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Laser Spectroscopy of the $\tilde{A}\,^1A'$–$\tilde{X}\,^1A'$ System of CuOH and CuOD

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The $\tilde{A}\,^1A'$–$\tilde{X}\,^1A'$ electronic transition of CuOH and CuOD in the red at 6285 Å has been measured at high resolution by laser excitation spectroscopy. Effective spectroscopic constants for ^{63}CuOH, ^{65}CuOH, ^{63}CuOD, and ^{65}CuOD have been determined from rotational analyses of the unperturbed K_a subbands and a partial r_s structure was evaluated for the molecule. The geometric parameters in the excited $\tilde{A}\,^1A'$ state are

$$r_{\text{Cu-O}} = 1.7748(32)\ \text{Å}, \quad r_{\text{O-H}} = 1.0348(40)\ \text{Å}, \quad \text{and} \quad \angle\text{CuOH} = 111.0(16)°.$$

INTRODUCTION

While considerable spectroscopic effort has been devoted to the study of diatomics containing transition metals, particularly hydrides and oxides, there have been few studies of polyatomics. It was the initial aim of this work to investigate the chemiluminescence spectra of copper-containing polyatomics using a hollow cathode sputtering source similar to that developed by Trkula *et al.* (*1*). Trkula and Harris used this source to produce CuOH using H_2O and D_2O as oxidants and they rotationally analyzed the green system by high-resolution laser-excitation spectroscopy (*2*). We repeated this work to test our source and obtained a spectrum in the green which agreed very well with the chemiluminescence spectrum reported by Trkula and Harris (*2*).

However, two additional features were observed in the red; one with a closed parallel structure and the other more open. Antić-Javanović and Pesić reported a red transition in their work on flames containing copper salts (*3*) in 1969, and more recently Parson and co-workers have observed these two red systems in the chemiluminescence spectra of the reactions of excited Cu atoms with H_2O_2 (*4*). The structure of the more open band closed up on deuteration, indicating that the molecule responsible for this band contained hydrogen. The ratios of the intensities of both red systems to the green system were found to be insensitive to the discharge conditions and this led us to conclude that both red systems were due to CuOH. Furthermore, we obtained high-resolution laser-excitation spectra of these red systems, confirming that both involve transitions from the ground electronic state.

During the course of analyzing these red spectra, it became apparent that better ground state rotational constants were needed to form more accurate ground state combination differences, and so we remeasured the green system at high resolution (*5*). Armed with this improved set of ground state combination differences, we have

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been able to assign some rotational structure in both systems, and work is currently in progress on the more open transition at 6640 Å. We present here the high-resolution analysis of the parallel system at 6285 Å for CuOH and CuOD.

EXPERIMENTAL DETAILS

In the course of this work, it was found that the hollow cathode sputtering source produced relatively noisy spectra, and so we investigated alternate sources of copper atoms. Ultimately, the best source proved to be a conventional Broida oven (*6*) equipped with a graphite crucible for the high temperatures necessary to melt copper. The copper vapor was then entrained in a flow of argon which entered at the top of the crucible, and this flow was channeled into the oxidant region through a graphite funnel. It was found that hydrogen peroxide produced far more CuOH than water, and so all spectra were recorded using H_2O_2 or D_2O_2 as the oxidant.

The laser used in this study was a single-frequency Coherent 699-29 ring dye laser operating with Kiton Red dye and pumped by a Coherent Innova 20 argon ion laser. The laser beam was aligned horizontally in the oxidant flame, and the laser-induced fluorescence at right angles to the beam was detected by a photomultiplier tube. Because the spectra were very weak, it was necessary to reduce the amount of stray laser light inside the oven to obtain a good signal. This was achieved by placing two 3-mm circular apertures in the path of the laser, one on either side of the photomultiplier tube, and by placing a 4-mm slit over the photomultiplier tube ~1 cm away from

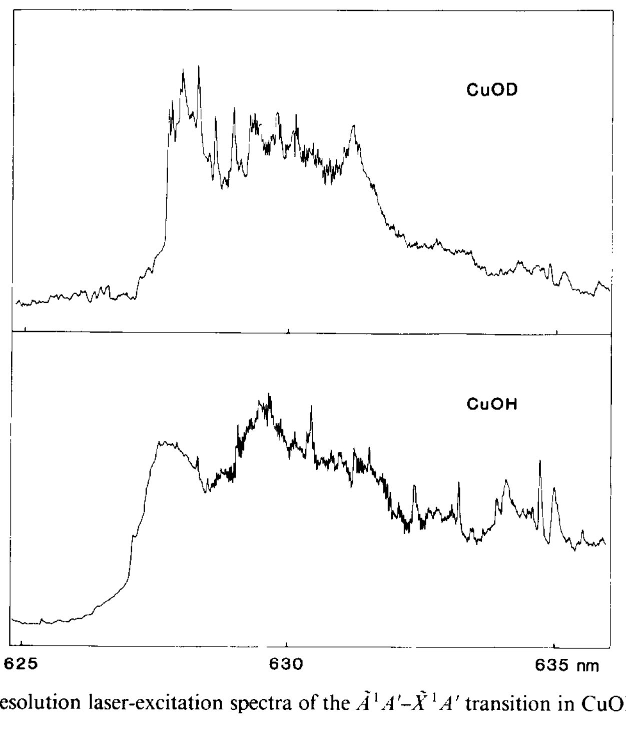

FIG. 1. Low-resolution laser-excitation spectra of the $\tilde{A}\,^1A'$–$\tilde{X}\,^1A'$ transition in CuOH and CuOD.

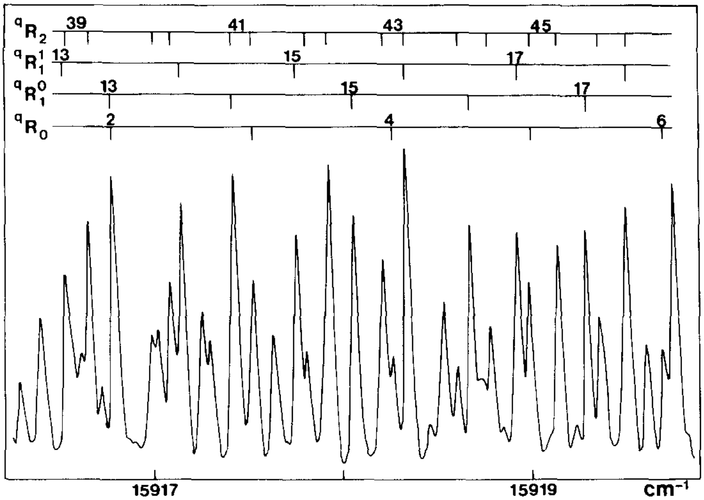

FIG. 2. A portion of the high-resolution spectrum of CuOH in the *R*-branch region.

the laser beam. The laser was amplitude modulated at 700 Hz using a mechanical chopper and the signal was detected using a lock-in amplifier and stored as a function of frequency using the Coherent Autoscan system. The wavenumber scale was calibrated by simultaneously recording the I_2 spectrum with each scan, and comparing these wavenumbers with the published line list after applying the 0.0056 cm^{-1} correction (*7, 8*). The spectra were then transferred to a 386 personal computer where individual lines were fit to Voigt profiles using PC-DECOMP.

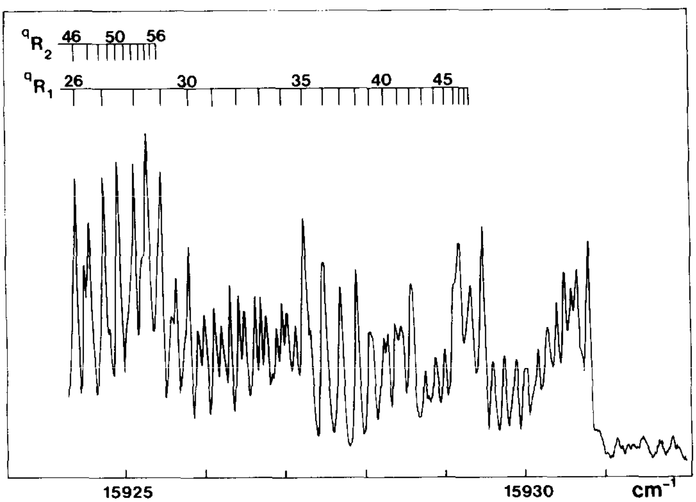

FIG. 3. A portion of the high-resolution spectrum of CuOD in the *R*-branch region showing several bandheads. The first head at 15 931 cm^{-1} probably belongs to the K_a = 0 subband but the presence of massive perturbations prevented a definite assignment.

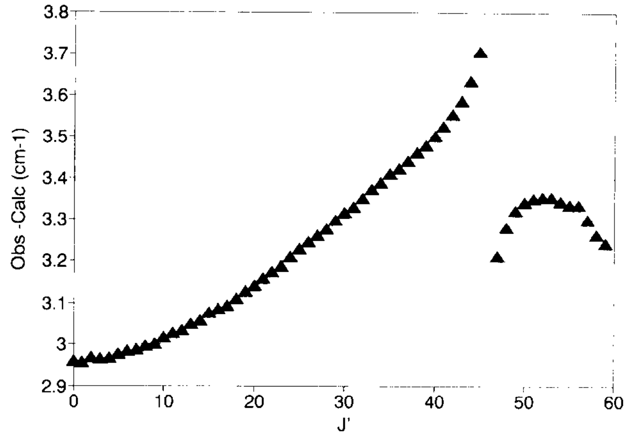

FIG. 4. The observed − calculated line positions using the constants of Table I are plotted against J for the upper $K_a = 0$ stack of CuOH showing a global and a local perturbation.

The initial spectra of CuOH were recorded through a 700-nm blue-pass filter and 620-nm red-pass filter combination to reduce the black body radiation coming from the oven. These spectra recorded at ~6 Torr contained a number of "glitches" caused by small pieces of copper carried from the oven and scattering laser light into the photomultiplier tube. This problem was solved by replacing the 620-nm red-pass filter with a 640-nm red-pass filter. This reduced the filter band pass to the wavelength region occupied by the second red system. Subsequent spectra (the rest of CuOH and all of CuOD) were recorded at higher pressures (>10 Torr) to enhance the collisional relaxation from the first (6285 Å) to the second (6640Å) red system. Although this improved the signal-to-noise ratio and eliminated the scattered laser light there was an increase in the width of each line because of pressure broadening. When these

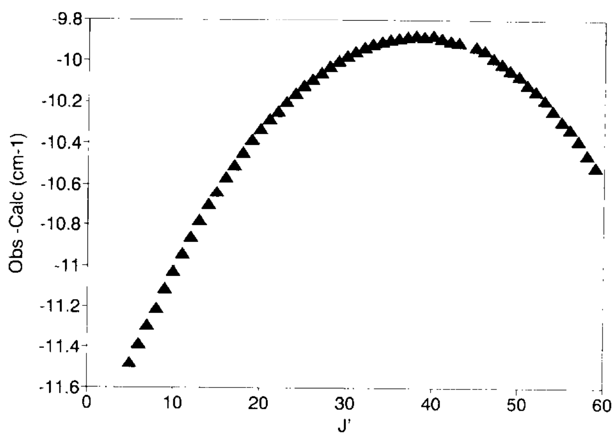

FIG. 5. The observed − calculated line positions using the constants of Table I are plotted against J for the upper $K_a = 3$ stack of CuOH showing a global perturbation that resembles a parabola.

spectra were measured in PC-DECOMP the typical widths (FWHM) for lines in the initial spectra were 0.045 cm^{-1} compared to 0.055 cm^{-1} for the higher-pressure data.

RESULTS

The low-resolution laser-excitation spectra of CuOH and CuOD are displayed in Fig. 1. The main features of both spectra are *PR* rotational contours degraded to the red, implying that both transitions are predominantly *a*-type. The spectrum of CuOH also shows some sharp structure from 6300 to 6350 Å, and we assign this to a band (010–000) associated with the Cu–O–H bending mode of the second red system at 6640 Å.

The spectrum of CuOD shows some sharp features near 6290 Å and we assign these as ${}^qR_{K_a}$ subband heads of the $\tilde{A}^1A'$–$\tilde{X}^1A'$ transition from the high-resolution analysis. The broad feature near 6310 Å we assign as the ${}^qR_{K_a}$ subband heads of a sequence band (001–001) in the Cu–O stretch. The corresponding sequence band is also slightly evident in the CuOH spectrum.

Portions of the high-resolution spectra are displayed in Figs. 2 and 3 for CuOH and CuOD, respectively. Both figures show the high density of lines in the *R*-branch regions of the spectra. Figure 3 shows the rotational assignments for two of the ${}^qR_{K_a}$ subband heads in the CuOD spectrum; the structure near 15 931 cm^{-1} is probably due to the $K_a = 0$ subband, but has not been assigned because this subband is very perturbed.

Analysis of the high-resolution spectra proceeded routinely through use of PC-LOOMIS, a computer program which takes the measured peak positions and intensities (from PC-DECOMP) as input and produces interactive color Loomis–Wood plots. This program enabled *PR* subbands for different K_a to be picked out, and these were assigned *J* and K_a values from ground state combination differences. In this way, *PR* branches were assigned up to $K_a = 4$ in CuOH and $K_a = 5$ in CuOD, a total of 2075 lines for the four isotopic species ^{63}CuOH, ^{65}CuOH, ^{63}CuOD, and ^{65}CuOD. The K_a

TABLE I

Spectroscopic Constants for the $\tilde{A}^1A'$ State of CuOH (in cm^{-1})

Constant		^{63}CuOH	^{65}CuOH	^{63}CuOD	^{65}CuOD
E		15911.5456(11)	15911.5005(16)	15911.0949(34)	15911.0628(55)
A		18.31604(42)	18.29864(56)	10.7142(20)	10.7040(34)
B		0.3881545(70)	0.385676(11)	0.360814(20)	0.358041(34)
C		0.3782373(70)	0.375835(11)	0.346393(20)	0.344775(34)
Δ_J	$\times 10^{-7}$	5.0522(64)	5.040(11)	4.7292(76)	5.549(27)
Δ_{JK}	$\times 10^{-4}$	-1.9863(41)	-1.9503(78)	-0.1780(61)	-0.064(14)
Δ_K	$\times 10^{-2}$	1.8358(23)	1.7473(30)	0.282(32)	0.199(55)
δ_J	$\times 10^{-7}$	0.200(17)	0.54(21)	3.903(84)	2.236(85)
δ_K	$\times 10^{-4}$	2.705(31)	2.866(52)	0.400‡	0.168‡
H_{JJK}	$\times 10^{-9}$	2.51(18)	1.64(38)		
H_{JKK}	$\times 10^{-5}$	-1.2868(19)	-1.2472(29)	-0.0962(17)	-0.0616(40)
H_K	$\times 10^{-3}$			1.393(19)	1.383(33)
h_J	$\times 10^{-11}$	-0.370(39)	-0.670(52)	5.81(24)	
L_K	$\times 10^{-5}$			3.100(37)	3.150(63)
σ		0.0052	0.0057	0.0070	0.0083
N		462	331	397	244

TABLE II

Observed Line Positions (cm^{-1}) for ^{63}CuOH (O–C Units of 10^{-3} cm^{-1})

J'	Ka'	Kc'		J"	Ka"	Kc"	OBS	O-C
0	0	0	-	1	0	1	15913.731*	2963
1	0	1	-	2	0	2	15912.940*	2958
2	0	2	-	3	0	3	15912.156*	2972
4	0	4	-	5	0	5	15910.531*	2974
5	0	5	-	6	0	6	15909.705*	2977
6	0	6	-	7	0	7	15908.873*	2984
7	0	7	-	8	0	8	15908.028*	2988
8	0	8	-	9	0	9	15907.179*	2999
9	0	9	-	10	0	10	15906.316*	3006
10	0	10	-	11	0	11	15905.451*	3021
11	0	11	-	12	0	12	15904.569*	3030
12	0	12	-	13	0	13	15903.674*	3035
13	0	13	-	14	0	14	15902.785*	3057
14	0	14	-	15	0	15	15901.869*	3063
15	0	15	-	16	0	16	15900.954*	3078
16	0	16	-	17	0	17	15900.019*	3085
17	0	17	-	18	0	18	15899.077*	3093
18	0	18	-	19	0	19	15898.134*	3111
19	0	19	-	20	0	20	15897.183*	3131
20	0	20	-	21	0	21	15896.216*	3146
21	0	21	-	22	0	22	15895.239*	3159
22	0	22	-	23	0	23	15894.254*	3176
23	0	23	-	24	0	24	15893.253*	3185
24	0	24	-	25	0	25	15892.256*	3208
25	0	25	-	26	0	26	15891.245*	3227
26	0	26	-	27	0	27	15890.225*	3246
27	0	27	-	28	0	28	15889.192*	3263
28	0	28	-	29	0	29	15888.144*	3274
29	0	29	-	30	0	30	15887.101*	3298
30	0	30	-	31	0	31	15886.042*	3317
31	0	31	-	32	0	32	15884.968*	3330
32	0	32	-	33	0	33	15883.892*	3351
33	0	33	-	34	0	34	15882.811*	3375
34	0	34	-	35	0	35	15881.708*	3388
35	0	35	-	36	0	36	15880.611*	3414
36	0	36	-	37	0	37	15879.489*	3425
38	0	38	-	39	0	39	15877.235*	3463
39	0	39	-	40	0	40	15876.092*	3480
40	0	40	-	41	0	41	15874.945*	3502
41	0	41	-	42	0	42	15873.793*	3527
43	0	43	-	44	0	44	15871.476*	3589
44	0	44	-	45	0	45	15870.321*	3637
45	0	45	-	46	0	46	15869.189*	3715
48	0	48	-	49	0	49	15865.083*	3289
49	0	49	-	50	0	50	15863.883*	3331
50	0	50	-	51	0	51	15862.653*	3352
51	0	51	-	52	0	52	15861.403*	3365
52	0	52	-	53	0	53	15860.149*	3369
53	0	53	-	54	0	54	15858.872*	3365
54	0	54	-	55	0	55	15857.584*	3356
55	0	55	-	56	0	56	15856.289*	3347
56	0	56	-	57	0	57	15854.991*	3341
57	0	57	-	58	0	58	15853.661*	3311
58	0	58	-	59	0	59	15852.306*	3261
59	0	59	-	60	0	60	15850.989*	3256
1	0	1	-	0	0	0	15915.271*	2959
2	0	2	-	1	0	1	15916.039*	2971
3	0	3	-	2	0	2	15916.782*	2968
4	0	4	-	3	0	3	15917.514*	2966
5	0	5	-	4	0	4	15918.254*	2981
6	0	6	-	5	0	5	15918.976*	2989
7	0	7	-	6	0	6	15919.682*	2991
8	0	8	-	7	0	7	15920.382*	2999
9	0	9	-	8	0	8	15921.066*	3000
10	0	10	-	9	0	9	15921.755*	3018
11	0	11	-	10	0	10	15922.426*	3027
12	0	12	-	11	0	11	15923.086*	3037
13	0	13	-	12	0	12	15923.735*	3045
14	0	14	-	13	0	13	15924.377*	3057
15	0	15	-	14	0	14	15925.016*	3078
16	0	16	-	15	0	15	15925.636*	3089
17	0	17	-	16	0	16	15926.242*	3098
18	0	18	-	17	0	17	15926.845*	3113
19	0	19	-	18	0	18	15927.437*	3128
20	0	20	-	19	0	19	15928.015*	3140
21	0	21	-	20	0	20	15928.590*	3159
23	0	23	-	22	0	22	15929.704*	3192
24	0	24	-	23	0	23	15930.248*	3212
25	0	25	-	24	0	24	15930.781*	3232
26	0	26	-	25	0	25	15931.300*	3246
27	0	27	-	26	0	26	15931.808*	3262
28	0	28	-	27	0	27	15932.312*	3283
29	0	29	-	28	0	28	15932.799*	3298
30	0	30	-	29	0	29	15933.278*	3315
31	0	31	-	30	0	30	15933.747*	3333
32	0	32	-	31	0	31	15934.210*	3354
33	0	33	-	32	0	32	15934.658*	3371
34	0	34	-	33	0	33	15935.099*	3392
35	0	35	-	34	0	34	15935.528*	3410
36	0	36	-	35	0	35	15935.942*	3424
37	0	37	-	36	0	36	15936.352*	3443
38	0	38	-	37	0	37	15936.753*	3463
39	0	39	-	38	0	38	15937.144*	3484
40	0	40	-	39	0	39	15937.526*	3507
41	0	41	-	40	0	40	15937.898*	3528
42	0	42	-	41	0	41	15938.268*	3557

J'	Ka'	Kc'		J"	Ka"	Kc"	OBS	O-C
43	0	43	-	42	0	42	15938.632*	359
44	0	44	-	43	0	43	15939.006*	3644
45	0	45	-	44	0	44	15939.381*	3706
47	0	47	-	46	0	46	15939.487*	3218
48	0	48	-	47	0	47	15939.836*	3283
49	0	49	-	48	0	48	15940.150*	3324
50	0	50	-	49	0	49	15940.436*	3345
51	0	51	-	50	0	50	15940.702*	3355
52	0	52	-	51	0	51	15940.947*	3353
53	0	53	-	52	0	52	15941.189*	3358
54	0	54	-	53	0	53	15941.407*	3347
55	0	55	-	54	0	54	15941.619*	3338
56	0	56	-	55	0	55	15941.836*	3342
57	0	57	-	56	0	56	15942.000*	3302
58	0	58	-	57	0	57	15942.172*	3279
59	0	59	-	58	0	58	15942.321*	3239
60	0	60	-	59	0	59	15942.486*	3224
5	1	4	-	6	1	5	15902.021	11
6	1	5	-	7	1	6	15901.191*	17
7	1	6	-	8	1	7	15900.344*	15
8	1	7	-	9	1	8	15899.481	7
9	1	8	-	10	1	9	15898.621	10
10	1	9	-	11	1	10	15897.743	5
11	1	10	-	12	1	11	15896.862	5
12	1	11	-	13	1	12	15895.969	3
13	1	12	-	14	1	13	15895.064	-2
14	1	13	-	15	1	14	15894.169*	12
15	1	14	-	16	1	15	15893.253*	14
16	1	15	-	17	1	16	15892.311	-2
17	1	16	-	18	1	17	15891.378	-0
18	1	17	-	19	1	18	15890.434	0
19	1	18	-	20	1	19	15889.482	1
20	1	19	-	21	1	20	15888.520	0
21	1	20	-	22	1	21	15887.550	0
22	1	21	-	23	1	22	15886.574	2
23	1	22	-	24	1	23	15885.583	-1
24	1	23	-	25	1	24	15884.578	-10
25	1	24	-	26	1	25	15883.583	-2
26	1	25	-	27	1	26	15882.573	1
27	1	26	-	28	1	27	15881.555	3
28	1	27	-	29	1	28	15880.520	-2
29	1	28	-	30	1	29	15879.489	4
30	1	29	-	31	1	30	15878.440	-0
31	1	30	-	32	1	31	15877.381	-6
32	1	31	-	33	1	32	15876.318	-7
33	1	32	-	34	1	33	15875.259	3
34	1	33	-	35	1	34	15874.178	-2
35	1	34	-	36	1	35	15873.088	-6
36	1	35	-	37	1	36	15872.003	1
37	1	36	-	38	1	37	15870.906	4
38	1	37	-	39	1	38	15869.789	-4
39	1	38	-	40	1	39	15868.668	-10
40	1	39	-	41	1	40	15867.554	-2
41	1	40	-	42	1	41	15866.423	-3
42	1	41	-	43	1	42	15865.289	2
43	1	42	-	44	1	43	15864.144	2
44	1	43	-	45	1	44	15862.993	2
45	1	44	-	46	1	45	15861.835	4
46	1	45	-	47	1	46	15860.675	10
47	1	46	-	48	1	47	15859.501	9
48	1	47	-	49	1	48	15858.315	3
49	1	48	-	50	1	49	15857.131	6
51	1	50	-	52	1	51	15854.733	3
52	1	51	-	53	1	52	15853.534	11
53	1	52	-	54	1	53	15852.306	-3
54	1	53	-	55	1	54	15851.084	-5
55	1	54	-	56	1	55	15849.859	-4
56	1	55	-	57	1	56	15848.622	-7
3	1	2	-	2	1	1	15909.125	7
4	1	3	-	3	1	2	15909.868	7
5	1	4	-	4	1	3	15910.603	8
6	1	5	-	5	1	4	15911.328	9
7	1	6	-	6	1	5	15912.036	2
8	1	7	-	7	1	6	15912.743	3
9	1	8	-	8	1	7	15913.431	-5
10	1	9	-	9	1	8	15914.127	4
11	1	10	-	10	1	9	15914.797	-4
12	1	11	-	11	1	10	15915.472	3
13	1	12	-	12	1	11	15916.132	4
14	1	13	-	13	1	12	15916.782	5
15	1	14	-	14	1	13	15917.415	-2
16	1	15	-	15	1	14	15918.051	3
17	1	16	-	16	1	15	15918.667	-2
18	1	17	-	17	1	16	15919.281	-1
19	1	18	-	18	1	17	15919.892	8
20	1	19	-	19	1	18	15920.471	-7
21	1	20	-	20	1	19	15921.066	3
22	1	21	-	21	1	20	15921.650*	12
23	1	22	-	22	1	21	15922.190*	-14
24	1	23	-	23	1	22	15922.760	-1
25	1	24	-	24	1	23	15923.310	1
26	1	25	-	25	1	24	15923.841	-7
27	1	26	-	26	1	25	15924.377	-1
28	1	27	-	27	1	26	15924.895	-3
29	1	28	-	28	1	27	15925.409	-0
30	1	29	-	29	1	28	15925.911	-1

J'	Ka'	Kc'		J"	Ka"	Kc"	OBS	O-C
31	1	30	-	30	1	29	15926.400	-6
32	1	31	-	31	1	30	15926.888	-2
33	1	32	-	32	1	31	15927.364	-2
34	1	33	-	33	1	32	15927.829	-4
35	1	34	-	34	1	33	15928.291	-0
36	1	35	-	35	1	34	15928.746	5
37	1	36	-	36	1	35	15929.171	-10
38	1	37	-	37	1	36	15929.613	0
39	1	38	-	38	1	37	15930.034	-2
40	1	39	-	39	1	38	15930.461	10
41	1	40	-	40	1	39	15930.862	5
42	1	41	-	41	1	40	15931.256	1
43	1	42	-	42	1	41	15931.644	1
44	1	43	-	43	1	42	15932.026	2
45	1	44	-	44	1	43	15932.399	3
46	1	45	-	45	1	44	15932.764	5
47	1	46	-	46	1	45	15933.109	-6
48	1	47	-	47	1	46	15933.461	-1
49	1	48	-	48	1	47	15933.796	-4
50	1	49	-	49	1	48	15934.131	-1
51	1	50	-	50	1	49	15934.460	7
52	1	51	-	51	1	50	15934.764	-4
53	1	52	-	52	1	51	15935.067	-6
54	1	53	-	53	1	52	15935.344*	-27
3	1	3	-	4	1	4	15903.674	-3
4	1	4	-	5	1	5	15902.859	-2
5	1	5	-	6	1	6	15902.021*	-14
6	1	6	-	7	1	7	15901.191	-7
7	1	7	-	8	1	8	15900.344	-7
8	1	8	-	9	1	9	15899.481*	-12
9	1	9	-	10	1	10	15898.621	-4
10	1	10	-	11	1	11	15897.743	-3
11	1	11	-	12	1	12	15896.862	4
12	1	12	-	13	1	13	15895.969	11
13	1	13	-	14	1	14	15895.064*	15
14	1	14	-	15	1	15	15894.134	6
15	1	15	-	16	1	16	15893.196	-2
16	1	16	-	17	1	17	15892.256	-2
17	1	17	-	18	1	18	15891.301	-7
18	1	18	-	19	1	19	15890.339	-8
19	1	19	-	20	1	20	15889.373	-4
20	1	20	-	21	1	21	15888.393	-3
21	1	21	-	22	1	22	15887.412	5
22	1	22	-	23	1	23	15886.406	-0
23	1	23	-	24	1	24	15885.392	-4
24	1	24	-	25	1	25	15884.370	-7
25	1	25	-	26	1	26	15883.350	3
26	1	26	-	27	1	27	15882.307	-2
27	1	27	-	28	1	28	15881.257	-3
28	1	28	-	29	1	29	15880.202	-0
29	1	29	-	30	1	30	15879.137	1
30	1	30	-	31	1	31	15878.056	-3
31	1	31	-	32	1	32	15876.973	-1
32	1	32	-	33	1	33	15875.881	0
33	1	33	-	34	1	34	15874.783	6
34	1	34	-	35	1	35	15873.652*	-13
35	1	35	-	36	1	36	15872.543	-2
36	1	36	-	37	1	37	15871.415	-1
37	1	37	-	38	1	38	15870.281	4
38	1	38	-	39	1	39	15869.135	4
39	1	39	-	40	1	40	15867.980	3
40	1	40	-	41	1	41	15866.814	-1
41	1	41	-	42	1	42	15865.645	0
42	1	42	-	43	1	43	15864.469	3
43	1	43	-	44	1	44	15863.281	1
44	1	44	-	45	1	45	15862.083	-4
45	1	45	-	46	1	46	15860.892	5
46	1	46	-	47	1	47	15859.677	-2
47	1	47	-	48	1	48	15858.468	5
48	1	48	-	49	1	49	15857.245	4
50	1	50	-	51	1	51	15854.781	3
51	1	51	-	52	1	52	15853.534	-2
52	1	52	-	53	1	53	15852.306*	18
53	1	53	-	54	1	54	15851.029	-6
54	1	54	-	55	1	55	15849.774	-1
55	1	55	-	56	1	56	15848.512	2
56	1	56	-	57	1	57	15847.246	7
4	1	4	-	3	1	3	15909.804*	-13
5	1	5	-	4	1	4	15910.531	-6
6	1	6	-	5	1	5	15911.244	-2
7	1	7	-	6	1	6	15911.935	-9
8	1	8	-	7	1	7	15912.638	6
9	1	9	-	8	1	8	15913.307	-2
10	1	10	-	9	1	9	15913.971	-3
11	1	11	-	10	1	10	15914.630	0
12	1	12	-	11	1	11	15915.271	-4
14	1	14	-	13	1	13	15916.538	6
15	1	15	-	14	1	14	15917.141	-3
16	1	16	-	15	1	15	15917.746	-0
17	1	17	-	16	1	16	15918.331	-7
18	1	18	-	17	1	17	15918.915	-4
19	1	19	-	18	1	18	15919.492	2
20	1	20	-	19	1	19	15920.046	-4
21	1	21	-	20	1	20	15920.603	4
22	1	22	-	21	1	21	15921.140	2
23	1	23	-	22	1	22	15921.650*	-17

J'	Ka'	Kc'		J"	Ka"	Kc"	OBS	O-C
24	1	24	-	23	1	23	15922.190	4
25	1	25	-	24	1	24	15922.687	-6
26	1	26	-	25	1	25	15923.187	-4
27	1	27	-	26	1	26	15923.672	-7
28	1	28	-	27	1	27	15924.156	-0
29	1	29	-	28	1	28	15924.622	-2
30	1	30	-	29	1	29	15925.080	-1
31	1	31	-	30	1	30	15925.522	-6
32	1	32	-	31	1	31	15925.966	0
33	1	33	-	32	1	32	15926.400	6
34	1	34	-	33	1	33	15926.812	0
35	1	35	-	34	1	34	15927.220	0
36	1	36	-	35	1	35	15927.624	6
37	1	37	-	36	1	36	15928.015	7
38	1	38	-	37	1	37	15928.391	3
39	1	39	-	38	1	38	15928.746*	-12
40	1	40	-	39	1	39	15929.132*	13
41	1	41	-	40	1	40	15929.471	-0
42	1	42	-	41	1	41	15929.823	8
43	1	43	-	42	1	42	15930.149	0
44	1	44	-	43	1	43	15930.461*	-14
45	1	45	-	44	1	44	15930.781	-10
46	1	46	-	45	1	45	15931.099	-2
47	1	47	-	46	1	46	15931.409	9
48	1	48	-	47	1	47	15931.685	-7
49	1	49	-	48	1	48	15931.971	-5
50	1	50	-	49	1	49	15932.246	-6
51	1	51	-	50	1	50	15932.528	8
53	1	53	-	52	1	52	15933.034	0
54	1	54	-	53	1	53	15933.278	-1
55	1	55	-	54	1	54	15933.511	-7
56	1	56	-	55	1	55	15933.747	-3
57	1	57	-	56	1	56	15933.979	4
58	1	58	-	57	1	57	15934.210*	16
59	1	59	-	58	1	58	15934.405	-2
60	1	60	-	59	1	59	15934.611	-2
4	2	2	-	5	2	3	15888.764	-5
5	2	3	-	6	2	4	15887.948	-0
7	2	5	-	8	2	6	15886.277	-2
8	2	6	-	9	2	7	15885.430	-2
9	2	7	-	10	2	8	15884.578	2
10	2	8	-	11	2	9	15883.710	-1
11	2	9	-	12	2	10	15882.842	5
12	2	10	-	13	2	11	15881.948	-7
13	2	11	-	14	2	12	15881.058	-6
14	2	12	-	15	2	13	15880.161	-4
15	2	13	-	16	2	14	15879.253	-4
16	2	14	-	17	2	15	15878.342	1
17	2	15	-	18	2	16	15877.414	-2
18	2	16	-	19	2	17	15876.481	-2
19	2	17	-	20	2	18	15875.550	7
20	2	18	-	21	2	19	15874.596	3
22	2	20	-	23	2	21	15872.656*	-15
23	2	21	-	24	2	22	15871.693	-5
24	2	22	-	25	2	23	15870.721	4
25	2	23	-	26	2	24	15869.724	-4
26	2	24	-	27	2	25	15868.729	-2
27	2	25	-	28	2	26	15867.727	-1
28	2	26	-	29	2	27	15866.713	-3
29	2	27	-	30	2	28	15865.691	-6
30	2	28	-	31	2	29	15864.668	-2
31	2	29	-	32	2	30	15863.631	-5
32	2	30	-	33	2	31	15862.589	-6
33	2	31	-	34	2	32	15861.550	2
34	2	32	-	35	2	33	15860.497	4
35	2	33	-	36	2	34	15859.438	7
36	2	34	-	37	2	35	15858.374	11
37	2	35	-	38	2	36	15857.300*	12
38	2	36	-	39	2	37	15856.212	6
39	2	37	-	40	2	38	15855.127	10
40	2	38	-	41	2	39	15854.018	-5
41	2	39	-	42	2	40	15852.927	5
42	2	40	-	43	2	41	15851.821	6
43	2	41	-	44	2	42	15850.708	6
44	2	42	-	45	2	43	15849.582	-1
45	2	43	-	46	2	44	15848.449	9
46	2	44	-	47	2	45	15847.319	9
47	2	45	-	48	2	46	15846.169*	-22
48	2	46	-	49	2	47	15845.035*	-15
49	2	47	-	50	2	48	15843.895	-7
51	2	49	-	52	2	50	15841.570*	-21
52	2	50	-	53	2	51	15840.404*	-24
53	2	51	-	54	2	52	15839.227*	-33
54	2	52	-	55	2	53	15838.045*	-41
55	2	53	-	56	2	54	15836.851*	57
56	2	54	-	57	2	55	15835.653*	-72
57	2	55	-	58	2	56	15834.465*	-72
58	2	56	-	59	2	57	15833.258*	-86
4	2	2	-	3	2	1	15895.757	-1
5	2	3	-	4	2	2	15896.492	3
7	2	5	-	6	2	4	15897.923	3
8	2	6	-	7	2	5	15898.621	-9
9	2	7	-	8	2	6	15899.323	-3
10	2	8	-	9	2	7	15900.019	6
11	2	9	-	10	2	8	15900.692	1
12	2	10	-	11	2	9	15901.356	-4

Note. (*) Line not included in the fit.

TABLE II—*Continued*

J'	Ka'	Kc'		J"	Ka"	Kc"	OBS	O-C
13	2	11	-	12	2	10	15902.021	1
14	2	12	-	13	2	11	15902.673	2
15	2	13	-	14	2	12	15903.314	0
16	2	14	-	15	2	13	15903.948	1
17	2	15	-	16	2	14	15904.569	-4
18	2	16	-	17	2	15	15905.189	-0
19	2	17	-	18	2	16	15905.796	-0
20	2	18	-	19	2	17	15906.395	-0
21	2	19	-	20	2	18	15906.982	-4
22	2	20	-	21	2	19	15907.563	-4
23	2	21	-	22	2	20	15908.136	-5
24	2	22	-	23	2	21	15908.699	-7
25	2	23	-	24	2	22	15909.259	-3
26	2	24	-	25	2	23	15909.804	-6
27	2	25	-	26	2	24	15910.349	-1
28	2	26	-	27	2	25	15910.883	1
29	2	27	-	28	2	26	15911.399	-7
30	2	28	-	29	2	27	15911.935*	14
31	2	29	-	30	2	28	15912.434	5
32	2	30	-	31	2	29	15912.940	12
33	2	31	-	32	2	30	15913.431	11
34	2	32	-	33	2	31	15913.906	3
35	2	33	-	34	2	32	15914.389	9
36	2	34	-	35	2	33	15914.854	6
37	2	35	-	36	2	34	15915.301	-8
39	2	37	-	38	2	36	15916.215	7
40	2	38	-	39	2	37	15916.653	6
41	2	39	-	40	2	38	15917.081	3
42	2	40	-	41	2	39	15917.514*	13
43	2	41	-	42	2	40	15917.919	0
44	2	42	-	43	2	41	15918.331	3
45	2	43	-	44	2	42	15918.720	-11
46	2	44	-	45	2	43	15919.132	5
47	2	45	-	46	2	44	15919.492*	-25
48	2	46	-	47	2	45	15919.892	-6
49	2	47	-	48	2	46	15920.274	-0
50	2	48	-	49	2	47	15920.603*	-40
51	2	49	-	50	2	48	15920.978	-28
52	2	50	-	51	2	49	15921.329*	-32
4	2	3	-	5	2	4	15888.764	-5
5	2	4	-	6	2	5	15887.948	-0
7	2	6	-	8	2	7	15886.277	-2
8	2	7	-	9	2	8	15885.430	-2
9	2	8	-	10	2	9	15884.578	2
10	2	9	-	11	2	10	15883.710	-1
11	2	10	-	12	2	11	15882.842	5
12	2	11	-	13	2	12	15881.948	-7
13	2	12	-	14	2	13	15881.058	-6
14	2	13	-	15	2	14	15880.161	-4
15	2	14	-	16	2	15	15879.253	-4
16	2	15	-	17	2	16	15878.342	2
17	2	16	-	18	2	17	15877.414	-1
18	2	17	-	19	2	18	15876.481	-1
19	2	18	-	20	2	19	15875.550	9
20	2	19	-	21	2	20	15874.596	5
23	2	22	-	24	2	23	15871.693	-0
24	2	23	-	25	2	24	15870.721	9
25	2	24	-	26	2	25	15869.724	3
26	2	25	-	27	2	26	15868.729	5
27	2	26	-	28	2	27	15867.727	9
28	2	27	-	29	2	28	15866.713	8
29	2	28	-	30	2	29	15865.691	7
30	2	29	-	31	2	30	15864.668*	13
31	2	30	-	32	2	31	15863.631	12
32	2	31	-	33	2	32	15862.589*	13
33	2	32	-	34	2	33	15861.518	-8
34	2	33	-	35	2	34	15860.462	-6
35	2	34	-	36	2	35	15859.398	-6
37	2	36	-	38	2	37	15857.245	-8
38	2	37	-	39	2	38	15856.166	-2
39	2	38	-	40	2	39	15855.072	-3
40	2	39	-	41	2	40	15853.973	-3
41	2	40	-	42	2	41	15852.858*	-13
42	2	41	-	43	2	42	15851.758	-1
43	2	42	-	44	2	43	15850.637	-4
44	2	43	-	45	2	44	15849.509	-8
45	2	44	-	46	2	45	15848.383	-3
46	2	45	-	47	2	46	15847.246	-4
47	2	46	-	48	2	47	15846.109	2
48	2	47	-	49	2	48	15844.958	-2
49	2	48	-	50	2	49	15843.804	-3
50	2	49	-	51	2	50	15842.651	3

J'	Ka'	Kc'		J"	Ka"	Kc"	OBS	O-C
51	2	50	-	52	2	51	15841.482	-1
52	2	51	-	53	2	52	15840.320	7
53	2	52	-	54	2	53	15839.144	6
54	2	53	-	55	2	54	15837.965	6
55	2	54	-	56	2	55	15836.779	5
56	2	55	-	57	2	56	15835.596	11
4	2	3	-	3	2	2	15895.757	-1
5	2	4	-	4	2	3	15896.492	3
6	2	5	-	5	2	4	15897.227*	15
7	2	6	-	6	2	5	15897.923	-3
8	2	7	-	7	2	6	15898.621	-9
9	2	8	-	8	2	7	15899.323	-2
10	2	9	-	9	2	8	15900.019	7
11	2	10	-	10	2	9	15900.692	2
12	2	11	-	11	2	10	15901.356	-2
13	2	12	-	12	2	11	15902.021	3
14	2	13	-	13	2	12	15902.673	4
15	2	14	-	14	2	13	15903.314	3
16	2	15	-	15	2	14	15903.948	4
17	2	16	-	16	2	15	15904.569	0
18	2	17	-	17	2	16	15905.189	5
19	2	18	-	18	2	17	15905.796	6
20	2	19	-	19	2	18	15906.395	7
21	2	20	-	20	2	19	15906.982	5
22	2	21	-	21	2	20	15907.563	6
23	2	22	-	22	2	21	15908.136	7
24	2	23	-	23	2	22	15908.699	7
25	2	24	-	24	2	23	15909.259*	13
26	2	25	-	25	2	24	15909.804*	13
30	2	29	-	29	2	28	15911.895	6
31	2	30	-	30	2	29	15912.393	-0
32	2	31	-	31	2	30	15912.891	2
33	2	32	-	32	2	31	15913.371	-5
34	2	33	-	33	2	32	15913.852	-2
35	2	34	-	34	2	33	15914.319	-7
37	2	36	-	36	2	35	15915.238	-5
39	2	38	-	38	2	37	15916.132	2
41	2	40	-	40	2	39	15916.978	-7
43	2	42	-	42	2	41	15917.802	-7
44	2	43	-	43	2	42	15918.203	-8
45	2	44	-	44	2	43	15918.594	-11
46	2	45	-	45	2	44	15918.976*	-16
47	2	46	-	46	2	45	15919.354*	-17
48	2	47	-	47	2	46	15919.742	-2
49	2	48	-	48	2	47	15920.104	-6
50	2	49	-	49	2	48	15920.471	3
51	2	50	-	50	2	49	15920.824	4
53	2	52	-	52	2	51	15921.502	-1
54	2	53	-	53	2	52	15921.834	-2
5	3	2	-	6	3	3	15853.116*	-11469
6	3	3	-	7	3	4	15852.377*	-11383
7	3	4	-	8	3	5	15851.633*	-11294
8	3	5	-	9	3	6	15850.877*	-11207
9	3	6	-	10	3	7	15850.122*	-11113
10	3	7	-	11	3	8	15849.349*	-11028
11	3	8	-	12	3	9	15848.564*	-10948
12	3	9	-	13	3	10	15847.782*	-10856
13	3	10	-	14	3	11	15846.981*	-10776
14	3	11	-	15	3	12	15846.169*	-10696
15	3	12	-	16	3	13	15845.334*	-10635
16	3	13	-	17	3	14	15844.500*	-10565
17	3	14	-	18	3	15	15843.649*	-10502
18	3	15	-	19	3	16	15842.787*	-10444
19	3	16	-	20	3	17	15841.922*	-10380
20	3	17	-	21	3	18	15841.033*	-10333
21	3	18	-	22	3	19	15840.141*	-10282
22	3	19	-	23	3	20	15839.227*	-10245
23	3	20	-	24	3	21	15838.314*	-10199
24	3	21	-	25	3	22	15837.389*	-10158
25	3	22	-	26	3	23	15836.457*	-10117
26	3	23	-	27	3	24	15835.506*	-10087
27	3	24	-	28	3	25	15834.551*	-10055
28	3	25	-	29	3	26	15833.583*	-10027
29	3	26	-	30	3	27	15832.611*	-9997
30	3	27	-	31	3	28	15831.624*	-9974
31	3	28	-	32	3	29	15830.631*	-9952
32	3	29	-	33	3	30	15829.626*	-9933
33	3	30	-	34	3	31	15828.617*	-9913
34	3	31	-	35	3	32	15827.587*	-9905
35	3	32	-	36	3	33	15826.553*	-9897
36	3	33	-	37	3	34	15825.508*	-9891
37	3	34	-	38	3	35	15824.460*	-9882

J'	Ka'	Kc'		J"	Ka"	Kc"	OBS	O-C
38	3	35	-	39	3	36	15823.407*	-9873
39	3	36	-	40	3	37	15822.341*	-9869
40	3	37	-	41	3	38	15821.265*	-9870
41	3	38	-	42	3	39	15820.172*	-9881
42	3	39	-	43	3	40	15819.071*	-9894
43	3	40	-	44	3	41	15817.963*	-9907
45	3	42	-	46	3	43	15815.734*	-9930
46	3	43	-	47	3	44	15814.603*	-9949
47	3	44	-	48	3	45	15813.458*	-9977
48	3	45	-	49	3	46	15812.307*	-10005
49	3	46	-	50	3	47	15811.149*	-10033
50	3	47	-	51	3	48	15809.979*	-10069
51	3	48	-	52	3	49	15808.802*	-10106
52	3	49	-	53	3	50	15807.621*	-10142
53	3	50	-	54	3	51	15806.430*	-10183
54	3	51	-	55	3	52	15805.226*	-10231
55	3	52	-	56	3	53	15804.011*	-10286
56	3	53	-	57	3	54	15802.804*	-10327
57	3	54	-	58	3	55	15801.578*	-10383
58	3	55	-	59	3	56	15800.338*	-10447
59	3	56	-	60	3	57	15799.106*	-10500
5	3	2	-	4	3	1	15861.642*	-11480
6	3	3	-	5	3	2	15862.464*	-11384
7	3	4	-	6	3	3	15863.281*	-11285
8	3	5	-	7	3	4	15864.070*	-11206
9	3	6	-	8	3	5	15864.866*	-11113
10	3	7	-	9	3	6	15865.645*	-11027
11	3	8	-	10	3	7	15866.423*	-10934
12	3	9	-	11	3	8	15867.176*	-10857
13	3	10	-	12	3	9	15867.928*	-10773
14	3	11	-	13	3	10	15868.668*	-10694
15	3	12	-	14	3	11	15869.375*	-10638
16	3	13	-	15	3	12	15870.092*	-10564
17	3	14	-	16	3	13	15870.787*	-10505
18	3	15	-	17	3	14	15871.476*	-10443
19	3	16	-	18	3	15	15872.154*	-10384
20	3	17	-	19	3	16	15872.818*	-10331
21	3	18	-	20	3	17	15873.467*	-10284
22	3	19	-	21	3	18	15874.104*	-10242
23	3	20	-	22	3	19	15874.739*	-10194
24	3	21	-	23	3	20	15875.354*	-10157
25	3	22	-	24	3	21	15875.961*	-10120
26	3	23	-	25	3	22	15876.557*	-10087
27	3	24	-	26	3	23	15877.139*	-10060
28	3	25	-	27	3	24	15877.718*	-10027
29	3	26	-	28	3	25	15878.281*	-10003
30	3	27	-	29	3	26	15878.837*	-9977
31	3	28	-	30	3	27	15879.381*	-9956
32	3	29	-	31	3	28	15879.919*	-9934
33	3	30	-	32	3	29	15880.439*	-9921
34	3	31	-	33	3	30	15880.952*	-9908
35	3	32	-	34	3	31	15881.456*	-9896
36	3	33	-	35	3	32	15881.948*	-9889
37	3	34	-	36	3	33	15882.431*	-9883
38	3	35	-	37	3	34	15882.906*	-9877
39	3	36	-	38	3	35	15883.350*	-9895
40	3	37	-	39	3	36	15883.815*	-9885
41	3	38	-	40	3	37	15884.250*	-9897
42	3	39	-	41	3	38	15884.676*	-9911
43	3	40	-	42	3	39	15885.108*	-9912
45	3	42	-	44	3	41	15885.930*	-9934
46	3	43	-	45	3	42	15886.324*	-9951
47	3	44	-	46	3	43	15886.684*	-9996
48	3	45	-	47	3	44	15887.055*	-10022
49	3	46	-	48	3	45	15887.412*	-10057
50	3	47	-	49	3	46	15887.777*	-10075
51	3	48	-	50	3	47	15888.106*	-10123
52	3	49	-	51	3	48	15888.449*	-10150
53	3	50	-	52	3	49	15888.764*	-10198
54	3	51	-	53	3	50	15889.071*	-10249
55	3	52	-	54	3	51	15889.373*	-10297
56	3	53	-	55	3	52	15889.684*	-10331
57	3	54	-	56	3	53	15889.964*	-10388
58	3	55	-	57	3	54	15890.225*	-10458
59	3	56	-	58	3	55	15890.487*	-10520
60	3	57	-	59	3	56	15890.736*	-10590
4	4	0	-	5	4	1	15832.741	1
5	4	1	-	6	4	2	15831.915	-3
6	4	2	-	7	4	3	15831.092	6
7	4	3	-	8	4	4	15830.235	-9
8	4	4	-	9	4	5	15829.391	-3
9	4	5	-	10	4	6	15828.546*	13

J'	Ka'	Kc'		J"	Ka"	Kc"	OBS	O-C
10	4	6	-	11	4	7	15827.657	7
11	4	7	-	12	4	8	15826.778	-7
12	4	8	-	13	4	9	15825.897	1
13	4	9	-	14	4	10	15824.993	8
14	4	10	-	15	4	11	15824.088	-7
15	4	11	-	16	4	12	15823.182	3
16	4	12	-	17	4	13	15822.263	8
17	4	13	-	18	4	14	15821.331	10
18	4	14	-	19	4	15	15820.390	11
19	4	15	-	20	4	16	15819.427	-0
20	4	16	-	21	4	17	15818.469	2
21	4	17	-	22	4	18	15817.502	4
22	4	18	-	23	4	19	15816.528	9
23	4	19	-	24	4	20	15815.540	9
24	4	20	-	25	4	21	15814.540	5
25	4	21	-	26	4	22	15813.538	7
26	4	22	-	27	4	23	15812.521	4
27	4	23	-	28	4	24	15811.502	7
28	4	24	-	29	4	25	15810.475	11
29	4	25	-	30	4	26	15809.424	0
30	4	26	-	31	4	27	15808.377	1
31	4	27	-	32	4	28	15807.325	6
32	4	28	-	33	4	29	15806.256	3
33	4	29	-	34	4	30	15805.183	3
34	4	30	-	35	4	31	15804.096	-1
35	4	31	-	36	4	32	15803.008	1
36	4	32	-	37	4	33	15801.904	3
37	4	33	-	38	4	34	15800.801	1
38	4	34	-	39	4	35	15799.681	4
39	4	35	-	40	4	36	15798.559	2
40	4	36	-	41	4	37	15797.425	-4
41	4	37	-	42	4	38	15796.281	-8
44	4	40	-	45	4	41	15792.831	11
45	4	41	-	46	4	42	15791.649	2
47	4	43	-	48	4	44	15789.284	6
48	4	44	-	49	4	45	15788.078	-4
49	4	45	-	50	4	46	15786.873	-4
50	4	46	-	51	4	47	15785.670	5
51	4	47	-	52	4	48	15784.461*	16
8	4	4	-	7	4	3	15842.581	4
10	4	6	-	9	4	5	15843.949	2
11	4	7	-	10	4	6	15844.608	-10
12	4	8	-	11	4	7	15845.273	-7
13	4	9	-	12	4	8	15845.924	-8
14	4	10	-	13	4	9	15846.571	-3
15	4	11	-	14	4	10	15847.192*	14
16	4	12	-	15	4	11	15847.833	3
17	4	13	-	16	4	12	15848.449	5
18	4	14	-	17	4	13	15849.040	-8
19	4	15	-	18	4	14	15849.644	1
20	4	16	-	19	4	15	15850.229	1
21	4	17	-	20	4	16	15850.802	-1
22	4	18	-	21	4	17	15851.365	-5
23	4	19	-	22	4	18	15851.926	-1
24	4	20	-	23	4	19	15852.473	-0
25	4	21	-	24	4	20	15853.010	2
26	4	22	-	25	4	21	15853.534	6
27	4	23	-	26	4	22	15854.056	3
28	4	24	-	27	4	23	15854.570	2
29	4	25	-	28	4	24	15855.072	4
30	4	26	-	29	4	25	15855.561	2
31	4	27	-	30	4	26	15856.033	-6
32	4	28	-	31	4	27	15856.514	3
33	4	29	-	32	4	28	15856.975	1
34	4	30	-	33	4	29	15857.422	-5
35	4	31	-	34	4	30	15857.870	-1
36	4	32	-	35	4	31	15858.315	10
37	4	33	-	36	4	32	15858.725	-6
38	4	34	-	37	4	33	15859.142	-4
39	4	35	-	38	4	34	15859.548	-5
40	4	36	-	39	4	35	15859.937*	13
41	4	37	-	40	4	36	15860.327	-10
42	4	38	-	41	4	37	15860.708	-6
44	4	40	-	43	4	39	15861.451	6
45	4	41	-	44	4	40	15861.789	7
46	4	42	-	45	4	41	15862.132	-6
47	4	43	-	46	4	42	15862.464	-6
48	4	44	-	47	4	43	15862.786	-7
49	4	45	-	48	4	44	15863.100	-7
50	4	46	-	49	4	45	15863.412	-0
51	4	47	-	50	4	46	15863.718	-1
52	4	48	-	51	4	47	15864.004	-1

= 0 and $K_a = 3$ stacks in the upper state for CuOH were found to be perturbed and plots of the observed minus calculated line positions plotted against the upper state J quantum number are pictured in Figs. 4 and 5. The situation for CuOD is worse: no PR branches could be found connecting to $K_a = 0$ or to the lower asymmetry component ($\gamma = K_a + K_c - J = 1$) of the $K_a = 1$ stack. Presumably these stacks are very perturbed.

The unperturbed, assigned transitions were fit to a model which described the energies of both ground and upper electronic states with a Watson A reduced Hamiltonian

TABLE III

Observed Line Positions (cm^{-1}) for $^{65}CuOH$ (O–C Units of 10^{-3} cm^{-1})

J'	Ka'	Kc'	J''	Ka''	Kc''	OBS	O-C	J'	Ka'	Kc'	J''	Ka''	Kc''	OBS	O-C	J'	Ka'	Kc'	J''	Ka''	Kc''	OBS	O-C	J'	Ka'	Kc'	J''	Ka''	Kc''	OBS	O-C
3	0	3	4	0	4	15911.328*	2977	39	1	38	40	1	39	15868.867	5	36	1	36	37	1	37	15871.592	10	50	2	48	51	2	49	15842.932	-7
4	0	4	5	0	5	15910.531*	2994	40	1	39	41	1	40	15867.727*	-19	37	1	37	38	1	38	15870.451	-1	51	2	49	52	2	50	15841.792	6
5	0	5	6	0	6	15909.705*	2991	41	1	40	42	1	41	15866.630	7	38	1	38	39	1	39	15869.320	6	3	2	1	2	2	0	15894.910	4
6	0	6	7	0	7	15908.873*	2993	42	1	41	43	1	42	15865.489	-3	39	1	39	40	1	40	15868.168	1	4	2	2	3	2	1	15895.657*	16
7	0	7	8	0	8	15908.028*	2992	43	1	42	44	1	43	15864.353	-1	40	1	40	41	1	41	15867.016	2	5	2	3	4	2	2	15896.364	-4
8	0	8	9	0	9	15907.179*	2997	44	1	43	45	1	44	15863.207	-2	41	1	41	42	1	42	15865.855	3	6	2	4	5	2	3	15897.081	-6
9	0	9	10	0	10	15906.316*	2998	45	1	44	46	1	45	15862.038*	-19	42	1	42	43	1	43	15864.668*	-14	7	2	5	6	2	4	15897.787	-8
10	0	10	11	0	11	15905.451*	3008	46	1	45	47	1	46	15860.892	-5	43	1	43	44	1	44	15863.493*	-13	8	2	6	7	2	5	15898.490	-5
11	0	11	12	0	12	15904.569*	3011	47	1	46	48	1	47	15859.735	4	44	1	44	45	1	45	15862.322	1	9	2	7	8	2	6	15899.191	4
12	0	12	13	0	13	15903.674*	3011	48	1	47	49	1	48	15858.568	11	45	1	45	46	1	46	15861.129	-2	10	2	8	9	2	7	15899.880	11
13	0	13	14	0	14	15902.785*	3027	49	1	48	50	1	49	15857.371	-5	46	1	46	47	1	47	15859.937	5	11	2	9	10	2	8	15900.539	-4
14	0	14	15	0	15	15901.869*	3026	50	1	49	51	1	50	15856.166*	-23	47	1	47	48	1	48	15858.725	-3	12	2	10	11	2	9	15901.191*	-17
15	0	15	16	0	16	15900.988*	3070	51	1	50	52	1	51	15854.991	-2	48	1	48	49	1	49	15857.509	-7	13	2	11	12	2	10	15901.869	6
16	0	16	17	0	17	15900.057*	3074	53	1	52	54	1	53	15852.588	5	49	1	49	50	1	50	15856.289	-9	14	2	12	13	2	11	15902.507	-4
17	0	17	18	0	18	15899.118*	3080	54	1	53	55	1	54	15851.365	-2	50	1	50	51	1	51	15855.072	-2	15	2	13	14	2	12	15903.155	6
18	0	18	19	0	19	15898.184*	3101	55	1	54	56	1	55	15850.122*	-22	51	1	51	52	1	52	15853.813*	-31	16	2	14	15	2	13	15903.770	-8
19	0	19	20	0	20	15897.227*	3109	56	1	55	57	1	56	15848.903	-12	52	1	52	53	1	53	15852.588*	-22	17	2	15	16	2	14	15904.401	3
20	0	20	21	0	21	15896.261*	3137	57	1	56	58	1	57	15847.678	-0	6	1	6	5	1	5	15911.162	4	18	2	16	17	2	15	15905.011	-0
21	0	21	22	0	22	15895.307*	3148	58	1	57	59	1	58	15846.429	-7	7	1	7	6	1	6	15911.856	4	19	2	17	18	2	16	15905.612	-3
22	0	22	23	0	23	15894.324*	3159	59	1	58	60	1	59	15845.166*	-20	8	1	8	7	1	7	15912.537	3	20	2	18	19	2	17	15906.205	-4
23	0	23	24	0	24	15893.336*	3175	7	1	6	6	1	5	15911.935	-5	9	1	9	8	1	8	15913.196	-11	21	2	19	20	2	18	15906.791	-5
24	0	24	25	0	25	15892.346*	3199	8	1	7	7	1	6	15912.638	-3	10	1	10	9	1	9	15913.852*	-17	22	2	20	21	2	19	15907.371	-2
25	0	25	26	0	26	15891.336*	3211	10	1	9	9	1	8	15914.013	-2	11	1	11	10	1	10	15914.526	6	23	2	21	22	2	20	15907.936	-6
27	0	27	28	0	28	15889.299*	3249	11	1	10	10	1	9	15914.696	8	12	1	12	11	1	11	15915.163	2	24	2	22	23	2	21	15908.496	-7
28	0	28	29	0	29	15888.265*	3267	12	1	11	11	1	10	15915.356	4	13	1	13	12	1	12	15915.775*	-16	25	2	23	24	2	22	15909.056	0
29	0	29	30	0	30	15887.218*	3281	13	1	12	12	1	11	15915.988*	-18	14	1	14	13	1	13	15916.405	-5	26	2	24	25	2	23	15909.588	-12
30	0	30	31	0	31	15886.168*	3301	14	1	13	13	1	12	15916.653	1	15	1	15	14	1	14	15917.016	-3	27	2	25	26	2	24	15910.142	6
31	0	31	32	0	32	15885.108*	3321	15	1	14	14	1	13	15917.291	4	16	1	16	15	1	15	15917.623	6	28	2	26	27	2	25	15910.655	-8
32	0	32	33	0	33	15884.031*	3333	16	1	15	15	1	14	15917.919	4	17	1	17	16	1	16	15918.203	-3	29	2	27	28	2	26	15911.197*	14
34	0	34	35	0	35	15881.877*	3384	17	1	16	16	1	15	15918.523	-9	18	1	18	17	1	17	15918.776	-6	30	2	28	29	2	27	15911.700	6
35	0	35	36	0	36	15880.767*	3390	18	1	17	17	1	16	15919.132	-8	19	1	19	18	1	18	15919.354	5	31	2	29	30	2	28	15912.203	5
36	0	36	37	0	37	15879.658*	3406	19	1	18	18	1	17	15919.742	3	20	1	20	19	1	19	15919.892*	-14	33	2	31	32	2	30	15913.196*	15
37	0	37	38	0	38	15878.555*	3437	20	1	19	19	1	18	15920.329	1	22	1	22	21	1	21	15920.978	-9	34	2	32	33	2	31	15913.662	1
1	0	1	0	0	0	15915.238*	2976	21	1	20	20	1	19	15920.915	5	23	1	23	22	1	22	15921.502	-10	35	2	33	34	2	32	15914.127	-7
2	0	2	1	0	1	15915.988*	2975	22	1	21	21	1	20	15921.502*	21	24	1	24	23	1	23	15922.034	6	37	2	35	36	2	34	15915.060	5
3	0	3	2	0	2	15916.714*	2960	23	1	22	22	1	21	15922.034	-10	25	1	25	24	1	24	15922.526	-6	38	2	36	37	2	35	15915.510	6
6	0	6	5	0	5	15918.882*	2968	24	1	23	23	1	22	15922.597	-0	27	1	27	26	1	26	15923.511	-1	41	2	39	40	2	38	15916.814	7
7	0	7	6	0	6	15919.598*	2985	26	1	25	25	1	24	15923.672	-4	28	1	28	27	1	27	15923.985	-1	42	2	40	41	2	39	15917.244*	17
9	0	9	8	0	8	15920.978*	2999	27	1	26	26	1	25	15924.199	-4	29	1	29	28	1	28	15924.457	7	4	2	3	5	2	4	15888.696	-1
10	0	10	9	0	9	15921.650*	3004	28	1	27	27	1	26	15924.719	-1	30	1	30	29	1	29	15924.895	-9	5	2	4	6	2	5	15887.895*	13
11	0	11	10	0	10	15922.320*	3016	29	1	28	28	1	27	15925.229	-0	31	1	31	30	1	30	15925.355	6	6	2	5	7	2	6	15887.055	-2
12	0	12	11	0	11	15922.970*	3020	30	1	29	29	1	28	15925.728	-0	32	1	32	31	1	31	15925.783	-0	7	2	6	8	2	7	15886.216	-8
13	0	13	12	0	12	15923.620*	3034	31	1	30	30	1	29	15926.212	-7	33	1	33	32	1	32	15926.212	4	8	2	7	9	2	8	15885.392	10
14	0	14	13	0	13	15924.258*	3047	32	1	31	31	1	30	15926.699	-1	34	1	34	33	1	33	15926.629	5	9	2	8	10	2	9	15884.528	-3
15	0	15	14	0	14	15924.895*	3068	33	1	32	32	1	31	15927.172	-2	35	1	35	34	1	34	15927.029	-0	10	2	9	11	2	10	15883.670	-1
16	0	16	15	0	15	15925.522*	3091	34	1	33	33	1	32	15927.624*	-14	36	1	36	35	1	35	15927.437	12	11	2	10	12	2	11	15882.811	8
17	0	17	16	0	16	15926.115*	3089	35	1	34	34	1	33	15928.086	-7	37	1	37	36	1	36	15927.829*	16	12	2	11	13	2	12	15881.948*	22
18	0	18	17	0	17	15926.698*	3090	36	1	35	35	1	34	15928.544	4	38	1	38	37	1	37	15928.190	-0	13	2	12	14	2	13	15881.058*	17
19	0	19	18	0	18	15927.299*	3115	37	1	36	36	1	35	15928.992*	14	41	1	41	40	1	40	15929.273	4	14	2	13	15	2	14	15880.161*	14
20	0	20	19	0	19	15927.873*	3127	38	1	37	37	1	36	15929.404	-4	42	1	42	41	1	41	15929.613	3	15	2	14	16	2	15	15879.253	8
21	0	21	20	0	20	15928.442*	3144	39	1	38	38	1	37	15929.823	-5	43	1	43	42	1	42	15929.946	2	16	2	15	17	2	16	15878.342	8
22	0	22	21	0	21	15928.992*	3151	40	1	39	39	1	38	15930.248	8	44	1	44	43	1	43	15930.248*	-20	17	2	16	18	2	17	15877.414	-1
23	0	23	22	0	22	15929.547*	3175	41	1	40	40	1	39	15930.622*	-21	4	2	2	5	2	3	15888.696	-1	18	2	17	19	2	18	15876.481	-6
24	0	24	23	0	23	15930.064*	3191	42	1	41	41	1	40	15931.035	-3	5	2	3	6	2	4	15887.895*	13	19	2	18	20	2	19	15875.550	-2
25	0	25	24	0	24	15930.622*	3218	43	1	42	42	1	41	15931.409*	-15	6	2	4	7	2	5	15887.055	-2	20	2	19	21	2	20	15874.596	-12
26	0	26	25	0	25	15931.132*	3227	44	1	43	43	1	42	15931.808	6	7	2	5	8	2	6	15886.216	-8	21	2	20	22	2	21	15873.652	-4
27	0	27	26	0	26	15931.644*	3250	45	1	44	44	1	43	15932.174	3	8	2	6	9	2	7	15885.392	10	22	2	21	23	2	22	15872.697	2
28	0	28	27	0	27	15932.145*	3270	46	1	45	45	1	44	15932.528	-4	9	2	7	10	2	8	15884.528	-3	23	2	22	24	2	23	15871.739	11
29	0	29	28	0	28	15932.629*	3285	47	1	46	46	1	45	15932.890	6	10	2	8	11	2	9	15883.670	-1	25	2	24	26	2	25	15869.789*	22
30	0	30	29	0	29	15933.109*	3305	49	1	48	48	1	47	15933.568	4	11	2	9	12	2	10	15882.811	8	26	2	25	27	2	26	15868.763	7
31	0	31	30	0	30	15933.568*	3315	50	1	49	49	1	48	15933.891	1	12	2	10	13	2	11	15881.948*	22	27	2	26	28	2	27	15867.784	7
32	0	32	31	0	31	15934.024*	3333	51	1	50	50	1	49	15934.210	1	13	2	11	14	2	12	15881.058*	17	28	2	27	29	2	28	15866.772	3
33	0	33	32	0	32	15934.460*	3340	52	1	51	51	1	50	15934.520	2	14	2	12	15	2	13	15880.161*	14	32	2	31	33	2	32	15862.653	-11
34	0	34	33	0	33	15934.907*	3368	53	1	52	52	1	51	15934.824	5	15	2	13	16	2	14	15879.253	8	33	2	32	34	2	33	15861.608*	-13
35	0	35	34	0	34	15935.344*	3396	54	1	53	53	1	52	15935.099*	-13	16	2	14	17	2	15	15878.342	8	34	2	33	35	2	34	15860.564	-5
36	0	36	35	0	35	15935.757*	3411	55	1	54	54	1	53	15935.394	-3	17	2	15	18	2	16	15877.414	-1	35	2	34	36	2	35	15859.501	-9
37	0	37	36	0	36	15936.165*	3430	56	1	55	55	1	54	15935.663	-10	18	2	16	19	2	17	15876.481	-7	36	2	35	37	2	36	15858.436	-9
38	0	38	37	0	37	15936.557*	3444	57	1	56	56	1	55	15935.942	2	19	2	17	20	2	18	15875.550	-3	37	2	36	38	2	37	15857.371	-0
39	0	39	38	0	38	15936.939*	3457	58	1	57	57	1	56	15936.196	-4	20	2	18	21	2	19	15874.596*	-14	38	2	37	39	2	38	15856.289	-3
40	0	40	39	0	39	15937.307*	3466	59	1	58	58	1	57	15936.455	5	21	2	19	22	2	20	15873.652	-6	39	2	38	40	2	39	15855.204	-2
41	0	41	40	0	40	15937.665*	3495	60	1	59	59	1	58	15936.700	8	22	2	20	23	2	21	15872.697	-2	40	2	39	41	2	40	15854.106	-7
42	0	42	41	0	41	15938.045*	3516	8	1	8	9	1	9	15899.481	2	23	2	21	24	2	22	15871.739	7	41	2	40	42	2	41	15853.010	-4
43	0	43	42	0	42	15938.405*	3546	9	1	9	10	1	10	15898.621	4	25	2	23	26	2	24	15869.789*	16	42	2	41	43	2	42	15851.926*	18
44	0	44	43	0	43	15938.758*	3579	10	1	10	11	1	11	15897.743	-1	26	2	24	27	2	25	15868.783	-0	43	2	42	44	2	43	15850.802	7
45	0	45	44	0	44	15939.113*	3623	11	1	11	12	1	12	15896.862	1	27	2	25	28	2	26	15867.784	-2	45	2	44	46	2	45	15848.564	11
16	1	15	17	1	16	15892.346	2	12	1	12	13	1	13	15895.969	2	28	2	26	29	2	27	15866.772	-8	46	2	45	47	2	46	15847.417	-5
17	1	16	18	1	17	15891.423	8	13	1	13	14	1	14	15895.064	0	29	2	27	30	2	28	15865.766	-1	47	2	46	48	2	47	15846.289	-3
18	1	17	19	1	18	15890.487	10	14	1	14	15	1	15	15894.134*	-15	30	2	28	31	2	29	15864.745	-1	48	2	47	49	2	48	15845.166*	22
19	1	18	20	1	19	15889.535	5	17	1	17	18	1	18	15891.336	-11	31	2	29	32	2	30	15863.718	-0	49	2	48	50	2	49	15844.009*	13
20	1	19	21	1	20	15888.577	3	18	1	18	19	1	19	15890.393	1	32	2	30	33	2	31	15862.679	-5	50	2	49	51	2	50	15842.853	10
21	1	20	22	1	21	15887.609	-2	19	1	19	20	1	20	15889.423	-5	33	2	31	34	2	32	15861.642	1	51	2	50	52	2	51	15841.714*	30
22	1	21	23	1	22	15886.640	1	20	1	20	21	1	21	15888.449	-4	34	2	32	35	2	33	15860.605*	13	3	2	2	2	2	1	15894.910	4
23	1	22	24	1	23	15885.656	-2	21	1	21	22	1	22	15887.469	-1	35	2	33	36	2	34	15859.548	11	4	2	3	3	2	2	15895.657*	16
24	1	23	25	1	24	15884.676	8	22	1	22	23	1	23	15886.477	2	36	2	34	37	2	35	15858.468	-6	5	2	4	4	2	3	15896.364	-4
25	1	24	26	1	25	15883.670	-1	23	1	23	24	1	24	15885.474	2	37	2	35	38	2	36	15857.422*	17	6	2	5	5	2	4	15897.081	-6
26	1	25	27	1	26	15882.664	-1	24	1	24	25	1	25	15884.455	-4	38	2	36	39	2	37	15856.330	1	7	2	6	6	2	5	15897.787	-8
27	1	26	28	1	27	15881.649	-2	25	1	25	26	1	26	15883.439	2	39	2	37	40	2	38	15855.262*	15	8	2	7	7	2	6	15898.490	-5
29	1	28	30	1	29	15879.596	-2	26	1	26	27	1	27	15882.398	-6	40	2	38	41	2	39	15854.168	9	9	2	8	8	2	7	15899.191	4
30	1	29	31	1	30	15878.555	-5	27	1	27	28	1	28	15881.362	-1	41	2	39	42	2	40	15853.067	4	10	2	9	9	2	8	15899.880	12
31	1	30	32	1	31	15877.515	1	28	1	28	29	1	29	15880.307	-5	43	2	41	44	2	42	15850.877*	23	11	2	10	10	2	9	15900.539	-3
33	1	32	34	1	33	15875.403	6	29	1	29	30	1	30	15879.253	1	44	2	42	45	2	43	15849.736	-5	12	2	11	11	2	10	15901.191*	-15
34	1	33	35	1	34	15874.327	0	30	1	30	31	1	31	15878.178	-5	45	2	43	46	2	44	15848.622	-0	13	2	12	12	2	11	15901.869	7
35	1	34	36	1	35	15873.245	-4	31	1	31	32	1	32	15877.092*	-13	46	2	44	47	2	45	15847.514*	17	14	2	13	13	2	12	15902.507	-2
36	1	35	37	1	36	15872.154	-10	32	1	32	33	1	33	15876.018	0	47	2	45	48	2	46	15846.364	-2	15	2	14	14	2	13	15903.155	9
37	1	36	38	1	37	15871.082	11	34	1	34	35	1	35	15873.822	5	48	2	46	49	2	47	15845.232	3	16	2	15	15	2	14	15903.770	-5
38	1	37	39	1	38	15869.968	-1	35	1	35	36	1	36	15872.697	-6	49	2	47	50	2	48	15844.086	-2	17	2	16	16	2	15	15904.401	7

Note. (*) Line not included in the fit.

TABLE III—*Continued*

J'	Ka'	Kc'		J"	Ka"	Kc"	OBS	O-C	J'	Ka'	Kc'		J"	Ka"	Kc"	OBS	O-C	J'	Ka'	Kc'		J"	Ka"	Kc"	OBS	O-C	J'	Ka'	Kc'		J"	Ka"	Kc"	OBS	O-C
18	2	17	-	17	2	16	15905.011	5	26	3	23	-	27	3	24	15835.363*	-10256	20	3	17	-	19	3	16	15872.407*	-10531	27	4	23	-	28	4	24	15811.596	7
19	2	18	-	18	2	17	15905.612	3	27	3	24	-	28	3	25	15834.418*	-10220	21	3	18	-	20	3	17	15873.037*	-10500	28	4	24	-	29	4	25	15810.567	2
20	2	19	-	19	2	18	15906.205	3	28	3	25	-	29	3	26	15833.467*	-10181	23	3	20	-	22	3	19	15874.327*	-10382	29	4	25	-	30	4	26	15809.531	-1
21	2	20	-	20	2	19	15906.791	4	29	3	26	-	30	3	27	15832.502*	-10149	24	3	21	-	23	3	20	15874.945*	-10338	30	4	26	-	31	4	27	15808.487	-3
22	2	21	-	21	2	20	15907.371	6	30	3	27	-	31	3	28	15831.525*	-10123	25	3	22	-	24	3	21	15875.550*	-10300	31	4	27	-	32	4	28	15807.446	5
23	2	22	-	22	2	21	15907.936	5	31	3	28	-	32	3	29	15830.549*	-10089	26	3	23	-	25	3	22	15876.147*	-10261	32	4	28	-	33	4	29	15806.381	-1
24	2	23	-	23	2	22	15908.496	7	32	3	29	-	33	3	30	15829.564*	-10065	27	3	24	-	26	3	23	15876.737*	-10221	33	4	29	-	34	4	30	15805.311	-4
25	2	24	-	24	2	23	15909.056*	16	33	3	30	-	34	3	31	15828.546*	-10049	28	3	25	-	27	3	24	15877.313*	-10188	34	4	30	-	35	4	31	15804.237	-2
26	2	25	-	25	2	24	15909.588	6	34	3	31	-	35	3	32	15827.535*	-10028	29	3	26	-	28	3	25	15877.878*	-10158	35	4	31	-	36	4	32	15803.154	-0
27	2	26	-	26	2	25	15910.142*	27	35	3	32	-	36	3	33	15826.514*	-10011	30	3	27	-	29	3	26	15878.440*	-10122	36	4	32	-	37	4	33	15802.060	-2
28	2	27	-	27	2	26	15910.655*	16	36	3	33	-	37	3	34	15825.508*	-9972	31	3	28	-	30	3	27	15878.960*	-10100	37	4	33	-	38	4	34	15800.959	-1
29	2	28	-	28	2	27	15911.162	6	37	3	34	-	38	3	35	15824.460*	-9968	32	3	29	-	31	3	28	15879.489*	-10102	38	4	34	-	39	4	35	15799.845	-5
30	2	29	-	29	2	28	15911.661	-3	38	3	35	-	39	3	36	15823.407*	-9964	32	3	29	-	31	3	28	15879.537*	-10054	39	4	35	-	40	4	36	15798.732	-0
31	2	30	-	30	2	29	15912.156	-8	39	3	36	-	40	3	37	15822.341*	-9984	33	3	30	-	32	3	29	15880.042*	-10052	40	4	36	-	41	4	37	15797.600	-4
32	2	31	-	31	2	30	15912.638*	-17	40	3	37	-	41	3	38	15821.265*	-9970	34	3	31	-	33	3	30	15880.520*	-10069	5	4	1	-	4	4	0	15840.320*	-18
33	2	32	-	32	2	31	15913.131	-8	41	3	38	-	42	3	39	15820.214*	-9943	35	3	32	-	34	3	31	15881.058*	-10019	6	4	2	-	5	4	1	15841.033*	-20
34	2	33	-	33	2	32	15913.613	-1	42	3	39	-	43	3	40	15819.130*	-9943	36	3	33	-	35	3	32	15881.555*	-10002	13	4	9	-	12	4	8	15845.803	11
35	2	34	-	34	2	33	15914.076	-5	43	3	40	-	44	3	41	15818.032*	-9951	37	3	34	-	36	3	33	15882.047*	-9981	14	4	10	-	13	4	9	15846.429	-3
36	2	35	-	35	2	34	15914.526*	-14	44	3	41	-	45	3	42	15816.926*	-9960	38	3	35	-	37	3	34	15882.516*	-9977	15	4	11	-	14	4	10	15847.069	8
37	2	36	-	36	2	35	15914.982	-9	45	3	42	-	46	3	43	15815.835*	-9949	40	3	37	-	39	3	36	15883.439*	-9960	16	4	12	-	15	4	11	15847.678	3
38	2	37	-	37	2	36	15915.426	-9	46	3	43	-	47	3	44	15814.702*	-9974	41	3	38	-	40	3	37	15883.892*	-9949	17	4	13	-	16	4	12	15848.293	0
40	2	39	-	39	2	38	15916.295	-2	47	3	44	-	48	3	45	15813.538*	-10023	42	3	39	-	41	3	38	15884.313*	-9961	18	4	14	-	17	4	13	15848.903	9
41	2	40	-	40	2	39	15916.714	-3	48	3	45	-	49	3	46	15812.439*	-10001	43	3	40	-	42	3	39	15884.741*	-9961	20	4	16	-	19	4	15	15850.069	1
42	2	41	-	41	2	40	15917.141	12	49	3	46	-	50	3	47	15811.292*	-10021	45	3	42	-	44	3	41	15885.162*	-10371	21	4	17	-	20	4	16	15850.637	-4
5	3	2	-	6	3	3	15852.823*	-11670	50	3	47	-	51	3	48	15810.142*	-10039	45	3	42	-	44	3	41	15885.583*	-9950	22	4	18	-	21	4	17	15851.205	-0
6	3	3	-	7	3	4	15852.110*	-11563	51	3	48	-	52	3	49	15808.969*	-10075	46	3	43	-	45	3	42	15885.967*	-9971	23	4	19	-	22	4	18	15851.758	1
7	3	4	-	8	3	5	15851.365*	-11480	52	3	49	-	53	3	50	15807.801*	-10100	4	4	0	-	5	4	1	15832.685	7	24	4	20	-	23	4	19	15852.306	2
8	3	5	-	9	3	6	15850.637*	-11371	53	3	50	-	54	3	51	15806.621*	-10130	5	4	1	-	6	4	2	15831.861	-1	25	4	21	-	24	4	20	15852.823*	-16
9	3	6	-	10	3	7	15849.859*	-11306	54	3	51	-	55	3	52	15805.421*	-10175	6	4	2	-	7	4	3	15831.018*	-17	26	4	22	-	25	4	21	15853.362	-2
10	3	7	-	11	3	8	15849.089*	-11223	55	3	52	-	56	3	53	15804.237*	-10199	8	4	4	-	9	4	5	15829.345	-11	27	4	23	-	26	4	22	15853.875	-5
11	3	8	-	12	3	9	15848.293*	-11159	56	3	53	-	57	3	54	15803.006*	-10263	9	4	5	-	10	4	6	15828.494	-8	28	4	24	-	27	4	23	15854.389	2
12	3	9	-	13	3	10	15847.546*	-11038	57	3	54	-	58	3	55	15801.816*	-10284	13	4	9	-	14	4	10	15824.993	-2	29	4	25	-	28	4	24	15854.886	2
13	3	10	-	14	3	11	15846.740*	-10968	6	3	3	-	5	3	2	15862.132*	-11585	14	4	10	-	15	4	11	15824.088	-8	30	4	26	-	29	4	25	15855.372	0
14	3	11	-	15	3	12	15845.924*	-10900	7	3	4	-	6	3	3	15862.926*	-11485	15	4	11	-	16	4	12	15823.182	-5	32	4	28	-	31	4	27	15856.330	12
15	3	12	-	16	3	13	15845.116*	-10817	8	3	5	-	7	3	4	15863.718*	-11398	16	4	12	-	17	4	13	15822.263	-6	33	4	29	-	32	4	28	15856.773	-4
16	3	13	-	17	3	14	15844.270*	-10763	9	3	6	-	8	3	5	15864.506*	-11305	17	4	13	-	18	4	14	15821.331	-12	34	4	30	-	33	4	29	15857.245*	18
17	3	14	-	18	3	15	15843.431*	-10695	10	3	7	-	9	3	6	15865.289*	-11213	18	4	14	-	19	4	15	15820.390*	-18	35	4	31	-	34	4	30	15857.669	1
18	3	15	-	19	3	16	15842.581*	-10630	12	3	9	-	11	3	8	15866.814*	-11041	19	4	15	-	20	4	16	15819.464	1	36	4	32	-	35	4	31	15858.101	3
19	3	16	-	20	3	17	15841.714*	-10574	13	3	10	-	12	3	9	15867.554*	-10965	20	4	16	-	21	4	17	15818.521	12	37	4	33	-	36	4	32	15858.514	-5
20	3	17	-	21	3	18	15840.833*	-10525	14	3	11	-	13	3	10	15868.275*	-10900	21	4	17	-	22	4	18	15817.556	8	38	4	34	-	37	4	33	15858.927	-3
21	3	18	-	22	3	19	15839.955*	-10465	15	3	12	-	14	3	11	15868.994*	-10828	22	4	18	-	23	4	19	15816.590*	13	39	4	35	-	38	4	34	15859.328	-4
22	3	19	-	23	3	20	15839.048*	-10427	16	3	13	-	15	3	12	15869.724*	-10738	23	4	19	-	24	4	20	15815.603	6	40	4	36	-	39	4	35	15859.735	11
23	3	20	-	24	3	21	15838.142*	-10381	17	3	14	-	16	3	13	15870.391*	-10702	24	4	20	-	25	4	21	15814.603	-4	42	4	38	-	41	4	37	15860.497*	17
24	3	21	-	25	3	22	15837.230*	-10332	18	3	15	-	17	3	14	15871.062*	-10635	25	4	21	-	26	4	22	15813.608	-2									
25	3	22	-	26	3	23	15836.302*	-10293	19	3	16	-	18	3	15	15871.739*	-10593	26	4	22	-	27	4	23	15812.610	6									

in the I^r representation (*9*). In this fit, the ground state constants were kept fixed at the values determined from our previous analysis of the $\tilde{B}\,{}^1A''$–$\tilde{X}\,{}^1A'$ system (*5*). The effective rotational constants from these final fits (one standard deviation uncertainty in parentheses) are given in Table I, and the transitions and deviations from the fit for ^{63}CuOH, ^{65}CuOH, ^{63}CuOD, and ^{65}CuOD are given in Tables II–V, respectively. From these constants, we have predicted the wavenumbers for *b*-type transitions between the two states (allowed by the C_s symmetry of the molecule), but have found no such lines in the spectra. This means that the transition dipole moment is very close to the *a*-axis which is close to the Cu–O bond. For example in ^{63}CuOH, the *a*-axis is at an angle of 4° to the Cu–O bond.

A partial r_s structure has also been determined for the upper state from these rotational constants. For this determination, Kraitchman's equations (*10, 11*) for single isotopic substitutions were used to locate the copper and hydrogen nuclei relative to the center of mass of the "parent." It was necessary to impose one extra constraint to determine the coordinates of the oxygen nucleus (for which no isotopic data were measured). This could come either from the definition of the center of mass, or from the moment of inertia equation. However, the small *b* coordinate for the copper nucleus was badly determined, and so we chose to use the moment of inertia equation (which depends on the square of b_{Cu}—a very small number) to determine the position of the oxygen nucleus. This gave more consistent results than when the definition of the center of mass was used as the constraint. Each of the isotopomers was taken in turn as the "parent," and the average value for each molecular parameter is presented together with one standard deviation from this averaging procedure in Table VI. For

TABLE IV

Observed Line Positions (cm^{-1}) for $^{63}CuOD$ (O–C Units of 10^{-3} cm^{-1})

J'	Ka'	Kc'		J"	Ka"	Kc"	OBS	O-C
3	1	2	-	4	1	3	15906.425	3
4	1	3	-	5	1	4	15905.649	-0
5	1	4	-	6	1	5	15904.858	-7
6	1	5	-	7	1	6	15904.065	-5
7	1	6	-	8	1	7	15903.256	-7
8	1	7	-	9	1	8	15902.436	-8
9	1	8	-	10	1	9	15901.612	-2
10	1	9	-	11	1	10	15900.770	-1
11	1	10	-	12	1	11	15899.913	-4
12	1	11	-	13	1	12	15899.061	10
13	1	12	-	14	1	13	15898.188*	16
14	1	13	-	15	1	14	15897.284	2
15	1	14	-	16	1	15	15896.373	-7
16	1	15	-	17	1	16	15895.449*	-15
17	1	16	-	18	1	17	15894.539	2
18	1	17	-	19	1	18	15893.596	-1
19	1	18	-	20	1	19	15892.651	6
20	1	19	-	21	1	20	15891.671	-8
21	1	20	-	22	1	21	15890.703	2
22	1	21	-	23	1	22	15889.694*	-16
23	1	22	-	24	1	23	15888.700	-7
24	1	23	-	25	1	24	15887.673*	-17
25	1	24	-	26	1	25	15886.661	2
26	1	25	-	27	1	26	15885.620	4
27	1	26	-	28	1	27	15884.570	11
28	1	27	-	29	1	28	15883.480	-9
29	1	28	-	30	1	29	15882.412	7
30	1	29	-	31	1	30	15881.304	-4
31	1	30	-	32	1	31	15880.169	-9
33	1	32	-	34	1	33	15877.925	-11
34	1	33	-	35	1	34	15876.778	-8
35	1	34	-	36	1	35	15875.622	0
36	1	35	-	37	1	36	15874.442	-2
37	1	36	-	38	1	37	15873.239	-13
38	1	37	-	39	1	38	15872.019*	-29
39	1	38	-	40	1	39	15870.805*	-25
40	1	39	-	41	1	40	15869.573*	-27
6	1	5	-	5	1	4	15913.501	-5
7	1	6	-	6	1	5	15914.140	-9
8	1	7	-	7	1	6	15914.780	-2
9	1	8	-	8	1	7	15915.425*	22
10	1	9	-	9	1	8	15916.019	9
11	1	10	-	10	1	9	15916.612	6
12	1	11	-	11	1	10	15917.196	6
13	1	12	-	12	1	11	15917.768	8
14	1	13	-	13	1	12	15918.330	10
15	1	14	-	14	1	13	15918.870	4
16	1	15	-	15	1	14	15919.410	11
17	1	16	-	16	1	15	15919.934*	16
18	1	17	-	17	1	16	15920.430	4
19	1	18	-	18	1	17	15920.925	4
20	1	19	-	19	1	18	15921.407	6
21	1	20	-	20	1	19	15921.868	0
22	1	21	-	21	1	20	15922.320	-2
23	1	22	-	22	1	21	15922.752	-10
24	1	23	-	23	1	22	15923.190	1
25	1	24	-	24	1	23	15923.609	8
26	1	25	-	25	1	24	15923.996	-4
27	1	26	-	26	1	25	15924.377	-7
28	1	27	-	27	1	26	15924.731*	-23
29	1	28	-	28	1	27	15925.105	-5
30	1	29	-	29	1	28	15925.444	-8
31	1	30	-	30	1	29	15925.785	5
32	1	31	-	31	1	30	15926.101	8
33	1	32	-	32	1	31	15926.397	6
34	1	33	-	33	1	32	15926.676	1
35	1	34	-	34	1	33	15926.947	3
36	1	35	-	35	1	34	15927.200	0
37	1	36	-	36	1	35	15927.444	5
38	1	37	-	37	1	36	15927.673	7
39	1	38	-	38	1	37	15927.870	-8
40	1	39	-	39	1	38	15928.078	2
41	1	40	-	40	1	39	15928.267	7
42	1	41	-	41	1	40	15928.415	-14
43	1	42	-	42	1	41	15928.579	-5
44	1	43	-	43	1	42	15928.736	10
45	1	44	-	44	1	43	15928.861	5
46	1	45	-	45	1	44	15928.975	3
47	1	46	-	46	1	45	15929.083	9
48	1	47	-	47	1	46	15929.158	-6
49	1	48	-	48	1	47	15929.245	4
50	1	49	-	49	1	48	15929.304	-3
3	2	1	-	4	2	2	15901.419*	-35
4	2	2	-	5	2	3	15900.666	-16
5	2	3	-	6	2	4	15899.862*	-37
6	2	4	-	7	2	5	15899.061*	-41
7	2	5	-	8	2	6	15898.269*	-25
8	2	6	-	9	2	7	15897.434*	-38
9	2	7	-	10	2	8	15896.620	-17
10	2	8	-	11	2	9	15895.776	-15
11	2	9	-	12	2	10	15894.918	-13
12	2	10	-	13	2	11	15894.061	1
13	2	11	-	14	2	12	15893.178	2
14	2	12	-	15	2	13	15892.282	2
15	2	13	-	16	2	14	15891.368	-4
16	2	14	-	17	2	15	15890.465	14
17	2	15	-	18	2	16	15889.516	-4
18	2	16	-	19	2	17	15888.577	2
19	2	17	-	20	2	18	15887.623	4
20	2	18	-	21	2	19	15886.661	10
21	2	19	-	22	2	20	15885.690	20
22	2	20	-	23	2	21	15884.708*	29
23	2	21	-	24	2	22	15883.696	20
24	2	22	-	25	2	23	15882.680	19
25	2	23	-	26	2	24	15881.657*	23
26	2	24	-	27	2	25	15880.603	7
27	2	25	-	28	2	26	15879.539	-7
28	2	26	-	29	2	27	15878.481	-3
29	2	27	-	30	2	28	15877.414	4
30	2	28	-	31	2	29	15876.310*	-16
31	2	29	-	32	2	30	15875.227	-3
32	2	30	-	33	2	31	15874.107	-15
33	2	31	-	34	2	32	15872.996	-6
34	2	32	-	35	2	33	15871.863	-8
35	2	33	-	36	2	34	15870.724	-4
36	2	34	-	37	2	35	15869.573	-1
37	2	35	-	38	2	36	15868.402	-5
38	2	36	-	39	2	37	15867.239	9
39	2	37	-	40	2	38	15866.047	7
40	2	38	-	41	2	39	15864.856*	17
41	2	39	-	42	2	40	15863.653*	27
42	2	40	-	43	2	41	15862.449*	46
43	2	41	-	44	2	42	15861.213*	47
44	2	42	-	45	2	43	15859.965*	48
45	2	43	-	46	2	44	15858.704*	43
46	2	44	-	47	2	45	15857.454*	63
47	2	45	-	48	2	46	15856.190*	80
48	2	46	-	49	2	47	15854.923*	104
49	2	47	-	50	2	48	15853.627*	111
50	2	48	-	51	2	49	15852.320*	116
51	2	49	-	52	2	50	15851.033*	151
52	2	50	-	53	2	51	15849.701*	152
53	2	51	-	54	2	52	15848.377*	169
54	2	52	-	55	2	53	15847.014*	156
55	2	53	-	56	2	54	15845.678*	178
56	2	54	-	57	2	55	15844.328*	194
57	2	55	-	58	2	56	15842.950*	189
58	2	56	-	59	2	57	15841.576*	193
59	2	57	-	60	2	58	15840.186*	187
3	2	2	-	4	2	3	15901.419*	-36
4	2	3	-	5	2	4	15900.666	-16
5	2	4	-	6	2	5	15899.862*	-37
6	2	5	-	7	2	6	15899.061*	-41
7	2	6	-	8	2	7	15898.269*	-24
8	2	7	-	9	2	8	15897.434*	-37
9	2	8	-	10	2	9	15896.620	-16
10	2	9	-	11	2	10	15895.776	-14
11	2	10	-	12	2	11	15894.918	-11
12	2	11	-	13	2	12	15894.061	4
13	2	12	-	14	2	13	15893.178	7
14	2	13	-	15	2	14	15892.282	8
15	2	14	-	16	2	15	15891.368	5
16	2	15	-	17	2	16	15890.465*	24
17	2	16	-	18	2	17	15889.516	10
18	2	17	-	19	2	18	15888.577	19
19	2	18	-	20	2	19	15887.623*	26
20	2	19	-	21	2	20	15886.661*	36
21	2	20	-	22	2	21	15885.690*	51
22	2	21	-	23	2	22	15884.708*	66
23	2	22	-	24	2	23	15883.696*	64
24	2	23	-	25	2	24	15882.680*	70
25	2	24	-	26	2	25	15881.657*	81
26	2	25	-	27	2	26	15880.648*	119
27	2	26	-	28	2	27	15879.621*	150
28	2	27	-	29	2	28	15878.575*	176
29	2	28	-	30	2	29	15877.526*	210
30	2	29	-	31	2	30	15876.470*	248
31	2	30	-	32	2	31	15875.421*	307
32	2	31	-	33	2	32	15874.383*	388
33	2	32	-	34	2	33	15873.373*	509
7	2	5	-	6	2	4	15909.066*	-28
8	2	6	-	7	2	5	15909.700	-12
9	2	7	-	8	2	6	15910.301	-17
10	2	8	-	9	2	7	15910.908	-3
11	2	9	-	10	2	8	15911.482	-9
12	2	10	-	11	2	9	15912.050	-9
13	2	11	-	12	2	10	15912.611	-3
14	2	12	-	13	2	11	15913.157	-1
15	2	13	-	14	2	12	15913.686	-2
16	2	14	-	15	2	13	15914.207	-0
17	2	15	-	16	2	14	15914.711	-2
18	2	16	-	17	2	15	15915.205	-3
19	2	17	-	18	2	16	15915.688	-2
20	2	18	-	19	2	17	15916.151	-8
21	2	19	-	20	2	18	15916.612	-5
22	2	20	-	21	2	19	15917.063	-0
26	2	24	-	25	2	23	15918.737	10
27	2	25	-	26	2	24	15919.126	13
28	2	26	-	27	2	25	15919.502	15
29	2	27	-	28	2	26	15919.847	-2
30	2	28	-	29	2	27	15920.204	4
31	2	29	-	30	2	28	15920.545	7
32	2	30	-	31	2	29	15920.865	1
33	2	31	-	32	2	30	15921.176	-2
34	2	32	-	33	2	31	15921.478	-2
35	2	33	-	34	2	32	15921.776	5
37	2	35	-	36	2	34	15922.320	6
38	2	36	-	37	2	35	15922.581	13
39	2	37	-	38	2	36	15922.829*	20
40	2	38	-	39	2	37	15923.059*	21
41	2	39	-	40	2	38	15923.291*	36
42	2	40	-	41	2	39	15923.495*	35
43	2	41	-	42	2	40	15923.711*	59
44	2	42	-	43	2	41	15923.906*	73
45	2	43	-	44	2	42	15924.070*	70
46	2	44	-	45	2	43	15924.229*	72
47	2	45	-	46	2	44	15924.377*	76
48	2	46	-	47	2	45	15924.545*	110
49	2	47	-	48	2	46	15924.676*	121
50	2	48	-	49	2	47	15924.806*	140
51	2	49	-	50	2	48	15924.897*	132
52	2	50	-	51	2	49	15925.002*	149
53	2	51	-	52	2	50	15925.105*	173
54	2	52	-	53	2	51	15925.194*	193
55	2	53	-	54	2	52	15925.262*	202
56	2	54	-	55	2	53	15925.324*	214
57	2	55	-	56	2	54	15925.392*	239
7	2	6	-	6	2	5	15909.066*	-27
8	2	7	-	7	2	6	15909.700	-10
9	2	8	-	8	2	7	15910.301	-14
10	2	9	-	9	2	8	15910.908	2
11	2	10	-	10	2	9	15911.482	-3
12	2	11	-	11	2	10	15912.050	-1
13	2	12	-	12	2	11	15912.611	8
14	2	13	-	13	2	12	15913.157	13
15	2	14	-	14	2	13	15913.686	16
16	2	15	-	15	2	14	15914.207*	22
17	2	16	-	16	2	15	15914.711*	25
18	2	17	-	17	2	16	15915.205*	31
19	2	18	-	18	2	17	15915.688*	39
20	2	19	-	19	2	18	15916.151*	40
21	2	20	-	20	2	19	15916.612*	52
22	2	21	-	21	2	20	15917.063*	67
23	2	22	-	22	2	21	15917.503*	84
24	2	23	-	23	2	22	15917.923*	93
25	2	24	-	24	2	23	15918.330*	102
26	2	25	-	25	2	24	15918.737*	125
27	2	26	-	26	2	25	15919.126*	142
28	2	27	-	27	2	26	15919.502*	159
29	2	28	-	28	2	27	15919.900*	212
30	2	29	-	29	2	28	15920.284*	262
31	2	30	-	30	2	29	15920.673*	331
32	2	31	-	31	2	30	15921.033*	383
33	2	32	-	32	2	31	15921.407*	463
11	3	8	-	12	3	9	15887.367	-14
12	3	9	-	13	3	10	15886.506	-5
13	3	10	-	14	3	11	15885.620	-9
15	3	12	-	16	3	13	15883.836	7
16	3	13	-	17	3	14	15882.913	3
17	3	14	-	18	3	15	15881.966	-13
18	3	15	-	19	3	16	15881.053*	17
19	3	16	-	20	3	17	15880.062	0
20	3	17	-	21	3	18	15879.114	-1
21	3	18	-	22	3	19	15878.137	1
22	3	19	-	23	3	20	15877.154	9
23	3	20	-	24	3	21	15876.143	1
24	3	21	-	25	3	22	15875.132	5
25	3	22	-	26	3	23	15874.107	7
26	3	23	-	27	3	24	15873.059	-3
27	3	24	-	28	3	25	15872.019	8
28	3	25	-	29	3	26	15870.947	-3
29	3	26	-	30	3	27	15869.874	-2
30	3	27	-	31	3	28	15868.788	-3
31	3	28	-	32	3	29	15867.698	4
32	3	29	-	33	3	30	15866.591	6
34	3	31	-	35	3	32	15864.332	-1
35	3	32	-	36	3	33	15863.181	-8
36	3	33	-	37	3	34	15862.027	-8
37	3	34	-	38	3	35	15860.865	-4
38	3	35	-	39	3	36	15859.685	-7
39	3	36	-	40	3	37	15858.490	-14
40	3	37	-	41	3	38	15857.290	-14
41	3	38	-	42	3	39	15856.088	-4
42	3	39	-	43	3	40	15854.865	-5
43	3	40	-	44	3	41	15853.627	-10
44	3	41	-	45	3	42	15852.375*	-18
45	3	42	-	46	3	43	15851.132	-6
46	3	43	-	47	3	44	15849.867	-5
47	3	44	-	48	3	45	15848.587	-8
48	3	45	-	49	3	46	15847.301	-7
49	3	46	-	50	3	47	15846.013	3
50	3	47	-	51	3	48	15844.695	-7
51	3	48	-	52	3	49	15843.378	-5
52	3	49	-	53	3	50	15842.049	-5
53	3	50	-	54	3	51	15840.706	-10
54	3	51	-	55	3	52	15839.362	-5
55	3	52	-	56	3	53	15838.001	-8
56	3	53	-	57	3	54	15836.641	-2
57	3	54	-	58	3	55	15835.256	-10
58	3	55	-	59	3	56	15833.873	-9
59	3	56	-	60	3	57	15832.467*	-22
5	3	2	-	4	3	1	15900.263	6
6	3	3	-	5	3	2	15900.908	6
7	3	4	-	6	3	3	15901.533	-0
8	3	5	-	7	3	4	15902.154	2
9	3	6	-	8	3	5	15902.750	-9
10	3	7	-	9	3	6	15903.332*	-21
11	3	8	-	10	3	7	15903.932	-2
12	3	9	-	11	3	8	15904.503	-0
13	3	10	-	12	3	9	15905.057	-2
14	3	11	-	13	3	10	15905.600	-2
15	3	12	-	14	3	11	15906.134	0
16	3	13	-	15	3	12	15906.654	2
17	3	14	-	16	3	13	15907.170	12
18	3	15	-	17	3	14	15907.654	3
19	3	16	-	18	3	15	15908.134	2
20	3	17	-	19	3	16	15908.610	9
21	3	18	-	20	3	17	15909.066	9
22	3	19	-	21	3	18	15909.504	4
23	3	20	-	22	3	19	15909.940	8
24	3	21	-	23	3	20	15910.356	5
25	3	22	-	24	3	21	15910.763	6
26	3	23	-	25	3	22	15911.157	6
27	3	24	-	26	3	23	15911.536	3
28	3	25	-	27	3	24	15911.905	3
29	3	26	-	28	3	25	15912.265	7
30	3	27	-	29	3	26	15912.611	8
31	3	28	-	30	3	27	15912.940	5
32	3	29	-	31	3	28	15913.261	6
33	3	30	-	32	3	29	15913.567	4
34	3	31	-	33	3	30	15913.858	-0
35	3	32	-	34	3	31	15914.140	-1
36	3	33	-	35	3	32	15914.411	-1
37	3	34	-	36	3	33	15914.665	-6
38	3	35	-	37	3	34	15914.910	-8
39	3	36	-	38	3	35	15915.151	-2
40	3	37	-	39	3	36	15915.377	1
41	3	38	-	40	3	37	15915.592	6
42	3	39	-	41	3	38	15915.787	3
43	3	40	-	42	3	39	15915.964	-6
44	3	41	-	43	3	40	15916.151	6
45	3	42	-	44	3	41	15916.300	-7
46	3	43	-	45	3	42	15916.473	14
47	3	44	-	46	3	43	15916.612	14
48	3	45	-	47	3	44	15916.737	12
49	3	46	-	48	3	45	15916.852	12
50	3	47	-	49	3	46	15916.938	-7
51	3	48	-	50	3	47	15917.063*	25
52	3	49	-	51	3	48	15917.132	12
53	3	50	-	52	3	49	15917.196	5
54	3	51	-	53	3	50	15917.262	12
55	3	52	-	54	3	51	15917.334*	35
56	3	53	-	55	3	52	15917.374*	36
8	4	4	-	9	4	5	15881.437	-8
9	4	5	-	10	4	6	15880.603	-11
10	4	6	-	11	4	7	15879.785	14
11	4	7	-	12	4	8	15878.917	2
12	4	8	-	13	4	9	15878.034	-13
13	4	9	-	14	4	10	15877.154	-13
14	4	10	-	15	4	11	15876.268	-7
15	4	11	-	16	4	12	15875.370	-0
16	4	12	-	17	4	13	15874.442	-12
17	4	13	-	18	4	14	15873.538	12
18	4	14	-	19	4	15	15872.580	-6
19	4	15	-	20	4	16	15871.637	4
20	4	16	-	21	4	17	15870.679	11
21	4	17	-	22	4	18	15869.680	-12
22	4	18	-	23	4	19	15868.702	-1
23	4	19	-	24	4	20	15867.698	-6
24	4	20	-	25	4	21	15866.701	10
25	4	21	-	26	4	22	15865.661	-6
26	4	22	-	27	4	23	15864.626	-5
27	4	23	-	28	4	24	15863.580	-4
28	4	24	-	29	4	25	15862.522	-4
29	4	25	-	30	4	26	15861.453	-2
30	4	26	-	31	4	27	15860.366	-7
31	4	27	-	32	4	28	15859.275	-4
32	4	28	-	33	4	29	15858.166	-7
33	4	29	-	34	4	30	15857.049	-7
34	4	30	-	35	4	31	15855.928	-0
35	4	31	-	36	4	32	15854.785	-4
36	4	32	-	37	4	33	15853.627	-10
37	4	33	-	38	4	34	15852.473	-3
38	4	34	-	39	4	35	15851.302	0
39	4	35	-	40	4	36	15850.117	0
40	4	36	-	41	4	37	15848.926	5
41	4	37	-	42	4	38	15847.718	4
42	4	38	-	43	4	39	15846.488	-7
43	4	39	-	44	4	40	15845.253	-13
44	4	40	-	45	4	41	15844.016	-10
45	4	41	-	46	4	42	15842.779	4
46	4	42	-	47	4	43	15841.505	-8
47	4	43	-	48	4	44	15840.239	-2
48	4	44	-	49	4	45	15838.962	5

Note. (*) Line not included in the fit.

TABLE IV—*Continued*

J'	Ka'	Kc'		J"	Ka"	Kc"	OBS	O-C	J'	Ka'	Kc'		J"	Ka"	Kc"	OBS	O-C	J'	Ka'	Kc'		J"	Ka"	Kc"	OBS	O-C	J'	Ka'	Kc'		J"	Ka"	Kc"	OBS	O-C
49	4	45	-	50	4	46	15837.662	-1	35	4	31	-	34	4	30	15905.721	5	25	5	20	-	26	5	21	15857.456	11	17	5	12	-	16	5	11	15890.500*	19
50	4	46	-	51	4	47	15836.362	4	36	4	32	-	35	4	31	15905.996	7	26	5	21	-	27	5	22	15856.406	0	18	5	13	-	17	5	12	15890.979	5
51	4	47	-	52	4	48	15835.053	9	37	4	33	-	36	4	32	15906.249	-1	27	5	22	-	28	5	23	15855.360	4	19	5	14	-	18	5	13	15891.458	5
52	4	48	-	53	4	49	15833.711	-7	38	4	34	-	37	4	33	15906.504	5	28	5	23	-	29	5	24	15854.296	2	20	5	15	-	19	5	14	15891.927	6
53	4	49	-	54	4	50	15832.382	-1	39	4	35	-	38	4	34	15906.739	3	29	5	24	-	30	5	25	15853.222	2	21	5	16	-	20	5	15	15892.384	7
54	4	50	-	55	4	51	15831.049	11	40	4	36	-	39	4	35	15906.969	8	30	5	25	-	31	5	26	15852.127	-7	22	5	17	-	21	5	16	15892.826	8
55	4	51	-	56	4	52	15829.696	14	41	4	37	-	40	4	36	15907.170	-3	31	5	26	-	32	5	27	15851.034	-3	23	5	18	-	22	5	17	15893.251	2
56	4	52	-	57	4	53	15828.314	-3	42	4	38	-	41	4	37	15907.373	-1	32	5	27	-	33	5	28	15849.924	-4	25	5	20	-	24	5	19	15894.061	-10
57	4	53	-	58	4	54	15826.949	7	43	4	39	-	42	4	38	15907.560	-3	33	5	28	-	34	5	29	15848.796	-11	26	5	21	-	25	5	20	15894.457	-6
58	4	54	-	59	4	55	15825.555	-3	44	4	40	-	43	4	39	15907.731	-9	34	5	29	-	35	5	30	15847.664	-11	27	5	22	-	26	5	21	15894.651	8
59	4	55	-	60	4	56	15824.170	6	45	4	41	-	44	4	40	15907.907	3	35	5	30	-	36	5	31	15846.540	9	28	5	23	-	27	5	22	15895.211	-0
11	4	7	-	10	4	6	15895.488*	25	46	4	42	-	45	4	41	15908.053	-4	36	5	31	-	37	5	32	15845.362	-13	29	5	24	-	28	5	23	15895.561	-4
12	4	8	-	11	4	7	15896.039	6	47	4	43	-	46	4	42	15908.194	-4	37	5	32	-	38	5	33	15844.201	-8	30	5	25	-	29	5	24	15895.909	1
13	4	9	-	12	4	8	15896.620*	30	48	4	44	-	47	4	43	15908.345*	18	38	5	33	-	39	5	34	15843.019	-12	31	5	26	-	30	5	25	15896.239	0
14	4	10	-	13	4	9	15897.151*	16	49	4	45	-	48	4	44	15908.469*	24	39	5	34	-	40	5	35	15841.840	-1	32	5	27	-	31	5	26	15896.563	8
15	4	11	-	14	4	10	15897.688*	21	50	4	46	-	49	4	45	15908.556	5	40	5	35	-	41	5	36	15840.639	-2	33	5	28	-	32	5	27	15896.863	2
16	4	12	-	15	4	11	15898.188	0	51	4	47	-	50	4	46	15908.675*	31	41	5	36	-	42	5	37	15839.421	-7	34	5	29	-	33	5	28	15897.151	-3
17	4	13	-	16	4	12	15898.701	5	52	4	48	-	51	4	47	15908.746*	19	42	5	37	-	43	5	38	15838.208	3	35	5	30	-	34	5	29	15897.439	5
18	4	14	-	17	4	13	15899.203	12	53	4	49	-	52	4	48	15908.807	8	43	5	38	-	44	5	39	15836.987*	17	36	5	31	-	35	5	30	15897.689	13
19	4	15	-	18	4	14	15899.665	-9	54	4	50	-	53	4	49	15908.861	2	44	5	39	-	45	5	40	15835.728	4	37	5	32	-	36	5	31	15897.966	7
20	4	16	-	19	4	15	15900.138	-6	8	5	3	-	9	5	4	15873.240	-11	45	5	40	-	46	5	41	15834.479	11	38	5	33	-	37	5	32	15898.188	-14
21	4	17	-	20	4	16	15900.604	3	9	5	4	-	10	5	5	15872.414	-5	46	5	41	-	47	5	42	15833.190	-11	39	5	34	-	38	5	33	15898.435	2
22	4	18	-	21	4	17	15901.055	8	10	5	5	-	11	5	6	15871.557*	-18	47	5	42	-	48	5	43	15831.917	-5	40	5	35	-	39	5	34	15898.659	7
23	4	19	-	22	4	18	15901.488	7	11	5	6	-	12	5	7	15870.724	5	48	5	43	-	49	5	44	15830.636	4	41	5	36	-	40	5	35	15898.861	2
24	4	20	-	23	4	19	15901.911	10	14	5	9	-	15	5	10	15868.071	-4	49	5	44	-	50	5	45	15829.337	4	42	5	37	-	41	5	36	15899.060	6
25	4	21	-	24	4	20	15902.315	5	15	5	10	-	16	5	11	15867.161	-8	50	5	45	-	51	5	46	15828.022	1	43	5	38	-	42	5	37	15899.255*	19
26	4	22	-	25	4	21	15902.708	3	16	5	11	-	17	5	12	15866.256	5	51	5	46	-	52	5	47	15826.701	1	44	5	39	-	43	5	38	15899.413	7
27	4	23	-	26	4	22	15903.090	1	17	5	12	-	18	5	13	15865.319	-3	52	5	47	-	53	5	48	15825.365	-3	45	5	40	-	44	5	39	15899.569	5
28	4	24	-	27	4	23	15903.465	4	18	5	13	-	19	5	14	15864.386	7	53	5	48	-	54	5	49	15824.025	-1	46	5	41	-	45	5	40	15899.725*	16
29	4	25	-	28	4	24	15903.820	1	19	5	14	-	20	5	15	15863.439	14	54	5	49	-	55	5	50	15822.673	0	47	5	42	-	46	5	41	15899.865*	21
30	4	26	-	29	4	25	15904.167	1	20	5	15	-	21	5	16	15862.447	-11	55	5	50	-	56	5	51	15821.310	1	48	5	43	-	47	5	42	15899.989*	23
31	4	27	-	30	4	26	15904.503	2	21	5	16	-	22	5	17	15861.499*	20	56	5	51	-	57	5	52	15819.933	-3	49	5	44	-	48	5	43	15900.095*	19
32	4	28	-	31	4	27	15904.824	1	22	5	17	-	23	5	18	15860.498	10	13	5	8	-	12	5	7	15888.384	0	50	5	45	-	49	5	44	15900.201*	27
33	4	29	-	32	4	28	15905.139	6	23	5	18	-	24	5	19	15859.484	-2	14	5	9	-	13	5	8	15888.937	10									
34	4	30	-	33	4	29	15905.456*	26	24	5	19	-	25	5	20	15858.464	-7	16	5	11	-	15	5	10	15890.001*	26									

comparison this table also shows the partial r_s structures determined from our previous paper (5) for the $\tilde{B}\,^1A''$ and $\tilde{X}\,^1A'$ states. The errors on the geometrical parameters are largest for the $\tilde{A}\,^1A'$ state, presumably because some global perturbations were absorbed into the values for the rotational constants obtained from our fit. In particular, the B and C constants for CuOD were obtained from fitting just the upper asymmetry component of the $K_a = 1$ PR subbands—the lower component is very perturbed. We have no way of knowing the extent of global perturbation of this upper component.

DISCUSSION

A simple zeroth-order, ionic picture of the bonding in the ground state of CuOH consists of a Cu^+ (^1S, $3d^{10}$) cation perturbed by the ligand field of an OH^- ($^1\Sigma^+$) anion. The lowest excited states would then arise from the Cu^+ (^1D, ^3D, $3d^94s$) cation formed by the $4s \leftarrow 3d$ promotion. This model predicts that CuOH should resemble the isoelectronic CuF (12, 13) with an $\tilde{X}\,^1\Sigma^+$ ground state and the $^1\Delta$, $^3\Delta$, $^1\Pi$, $^3\Pi$, $^1\Sigma^+$, $^3\Sigma^+$ excited states arising from the Cu d-hole.

The true bonding in CuOH must involve a substantial amount of covalent character in the Cu–O bond of CuOH because the ground and all of the known excited states of CuOH are strongly bent with an angle of 110–118° (Table VI) compared to the angle of 104.5° for H_2O. The simplistic ionic model also cannot explain the large increase (~8%) in the O–H bond length between the $\tilde{X}\,^1A'$ and $\tilde{A}\,^1A'$ states. The only appropriate model is therefore one in which covalent bonding and electron correlation are fully taken into account.

It is interesting to try to correlate the observed excited CuOH states with those of the isoelectronic CuF molecule (as well as back to the hypothetical linear CuOH molecule). For example, the green $\tilde{B}\,^1A''$–$\tilde{X}\,^1A'$ transition seems to correlate to the $C^1\Pi$–$X^1\Sigma^+$ transition of CuF (12, 13). The $\tilde{A}\,^1A'$ state of CuOH probably correlates

TABLE V

Observed Line Positions (cm^{-1}) for $^{65}CuOD$ (O–C Units of 10^{-3} cm^{-1})

J'	Ka'	Kc'		J"	Ka"	Kc"	OBS	O-C
5	1	4	-	6	1	5	15904.857	10
6	1	5	-	7	1	6	15904.065	10
7	1	6	-	8	1	7	15903.253	1
8	1	7	-	9	1	8	15902.436	-1
9	1	8	-	10	1	9	15901.612	1
10	1	9	-	11	1	10	15900.771	-1
11	1	10	-	12	1	11	15899.916	-6
12	1	11	-	13	1	12	15899.060	0
13	1	12	-	14	1	13	15898.188	3
14	1	13	-	15	1	14	15897.286	-14
16	1	15	-	17	1	16	15895.495	4
18	1	17	-	19	1	18	15893.647	13
20	1	19	-	21	1	20	15891.732	5
21	1	20	-	22	1	21	15890.767	12
22	1	21	-	23	1	22	15889.766	-4
23	1	22	-	24	1	23	15888.779	5
24	1	23	-	25	1	24	15887.750	-13
25	1	24	-	26	1	25	15886.723*	-18
26	1	25	-	27	1	26	15885.691	-14
27	1	26	-	28	1	27	15884.655	-1
29	1	28	-	30	1	29	15882.528	8
30	1	29	-	31	1	30	15881.437	5
31	1	30	-	32	1	31	15880.319	-11
33	1	32	-	34	1	33	15878.076	-10
34	1	33	-	35	1	34	15876.956	12
35	1	34	-	36	1	35	15875.778	-10
36	1	35	-	37	1	36	15874.615	-2
37	1	36	-	38	1	37	15873.437	4
38	1	37	-	39	1	38	15872.225	-9
12	1	11	-	11	1	10	15917.063	-15
13	1	12	-	12	1	11	15917.641	-3
14	1	13	-	13	1	12	15918.190	-7
15	1	14	-	14	1	13	15918.737	0
16	1	15	-	15	1	14	15919.262	-3
17	1	16	-	16	1	15	15919.773	-7
18	1	17	-	17	1	16	15920.283	1
19	1	18	-	18	1	17	15920.772	1
20	1	19	-	19	1	18	15921.227*	-21
21	1	20	-	20	1	19	15921.722	11
22	1	21	-	21	1	20	15922.158	-3
23	1	22	-	22	1	21	15922.581	-17
24	1	23	-	23	1	22	15923.025	4
25	1	24	-	24	1	23	15923.430	0
26	1	25	-	25	1	24	15923.842	16
27	1	26	-	26	1	25	15924.228*	20
28	1	27	-	27	1	26	15924.596*	20
29	1	28	-	28	1	27	15924.940	11
30	1	29	-	29	1	28	15925.262	-7
32	1	31	-	31	1	30	15925.899	-5
33	1	32	-	32	1	31	15926.206	6
34	1	33	-	33	1	32	15926.479	-2
35	1	34	-	34	1	33	15926.747	0
36	1	35	-	35	1	34	15927.011	13
37	1	36	-	36	1	35	15927.239	5
15	2	14	-	16	2	15	15891.404	4
16	2	15	-	17	2	16	15890.500	15
17	2	16	-	18	2	17	15889.572	14
18	2	17	-	19	2	18	15888.633	14
19	2	18	-	20	2	19	15887.672	4
20	2	19	-	21	2	20	15886.723	18
15	2	13	-	16	2	14	15891.404	-1
16	2	14	-	17	2	15	15890.500	8
17	2	15	-	18	2	16	15889.572	5
18	2	16	-	19	2	17	15888.633	3
19	2	17	-	20	2	18	15887.672	-9
20	2	18	-	21	2	19	15886.723	1
21	2	19	-	22	2	20	15885.759	9
22	2	20	-	23	2	21	15884.756	-9
24	2	22	-	25	2	23	15882.767	4
25	2	23	-	26	2	24	15881.774*	30

J'	Ka'	Kc'		J"	Ka"	Kc"	OBS	O-C
26	2	24	-	27	2	25	15880.734	20
27	2	25	-	28	2	26	15879.707*	35
7	2	6	-	6	2	5	15908.995	-5
8	2	7	-	7	2	6	15909.601	-14
9	2	8	-	8	2	7	15910.214	-2
10	2	9	-	9	2	8	15910.804	-1
11	2	10	-	10	2	9	15911.383	1
12	2	11	-	11	2	10	15911.936	-9
13	2	12	-	12	2	11	15912.503	7
14	2	13	-	13	2	12	15913.030	-3
15	2	14	-	14	2	13	15913.567	8
16	2	15	-	15	2	14	15914.081	9
17	2	16	-	16	2	15	15914.582	11
18	2	17	-	17	2	16	15915.074	16
19	2	18	-	18	2	17	15915.562*	30
20	2	19	-	19	2	18	15916.019*	26
7	2	5	-	6	2	4	15908.995	-6
8	2	6	-	7	2	5	15909.601	-15
9	2	7	-	8	2	6	15910.214	-4
10	2	8	-	9	2	7	15910.804	-5
11	2	9	-	10	2	8	15911.383	-4
12	2	10	-	11	2	9	15911.936	-16
13	2	11	-	12	2	10	15912.503	-2
14	2	12	-	13	2	11	15913.030	-15
15	2	13	-	14	2	12	15913.567	-6
16	2	14	-	15	2	13	15914.081	-9
17	2	15	-	16	2	14	15914.582	-11
18	2	16	-	17	2	15	15915.074	-11
19	2	17	-	18	2	16	15915.562	-3
20	2	18	-	19	2	17	15916.019	-13
21	2	19	-	20	2	18	15916.473	-15
22	2	20	-	21	2	19	15916.937	6
23	2	21	-	22	2	20	15917.374	11
24	2	22	-	23	2	21	15917.768	-14
25	2	23	-	24	2	22	15918.190	-0
26	2	24	-	25	2	23	15918.589	4
27	2	25	-	26	2	24	15918.973	5
28	2	26	-	27	2	25	15919.349	9
29	2	27	-	28	2	26	15919.701	1
30	2	28	-	29	2	27	15920.049	3
31	2	29	-	30	2	28	15920.375	-6
7	3	4	-	8	3	5	15890.705	-4
8	3	5	-	9	3	6	15889.890	-4
9	3	6	-	10	3	7	15889.065	-4
10	3	7	-	11	3	8	15888.227	-3
11	3	8	-	12	3	9	15887.366	-12
12	3	9	-	13	3	10	15886.505	-10
14	3	11	-	15	3	12	15884.756	3
17	3	14	-	18	3	15	15882.029	10
18	3	15	-	19	3	16	15881.097	15
19	3	16	-	20	3	17	15880.133	-2
20	3	17	-	21	3	18	15879.184	9
21	3	18	-	22	3	19	15878.209	5
22	3	19	-	23	3	20	15877.199*	-21
22	3	19	-	23	3	20	15877.234	14
23	3	20	-	24	3	21	15876.221	-4
24	3	21	-	25	3	22	15875.226	8
25	3	22	-	26	3	23	15874.199	-0
26	3	23	-	27	3	24	15873.148*	-20
27	3	24	-	28	3	25	15872.117	-9
28	3	25	-	29	3	26	15871.072	0
29	3	26	-	30	3	27	15869.998	-8
30	3	27	-	31	3	28	15868.930	2
31	3	28	-	32	3	29	15867.835	-4
33	3	30	-	34	3	31	15865.613	-13
34	3	31	-	35	3	32	15864.489	-13
35	3	32	-	36	3	33	15863.340*	-27
36	3	33	-	37	3	34	15862.210	-10
37	3	34	-	38	3	35	15861.055	-6
38	3	35	-	39	3	36	15859.881	-11

J'	Ka'	Kc'		J"	Ka"	Kc"	OBS	O-C
39	3	36	-	40	3	37	15858.707	-3
40	3	37	-	41	3	38	15857.507	-10
41	3	38	-	42	3	39	15856.298	-15
42	3	39	-	43	3	40	15855.083	-14
43	3	40	-	44	3	41	15853.866	-4
11	3	8	-	10	3	7	15903.820	-3
12	3	9	-	11	3	8	15904.382	-7
14	3	11	-	13	3	10	15905.456*	-27
15	3	12	-	14	3	11	15905.986	-15
16	3	13	-	15	3	12	15906.506*	-21
17	3	14	-	16	3	13	15907.028	-1
18	3	15	-	17	3	14	15907.515	-5
19	3	16	-	18	3	15	15908.000	2
20	3	17	-	19	3	16	15908.468	4
21	3	18	-	20	3	17	15908.924	7
22	3	19	-	21	3	18	15909.368	10
23	3	20	-	22	3	19	15909.793	6
24	3	21	-	23	3	20	15910.214	12
25	3	22	-	24	3	21	15910.623	16
26	3	23	-	25	3	22	15910.999	2
27	3	24	-	26	3	23	15911.383	6
28	3	25	-	27	3	24	15911.744	2
29	3	26	-	28	3	25	15912.104	8
30	3	27	-	29	3	26	15912.442	4
31	3	28	-	30	3	27	15912.768	1
32	3	29	-	31	3	28	15913.091	8
33	3	30	-	32	3	29	15913.402	14
34	3	31	-	33	3	30	15913.686	6
35	3	32	-	34	3	31	15913.975	16
36	3	33	-	35	3	32	15914.245*	19
37	3	34	-	36	3	33	15914.501*	20
39	3	36	-	38	3	35	15914.972*	19
40	3	37	-	39	3	36	15915.205*	35
10	4	6	-	11	4	7	15879.785	10
11	4	7	-	12	4	8	15878.920	-5
12	4	8	-	13	4	9	15878.076	14
13	4	9	-	14	4	10	15877.199	10
14	4	10	-	15	4	11	15876.316	13
15	4	11	-	16	4	12	15875.421	16
16	4	12	-	17	4	13	15874.499	4
18	4	14	-	19	4	15	15872.631	-8
19	4	15	-	20	4	16	15871.689	-4
20	4	16	-	21	4	17	15870.724	-11
21	4	17	-	22	4	18	15869.766	0
22	4	18	-	23	4	19	15868.788	4
23	4	19	-	24	4	20	15867.777	-14
24	4	20	-	25	4	21	15866.776	-9
25	4	21	-	26	4	22	15865.764	-5
26	4	22	-	27	4	23	15864.736	-1
27	4	23	-	28	4	24	15863.708	8
28	4	24	-	29	4	25	15862.643	-5
29	4	25	-	30	4	26	15861.565*	-18
30	4	26	-	31	4	27	15860.498	-10
31	4	27	-	32	4	28	15859.412	-10
32	4	28	-	33	4	29	15858.318	-6
33	4	29	-	34	4	30	15857.207	-6
34	4	30	-	35	4	31	15856.088	-4
35	4	31	-	36	4	32	15854.973	14
36	4	32	-	37	4	33	15853.806	-9
37	4	33	-	38	4	34	15852.640*	-18
38	4	34	-	39	4	35	15851.489	-2
39	4	35	-	40	4	36	15850.303	-10
40	4	36	-	41	4	37	15849.124	1
41	4	37	-	42	4	38	15847.925	3
42	4	38	-	43	4	39	15846.717	8
43	4	39	-	44	4	40	15845.520*	34
44	4	40	-	45	4	41	15844.261	11
45	4	41	-	46	4	42	15843.019	15
9	4	5	-	8	4	4	15894.181	-13
11	4	7	-	10	4	6	15895.374	10

J'	Ka'	Kc'		J"	Ka"	Kc"	OBS	O-C
12	4	8	-	11	4	7	15895.909*	-21
13	4	9	-	12	4	8	15896.469	-15
14	4	10	-	13	4	9	15897.025	-1
15	4	11	-	14	4	10	15897.553	-2
16	4	12	-	15	4	11	15898.051*	-20
17	4	13	-	16	4	12	15898.572	-3
18	4	14	-	17	4	13	15899.060	-8
19	4	15	-	18	4	14	15899.519*	-27
20	4	16	-	19	4	15	15899.989*	-25
21	4	17	-	20	4	16	15900.464	-4
22	4	18	-	21	4	17	15900.909	-1
23	4	19	-	22	4	18	15901.336	-4
24	4	20	-	23	4	19	15901.754	-3
25	4	21	-	24	4	20	15902.159	-3
26	4	22	-	25	4	21	15902.555	0
29	4	25	-	28	4	24	15903.664	7
30	4	26	-	29	4	25	15904.001	2
31	4	27	-	30	4	26	15904.334	4
32	4	28	-	31	4	27	15904.662	14
33	4	29	-	32	4	28	15904.962	8
34	4	30	-	33	4	29	15905.266*	19
35	4	31	-	34	4	30	15905.551*	23
36	4	32	-	35	4	31	15905.825*	29
37	4	33	-	36	4	32	15906.077*	26
14	5	9	-	15	5	10	15868.071*	19
15	5	10	-	16	5	11	15867.161	8
13	5	8	-	14	5	9	15868.930	-9
16	5	11	-	17	5	12	15866.256	14
17	5	12	-	18	5	13	15865.319	-1
18	5	13	-	19	5	14	15864.386	1
19	5	14	-	20	5	15	15863.439	1
21	5	16	-	22	5	17	15861.499	-9
23	5	18	-	24	5	19	15859.540	9
25	5	20	-	26	5	21	15857.507	2
26	5	21	-	27	5	22	15856.465	-10
27	5	22	-	28	5	23	15855.442	9
28	5	23	-	29	5	24	15854.366	-13
29	5	24	-	30	5	25	15853.308	-5
30	5	25	-	31	5	26	15852.225	-11
31	5	26	-	32	5	27	15851.133	-14
32	5	27	-	33	5	28	15850.022*	-24
33	5	28	-	34	5	29	15848.925	-9
34	5	29	-	35	5	30	15847.802	-8
35	5	30	-	36	5	31	15846.666	-8
36	5	31	-	37	5	32	15845.520	-7
38	5	33	-	39	5	34	15843.202	4
40	5	35	-	41	5	36	15840.833	9
41	5	36	-	42	5	37	15839.622	3
42	5	37	-	43	5	38	15838.400	-4
43	5	38	-	44	5	39	15837.180	4
44	5	39	-	45	5	40	15835.946	8
45	5	40	-	46	5	41	15834.699	11
22	5	17	-	21	5	16	15892.649	11
23	5	18	-	22	5	17	15893.084*	19
24	5	19	-	23	5	18	15893.491	10
25	5	20	-	24	5	19	15893.911*	28
26	5	21	-	25	5	20	15894.282	9
27	5	22	-	26	5	21	15894.671*	20
28	5	23	-	27	5	22	15895.024	8
29	5	24	-	28	5	23	15895.374	6
30	5	25	-	29	5	24	15895.697	-11
31	5	26	-	30	5	25	15896.041	6
32	5	27	-	31	5	26	15896.372*	22
33	5	28	-	32	5	27	15896.672*	19
34	5	29	-	33	5	28	15896.956	14
35	5	30	-	34	5	29	15897.220	0
36	5	31	-	35	5	30	15897.480	-4
38	5	33	-	37	5	32	15897.966	-11
39	5	34	-	38	5	33	15898.188	-16

Note. (*) Line not included in the fit.

with the $B^1\Sigma^+$ state of CuF at 19 717 cm^{-1} (*12, 13*). However, the $\tilde{A}^1A'$ state of CuOH could also correlate with the 0^+e spin component of the $b^3\Pi$ state (*14–16*) (called $A0^+$ in Refs. *12* and *13*) of CuF at 17 613 cm^{-1}. More experimental and, particularly, theoretical work is required before a clear description of the excited CuOH states emerges.

There is an ab initio calculation of the ground state geometry of the CuOH molecule at the SCF level (*17*) by Illas *et al.* They find a bent CuOH molecule with r_{Cu-O} = 1.818 Å, r_{O-H} = 0.960 Å, and ∠Cu–O–H = 131.9° slightly more stable than the linear form. Except for the r_{O-H} distance, there is only modest agreement between the predicted

TABLE VI

r_s Structure for CuOH

Parameter	$\tilde{X}\,^1A'$	$\tilde{A}\,^1A'$	$\tilde{B}\,^1A''$
r_{Cu-O} (Å)	1.76893(25)	1.7748(32)	1.78414(46)
r_{O-H} (Å)	0.9520(50)	1.0348(40)	0.9508(27)
$\angle_{CuOH}$ (°)	110.245(80)	111.0(16)	117.670(98)

values and those observed by experiment (Table VI). A similar calculation by Klimenko *et al.* (*18*) predicted r_{Cu-O} = 1.767 Å, r_{O-H} = 0.937 Å, and $\angle$Cu–O–H = 126°.

It is evident from the perturbations seen in the spectra that the $\tilde{A}\,^1A'$ state is interacting with a vibronic state associated with a lower-lying electronic state, presumably the state responsible for the other red system at 6640 Å. We also suspect that the O–H stretch of this state is responsible for the perturbations seen in the green system (*5*). Work is currently in progress on analyzing this other red system. This system almost certainly has an excited triplet state because we have seen resolved hyperfine structure at Doppler resolution. Our analysis of this system should enable us to place some of these rather speculative arguments about perturbations and electronic correlations on a more quantitative footing. Once again we appeal for a good ab initio calculation to be performed on the excited states of this fascinating molecule.

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