222	-0	11207.606	-0	11833.879	-2	11758.838	0	11177.086	-6	11102.054	5	11722.566	-4	11648.084	-9
56	10067.254	-12	9989.728	3	11942.096	3	11865.146	5	11279.278	6	11202.313	-7	11829.638	1	11753.266	0	11173.206	-7	11096.835	-7	11718.402	3	11642.603	-3
57			9985.016	-2	11937.710	4	11859.422	4	11275.232	-7	11196.953	3	11825.307	2	11747.610	2	11169.249	-1	11091.558	3	11714.128	-13	11637.029	-4
58	10060.479	10	9980.235	-4	11933.231	2	11853.608	1	11271.120	-1	11191.498	-2	11820.885	1	11741.862	-3	11165.209	3	11086.180	-6	11709.792	-4	11631.372	-1
59	10056.961	-1			11928.667	3	11847.710	1	11266.910	-12	11185.967	-0	11816.370	-6	11736.027	-7	11161.099	19	11080.732	-6	11705.373	11	11625.618	-10
60	10053.385	-0	9970.456	-15	11924.009	1	11841.731	8	11262.639	-1	11180.354	-0	11811.780	1	11730.117	1	11156.867	-5	11075.204	-5	11700.840	-3	11619.792	-5
61	10049.743	9	9965.478	-3	11919.264	-1	11835.660	11	11258.272	-3	11174.658	-1	11807.092	-3	11724.107	-6	11152.583	2	11069.593	-5	11696.233	-4	11613.873	-7
62	10046.014	1	9960.425	4	11914.431	-0	11829.483	-4	11253.818	-8	11168.892	9	11802.321	-2	11718.020	-3	11148.212	4	11063.905	-2	11691.537	-5	11607.889	11
63	10042.218	-1	9955.281	-9	11909.511	2	11823.238	-1	11249.296	1	11163.022	-2	11797.461	-1	11711.844	-2	11143.768	14	11058.128	-8	11686.759	-2	11601.787	-5
64	10038.345	-8	9950.097	8	11904.499	2	11816.901	-0	11244.677	-3	11157.084	-1	11792.512	-2	11705.587	4	11139.208	-8	11052.288	4	11681.883	-10	11595.607	-11
65	10034.417	2	9944.809	-8	11899.398	2	11810.477	-0	11239.980	-3	11151.066	2	11787.479	1	11699.230	-3	11134.604	6	11046.355	3	11676.939	1	11589.356	-4
66	10030.396	-9	9939.482	6	11894.206	-0	11803.977	12	11235.204	0	11144.957	-5	11782.355	1	11692.792	-5	11129.896	-1	11040.334	-5	11671.893	-3	11583.016	0
67	10026.327	3	9934.057	-7	11888.933	6	11797.362	-3	11230.341	1	11138.776	-3	11777.142	-0	11686.274	-1	11125.114	-1	11034.249	3	11666.766	-1	11576.589	2
68	10022.171	1	9928.578	-4	11883.559	1	11790.677	-2	11225.400	6	11132.517	2	11771.833	-9	11679.665	-1	11120.253	4	11028.064	-9	11661.551	-0	11570.079	7
69	10017.947	2	9923.032	3	11878.099	-1	11783.909	5	11220.357	-8	11126.169	-0	11766.455	1	11672.958	-12	11115.307	4	11021.821	1	11656.259	11	11563.484	12
70	10013.637	-11	9917.407	0	11872.555	1	11777.039	-2	11215.256	2	11119.741	-1	11760.978	-0	11666.189	-1	11110.273	-2	11015.488	2	11650.860	1	11556.790	2
71	10009.267	-11	9911.712	-2	11866.919	1	11770.091	-1	11210.054	-5	11113.242	8	11755.414	-0	11659.325	2	11105.164	-1	11009.072	-1	11645.387	4	11550.019	1
72	10004.849	11	9905.959	8	11861.188	-4	11763.058	3	11204.783	1	11106.642	-3	11749.762	-1	11652.367	-2	11099.976	3	11002.586	7	11639.828	8	11543.165	2
73	10000.329	3	9900.118	-1	11855.380	2	11755.935	5	11199.426	4	11099.976	1	11744.026	2	11645.331	2	11094.697	-3	10996.007	1	11634.181	10	11536.225	2
74	9995.734	-9	9894.223	5	11849.471	-3	11748.721	3	11193.979	0	11093.226	3	11738.198	2	11638.205	0	11089.348	5	10989.350	-2	11628.443	8	11529.202	3
75	9991.093	7	9888.254	9	11843.477	-4	11741.420	1	11188.455	3	11086.387	-4	11732.286	5	11630.985	-8	11083.908	1	10982.621	3	11622.617	5	11522.099	9
76	9986.363	4			11837.403	4	11734.036	3	11182.841	-3	11079.470	-7	11726.275	-4	11623.696	1	11078.396	7	10975.803	-2	11616.708	5	11514.900	4
77	9981.554	-6	9876.099	7	11831.234	6	11726.553	-5	11177.146	-6	11072.484	1	11720.189	1	11616.315	3	11072.789	0	10968.914	2	11610.713	5	11507.626	8
78	9976.681	-9			11824.968	0	11718.999	1	11171.378	0	11065.409	1	11714.007	-4	11608.842	-1	11067.111	3	10961.943	3	11604.624	-2	11500.262	8
79	9971.756	8	9863.667	7	11818.629	11	11711.348	-1	11165.520	-1	11058.253	1	11707.743	-2	11601.278	-10	11061.346	1	10954.885	-4	11598.466	8	11492.819	11
80			9857.339	-0	11812.175	-5	11703.624	10	11159.582	1	11051.017	2	11701.390	-1	11593.651	3			10947.762	5	11592.210	6	11485.281	5
81	9961:662	11	9850.957	7	11805.645	-8	11695.793	2	11153.560	2	11043.698	1	11694.952	2			11049.580	5	10940.547	0	11585.865	1		
82	9956.500	6	9844.488	-2	11799.038	2	11687.879	-2	11147.455	2	11036.299	-0	11688.421	-0	11578.106	-4	11043.568	-0	10933.257	1	11579.440	3	11469.972	12
83	9951.267	1			11792.325	-4	11679.886	1	11141.263	-2	11028.824	3	11681.804	-1	11570.220	8	11037.488	7	10925.884	-3	11572.930	5	11462.181	5
84	9945.952	-15			11785.534	-1	11671.797	-4	11134.997	2	11021.262	1	11675.103	2	11562.231	2	11031.319	8	10918.436	-3	11566.332	6	11454.306	-2
85	9940.598	0			11778.652	1	11663.627	-2	11128.638	-4	11013.618	-3	11668.309	-1	11554.161	1	11025.058	-3			11559.642	0	11446.352	-4
86	9935.170	13	9817.956	-5	11771.673	-4	11655.369	-2	11122.208	1	11005.899	-1	11661.423	-8	11546.012	5	11018.740	11			11552.871	-1	11438.311	-9
87	9929.632	-12	9811.156	0	11764.614	-1	11647.025	-2	11115.688	0	10998.100	0	11654.468	3	11537.769	2	11012.315	-2			11546.012	-3	11430.197	-3
88	9924.053	-6			11757.458	-6	11638.593	-2	11109.090	2	10990.226	7	11647.407	-4	11529.445	2	11005.806	-17			11539.070	-4	11421.989	-8
89	9918.394	-10	9797.340	2	11750.225	1	11630.078	2	11102.405	-0	10982.251	-6	11640.273	3			10999.231	-18			11532.046	0	11413.706	-4
90			9790.327	1	11742.893	-2	11621.471	0	11095.641	1	10974.210	-5	11633.045	2	11512.540	1	10992.586	-7			11524.923	-9	11405.320	-19
91	9906.889	10	9783.240	-4	11735.489	12	11612.777	-1	11088.791	-0	10966.091	-2	11625.718	-10	11503.969	9	10985.851	-5			11517.726	-7	11396.882	-3
92			9776.086	-6	11727.965	-4	11603.994	-6	11081.863	2	10957.889	-3	11618.326	0	11495.297	2	10979.040	1			11510.435	-13	11388.335	-12
93	9895.074	3	9768.871	-2	11720.370	-4	11595.131	-2	11074.851	2	10949.609	-0	11610.842	5	11486.544	-2	10972.144	3			11503.074	-3	11379.721	-6

TABLE I—*Continued*

	2-2				3-0				3-1				4-1				4-2				5-2			
J	Ree+Rff	O-C	Pee+Pff	O-C	Ree+Rff	O-C	Pee+Pff	O-C	Ree+Rff	O-C	Pee+Pff	O-C	Ree+Rff	O-C	Pee+Pff	O-C	Ree+Rff	O-C	Pee+Pff	O-C	Ree+Rff	O-C	Pee+Pff	O-C
94	9889.052	-6	9761.576	-8	11712.690	2	11586.181	-1	11067.755	-0	10941.245	-3	11603.265	5			10965.144	-17			11495.619	-3	11371.039	17
95	9882.974	-1			11704.920	5	11577.137	-5	11060.578	0	10932.805	-1	11595.607	10	11468.803	10	10958.094	-6			11488.076	-3	11362.244	10
96	9876.829	8	9746.807	8	11697.057	6	11568.016	-1	11053.313	-6	10924.283	-2	11587.846	-1	11459.789	-1	10950.951	-8					11353.349	-13
97	9870.589	-6	9739.317	13	11689.101	2	11558.802	-2	11045.976	-3	10915.678	-6	11580.018	8	11450.708	5	10943.729	-7			11472.727	-12	11344.391	-17
98					*11681.053*	-6	*11549.509*	*3*	*11038.556*	*-0*			*11572.080*	-6	*11441.528*	-2	*10936.435*	3			*11464.930*	-9	*11335.344*	*-25*
99							11540.124	3	11031.054	2			11564.081	4	11432.272	-3	10929.041	-7			11457.058	4	11326.245	-2
100					11664.712	1	11530.649	-1	11023.463	-2			11555.979	-1	11422.933	-1	10921.593	12			11449.104	20	11317.057	15
101					11656.401	-3	11521.054	-38	11015.795	-3			11547.803	6	11413.512	2							11307.761	7
102					11648.003	-5	11511.443	-5	11008.045	-3			11539.527	-0	11403.998	-4							11298.398	17
103					11639.524	0	11501.700	-16	11000.213	-4			11531.182	9										
104							11491.907	7	10992.303	-2			11522.730	-1	11384.727	-7								
105					11622.284	-4	11481.992	-6	10984.306	-5			11514.199	-4	11374.982	7								
106					11613.539	2	11472.008	-1	10976.232	-4			11505.579	-10										
107					11604.695	-3	11461.913	-21	10968.078	-2			11496.885	-6										
108					11595.773	3	11451.769	-4	10959.854	11			11488.111	5										
109					11586.751	-2	11441.528	2	10951.531	6														
110					11577.652	3	11431.199	6	10943.138	11														
111							11420.776	1	10934.651	4														
112							11410.282	12																

O-C Observed minus calculated line positions in units of 10-3 cm-1.

TABLE II

Observed Wavenumbers (in cm^{-1}) of the Bands of the $[10.3]^3\Phi_3$–$X^3\Phi_3$ Subband of CoF

	0-1								0-0							
J	Ree	O-C	Pee	O-C	Rff	O-C	Pff	O-C	Ree	O-C	Pee	O-C	Rff	O-C	Pff	O-C
7											10278.494	4			10278.494	4
8			9608.660	8			9608.660	8			10277.224	8			10277.224	8
9			9607.368	4			9607.368	4			10275.849	-22			10275.849	-22
10			9606.014	1			9606.014	1			10274.453	-3	10289.256	-5	10274.453	-3
11			9604.604	7	9620.811	-1	9604.604	7	10289.186	2	10272.968	-0	10289.186	2	10272.968	-0
12			9603.115	-1			9603.115	-1	10289.042	8	10271.407	-4	10289.042	8	10271.407	-4
13	9620.612	9	9601.570	-0	9620.612	9	9601.570	-0	10288.812	-2	10269.780	-1	10288.812	-2	10269.780	-1
14	9620.414	13	9599.964	3	9620.414	13	9599.964	3	10288.518	-4	10268.082	1	10288.518	-4	10268.082	1
15	9620.126	-8	9598.284	-2	9620.126	-8	9598.284	-2	10288.160	2	10266.302	-8	10288.160	2	10266.302	-8
16	9619.797	-7	9596.549	1	9619.797	-7	9596.549	1	10287.721	-3	10264.467	-2	10287.721	-3	10264.467	-2
17	9619.408	1	9594.741	-4	9619.408	1	9594.741	-4	10287.216	-3	10262.553	-3	10287.216	-3	10262.553	-3
18	9618.943	-3	9592.880	3	9618.943	-3	9592.880	3	10286.638	-4	10260.571	-1	10286.638	-4	10260.571	-1
19	9618.422	1	9590.941	-4	9618.422	1	9590.941	-4	10285.996	3	10258.515	-2	10285.996	3	10258.515	-2
20	9617.826	-3	9588.948	-0	9617.826	-3	9588.948	-0	10285.270	-3	10256.392	-0	10285.270	-4	10256.392	-0
21	9617.176	2	9586.884	-3	9617.176	2	9586.884	-3	10284.481	-1	10254.197	2	10284.481	-1	10254.197	1
22	9616.453	-0	9584.762	-0	9616.453	-0	9584.762	-0	10283.618	-1	10251.924	-5	10283.618	-1	10251.924	-5
23	9615.669	1	9582.573	-0	9615.669	1	9582.573	-0	10282.686	0	10249.590	-0	10282.686	0	10249.590	-0
24	9614.816	-1	9580.312	-8	9614.816	-1	9580.312	-8	10281.676	-3	10247.180	-2	10281.676	-4	10247.180	-2
25	9613.899	-3	9578.004	2	9613.899	-3	9578.004	2	10280.604	1	10244.717	15	10280.604	1	10244.717	15
26	9612.924	1	9575.621	2	9612.924	1	9575.621	1	10279.456	1	10242.154	2	10279.456	1	10242.154	2
27	9611.880	2	9573.173	-1	9611.880	2	9573.173	-1	10278.240	5	10239.528	-2	10278.240	4	10239.528	-3
28	9610.768	-0	9570.664	1	9610.768	-1	9570.664	1	10276.946	2	10236.838	-1	10276.946	1	10236.838	-1
29	9609.596	3	9568.089	1	9609.596	2	9568.089	0	10275.581	0	10234.075	-1	10275.581	-0	10234.075	-1
30	9608.354	0	9565.448	-1	9608.354	-1	9565.448	-2	10274.146	-1	10231.245	3	10274.146	-1	10231.245	2
31	9607.049	-0	9562.748	2	9607.049	-1	9562.748	1	10272.651	10	10228.339	1	10272.651	9	10228.339	1
32	9605.669	-12	9559.985	7	9605.684	2	9559.985	5	10271.068	4	10225.363	0	10271.068	3	10225.363	-1
33	9604.252	6	9557.152	4	9604.252	4	9557.152	2	10269.410	-5	10222.315	-2	10269.410	-6	10222.315	-3
34	9602.743	-3	9554.259	7	9602.743	-5	9554.259	5	10267.695	0	10219.202	2	10267.695	-1	10219.202	1
35	9601.187	4	9551.295	2	9601.187	2	9551.295	0	10265.904	1	10216.013	-0	10265.904	-1	10216.013	-1
36	9599.562	8	9548.273	3	9599.562	5	9548.273	1	10264.042	2	10212.755	-1	10264.042	0	10212.755	-2
37	9597.870	9	9545.193	10	9597.870	6	9545.193	7	10262.104	-1	10209.427	-0	10262.104	-3	10209.427	-2
38	9596.115	14	9542.041	10	9596.115	10	9542.041	7	10260.096	-3	10206.027	-1	10260.096	-4	10206.027	-3
39	9594.290	13	9538.832	16	9594.290	9 *	9538.832	12	10258.020	-0	10202.558	-1	10258.020	-2	10202.558	-3
40	9592.408	19	9535.550	13	9592.408	15 *	9535.550	9	10255.868	-3	10199.016	-2	10255.868	-5	10199.016	-4
41			9532.198	5	9590.464	24 *	9532.218	20 *	10253.651	1	10195.406	-1	10253.651	-1	10195.406	-4
42	9588.409	-8	9528.789	3	9588.466	43 *	9528.840	48 *	10251.356	0	10191.727	2	10251.356	-3	10191.727	-1
43	9586.323	-10	9525.309	-5	9586.387	47 *	9525.377	55 *	10248.991	-1	10187.968	-5	10248.991	-4	10187.968	-8
44	9584.185	1	9521.764	-16	9584.239	46 *	9521.850	62 *	10246.555	-0	10184.150	0	10246.555	-4	10184.150	-3
45	9581.961	-10	9518.169	-12	9582.055	75 *	9518.270	81 *	10244.047	0	10180.256	-0	10244.047	-4	10180.256	-5
46	9579.684	-8	9514.505	-13	9579.799	97 *	9514.609	80 *	10241.465	-2	10176.290	-2	10241.465	-7	10176.290	-7
47	9577.349	-0	9510.786	-6	9577.470	110 *	9510.915	112 *	10238.815	-0	10172.261	3	10238.815	-5	10172.261	-2
48	9574.934	-6	9506.987	-14	9575.086	133 *	9507.154	140 *	10236.092	0	10168.155	2	10236.092	-5	10168.155	-3
49	9572.462	-4	9503.144	-2	9572.652	171 *	9503.347	186 *	10233.300	3	10163.976	-1	10233.300	-2	10163.976	-7
50	9569.913	-15	9499.223	-5	9570.147	204 *	9499.456	212 *	10230.432	2	10159.729	-2	10230.432	-4	10159.729	-8
51	9567.322	-2	9495.240	-7	9567.602	260 *	9495.522	258 *	10227.492	1	10155.417	4	10227.492	-5	10155.417	-3
52	9564.649	-6	9491.196	-4	9564.999	324 *	9491.534	313 *	10224.486	5	10151.029	3	10224.486	-2	10151.029	-4
53	9561.920	-1	9487.093	2	9562.341	397 *	9487.510	397 *	10221.413	14	10146.573	4	10221.413	7	10146.573	-3
54	9559.116	-6	9482.920	2	9559.644	497 *	9483.441	499 *	10218.248	4	10142.045	5	10218.248	-4	10142.045	-3
55	9556.253	-4	9478.693	12	9555.525	-760 *	9477.956	-751 *	10215.023	4	10137.451	10	10215.023	-3	10137.451	2
56	9553.331	3	9474.382	3	9552.684	-675 *	9473.739	-671 *	10211.726	6	10132.777	5	10211.726	-2	10132.777	-2
57	9550.337	3	9470.010	-5	9549.767	-599 *	9469.446	-602 *	10208.360	9	10128.045	13	10208.360	1	10128.045	5
58	9547.282	8	9465.594	7	9546.754	-556 *	9465.072	-551 *	10204.915	5	10123.228	6	10204.915	-2	10123.228	-2
59	9544.162	13	9461.101	6	9543.684	-505 *	9460.626	-508 *	10201.407	11 *	10118.350	9	10201.407	3	10118.350	1

$$F_v(J) = T_v + B_vJ(J+1) - D_v[J(J+1)]^2 + H_v[J(J+1)]^3 + L_v[J(J+1)]^4$$
$$\pm \tfrac{1}{2}\{qJ(J+1) + q_D[J(J+1)]^2 + q_H[J(J+1)]^3 + q_L[J(J+1)]^4\}. \quad (1)$$

In the final fit the lines of the different subbands were weighted depending on the signal-to-noise ratio and the extent of blending. The perturbed transitions were not directly included in the fit but the corresponding combination differences for the unperturbed levels were included. The molecular constants for the ground and excited spin components of the three subbands of the $[10.3]^3\Phi_i$–$X^3\Phi_i$ transitions are presented in Tables IV, V, and VI.

The *e*/*f* parity assignment is difficult and we chose to put the *e*-parity level above the *f*-parity level for a given *J* in the $v = 0$ vibrational level of the $^3\Phi_2$ and $^3\Phi_3$ spin components.

DISCUSSION

The rotational constants obtained for the different vibrational levels of the ground and excited spin components (Tables IV, V, and VI) have been used to evaluate the

TABLE II—*Continued*

	0-1								0-0							
J	Ree	O-C	Pee	O-C	Rff	O-C	Pff	O-C	Ree	O-C	Pee	O-C	Rff	O-C	Pff	O-C
60	9540.969	10	9456.554	15	9540.532	-471 *	9456.106	-477 *	10197.823	11 *	10113.405	14	10197.823	4	10113.405	7
61	9537.725	20 *	9451.938	18 *	9537.319	-433 *	9451.530	-437 *	10194.150	-5 *	10108.383	14 *	10194.150	-11	10108.383	7
62			9447.232	-5 *	9534.016	-419 *	9446.872	-417 *	10190.397	-29 *	10103.319	41 *	10190.447	15	10103.274	-10
63	9531.033	34 *	9442.521	30 *	9530.653	-401 *	9442.150	-396 *	10186.643	17 *	10098.166	49 *	10186.643	12	10098.113	-9
64	9527.576	27 *	9437.710	29 *	9527.225	-384 *	9437.355	-386 *	10182.795	42 *	10092.912	26 *	10182.747	-10	10092.865	-24
65	9524.073	40 *	9432.844	37 *	9523.738	-361 *	9432.497	-375 *	10178.852	42 *	10087.620	36 *	10178.802	-9	10087.560	-25
66	9520.501	49 *	9427.921	51 *	9520.159	-363 *	9427.584	-357 *	10174.838	44 *	10082.256	44 *	10174.786	-7	10082.204	-8
67	9516.851	45 *	9422.921	52 *	9516.535	-347 *	9422.597	-349 *	10170.757	51 *	10076.809	40 *	10170.697	-7	10076.752	-15
68	9513.159	63 *	9417.864	58 *	9512.846	-332 *	9417.543	-344 *	10166.596	49 *	10071.309	51 *	10166.532	-9	10071.245	-7
69	9509.406	86 *	9412.753	75 *	9509.074	-333 *	9412.433	-334 *	10162.374	58 *	10065.734	58 *	10162.299	-8	10065.668	2
70	9505.567	88 *	9407.569	81 *	9505.258	-315 *	9407.247	-336 *	10158.083	69 *	10060.081	56 *	10158.002	1	10060.004	-7
71	9501.663	91 *	9402.318	84 *	9501.363	-311 *	9402.022	-314 *	10153.712	71 *	10054.375	72 *	10153.638	16	10054.280	-5
72	9497.703	101 *	9397.021	104 *	9497.406	-303 *	9396.713	-313 *	10149.273	76 *	10048.577	65 *	10149.177	5	10048.487	-1
73	9493.684	118 *	9391.652	114 *	9493.377	-304 *	9391.348	-305 *	10144.769	89 *	10042.731	79 *	10144.657	9 *	10042.625	4
74	9489.598	133 *	9386.216	120 *	9489.308	-280 *	9385.972	-246 *	10140.191	98 *	10036.813	91 *	10140.035	-18 *	10036.695	12
75	9485.453	152 *	9380.748	158 *	9485.159	-272 *	9380.439	-281 *	10135.540	106 *	10030.816	93 *	10135.415	30 *	10030.696	20 *
76	9481.246	176 *	9375.180	159 *	9480.951	-259 *	9374.881	-279 *	10130.823	118 *	10024.751	97 *	10130.690	44 *	10024.629	32 *
77	9476.970	194 *	9369.566	176 *	9476.681	-243 *	9369.265	-272 *	10126.027	123 *	10018.632	114 *	10125.889	55 *	10018.481	32 *
78	9472.651	234 *	9363.895	198 *	9472.367	-206 *	9363.599	-254 *	10121.184	152 *	10012.430	118 *	10121.006	56 *	10012.278	48 *
79	9468.260	266 *	9358.158	218 *	9467.999	-159 *	9357.881	-225 *	10116.301	211 *	10006.184	147 *	10116.109	116 *	10006.004	63 *
80	9463.843	337 *	9352.380	257 *	9463.638	-43 *	9352.082	-215 *	10111.405	327 *	9999.868	175 *	10111.123	157 *	9999.661	79 *
81	9459.402	447 *	9346.536	294 *	9459.328	190 *	9346.282	-144 *	10106.426	431 *	9993.497	215 *	10106.123	259 *	9993.269	117 *
82	9453.940	-400 *	9340.660	360 *	9453.940	-592 *	9340.445	-48 *	10100.576	-267 *	9987.125	322 *	10100.124	-567 *	9986.821	169 *
83	9449.373	-288 *	9334.722	426 *	9449.557	-306 *	9334.655	156 *	10095.497	-123 *	9980.687	431 *	10095.152	-294 *	9980.364	282 *
84	9444.693	-226 *	9327.877	-355 *	9444.949	-180 *	9327.831	-613 *	10090.245	-83 *	9973.428	-213 *	10089.945	-184 *	9972.883	-560 *
85	9439.929	-184 *	9321.840	-265 *	9440.209	-124 *	9322.036	-291 *	10084.919	-47 *	9966.821	-137 *	10084.608	-131 *	9966.444	-289 *
86	9435.089	-154 *	9315.722	-196 *	9435.384	-90 *	9315.983	-166 *	10079.485	-50 *	9960.125	-84 *	10079.188	-89 *	9959.811	-141 *
87	9430.200	-112 *	9309.521	-149 *	9430.495	-57 *	9309.799	-112 *	10074.015	-20 *	9953.337	-56 *	10073.666	-77 *	9952.985	-118 *
88	9425.208	-108 *	9303.222	-139 *	9425.517	-49 *	9303.539	-73 *	10068.452	-14 *	9946.476	-34 *	10068.078	-60 *	9946.100	-84 *
89	9420.177	-83 *	9296.891	-101 *	9420.484	-35 *	9297.194	-59 *	10062.829	0	9939.515	-46 *	10062.404	-55 *	9939.132	-61 *
90	9415.075	-65 *	9290.488	-76 *	9415.393	-16 *	9290.792	-42 *	10057.113	-11	9932.517	-30 *	10056.675	-34 *	9932.082	-52 *
91	9409.926	-34 *	9284.017	-59 *	9410.233	-5	9284.319	-36 *	10051.338	-15	9925.447	-21 *	10050.858	-29 *	9924.972	-33 *
92	9404.681	-37 *	9277.487	-41 *	9404.999	-6	9277.793	-24 *	10045.498	-14	9918.315	-8	10044.967	-27 *	9917.780	-27 *
93	9399.395	-20 *	9270.901	-22 *	9399.703	-7	9271.204	-16 *	10039.603	-3	9911.105	-10	10039.023	-6	9910.513	-26 *
94	9394.035	-17 *	9264.228	-32 *	9394.356	2	9264.554	-10	10033.632	-2	9903.831	-11	10032.979	-12	9903.195	-6 *
95	9388.624	-5	9257.524	-14 *	9388.938	-0	9257.857	6	10027.601	5	9896.484	-22	10026.889	6	9895.786	-9
96	9383.144	-2	9250.752	-8 *	9383.482	20	9251.068	-11	10021.496	3	9889.115	8	10020.701	-2	9888.323	4
97	9377.600	-3	9243.923	-2	9377.934	9	9244.263	14	10015.337	12			10014.449	-2	9880.775	1
98	9372.002	-1	9237.029	-4	9372.351	22	9237.359	-4	10009.099	7			10008.148	21	9873.178	17
99	9366.351	6	9230.090	3	9366.676	1							10001.746	13	9865.484	5
100	9360.631	2	9223.092	6	9360.955	-7	9223.436	14					9995.280	12	9857.726	-2
101	9354.867	10	9216.032	2	9355.199	8	9216.361	-7					9988.736	4	9849.909	1
102	9349.025	-4	9208.907	-15	9349.363	1	9209.254	-5					9982.129	4	9842.025	4
103	9343.136	-10	9201.759	-2	9343.474	-3	9202.066	-30					9975.436	-11	9834.068	3
104	9337.204	-4	9194.558	10									9968.694	-5	9826.034	-8
105			9187.310	26									9961.888	8	9817.956	6
106													9954.984	-8	9809.802	9
107													9948.026	-8	9801.563	-4
108															9793.271	-3

effective equilibrium molecular parameters provided in Table VII. The observation of many bands in the $^3\Phi_4$–$^3\Phi_4$ subband allows the determination of the equilibrium vibrational constant for the lowest energy spin component $X\,^3\Phi_4$. For the other spin components only the first vibrational interval $\Delta G(v + \frac{1}{2})$ was determined. The present experimental values of the ground state equilibrium rotational constants provide effective equilibrium internuclear distances of 1.735698(8), 1.734943(11), and 1.727557(28) Å for the $X\,^3\Phi_4$, $X\,^3\Phi_3$, and $X\,^3\Phi_2$ spin components, respectively.

Adam *et al.* (*12*) measured an approximate vibrational constant of 662.6 cm^{-1}. This value agrees only moderately well with our results, primarily because their value was extracted from low-resolution spectra measured by laser-induced fluorescence. The rotational constants in the work of Adam *et al.* (*12*) are also in moderate agreement with our values, if the measurement uncertainties are considered. In the preliminary work of Adam *et al.* (*12*) a pulsed dye laser of modest resolution was used so that our results provide considerable improvement in the ground state constants.

In the absence of any other experimental or theoretical work on CoF, it is reasonable to compare the present results with the spectroscopic data and ab initio predictions available for CoH (*14*). Indeed it will be interesting to study how closely the energy levels of CoH and CoF correspond. The theoretical work of Freindorf *et al.* (*14*) on

TABLE II—*Continued*

	1-0								2-0				2-1			
J	Ree	O-C	Pee	O-C	Rff	O-C	Pff	O-C	Ree+Rff	O-C	Pee+Pff	O-C	Ree+Rff	O-C	Pee+Pff	O-C
3	10865.320	17			10865.320	17										
4	10865.703	5			10865.703	5										
5	10866.004	-14			10866.004	-14										
6	10866.266	6	10857.151	-7	10866.266	6	10857.151	-7								
7	10866.421	-6	10855.929	4	10866.421	-6	10855.929	4			11428.171	16				
8	10866.525	7	10854.620	4	10866.525	7	10854.620	4			11426.825	12				
9			10853.244	14			10853.244	14	11438.618	9	11425.392	-0			10756.882	-4
10	10866.463	-7	10851.774	5	10866.463	-7	10851.774	5	11438.488	-10	11423.900	9	10770.062	7	10755.436	-12
11	10866.331	-0	10850.236	4	10866.331	-0	10850.236	4	11438.311	6	11422.313	4	10769.935	1	10753.946	9
12	10866.116	-1	10848.620	2	10866.116	-1	10848.620	2	11438.030	-3	11420.648	2	10769.737	-2	10752.339	-13
13	10865.824	-2	10846.929	-0	10865.824	-2	10846.929	-0	11437.683	3	11418.902	-1	10769.465	-4		
14	10865.454	-5	10845.160	-3	10865.454	-5	10845.160	-3	11437.249	3	11417.079	-1	10769.122	-4		
15	10865.015	-1	10843.330	8	10865.015	-1	10843.330	8	11436.729	-3	11415.171	-6	10768.701	-7	10747.148	-4
16	10864.494	-2	10841.406	1	10864.494	-2	10841.406	1	11436.133	-4	11413.193	0	10768.207	-9	10745.262	-10
17	10863.900	-0	10839.415	3	10863.900	-1	10839.415	3	11435.460	-2	11411.123	-6	10767.647	-4	10743.296	-22
18	10863.227	-2	10837.339	-4	10863.227	-2	10837.339	-5	11434.708	1	11408.984	-1	10767.000	-12	10741.283	-7
19	10862.480	-0	10835.199	-1	10862.480	-1	10835.199	-1	11433.874	2	11406.763	1	10766.303	4	10739.173	-15
20	10861.656	-0	10832.989	10	10861.656	-1	10832.989	10	11432.963	6	11404.457	-0	10765.531	17	10737.029	15
21	10860.755	-1	10830.682	-1	10860.755	-1	10830.682	-1	11431.978	16	11402.072	-3	10764.665	12	10734.758	-9
22	10859.774	-6	10828.312	0	10859.774	-6	10828.312	-0	11430.889	2	11399.611	-1	10763.720	-2	10732.448	2
23	10858.725	-1	10825.863	-2	10858.725	-2	10825.863	-2	11429.737	3	11397.076	5	10762.713	-3	10730.046	-8
24	10857.596	-2	10823.340	-2	10857.596	-3	10823.340	-2	11428.508	7	11394.437	-13	10761.641	2	10727.574	-13
25	10856.392	-1	10820.741	-2	10856.392	-2	10820.741	-3	11427.199	9	11391.754	3	10760.488	-2	10725.047	-3
26	10855.110	-2	10818.072	2	10855.110	-4	10818.072	1	11425.801	1	11388.982	9	10759.281	13	10722.433	-8
27	10853.755	0			10853.755	-2			11424.318	-14	11386.118	1	10757.978	3	10719.766	5
28	10852.323	1	10812.495	-1	10852.323	-1	10812.495	-3	11422.788	2	11383.186	2	10756.605	-5	10716.999	-9
29	10850.810	-3	10809.595	-0	10850.810	-6	10809.595	-2	11421.171	7	11380.176	3	10755.173	-3	10714.187	2
30	10849.232	3	10806.620	-1	10849.232	0	10806.620	-3			11377.088	3	10753.669	-1	10711.291	-1
31	10847.561	-7	10803.571	1	10847.561	-10	10803.571	-2	11417.687	0	11373.915	-6	10752.096	1	10708.320	-8
32	10845.838	6	10800.444	0	10845.838	2	10800.444	-3	11415.839	4	11370.684	4	10750.454	3	10705.300	4
33	10844.022	3	10797.246	2	10844.022	-2	10797.246	-2	11413.907	0	11367.365	2	10748.737	-1	10702.189	-5
34	10842.137	4	10793.970	2	10842.137	-0	10793.970	-2	11411.903	-1	11363.973	2	10746.956	0	10699.026	2
35	10840.173	4	10790.621	3	10840.173	-2	10790.621	-1	11409.829	2	11360.504	-1	10745.107	1	10695.788	4
36	10838.140	9	10787.199	6	10838.140	3	10787.199	1	11407.674	-1	11356.963	-2	10743.184	-6	10692.483	4
37	10836.026	7	10783.698	4	10836.026	1	10783.698	-1	11405.449	-2	11353.349	-1	10741.189	-17	10689.115	9
38	10833.837	6	10780.126	6	10833.837	-0	10780.126	-0	11403.151	-2	11349.663	-1			10685.672	6
39	10831.581	12	10776.477	5	10831.581	5	10776.477	-2	11400.779	-4	11345.900	-4			10682.171	10
40	10829.237	4	10772.756	5	10829.237	-3	10772.756	-2	11398.334	-7	11342.069	-3	10734.873	14	10678.606	16
41	10826.826	4	10768.962	6	10826.826	-4	10768.962	-1	11395.829	1	11338.174	5	10732.606	-8		
42	10824.345	6	10765.104	17	10824.345	-1	10765.104	9	11393.246	1	11334.194	-2	10730.300	-5	10671.234	-23
43	10821.782	0	10761.154	8	10821.782	-7	10761.154	-0	11390.581	-10	11330.160	8	10727.935	3	10667.480	-14
44			10757.137	5			10757.137	-3	11387.872	6	11326.037	-2	10725.489	-7	10663.645	-23
45	10816.457	6	10753.052	6	10816.457	0	10753.052	-2	11385.079	7	11321.860	4			10659.759	-21
46	10813.681	2	10748.899	10	10813.681	-2	10748.899	2	11382.221	11	11317.606	2			10655.804	-26
47	10810.832	-3	10744.660	-2	10810.832	-5	10744.660	-8	11379.287	9	11313.285	1				
48	10807.915	-7	10740.364	0	10807.915	-7	10740.364	-5			11308.893	-2				
49	10804.934	-5	10735.999	3	10804.934	-2	10735.999	-1	11373.214	8	11304.443	4				
50	10801.875	-15	10731.557	-4	10801.875	-8	10731.557	-4	11370.068	1	11299.919	4				
51	10798.762	-12	10727.054	-2	10798.762	1	10727.054	0	11366.871	13	11295.316	-7				
52	10795.575	-16	10722.472	-14	10795.575	3	10722.472	-8	11363.566	-13	11290.665	2				
53	10792.326	-19	10717.837	-14	10792.326	8	10717.837	-2	11360.218	-12	11285.935	-0				
54	10789.044	8	10713.143	-7	10788.998	-2	10713.136	4	11356.825	15	11281.137	-2				
55	10785.670	3	10708.386	-2	10785.615	-4	10708.370	9			11276.281	8				
56	10782.237	-1	10703.575	11	10782.179	2	10703.520	-8	11349.732	-17	11271.334	-3				
57	10778.750	-3	10698.678	-3	10778.683	8	10698.635	2	11346.121	16	11266.334	5				
58			10693.743	3			10693.676	-2			11261.242	-9				
59	10771.619	-2	10688.742	-2	10771.515	12	10688.671	5			11256.096	-0				
60	10767.983	4	10683.699	4	10767.851	15	10683.608	10								
61			10678.606	12	10764.120	2	10678.484	9								
62			10673.447	1	10760.346	-7	10673.315	13								
63					10756.509	-34	10668.086	7								
64							10662.794	-16								
65							10657.463	-35								

O-C Observed minus calculated line positions in units of 10-3 cm-1.

* Transitions affected by perturbations, not directly included in the final fit. See text for details.

CoH predicts a $^3\Phi$–$^3\Phi$ transition at about 13 150 cm^{-1}. Our recent observation of a $^3\Phi$–$^3\Phi$ transition of CoH at about 1 μm is consistent with this prediction and a similar transition is expected for CoF. This expectation is fulfilled with our present observation of the [10.3]$^3\Phi$–$X\,^3\Phi$ transition at 10 289 cm^{-1}.

At first sight the possible low-lying states of CoH and, presumably, CoF are very complex but a closer examination of the states predicted by Freindorf *et al.* (*14*) reveals a simple pattern. The ground state of the Co atom is an $a^4F(3d^74s^2)$ state which gives rise to $^3\Phi$, $^3\Delta$, $^3\Pi$, $^3\Sigma^-$, $^5\Phi$, $^5\Delta$, $^5\Pi$, and $^5\Sigma^-$ states when combined with a ^2S H atom. In the CoH molecule the first four states are calculated to be $^3\Phi$, $^3\Sigma^-$,

TABLE III

Observed Wavenumbers (in cm^{-1}) of the Bands of the $[10.3]^3\Phi_2$–$X^3\Phi_2$ Subband of CoF

	0-1								0-0								1-0							
J	**Ree**	**O-C**	**Pee**	**O-C**	**Rff**	**O-C**	**Pff**	**O-C**	**Ree**	**O-C**	**Pee**	**O-C**	**Rff**	**O-C**	**Pff**	**O-C**	**Ree**	**O-C**	**Pee**	**O-C**	**Rff**	**O-C**	**Pff**	**O-C**
5											10152.696	3			10152.696	3								
6											10151.555	-7			10151.555	-7			10728.777	-4			10728.777	-4
7											*10150.352*	-8			*10150.352*	-8			*10727.543*	*0*			*10727.543*	-0
8											10149.074	-12			10149.074	-12			10726.217	-12			10726.217	-12
9											10147.740	-3			10147.740	-3	10738.137	-3	10724.836	-2			10724.836	-2
10									10161.155	2	10146.330	2	10161.155	1	10146.330	1	10738.068	-3	10723.365	-5			10723.365	-6
11									10161.076	-3	10144.844	2	10161.076	-4	10144.844	1	10737.922	-3	10721.829	4	10737.922	-4	10721.829	3
12									10160.939	5	10143.291	5	10160.939	4	10143.291	4	10737.706	2	10720.204	-0	10737.706	1	10720.204	-1
13			9440.715	-4			9440.715	-5	10160.727	9	10141.654	-6	10160.727	8	10141.654	-7	10737.408	4	10718.504	-2	10737.408	2	10718.504	-3
14			9439.279	6	9459.754	12	9439.279	6	10160.438	8			10160.438	6			10737.029	1	10716.745	13	10737.029	-1	10716.745	11
15	9459.649	-2	9437.767	-6	9459.649	-3	9437.767	-6	10160.076	4	10138.193	-2	10160.076	2	10138.193	-3	10736.583	10	10714.886	5	10736.583	7	10714.886	3
16	9459.518	13			9459.518	12	9436.213	-5	10159.649	7	10136.350	-5	10159.649	3	10136.350	-7	10736.059	17	10712.953	1	10736.059	13	10712.953	-2
17	9459.328	24	9434.627	19	9459.328	22	9434.606	-3	10159.152	10	10134.447	1	10159.152	5	10134.447	-2	10735.441	7	10710.967	20	10735.441	2	10710.967	17
18	9459.051	2	9432.937	-6	9459.051	-0	9432.937	-7	10158.578	8	10132.467	1	10158.578	2	10132.467	-2	10734.758	10	10708.868	3	10734.758	4	10708.868	-1
19	9458.732	-5	9431.226	2	9458.732	-8	9431.226	1	10157.934	6	10130.419	5	10157.934	-0	10130.419	0	10733.990	6	10706.721	14	10733.990	-1	10706.730	19
20	9458.363	-6	9429.450	3	9458.363	-9	9429.450	2	10157.218	4	10128.299	7	10157.218	-4	10128.299	1	10733.148	6	10704.471	1	10733.148	-3	10704.471	-5
21	9457.956	12	9427.635	19	9457.949	1	9427.596	-22	10156.432	3	10126.090	-10	10156.432	-6	10126.111	4	10732.226	4	10702.165	8	10732.226	-7	10702.165	1
22	9457.463	-1	9425.721	-7	9457.463	-5	9425.721	-9	10155.575	3	10123.839	1	10155.575	-8	10123.839	-7	10731.229	5	10699.769	3	10731.229	-7	10699.769	-6
23	9456.920	-5	9423.787	3	9456.920	-10	9423.787	1	10154.648	3	10121.510	6	10154.648	-10	10121.510	-3	10730.151	3	10697.297	-1	10730.151	-11 *	10697.297	-12 *
24	9456.323	-6	9421.789	6	9456.325	-11	9421.789	3	10153.638	-8	10119.101	1	10153.638	-23 *	10119.101	-10 *	10728.993	0	10694.752	1	10728.993	-16 *	10694.752	-11 *
25	9455.678	3	9419.730	6	9455.678	-5	9419.730	2	10152.576	-0	10116.622	-2	10152.576	-17 *	10116.622	-15 *	10727.755	-3	10692.126	-2	10727.755	-22 *	10692.126	-16 *
26	9454.956	-7	9417.609	2	9454.956	-16	9417.609	-3	10151.428	-7	10114.075	-4	10151.428	-26 *	10114.075	-19 *	10726.432	-12	10689.419	-6	10726.432	-33 *	10689.419	-23 *
27	9454.191	-1	9415.439	7	9454.191	-11	9415.439	1	10150.214	-7	10111.465	3	10150.214	-29 *	10111.465	-15 *	10725.047	-3	10686.629	-15	10725.047	-27 *	10686.629	-34 *
28	9453.370	9	9413.197	-2	9453.371	-2	9413.197	-10	*10148.929*	-8	*10108.767*	-8	*10148.929*	-32 *	*10108.767*	-28 *	*10723.566*	*-10*	*10683.776*	-8	*10723.566*	-37 *	*10683.776*	-30 *
29	9452.471	0	9410.921	13	9452.471	-13	9410.921	4	10147.569	-12	10106.020	3	10147.569	-39 *	10105.987	-52 *	10722.010	-11	10680.836	-10	10722.010	-42 *	10680.836	-35 *
30	9451.530	9	9408.570	14	9451.530	-6	9408.570	3	10146.160	7	10103.195	6	10146.107	-76 *	10103.148	-65 *	10720.383	-3	10677.822	-6	10720.348	-72 *	10677.822	-34 *
31	9450.521	11	9406.155	10	9450.521	-6	9406.155	-2	10144.657	4	10100.286	-3	10144.575	-112 *	10100.216	-101 *	10718.668	-0	10674.729	-0	10718.582	-123 *	10674.699	-62 *
32	9449.461	24	9403.683	9	9449.461	4	9403.683	-5	10143.087	6	10097.322	4	10142.965	-153 *	10097.214	-137 *	10716.868	-1	10671.549	-3		*	10671.450	-137 *
33	9448.307	4	9401.151	8	9448.307	-19	9401.151	-9	10141.447	10	10094.288	11	10141.270	-208 *	10094.119	-194 *	10714.994	7	10668.294	2	10714.839	-193 *	10668.134	-197 *
34	9447.119	13	9398.552	3	9447.119	-13	9398.572	2	10139.719	-3	10091.170	6	10139.466	-300 *	10090.915	-288 *	10713.011	-11	10664.956	3	10712.779	-292 *	10664.712	-283 *
35	9445.853	7	9395.911	17	9445.860	-16	9395.911	-7	10137.940	8	10087.982	1	10137.541	-441 *	10087.560	-463 *	10710.967	-6	10661.541	10	10710.533	-494 *	10661.094	-483 *

O-C Observed minus calculated line positions in units of 10-3 cm-1.

* Transitions affected by perturbations, not directly included in the final fit. See text for details.

TABLE III—*Continued*

	0-1								0-0								1-0							
J	**Ree**	**O-C**	**Pee**	**O-C**	**Rff**	**O-C**	**Pff**	**O-C**	**Ree**	**O-C**	**Pee**	**O-C**	**Rff**	**O-C**	**Pff**	**O-C**	**Ree**	**O-C**	**Pee**	**O-C**	**Rff**	**O-C**	**Pff**	**O-C**
36	9444.540	16	9393.205	27	9444.540	-17	9393.205	0	10136.068	-4	10084.728	2	10136.650	525 *	10085.324	551 *	10708.852	11	10658.027	1	10709.436	537 *	10658.633	555 *
37	9443.134	-2	9390.401	2	9443.184	10	9390.444	14	10134.135	-3	10081.403	4	10134.495	300 *	10081.756	305 *	10706.627	4	10654.450	10	10706.988	303 *	10654.823	327 *
38			9387.569	13	9441.728	1	9387.581	-10	10132.125	-6	10077.997	-4	10132.397	205 *	10078.266	210 *	10704.322	3	10650.791	21	10704.589	202 *	10651.045	214 *
39	9440.160	-8	9384.651	1	9440.209	-6			10130.045	-5	10074.530	-2	10130.259	143 *	10074.742	150 *	10701.938	7	10647.023	6		*	10647.232	150 *
40	9438.578	-7	9381.667	-12	9438.640	2	9381.728	3	10127.894	-2	10070.987	-3	10128.045	79 *	10071.161	107 *	10699.463	7	10643.180	1	10699.641	110 *	10643.366	117 *
41					9436.983	-11	9378.702	6	10125.665	-3	10067.373	-2	10125.821	78 *	10067.530	86 *	10696.906	13	10639.263	7	10697.052	79 *	10639.440	110 *
42	9435.215	-4	9375.531	-10	9435.282	-2	9375.602	0	10123.364	-1	10063.686	-3	10123.547	102 *	10063.824	62 *	10694.232	-11	10635.256	8	10694.388	60 *	10635.423	96 *
43	9433.423	-10	9372.351	-23	9433.521	15	9372.442	-0	10120.988	0	10059.924	-5	10121.119	48 *	10060.081	74 *	10691.497	-8	10631.160	6	10691.656	63 *	10631.290	52 *
44	9431.576	-2	9369.141	2	9431.673	13	9369.240	25	10118.528	-7	10056.092	-4	10118.657	34 *	10056.225	46 *	10688.671	-7	10626.975	2	10688.803	33 *	10627.096	35 *
45	9429.649	-5	9365.821	-15	9429.746	2	9365.935	12	10116.003	-5	10052.189	-1	10116.109	11 *	10052.303	27 *	10685.760	-4	10622.709	3	10685.881	22 *	10622.823	25 *
46			9362.455	-9	9427.764	6	9362.556	-5	10113.405	2	10048.207	-1	10113.511	14 *	10048.315	16 *	10682.749	-10	10618.345	-7	10682.866	9 *	10618.484	36 *
47	9425.587	-3	9359.019	-3					10110.726	6	10044.144	-9	10110.835	16	10044.253	5	10679.670	4	10613.899	-10	10679.777	11	10614.011	3
48	9423.445	-4	9355.504	-6	9423.584	12	9355.645	13	10107.962	1	10040.026	4	10108.068	6	10040.127	6	10676.481	-2	10609.372	-7	10676.592	7	10609.481	-0
49	9421.238	4	9351.930	4			9352.060	-1	10105.120	-3	10035.817	1	10105.242	17	10035.918	0	10673.218	7	10604.751	-9	10673.315	2	10604.862	-3
50	9418.943	-0	9348.259	-10	9419.099	7	9348.424	6	10102.209	3	10031.527	-5	10102.314	5	10031.631	-5	10669.860	10	10600.047	-7	10669.947	-5	10600.148	-12
51	9416.565	-10	9344.541	4	9416.744	6	9344.696	-8	10099.211	3	10027.179	8	10099.315	2	10027.275	-3	10666.417	17	10595.259	1	10666.505	4	10595.350	-15
52	9414.128	-1	9340.729	-1	9414.301	-7	9340.917	2	10096.134	5	10022.734	3	10096.239	6	10022.838	-2	10662.891	29	10590.376	1	10662.963	4	10590.487	4
53	9411.614	12	9336.854	9	9411.800	1	9337.048	-2	10092.969	1	10018.220	7	10093.071	1	10018.314	-8			10585.422	18	10659.324	-6	10585.507	-3
54			9332.898	16	9409.203	-6	9333.104	-4	10089.725	1	10013.637	24	10089.824	1	10013.721	-2			10580.350	4			10580.444	-5
55			9328.867	28	9406.538	2					10008.952	19	10086.493	4	10009.034	-6							10575.281	-19
56							9324.980	-7	10082.976	-2	10004.169	1	10083.054	-14	10004.269	-5								
57					9400.934	-3	9320.796	-8	10079.482	8	9999.332	11	10079.552	-5	9999.426	2								
58							9316.545	9			9994.378	-8	10075.947	-7	9994.487	3								
59													10072.256	-3	9989.457	0								
60													10068.465	-2	9984.340	3								
61											9979.021	-30			9979.142	18								
62											9973.721	-35			9973.834	18								
63											9968.361	-3												
64											9962.874	0												

TABLE IV

Spectroscopic Constants[a] (in cm^{-1}) of the [10.3]$^3\Phi_4$–$X^3\Phi_4$ Subband of CoF

		$X^3\Phi_4$			
v	T_v	B_v	10^7 x D_v	10^{12} x H_v	10^{16} x L_v
0	0.0	0.3881194(17)	5.1295(15)	-0.1390(99)	0.0185(29)
1	672.70236(81)	0.3850322(18)	5.1649(31)	0.0225(37)	0.299(15)
2	1339.9254(12)	0.3814562(22)	4.3418(61)	-7.477(92)	2.425(47)

		[10.3]$^3\Phi_4$		
v	T_v	B_v	10^7 x D_v	10^{12} x H_v
0	10336.19750(57)	0.3516716(16)	5.17846(93)	--
1	10911.12802(67)	0.3490039(16)	5.14392(94)	--
2	11480.67399(59)	0.3463605(16)	5.10984(92)	--
3	12044.88132(62)	0.3437401(16)	5.07526(94)	--
4	12603.79033(99)	0.3411469(18)	5.0501(20)	0.50(10)
5	13157.4481(15)	0.3385774(22)	5.0323(38)	1.66(25)

[a]The numbers in parentheses are one standard deviation in the last digit.

$^3\Pi$, and $^3\Delta$ while the next four states are $^5\Phi$, $^5\Sigma^-$, $^5\Pi$, and $^5\Delta$, which are all within 7000 cm^{-1} of the ground state.

The first excited state of Co is the $b^4F(3d^84s^1)$ state, with the same symmetry as the ground state, at about 4000 cm^{-1} (*18*). This atomic state will give rise to a similar pattern of states near about 10 000 cm^{-1} (*14*). Of course, at 10 000 cm^{-1} there are also states correlating to other atomic limits present so that the energy level pattern becomes much more complicated. The $^3\Phi$–$^3\Phi$ transition that we have analyzed must correlate to the b^4F–a^4F atomic transition.

The [10.3]$^3\Phi$–$X^3\Phi$ transition of CoF is also similar to the $A^6\Sigma^+$–$X^6\Sigma^+$ transition of CrH near 1 μm (*19*). In the case of the Cr atom the ground state is the $a^7S(3d^53s^1)$

TABLE V

Spectroscopic Constants[a] (in cm^{-1}) of the [10.3]$^3\Phi_3$–$X^3\Phi_3$ Subband of CoF

			$X^3\Phi_3$				
v	T_v	B_v	10^7 x D_v	10^{10} x H_v	10^{14} x L_v	10^{12} x q_{Hv}	10^{16} x q_{Lv}
0	0.0	0.3882130(41)	5.257(10)	0.02121(94)	-0.02036(40)	0.900(35)	-1.990(34)
1	668.7960(11)	0.3850019(43)	5.468(12)	0.0399(14)	-0.0399(14)	1.227(32)	-0.869(27)

			[10.3]$^3\Phi_3$			
v	T_v	B_v	10^7 x D_v	10^{10} x H_v	10^{14} x L_v	10^{12} x q_{Hv}
0	10285.41877(74)	0.3526448(39)	5.1862(84)	-0.078(47)	--	0.024(15)
1	10862.9593(10)	0.3501149(60)	4.578(51)	-0.195(20)	1.123(27)	-4.06(28)
2	11435.2824(16)	0.3478860(83)	5.235(93)	2.147(43)	-3.189(66)	--

[a]The numbers in parentheses are one standard deviation in the list digit.

TABLE VI

Spectroscopic Constants[a] (in cm^{-1}) of the $[10.3]^3\Phi_2$–$X^3\Phi_2$ Subband of CoF

$X^3\Phi_2$

v	T_v	B_v	$10^7 \times D_v$	$10^{10} \times H_v$	$10^{14} \times L_v$	$10^8 \times q_{Dv}$	$10^{11} \times q_{Hv}$
0	0.0	0.388513(17)	4.14(12)	-0.510(34)	0.733(34)	0.50(19)	--
1	702.6036(40)	0.379222(22)	-4.54(18)	-1.500(74)	1.51(10)	-2.61(27)	1.492(73)

$[10.3]^3\Phi_2$

v	T_v	B_v	$10^7 \times D_v$	$10^{10} \times H_v$	$10^{14} \times L_v$	$10^8 \times q_{Dv}$	$10^{11} \times q_{Hv}$
0	10157.2863(13)	0.353072(16)	3.875(95)	-0.627(17)	--	-3.63(21)	0.990(33)
1	10734.4595(19)	0.350112(20)	3.50(23)	-2.81(12)	4.03(20)	-4.20(50)	1.21(18)

[a] The numbers in parentheses are one standard deviation in the last digit.

state while the first excited state is the $a^5S(3d^5 3s^1)$ state at 7573 cm^{-1}. The Cr ^7S state gives rise to $^6\Sigma^+$ and $^8\Sigma^+$ (repulsive) molecular states while the Cr ^5S state gives rise to $^4\Sigma^+$ and $^6\Sigma^+$ states. Hence the $A^6\Sigma^+$–$X^6\Sigma^+$ transition of CrH correlates to the forbidden atomic a^5S–a^7S transition.

Although the rotational constants for the three spin components have similar magnitudes, the vibrational intervals $[\Delta G(v + \frac{1}{2})]$ are considerably different for the $X^3\Phi_2$, $X^3\Phi_3$, and $X^3\Phi_4$ spin components (702.6, 668.8, and 672.7 cm^{-1}, respectively). This suggests that the electronic states of CoF have strong Hund's case (c) tendencies. This

TABLE VII

Equilibrium Constants (in cm^{-1}) of the $X^3\Phi$ and $[10.3]^3\Phi$ states of CoF

Constants[a]	$X^3\Phi_4$	$X^3\Phi_3$	$X^3\Phi_2$
B_e	0.3894797(34)	0.3898185(51)	0.393159(22)
α_e	0.0025984(45)	0.0032111(59)	0.009292(28)
γ_e	-0.0000611(5)	--	--
r_e(Å)	1.735698(8)	1.734943(11)	1.727557(28)
ω_e	678.1817(19)	[668.7960(11)][b]	[702.6036(40)][b]
$\omega_e x_e$	2.73967(84)	--	--

Constants[a]	$[10.3]^3\Phi_4$	$[10.3]^3\Phi_3$	$[10.3]^3\Phi_2$
B_e	0.3530152(89)	0.3540227(82)	0.354552(21)
α_e	0.0026928(8)	0.0001505(63)	0.002960(26)
γ_e	0.0000123(2)	--	--
r_e(Å)	1.823139(26)	1.820543(21)	1.819184(54)
ω_e	580.3556(17)	582.7580(27)	[577.3082(23)][b]
$\omega_e x_e$	2.72447(71)	2.6087(12)	--
$\omega_e y_e$	0.007257(84)	--	--

[a] The numbers in parentheses are one standard deviation in the last digit.

[b] $\Delta G_{1/2}$value.

is consistent with our treatment of the states as Hund's case (c) states in our fitting of the data. Some of the spin components require unphysical constants such as L in order to obtain a satisfactory fit. This is additional evidence for global perturbations of the different spin components.

An interesting result of this study is the observation of perturbations in the $v = 0$ and $v = 1$ vibrational levels of the $X^3\Phi_2$ and $X^3\Phi_3$ spin components, respectively. Although we do not have sufficient data to definitely characterize the nature of the perturbing states involved, the observation of perturbations in the ground $^3\Phi$ state is not surprising. Our observation of a large number of weak bands of CoF in the near infrared from 3000 to 9000 cm^{-1} is consistent with the predictions of Freindorf *et al.* (*14*). In the absence of $\Delta\Sigma \neq 0$ transitions, we are unable to locate the precise position of the $X^3\Phi_2$ and $X^3\Phi_3$ spin components. In CoH, however, the spin–orbit splitting between the $X^3\Phi_4$ and $X^3\Phi_3$ spin components is $-728\ \text{cm}^{-1}$. The most likely perturbing states are $^3\Sigma^-$, and $^3\Pi$, calculated to lie at 1130 and 1450 cm^{-1}, respectively, for CoH. The perturbation of the *f*-parity level for $v = 1$ of the $X^3\Phi_3$ spin component points to a $^3\Pi_{0-}$ perturber while the perturbation of $v = 0$ of the $X^3\Phi_2$ spin component is also consistent with a $^3\Pi_{0-}$ perturber. Additional experimental and theoretical work is required to obtain a definite assignment.

CONCLUSION

The emission spectrum of CoF has been investigated in the red and near-infrared regions. The molecules were made in a carbon tube furnace and the spectra were recorded with the 1-m Fourier transform spectrometer of the National Solar Observatory. The bands observed in the spectral region 9000–12500 cm^{-1} have been classified into three subbands assigned as the $^3\Phi_2$–$^3\Phi_2$, $^3\Phi_3$–$^3\Phi_3$, and $^3\Phi_4$–$^3\Phi_4$ subbands of a new $[10.3]^3\Phi_i$–$X^3\Phi_i$ transition. The use of a high-temperature source (~2300°C), results in the observation of many excited vibrational levels and very-high-J rotational lines. The rotational analysis of a total of 20 vibrational bands in the three subbands provides precise molecular constants for the ground and excited electronic states. The molecular parameters obtained have been used to extract effective equilibrium vibrational and rotational constants. The results are consistent with expectations based on the spectroscopic and theoretical information available for CoH.

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