

Supplementary material to paper:

Revised molecular constants and term values for the $X^2\Pi$ and $B^2\Sigma^+$ states of OH.

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Part 1: Term values (cm^{-1}) of the $v = 0$ – 13 levels of the $X^2\Pi$ state of the OH radical referred to the $X^2\Pi (v = 0) F_{1e}(J = 0.5)$ level.

Part 2: Term values (cm^{-1}) of the $v = 0$ and 1 levels of the $B^2\Sigma^+$ state of the OH radical referred to the $X^2\Pi (v = 0) F_{1e}(J = 0.5)$ level.

Part 3: Spectroscopic measurements (cm^{-1}) used in this work along with the observed-calculated values obtained from the fits.

Part 1: Rotational term values of the X²Π state of OH (cm-1)

J	v = 0				v = 1			
	F _{1e}	F _{1f}	F _{2e}	F _{2f}	F _{1e}	F _{1f}	F _{2e}	F _{2f}
0.5			126.29227	126.45013			3695.35565	3695.50644
1.5	0.00000	0.05559	187.49278	187.75295	3568.47111	3568.52242	3754.04184	3754.29215
2.5	83.72333	83.92457	288.77190	289.04440	3649.20403	3649.39071	3851.21086	3851.47669
3.5	201.93137	202.37960	429.27890	429.46249	3763.10849	3763.52636	3986.08574	3986.27137
4.5	355.12036	355.91494	608.19846	608.19391	3910.63341	3911.37729	4157.90489	4157.91562
5.5	543.59556	544.82929	824.81627	824.53095	4092.05852	4093.21743	4365.98772	4365.73469
6.5	767.48162	769.24032	1078.50960	1077.85790	4307.49774	4309.15407	4609.73220	4609.13318
7.5	1026.75520	1029.11839	1368.71581	1367.61839	4556.92563	4559.15570	4888.58942	4887.56827
8.5	1321.27599	1324.31772	1694.90251	1693.28555	4840.20469	4843.07943	5202.03751	5200.52350
9.5	1650.81037	1654.59981	2056.54543	2054.33998	5157.10696	5160.69243	5549.56149	5547.48874
10.5	2015.04818	2019.64993	2453.11330	2450.25495	5507.32966	5511.68740	5930.63914	5927.94627
11.5	2413.61422	2419.08853	2884.05802	2880.48675	5890.50619	5895.69340	6344.73172	6341.36170
12.5	2846.07642	2852.47917	3348.80855	3344.46864	6306.21397	6312.28353	6791.27799	6787.17805
13.5	3311.95163	3319.33433	3846.76713	3841.60718	6753.98008	6760.98054	7269.69052	7264.81218
14.5	3810.70998	3819.11972	4377.30707	4371.28010	7233.28550	7241.26104	7779.35354	7773.65266
15.5	4341.77829	4351.25760	4939.77176	4932.83525	7743.56845	7752.55873	8319.62181	8313.05868
16.5	4904.54283	4915.12958	5533.47421	5525.59023	8284.22704	8294.26713	8889.82022	8882.35962
17.5	5498.35166	5510.07898	6157.69727	6148.83255	8854.62156	8865.74186	9489.24383	9480.85517
18.5	6122.51669	6135.41287	6811.69410	6801.82011	9454.07652	9466.30261	10117.15832	10107.81565
19.5	6776.31563	6790.40400	7494.68887	7483.78190	10081.88239	10095.23500	10772.80057	10762.48272
20.5	7458.99367	7474.29255	8205.87770	8193.91893	10737.29734	10751.79222	11455.37952	11444.07013
21.5	8169.76520	8186.28784	8944.42970	8931.40522	11419.54877	11435.19665	12164.07706	12151.76463
22.5	8907.81539	8925.56991	9709.48802	9695.38889	12127.83479	12144.64135	12898.04903	12884.72694
23.5	9672.30172	9691.29109	10500.17110	10484.99331	12861.32570	12879.29150	13656.42621	13642.09278
24.5	10462.35546	10482.57752	11315.57377	11299.31828	13619.16530	13638.28577	14438.31546	14422.97390
25.5	11277.08314	11298.53056	12154.76850	12137.44123	14400.47223	14420.73767	15242.80065	15226.45911
26.5	12115.56795	12138.22825	13016.80660	12998.41835	15204.34118	15225.73676	16068.94377	16051.61530

27.5	12976.87106	13000.72665	13900.71940	13881.28582	16029.84414	16052.34988	16915.78588	16897.48839
28.5	13860.03293	13885.06118	14805.51934	14785.06092	16876.03143	16899.62227	17782.34802	17763.10428
29.5	14764.07457	14790.24780	15730.20115	15708.74311	17741.93278	17766.57855	18667.63211	18647.46968
30.5	15687.99871	15715.28430	16673.74284	16651.31506	18626.55824	18652.22374	19570.62162	19549.57285
31.5	16630.79089	16659.15131	17635.10668	17611.74364	19528.89903	19555.54400	20490.28229	20468.38425
32.5	17591.42051	17620.81341	18613.24009	18588.98081	20447.92818	20475.50741	21425.56259	21402.85706
33.5	18568.84175	18599.22002	19607.07643	19581.96437	21382.60117	21411.06443	22375.39405	22351.92748
34.5	19561.99439	19593.30623	20615.53567	20589.61866	22331.85623	22361.14836	23338.69140	23314.51490
35.5	20569.80455	20601.99352	21637.52490	21610.85512	23294.61455	23324.67542	24314.35246	24289.52180
36.5	21591.18520	21624.19029	22671.93873	22644.57258	24269.78019	24300.54474	25301.25774	25275.83336
37.5	22625.03660	22658.79230	23717.65941	23689.65755	25256.23977	25287.63794	26298.26975	26272.31679
38.5	23670.24650	23704.68279	24773.55682	24744.98411	26252.86172	26284.81847	27304.23181	27277.82018
39.5	24725.69006	24760.73249	25838.48814	25809.41361	27258.49527	27290.93045	28317.96652	28291.17097
40.5	25790.22964	25825.79930	26911.29714	26881.79406	28271.96878	28304.79711	29338.27352	29311.17379
41.5	26862.71410	26898.72762	27990.81319	27960.95907	29292.08770	29325.21863	30363.92670	30336.60763
42.5	27941.97778	27978.34733	29075.84973	29045.72639	30317.63171	30350.96928	31393.67055	31366.22230
43.5	29026.83909	29063.47231	30165.20218	30134.89588	31347.35113	31380.79381	32426.21552	32398.73379
44.5	30116.09839	30152.89832	31257.64521	31227.24676	32379.96235	32413.40283	33460.23237	33432.81867
45.5	31208.53530	31245.40030	32351.92921	32321.53411	33414.14212	33447.46708	34494.34504	34467.10702
46.5	32302.90517	32339.72881	33446.77572	33416.48442	34448.52056	34481.61039	35527.12207	35500.17386
47.5	33397.93462	33434.60551	34540.87183	34510.78990	35481.67249	35514.40100	36557.06608	36530.52874
48.5	34492.31583	34528.71748	35632.86306	35603.10151				
49.5	35584.69957	35620.71020	36721.34474	36692.02032				

J	v = 2				v = 3			
	F _{1e}	F _{1f}	F _{2e}	F _{2f}	F _{1e}	F _{1f}	F _{2e}	F _{2f}
0.5			7098.82558	7098.96912			10338.61744	10338.75352
1.5	6971.34602	6971.39319	7155.04106	7155.28101	10210.54532	10210.58846	10392.39668	10392.62572
2.5	7049.11770	7049.29020	7248.16530	7248.42355	10285.37339	10285.53199	10481.52673	10481.77648
3.5	7158.76759	7159.15564	7377.49066	7377.67709	10390.80107	10391.15962	10605.36490	10605.55090
4.5	7300.69837	7301.39211	7542.30756	7542.33211	10527.18575	10527.82956	10763.25179	10763.28881
5.5	7475.16362	7476.24815	7741.96890	7741.74662	10694.75424	10695.76432	10954.57337	10954.38051
6.5	7682.26542	7683.81964	7975.89339	7975.34552	10893.59550	10895.04711	11178.76905	11178.27112
7.5	7921.97508	7924.07201	8243.54577	8242.59943	11123.67627	11125.63904	11435.31694	11434.44440
8.5	8194.15682	8196.86419	8544.41429	8543.00191	11384.86115	11387.39952	11723.71487	11722.40337
9.5	8498.58727	8501.96797	8877.99261	8876.05143	11676.93002	11680.10368	12043.46430	12041.65419
10.5	8834.96995	8839.08240	9243.76672	9241.23844	11999.59135	12003.45551	12394.05824	12391.69434
11.5	9202.94573	9207.84399	9641.20611	9638.03675	12352.49200	12357.09758	12774.97306	12772.00446
12.5	9602.10028	9607.83415	10069.75807	10065.89789	12735.22434	12740.61798	13185.66295	13182.04292
13.5	10031.96956	10038.58454	10528.84408	10524.24758	13147.33145	13153.55553	13625.55639	13621.24245
14.5	10492.04392	10499.58113	11017.85761	11012.48359	13588.31111	13595.40365	14094.05401	14089.00790
15.5	10981.77128	10990.26742	11536.16300	11529.97462	14057.61883	14065.61345	14590.52733	14584.71515
16.5	11500.55979	11510.04697	12083.09494	12076.05982	14554.67039	14563.59616	15114.31820	15107.71048
17.5	12047.77995	12058.28567	12657.95846	12650.04876	15078.84390	15088.72525	15664.73868	15657.31044
18.5	12622.76657	12634.31356	13260.02924	13251.22173	15629.48155	15640.33818	16241.07118	16232.80205
19.5	13224.82045	13237.42660	13888.55412	13878.83027	16205.89122	16217.73798	16842.56885	16833.44315
20.5	13853.20997	13866.88825	14542.75179	14532.09782	16807.34790	16820.19470	17468.45608	17458.46289
21.5	14507.17248	14521.93088	15221.81353	15210.22049	17433.09494	17446.94669	18117.92909	18107.06233
22.5	15185.91572	15201.75717	15924.90411	15912.36789	18082.34528	18097.20175	18790.15653	18778.41502
23.5	15888.61908	15905.54141	16651.16257	16637.68395	18754.28245	18770.13826	19484.28013	19471.66763
24.5	16614.43477	16632.43067	17399.70314	17385.28780	19448.06158	19464.90611	20199.41521	20185.94050
25.5	17362.48897	17381.54596	18169.61602	18154.27455	20162.81023	20180.62755	20934.65127	20920.32815
26.5	18131.88286	18151.98326	18959.96817	18943.71611	20897.62909	20916.39794	21689.05228	21673.89967
27.5	18921.69356	18942.81448	19769.80402	19752.66181	21651.59261	21671.28628	22461.65703	22445.69897
28.5	19730.97494	19753.08826	20598.14604	20580.13909	22423.74930	22444.33563	23251.47915	23234.74488
29.5	20558.75837	20581.83072	21443.99524	21425.15386	23213.12204	23234.56331	24057.50701	24040.03100
30.5	21404.05325	21428.04599	22306.33144	22286.69091	24018.70792	24040.96080	24878.70324	24860.52530

31.5	22265.84738	22290.71656	23184.11342	23163.71397	24839.47798	24862.49344	25714.00402	25695.16934
32.5	23143.10719	23168.80353	24076.27875	24055.16561	25674.37651	25698.09968	26562.31789	26542.87720
33.5	24034.77762	24061.24644	24981.74339	24959.96684	26522.31991	26546.68999	27422.52410	27402.53374
34.5	24939.78179	24966.96296	25899.40097	25877.01637	27382.19514	27407.14525	28293.47037	28272.99249
35.5	25857.02027	25884.84810	26828.12154	26805.18949	28252.85753	28278.31448	29173.96994	29153.07267
36.5	26785.37001	26813.77314	27766.75000	27743.33639	29133.12785	29159.01198	30062.79777	30041.55550
37.5	27723.68265	27752.58393	28714.10377	28690.28000	30021.78863	30048.01354	30958.68582	30937.17942
38.5	28670.78241	28700.09867	29668.96992	29644.81304	30917.57940	30944.05163	31860.31703	31838.63422
39.5	29625.46314	29655.10500	30630.10138	30605.69436	31819.19082	31845.80951	32766.31801	32744.55371
40.5	30586.48459	30616.35623	31596.21216	31571.64418	32725.25730	32751.91382	33675.25003	33653.50684
41.5	31552.56778	31582.56659	32565.97150	32541.33829	33634.34813	33660.92559	34585.59810	34563.98680
42.5	32522.38908	32552.40532	33537.99660	33513.40081	34544.95654	34571.32927	35495.75777	35474.39789
43.5	33494.57300	33524.48941	34510.84369	34486.39538	35455.48652	35481.51953	36404.01927	36383.03977
44.5	34467.68335	34497.37468	35482.99732	35458.81448	36364.23699	36389.78527	37308.54857	37288.08855
45.5	35440.21251	35469.54499	36452.85730	36429.06647				
46.5	36410.56845	36439.39919	37418.72319	37395.46008				

J	v = 4				v = 5			
	F _{1e}	F _{1f}	F _{2e}	F _{2f}	F _{1e}	F _{1f}	F _{2e}	F _{2f}
0.5			13415.81989	13415.94816			16330.52332	16330.64336
1.5	13287.16488	13287.20414	13467.18645	13467.40376	16201.30672	16201.34217	16379.48655	16379.69118
2.5	13359.05257	13359.19759	13552.35511	13552.59498	16270.23873	16270.37028	16460.70337	16460.93190
3.5	13460.26959	13460.59907	13670.74376	13670.92753	16367.23015	16367.53054	16573.64810	16573.82777
4.5	13591.12902	13591.72323	13821.74115	13821.78858	16492.55056	16493.09476	16717.75556	16717.81136
5.5	13751.83010	13752.76574	14004.76567	14004.60013	16646.37072	16647.23084	16892.47578	16892.33550
6.5	13942.44720	13943.79572	14219.27710	14218.82717	16828.74876	16829.99217	17097.28841	17096.88458
7.5	14162.94089	14164.76830	14464.76643	14463.96612	17039.63707	17041.32601	17331.69662	17330.96684
8.5	14413.17450	14415.54177	14740.74026	14739.52863	17278.89570	17281.08750	17595.21460	17594.10135
9.5	14692.92952	14695.89288	15046.70661	15045.02741	17546.30551	17549.05288	17887.35532	17885.80567
10.5	15001.91766	15005.52886	15382.16407	15379.96546	17841.57910	17844.93029	18207.62086	18205.58618
11.5	15339.78992	15344.09641	15746.59404	15743.82846	18164.36905	18168.36808	18555.49519	18552.93108
12.5	15706.14335	15711.18830	16139.45550	16136.07959	18514.27424	18518.96088	18930.43932	18927.30549
13.5	16100.52595	16106.34821	16560.18157	16556.15618	18890.84452	18896.25433	19331.88791	19328.14817
14.5	16522.44044	16529.07454	17008.17728	17003.46753	19293.58429	19299.74856	19759.24721	19754.86949
15.5	16971.34720	16978.82321	17482.81831	17477.39362	19721.95530	19728.90104	20211.89374	20206.85013
16.5	17446.66658	17455.01002	17983.45023	17977.28447	20175.37895	20183.12878	20689.17363	20683.44040
17.5	17947.78080	17957.01254	18509.38826	18502.45977	20653.23813	20661.81025	21190.40233	21183.95999
18.5	18474.03560	18484.17175	19059.91720	19052.20895	21154.87884	21164.28701	21714.86469	21707.69796
19.5	19024.74157	19035.79338	19634.29165	19625.79124	21679.61163	21689.86513	22261.81519	22253.91303
20.5	19599.17541	19611.14915	20231.73620	20222.43602	22226.71284	22237.81649	22830.47835	22821.83389
21.5	20196.58092	20209.47783	20851.44579	20841.34304	22795.42578	22807.37998	23420.04919	23410.65972
22.5	20816.16993	20829.98611	21492.58601	21481.68279	23384.96180	23397.76256	24029.69382	24019.56066
23.5	21457.12306	21471.84941	22154.29333	22142.59667				
24.5	22118.59032	22134.21245	22835.67530	22823.19725				
25.5	22799.69160	22816.18974	23535.81059	23522.56825				
26.5	23499.51685	23516.86585	24253.74888	24239.76445				
27.5	24217.12624	24235.29544	24988.51050	24973.81135				
28.5	24951.54990	24970.50308	25739.08583	25723.70455				
29.5	25701.78743	25721.48272	26504.43439	26488.40885				
30.5	26466.80710	26487.19690	27283.48344	27266.85691				

31.5	27245.54455	27266.57541	28075.12621	28057.94741
32.5	28036.90106	28058.51355	28878.21942	28860.54269
33.5	28839.74117	28861.86975	29691.58020	29673.46564
34.5	29652.88965	29675.46246	30513.98212	30495.49575
35.5	30475.12755	30498.06623	31344.15020	31325.36420
36.5	31305.18730	31328.40674	32180.75477	32161.74774

J	v = 6				v = 7			
	F _{1e}	F _{1f}	F _{2e}	F _{2f}	F _{1e}	F _{1f}	F _{2e}	F _{2f}
0.5			19081.59516	19081.70612			21666.39096	21666.49165
1.5	18951.85774	18951.88947	19128.14781	19128.33797	21536.19957	21536.22759	21710.50318	21710.67651
2.5	19017.79516	19017.91347	19205.39475	19205.60921	21599.07288	21599.17786	21783.72481	21783.92172
3.5	19110.51235	19110.78385	19312.86236	19313.03446	21687.42359	21687.66570	21885.63006	21885.79025
4.5	19230.23596	19230.73004	19450.02904	19450.08927	21801.43568	21801.87831	22015.73821	22015.79803
5.5	19377.10709	19377.89096	19616.37513	19616.25614	21941.21894	21941.92400	22173.55838	22173.45567
6.5	19551.16554	19552.30215	19811.39926	19811.03791	22106.79223	22107.81786	22358.60676	22358.28302
7.5	19752.35313	19753.90061	20034.61561	20033.95353	22298.08367	22299.48354	22570.40677	22569.80788
8.5	19980.52406	19982.53572	20285.54430	20284.52787	22514.93815	22516.76130	22808.48207	22807.55845
9.5	20235.45595	20237.98051	20563.70117	20562.28128	22757.12630	22759.41726	23072.34816	23071.05462
10.5	20516.85941	20519.94116	20868.58909	20866.72096	23024.35260	23027.15153	23361.50484	23359.80046
11.5	20824.38550	20828.06442	21199.69148	21197.33452	23316.26203	23319.60473	23675.43022	23673.27825
12.5	21157.63147	21161.94328	21556.46755	21553.58533	23632.44512	23636.36313	24013.57632	24010.94415
13.5	21516.14510	21521.12125	21938.34914	21934.90930	23972.44183	23976.96239	24375.36586	24372.22496
14.5	21899.42793	21905.09559	22344.73843	22340.71278	24335.74452	24340.89052	24760.18995	24756.51596
15.5	22306.93788	22313.31988	22775.00663	22770.37106	24721.80016	24727.59014	25167.40660	25163.17927
16.5	22738.09120	22745.20600	23228.49300	23223.22761	25130.01208	25136.46013	25596.33955	25591.54284
17.5	23192.26413	23200.12579	23704.50444	23698.59347	25559.74131	25566.85706	26046.27761	26040.89963
18.5	23668.79426	23677.41239	24202.31521	24195.74706	26010.30764	26018.09621	26516.47411	26510.50716
19.5	24166.98161	24176.36140	24721.16691	24713.93410	26480.99045	26489.45249	27006.14657	26999.58712
20.5	24686.08961	24696.23186	25260.26851	25252.36763	26971.02939	26980.16106	27514.47649	27507.32508
21.5	25225.34592	25236.24710	25818.79649	25810.22809	27479.62489	27489.41794	28040.60915	28032.87032
22.5	25783.94313	25795.59547	26395.89501	26386.66347	28005.93850	28016.38038	28583.65340	28575.33560
23.5	26361.03934	26373.43096	26990.67602	26980.78940	28549.09324	28560.16715	29142.68156	29133.79692

J	v = 8				v = 9			
	F _{1e}	F _{1f}	F _{2e}	F _{2f}	F _{1e}	F _{1f}	F _{2e}	F _{2f}
0.5			24080.35243	24080.44141			26316.48202	26316.55644
1.5	23949.81989	23949.84423	24121.96592	24122.11944	26185.78987	26185.81046	26355.50011	26355.62821
2.5	24009.51852	24009.61014	24191.05934	24191.23425	26242.14781	26242.22568	26420.29797	26420.44280
3.5	24093.35220	24093.56454	24287.25010	24287.39268	26321.23537	26321.41673	26510.53138	26510.64631
4.5	24201.46205	24201.85207	24410.09503	24410.14793	26423.14996	26423.48463	26625.79073	26625.82538
5.5	24333.92444	24334.54811	24559.12967	24559.03639	26547.93141	26548.46876	26765.63466	26765.53893
6.5	24490.73386	24491.64390	24733.88554	24733.59270	26695.54523	26696.33189	26929.60659	26929.33298
7.5	24671.80068	24673.04564	24933.89258	24933.35086	26865.87837	26866.95717	27117.23880	27116.74338
8.5	24876.95597	24878.57994	25158.67455	25157.83892	27058.74160	27060.15115	27328.04970	27327.29258
9.5	25105.95841	25108.00100	25407.74224	25406.57199	27273.87427	27275.64884	27561.53858	27560.48401
10.5	25358.50094	25360.99732	25680.58701	25679.04566	27510.94939	27513.11885	27817.18001	27815.79637
11.5	25634.21627	25637.19724	25976.67527	25974.73053	27769.57787	27772.16769	28094.41868	28092.67848
12.5	25932.68121	25936.17318	26295.44422	26293.06795	28049.31185	28052.34312	28392.66509	28390.54496
13.5	26253.41992	26257.44490	26636.29845	26633.46664	28349.64705	28353.13639	28711.29184	28708.77253
14.5	26595.90620	26600.48178	26998.60739	26995.30021	28670.02422	28673.98378	29049.63051	29046.69690
15.5	26959.56520	26964.70446	27381.70326	27377.90501	29009.82993	29014.26735	29406.96882	29403.60993
16.5	27343.77444	27349.48597	27784.87932	27780.57852	29368.39668	29373.31505	29782.54805	29778.75701
17.5	27747.86450	27754.15232	28207.38849	28202.57781	29745.00250	29750.40034	30175.56041	30171.33447
18.5					30138.87001	30144.74130	30585.14646	30580.48690

J	v = 10				v = 11			
	F _{1e}	F _{1f}	F _{2e}	F _{2f}	F _{1e}	F _{1f}	F _{2e}	F _{2f}
0.5			28364.62447	28364.68071			30210.54999	30210.56871
1.5	28234.07165	28234.08845	28400.89888	28400.99439	30080.60072	30080.61331	30243.87655	30243.90109
2.5	28286.84639	28286.91018	28461.14731	28461.25153	30129.44851	30129.49655	30299.22121	30299.22809
3.5	28360.85023	28360.99953	28545.05811	28545.13199	30197.88711	30198.00008	30376.29627	30376.25508
4.5	28456.13495	28456.41169	28652.24995	28652.25080	30285.91834	30286.12868	30474.73940	30474.61644
5.5	28572.69936	28573.14538	28782.29952	28782.18457	30393.49223	30393.83244	30594.13563	30593.89685
6.5	28710.47355	28711.12836	28934.75670	28934.48528	30520.49283	30520.99348	30734.03072	30733.64367
7.5	28869.31312	28870.21275	29109.14944	29108.68410	30666.73167	30667.42016	30893.93640	30893.37150
8.5	29048.99928	29050.17574	29304.98250	29304.28961	30831.94621	30832.84605	31073.33056	31072.56181
9.5	29249.24153	29250.72250	29521.73336	29520.78329	31015.80093	31016.93124	31271.65454	31270.66001
10.5	29469.68078	29471.48951	29758.84705	29757.61434	31217.88920	31219.26438	31488.30942	31487.07158
11.5	29709.89204	29712.04726	30015.73110	30014.19446	31437.73526	31439.36469	31722.65198	31721.15801
12.5	29969.38630	29971.90215	30291.75065	30289.89305	31674.79569	31676.68345	31973.99095	31972.23304
13.5	30247.61136	30250.49733	30586.22384	30584.03249	31928.46043	31930.60500	32241.58354	32239.55916
14.5	30543.95181	30547.21266	30898.41733	30895.88376				
15.5	30857.72804	30861.36378	31227.54181	31224.66184				
16.5	31188.19446	31192.20028	31572.74727	31569.52104				

J	v = 12				v = 13			
	F _{1e}	F _{1f}	F _{2e}	F _{2f}	F _{1e}	F _{1f}	F _{2e}	F _{2f}
0.5			31834.96192	31834.96624			33212.43493	33212.36278
1.5	31706.38549	31706.39483	31864.97953	31864.97817	33086.40065	33086.40420	33238.74619	33238.59719
2.5	31750.79536	31750.83112	31914.82377	31914.79836	33125.67994	33125.69348	33282.39040	33282.15578
3.5	31812.95273	31813.03708	31984.22805	31984.15448	33180.57783	33180.60959	33343.10103	33342.76907
4.5	31892.80672	31892.96417	32072.84653	32072.69770	33250.97657	33251.03525	33420.52298	33420.08032
5.5	31990.25378	31990.50876	32180.27042	32180.01864	33336.69716	33336.79069	33514.22370	33513.65657
6.5	32105.12541	32105.50054	32306.03865	32305.65743	33437.48902	33437.62351	33623.70087	33622.99620
7.5	32237.18117	32237.69601	32449.64290	32449.10814	33553.02301	33553.20184	33748.38629	33747.53254
8.5	32386.10561	32386.77587	32610.52832	32609.81912	33682.88711	33683.11024	33887.64639	33886.63430
9.5	32551.50742	32552.34437	32788.09166	32787.19092	33826.58379	33826.84718	34040.78058	34039.60371
10.5	32732.91954	32733.92961	32981.67811	32980.57293	33983.52827	33983.82337	34207.01808	34205.67333
11.5	32929.79954	32930.98392	33190.57753	33189.25959	34153.04694	34153.36030	34385.51401	34384.00203
12.5	33141.52970	33142.88402	33414.02055	33412.48644	34334.37571	34334.68861	34575.34502	34573.67057

Part 2: Term values (cm⁻¹) of the B²Σ⁺ state of the OH radical.

J	v = 0		v = 1	
	F ₁	F ₂	F ₁	F ₂
0.5	68406.30207	-	69066.13331	-
1.5	68416.48701	68416.44757	69074.33939	69074.30732
2.5	68436.82124	68436.7559	69090.68843	69090.63637
3.5	68467.25961	68467.16896	69115.06923	69114.99926
4.5	68507.73381	68507.61868	69147.29756	69147.21258
5.5	68558.15152	68558.01297	69187.09499	69186.99874
6.5	68618.39532	68618.23464	69234.06073	69233.95777
7.5	68688.32130	68688.14003	69287.63632	69287.53206
8.5	68767.75747	68767.55737	69347.06337	69346.96404
9.5	68856.50180	68856.2849	69411.33416	69411.24681
10.5	68954.32007	68954.0886	69479.13524	69479.06776
11.5	69060.94340	69060.69982	69548.78397	69548.74509
12.5	69176.06547	69175.81252	69618.15800	69618.15727
13.5	69299.33960	69299.08022	69684.61771	69684.66550
14.5	69430.37541	69430.11278		
15.5	69568.73528	69568.47283		

Part 3: Spectroscopic measurements (cm⁻¹) used in this work along with the observed-calculated values obtained from the fits.

X²Π-X²Π

0-0	J	Obs (cm-1)	Obs-Calc
R _{2ff} (J)	8.5	361.0528	-0.00163
	10.5	430.2329	0.00111
	11.5	463.9818	-0.00009
	12.5	497.1382	-0.00034
	13.5	529.6722	-0.00072
	14.5	561.5549	-0.00025
	15.5	592.7528	-0.00218
	16.5	623.2427	0.00038
	17.5	652.9882	0.00065
	18.5	681.9623	0.00051
	19.5	710.1375	0.00047
	20.5	737.4865	0.00021
	21.5	763.9838	0.00013
	22.5	789.6044	-0.00002
	23.5	814.3245	-0.00047
	24.5	838.1225	-0.00044
	25.5	860.9762	-0.00092
	26.5	882.8664	-0.00108
	27.5	903.7738	-0.00130
	28.5	923.6811	-0.00108
	29.5	942.5709	-0.00105

	30.5	960.4276	-0.00098
	31.5	977.2366	-0.00057
	32.5	992.9833	-0.00026
	33.5	1007.6534	-0.00090
	34.5	1021.2372	0.00075
	35.5	1033.7189	0.00143
	36.5	1045.0867	0.00173
	37.5	1055.3280	0.00144
	38.5	1064.4308	0.00130
	39.5	1072.3812	0.00075
	40.5	1079.1654	0.00039
	41.5	1084.7673	-0.00002
	42.5	1089.1687	-0.00079
	43.5	1092.3491	-0.00178
	44.5	1094.2860	-0.00136
	45.5	1094.9520	0.00169
	46.5	1094.3060	0.00052
	47.5	1092.3120	0.00038
	48.5	1088.9184	-0.00041
	49.5	1084.0626	-0.00393
R _{2ee} (J)	11.5	464.7494	-0.00114
	12.5	497.9582	-0.00037
	13.5	530.5391	-0.00085
	14.5	562.4654	0.00072
	15.5	593.7027	0.00025
	16.5	624.2233	0.00023
	17.5	653.9973	0.00047
	18.5	682.9957	0.00093
	19.5	711.1895	0.00067
	20.5	738.5527	0.00070
	21.5	765.0587	0.00037

	22.5	790.6835	0.00042
	23.5	815.4031	0.00043
	24.5	839.1949	0.00017
	25.5	862.0381	-0.00001
	26.5	883.9125	-0.00029
	27.5	904.7994	-0.00054
	28.5	924.6813	-0.00051
	29.5	943.5411	-0.00059
	30.5	961.3633	-0.00054
	31.5	978.1329	-0.00051
	32.5	993.8359	-0.00044
	33.5	1008.4592	-0.00004
	34.5	1021.9894	0.00017
	35.5	1034.4141	0.00028
	36.5	1045.7211	0.00042
	37.5	1055.8975	0.00008
	38.5	1064.9316	0.00029
	39.5	1072.8093	0.00030
	41.5	1085.0355	-0.00104
	42.5	1089.3513	-0.00115
	43.5	1092.4380	-0.00504
	44.5	1094.2860	0.00200
	45.5	1094.8540	0.00749
	46.5	1094.0970	0.00089
	47.5	1091.9940	0.00277
R _{1ff} (J)	9.5	365.0486	-0.00153
	11.5	433.3901	-0.00054
	13.5	499.7817	-0.00368
	14.5	532.1376	-0.00028
	15.5	563.8706	-0.00139
	17.5	625.3347	0.00081

18.5	654.9924	0.00128
19.5	683.8895	0.00095
20.5	711.9962	0.00091
21.5	739.2828	0.00073
22.5	765.7217	0.00051
23.5	791.2870	0.00057
24.5	815.9532	0.00016
25.5	839.6977	0.00001
26.5	862.4982	-0.00021
27.5	884.3350	0.00048
28.5	905.1861	-0.00053
29.5	925.0355	-0.00099
30.5	943.8666	-0.00041
31.5	961.6617	-0.00040
32.5	978.4064	-0.00021
33.5	994.0862	-0.00001
34.5	1008.6871	-0.00019
35.5	1022.1973	0.00052
36.5	1034.6028	0.00079
37.5	1045.8912	0.00071
38.5	1056.0529	0.00320
39.5	1065.0677	0.00089
40.5	1072.9302	0.00188
41.5	1079.6190	-0.00072
42.5	1085.1245	-0.00048
43.5	1089.4257	-0.00031
44.5	1092.4993	-0.00268
45.5	1094.3240	-0.00451
46.5	1094.8700	-0.00670
47.5	1094.1120	0.00002
48.5	1091.9940	0.00128

R _{1ee} (J)	49.5	1088.4662	-0.00239
	9.5	364.2363	-0.00151
	11.5	432.4611	-0.00110
	13.5	498.7582	-0.00015
	14.5	531.0682	-0.00011
	15.5	562.7651	0.00056
	17.5	624.1660	0.00096
	18.5	653.7999	0.00096
	19.5	682.6790	0.00096
	20.5	710.7725	0.00097
	21.5	738.0508	0.00061
	22.5	764.4871	0.00078
	23.5	790.0542	0.00046
	24.5	814.7281	0.00041
	25.5	838.4850	0.00019
	26.5	861.3032	0.00010
	27.5	883.1618	-0.00007
	28.5	904.0415	-0.00014
	29.5	923.9239	-0.00024
	30.5	942.7919	-0.00028
	31.5	960.6296	-0.00002
	32.5	977.4214	0.00016
	33.5	993.1530	0.00035
	34.5	1007.8107	0.00054
	35.5	1021.3815	0.00085
	36.5	1033.8521	0.00070
	37.5	1045.2106	0.00071
	38.5	1055.4438	0.00023
	39.5	1064.5399	0.00032
	40.5	1072.4835	-0.00095
	41.5	1079.2615	-0.00219

	42.5	1084.8585	-0.00281
	43.5	1089.2583	-0.00100
	44.5	1092.4380	0.00109
	45.5	1094.3740	0.00412
	46.5	1095.0270	-0.00245
	47.5	1094.3820	0.00079
	48.5	1092.3850	0.00127
	49.5	1088.9882	0.00133
Q _{2fe} (J)	0.5	0.1578	-0.00006
	1.5	0.2602	0.00003
	2.5	0.2724	-0.00010
	3.5	0.1835	-0.00009
	4.5	-0.0046	-0.00006
	5.5	-0.2855	-0.00018
	6.5	-0.6517	0.00001
	7.5	-1.0974	0.00001
	8.5	-1.6169	0.00006
	9.5	-2.2053	0.00015
Q _{1fe} (J)	1.5	0.0556	0.00001
	2.5	0.2013	0.00007
	3.5	0.4483	0.00007
	4.5	0.7946	0.00003
	5.5	1.2338	0.00006
	6.5	1.7588	0.00010
	7.5	2.3633	0.00011
R _{1ee} (J)	1.5	83.7233	-0.00003
	2.5	118.2081	0.00006
R _{1ff} (J)	1.5	83.8690	0.00002
	2.5	118.4551	0.00007
R _{2ff} (J)	0.5	61.3029	0.00008

R _{2ee} (J)	1.5	101.2792	0.00008
R _{2ff} (J)	1.5	101.2914	-0.00005
	2.5	140.4182	0.00010
P _{21ff} (J)	1.5	126.3945	-0.00004
P _{21ee} (J)	2.5	103.7695	0.00006
P _{21ff} (J)	2.5	103.8284	0.00002

1-0	J	Obs (cm-1)	Obs-Calc
R _{1ff} (J)	1.5	3649.3325	-0.00262
	2.5	3679.6016	-0.00019
	3.5	3708.9973	-0.00039
	4.5	3737.3021	-0.00039
	5.5	3764.3246	-0.00018
	6.5	3789.9137	-0.00168
	7.5	3813.9597	-0.00133
	8.5	3836.3684	-0.00631
R _{2ff} (J)	0.5	3627.8421	0.00008
	1.5	3663.7210	-0.00274
	2.5	3697.2254	-0.00158
	3.5	3728.4518	-0.00133
	4.5	3757.5396	-0.00118
	5.5	3784.5942	-0.00803
	6.5	3809.7125	0.00213
P _{1ee} (J)	2.5	3484.7474	-0.00038
	3.5	3447.2720	-0.00066
	4.5	3407.9877	-0.00043
	5.5	3367.0375	-0.00035
	6.5	3324.5765	-0.00040
	7.5	3280.7416	-0.00094

	8.5	3235.6484	-0.00124
	9.5	3189.3943	-0.00002
	10.5	3142.0577	-0.00108
	11.5	3093.7146	-0.00084
	12.5	3044.4288	-0.00097
	13.5	2994.2621	-0.00024
	14.5	2943.2716	0.00150
	15.5	2891.5078	0.00059
	16.5	2839.0300	0.00438
$P_{2ee}(J)$	1.5	3507.8609	-0.00197
	2.5	3465.2668	-0.00314
	3.5	3421.9310	-0.00095
	4.5	3377.8870	-0.00029
	5.5	3333.0885	-0.00012
	6.5	3287.4779	-0.00022
	7.5	3241.0161	-0.00030
	8.5	3193.6858	-0.00111
	9.5	3145.4912	-0.00088
	10.5	3096.4480	-0.00020
	11.5	3046.5821	0.00097
	12.5	2995.9251	0.00193
	13.5	2944.5108	-0.00007
	14.5	2892.3835	0.00005
	15.5	2839.5801	-0.00168
$Q_{2ef}(J)$	0.5	3568.9053	-0.00021
	1.5	3566.2906	0.00171
	2.5	3562.1692	0.00274
	3.5	3556.6162	-0.00705
	4.5	3549.7129	0.00193
	5.5	3541.4562	-0.00057

Q _{1fe} (J)	1.5	3568.5220	-0.00042
	2.5	3565.6679	0.00052
	3.5	3561.5949	-0.00008
	4.5	3556.2629	0.00597
	5.5	3549.6309	0.00903
	6.5	3541.6732	0.00075
R _{1ee} (J)	1.5	3649.2014	-0.00263
	2.5	3679.3850	-0.00015
	3.5	3708.7018	-0.00024
	4.5	3736.9381	-0.00006
	5.5	3763.9021	-0.00008
	6.5	3789.4438	-0.00020
R _{2ee} (J)	0.5	3627.7493	-0.00027
	1.5	3663.7210	0.00292
	2.5	3697.3143	0.00045
	3.5	3728.6258	-0.00018
	4.5	3757.7886	-0.00066
	5.5	3784.9173	0.00136
	6.5	3810.0836	0.00378
P _{1ff} (J)	2.5	3484.5976	-0.00025
	3.5	3447.0108	-0.00031
	4.5	3407.6110	-0.00042
	5.5	3366.5476	-0.00040
	6.5	3323.9765	-0.00061
	7.5	3280.0358	0.00012
	8.5	3234.8370	-0.00099
	9.5	3188.4783	-0.00132
	10.5	3141.0414	-0.00109
	11.5	3092.5972	-0.00167
	12.5	3043.2142	-0.00003

	13.5	2992.9481	-0.00110
	14.5	2941.8635	0.00267
	15.5	2890.0070	0.00356
$P_{2ff}(J)$	1.5	3507.7547	0.00121
	2.5	3465.2462	-0.00156
	3.5	3422.0146	0.00040
	4.5	3378.0772	-0.00026
	5.5	3333.3837	-0.00097
	6.5	3287.8765	-0.00030
	7.5	3241.5153	0.00051
	8.5	3194.2817	-0.00102
	9.5	3146.1836	0.00008
	10.5	3097.2359	0.00211
	11.5	3047.4591	-0.00042
	12.5	2996.8928	-0.00026
	13.5	2945.5700	-0.00087
	14.5	2893.5308	-0.00128
	15.5	2840.8197	0.00229
	16.5	2787.4645	-0.00394
	17.5	2733.5285	0.00143
$Q_{2fe}(J)$	0.5	3569.2148	0.00063
	1.5	3566.8035	0.00412
	2.5	3562.7081	0.00331
	3.5	3556.9946	0.00213
	4.5	3549.7129	-0.00426
$Q_{1ef}(J)$	1.5	3568.4152	-0.00032
	2.5	3565.2800	0.00054
	3.5	3560.7295	0.00061
	4.5	3554.7194	0.00093
	5.5	3547.2334	0.00417

P _{1ee} (J)	6.5	3538.2538	-0.00362
	5.5	3367.0365	-0.00135
	6.5	3324.5747	-0.00220
	7.5	3280.7428	0.00026
	8.5	3235.6502	0.00056
	9.5	3189.3939	-0.00042
	10.5	3142.0606	0.00182
	11.5	3093.7161	0.00066
	13.5	2994.2630	0.00066
	14.5	2943.2709	0.00080
	16.5	2839.0245	-0.00112
	17.5	2785.8761	0.00072
	19.5	2677.7603	-0.00059
	20.5	2622.8889	0.00018
	22.5	2511.7348	0.00143
	23.5	2455.5310	-0.00207
	24.5	2398.9714	0.00116
	25.5	2342.0774	-0.00476
	29.5	2111.9576	0.00074
P _{2ee} (J)	4.5	3377.8860	-0.00129
	6.5	3287.4784	0.00028
	7.5	3241.0143	-0.00210
	9.5	3145.4907	-0.00138
	10.5	3096.4481	-0.00010
	11.5	3046.5797	-0.00143
	12.5	2995.9249	0.00173
	14.5	2892.3845	0.00105
	15.5	2839.5826	0.00082
	16.5	2786.1488	0.00120
	18.5	2677.5486	-0.00113
19.5	2622.4686	-0.00085	

	20.5	2566.9216	-0.00127
	22.5	2454.5876	-0.00144
	23.5	2397.8730	-0.00492
	24.5	2340.8525	0.00005
	27.5	2168.2319	0.00753
	28.5	2110.2578	-0.00874
P _{1ff} (J)	4.5	3407.6240	0.01258
	5.5	3366.5467	-0.00130
	6.5	3323.9724	-0.00471
	7.5	3280.0360	0.00032
	9.5	3188.4828	0.00318
	10.5	3141.0436	0.00111
	11.5	3092.6000	0.00113
	12.5	3043.2152	0.00097
	14.5	2941.8607	-0.00013
	15.5	2890.0042	0.00076
	17.5	2784.1893	0.00115
	18.5	2730.3295	0.00051
	19.5	2675.8994	0.00079
	20.5	2620.9397	-0.00275
	21.5	2565.5072	0.00282
	23.5	2453.3496	-0.00065
	24.5	2396.7126	-0.00138
	25.5	2339.7540	-0.00121
	26.5	2282.5107	0.00128
	27.5	2225.0093	-0.00080
	30.5	2051.2952	0.00095
P _{2ff} (J)	4.5	3378.0764	-0.00106
	6.5	3287.8791	0.00230
	9.5	3146.1845	0.00098
	10.5	3097.2331	-0.00069

11.5	3047.4577	-0.00182
12.5	2996.8950	0.00194
13.5	2945.5710	0.00013
14.5	2893.5317	-0.00038
15.5	2840.8189	0.00149
16.5	2787.4688	0.00036
17.5	2733.5276	0.00053
18.5	2679.0345	-0.00056
19.5	2624.0338	0.00005
23.5	2399.7314	-0.00223
25.5	2285.5336	0.00093
26.5	2228.0456	0.00484

1-1	J	Obs (cm-1)	Obs-Calc
R _{2ff} (J)	9.5	380.4589	0.00137
	10.5	413.4150	-0.00043
	11.5	445.8170	0.00065
	12.5	477.6328	-0.00133
	13.5	508.8397	-0.00078
	14.5	539.4059	-0.00012
	17.5	626.9606	0.00012
	18.5	654.6677	0.00063
	19.5	681.5875	0.00009
	20.5	707.6942	-0.00030
	21.5	732.9620	-0.00031
	22.5	757.3649	-0.00094
	23.5	780.8805	-0.00062
	24.5	803.4845	-0.00071
	25.5	825.1555	-0.00069
	27.5	865.6149	-0.00099

	29.5	902.1024	-0.00077
	30.5	918.8108	-0.00060
	31.5	934.4726	-0.00021
	32.5	949.0699	-0.00052
	33.5	962.5870	-0.00042
	34.5	975.0066	-0.00030
	35.5	986.3111	-0.00046
	36.5	996.4830	-0.00043
	37.5	1005.5027	-0.00069
	38.5	1013.3517	0.00091
	39.5	1020.0130	0.01019
	40.5	1025.4342	0.00035
	41.5	1029.6138	-0.00087
R _{2ee} (J)	10.5	414.0929	0.00032
	12.5	478.4138	0.00127
	13.5	509.6626	-0.00042
	14.5	540.2684	0.00013
	15.5	570.1988	0.00039
	17.5	627.9155	0.00102
	18.5	655.6429	0.00065
	19.5	682.5798	0.00085
	20.5	708.6978	0.00026
	21.5	733.9724	0.00044
	22.5	758.3776	0.00041
	23.5	781.8897	0.00046
	24.5	804.4853	0.00011
	25.5	826.1430	-0.00012
	26.5	846.8424	0.00029
	27.5	866.5621	-0.00005
	28.5	885.2841	0.00002
	29.5	902.9896	0.00009

	30.5	919.6615	0.00083
	31.5	935.2799	-0.00040
	32.5	949.8314	-0.00006
	33.5	963.2979	0.00055
	34.5	975.6603	-0.00076
	35.5	986.9053	0.00001
	36.5	997.0112	-0.00081
	37.5	1005.9626	0.00054
	38.5	1013.7344	-0.00030
	39.5	1020.3074	0.00040
	40.5	1025.6533	0.00012
R _{1ff} (J)	12.5	448.6947	-0.00232
	15.5	541.7078	-0.00060
	16.5	571.4700	-0.00473
	18.5	628.9321	-0.00029
	19.5	656.5538	-0.00342
	20.5	683.4048	0.00037
	21.5	709.4451	0.00040
	22.5	734.6503	0.00015
	23.5	758.9943	0.00003
	24.5	782.4518	-0.00010
	25.5	804.9989	-0.00019
	26.5	826.6127	-0.00042
	27.5	847.2722	-0.00018
	28.5	866.9560	-0.00029
	29.5	885.6448	-0.00039
	30.5	903.3198	-0.00047
	31.5	919.9632	-0.00020
	32.5	935.5571	0.00007
	33.5	950.0840	0.00007
	34.5	963.5276	0.00054

	35.5	975.8689	-0.00042
	36.5	987.0931	-0.00011
	37.5	997.1805	-0.00003
	38.5	1006.1125	0.00052
	39.5	1013.8661	-0.00056
	40.5	1020.4222	0.00068
	41.5	1025.7501	-0.00055
R _{1ee} (J)	11.5	415.7082	0.00042
	12.5	447.7646	-0.00151
	13.5	479.3051	-0.00033
	15.5	540.6572	-0.00139
	18.5	627.8060	0.00013
	19.5	655.4150	0.00005
	20.5	682.2518	0.00038
	21.5	708.2863	0.00028
	22.5	733.4913	0.00039
	23.5	757.8391	-0.00050
	24.5	781.3069	-0.00002
	25.5	803.8689	-0.00006
	26.5	825.5030	0.00004
	28.5	865.9011	-0.00025
	29.5	884.6256	0.00014
	30.5	902.3408	0.00003
	31.5	919.0290	-0.00016
	32.5	934.6734	0.00041
	33.5	949.2555	0.00044
	34.5	962.7585	0.00019
	35.5	975.1656	-0.00004
	36.5	986.4590	-0.00058
	37.5	996.6216	-0.00036
	38.5	1005.6341	0.00056

	39.5	1013.4731	-0.00041
	40.5	1020.1189	-0.00002
Q _{2fe} (J)	0.5	0.1507	-0.00009
	1.5	0.2503	-0.00001
	2.5	0.2658	-0.00003
Q _{1fe} (J)	1.5	0.0513	0.00000
	2.5	0.1867	0.00002
	3.5	0.4179	0.00003
	4.5	0.7438	-0.00008
	5.5	1.1589	-0.00001
	6.5	1.6564	0.00006
	7.5	2.2301	0.00002
R _{1ee} (J)	1.5	80.7329	-0.00002
	2.5	113.9044	-0.00006
R _{1ff} (J)	1.5	80.8683	0.00000
	2.5	114.1356	-0.00004
R _{2ee} (J)	0.5	58.6861	-0.00010
	1.5	97.1690	-0.00002
	2.5	134.8749	0.00001
R _{2ff} (J)	1.5	97.1845	-0.00003
	2.5	134.7946	-0.00009
P _{12ff} (J)	2.5	104.9016	0.00016

2-0	J	Obs (cm-1)	Obs-Calc
R _{1ff} (J)	1.5	7049.2349	0.00029
	2.5	7075.2315	0.00043
	3.5	7099.0139	0.00139
	4.5	7120.3333	0.00008
	5.5	7138.9909	0.00056

	6.5	7154.8316	-0.00009
	7.5	7167.7454	-0.00040
$R_{2ff}(J)$	0.5	7028.8318	0.00092
	1.5	7060.6725	0.00190
	2.5	7088.6337	0.00101
	3.5	7112.8700	0.00038
	4.5	7133.5534	0.00070
	5.5	7150.8142	-0.00037
	6.5	7164.7393	-0.00223
	7.5	7175.3856	0.00208
$P_{1ee}(J)$	2.5	6887.6230	0.00031
	3.5	6847.1863	-0.00003
	4.5	6803.6472	-0.00003
	5.5	6757.1028	-0.00001
	6.5	6707.6822	0.00020
	7.5	6655.5101	-0.00011
	8.5	6600.6987	-0.00039
	9.5	6543.3464	-0.00005
	10.5	6483.5383	-0.00079
	11.5	6421.3581	0.00237
$P_{2ee}(J)$	1.5	6911.3337	0.00090
	2.5	6866.2691	-0.00006
	3.5	6818.8863	-0.00010
	4.5	6769.2918	-0.00040
	5.5	6717.4912	-0.00009
	6.5	6663.4590	-0.00029
	7.5	6607.1775	-0.00009
	8.5	6548.6426	-0.00066
	9.5	6487.8693	0.00044
	10.5	6424.8831	0.00378

Q _{2ef} (J)	0.5	6972.3770	0.00156
	1.5	6967.2880	-0.00011
	2.5	6959.1217	0.00080
	3.5	6948.0271	-0.00107
Q _{1fe} (J)	1.5	6971.3936	0.00041
	2.5	6965.5674	0.00054
	3.5	6957.2248	0.00054
	4.5	6946.2719	0.00015
	5.5	6932.6518	-0.00080
R _{1ee} (J)	6.5	6916.3410	0.00299
	1.5	7049.1184	0.00070
	2.5	7075.0449	0.00064
	3.5	7098.7676	0.00060
	4.5	7120.0437	0.00044
	5.5	7138.6700	0.00014
	6.5	7154.4939	0.00045
	7.5	7167.3990	-0.00262
R _{2ee} (J)	8.5	7177.3047	-0.00659
	9.5	7184.1570	-0.00258
	0.5	7028.7490	0.00021
	1.5	7060.6725	-0.00002
	2.5	7088.7194	0.00064
	3.5	7113.0295	0.00085
	4.5	7133.7707	0.00026
	5.5	7151.0766	-0.00052
	6.5	7165.0360	-0.00016
P _{1ff} (J)	7.5	7175.7014	0.00292
	2.5	6887.4688	0.00018
	3.5	6846.9106	0.00000
	4.5	6803.2407	0.00000

	5.5	6756.5629	0.00008
	6.5	6707.0076	-0.00023
	7.5	6654.7012	-0.00005
	8.5	6599.7539	-0.00039
	9.5	6542.2629	-0.00148
	10.5	6482.3192	0.00116
	11.5	6419.9987	0.00483
$P_{2ff}(J)$	1.5	6911.2173	0.00113
	2.5	6866.2374	0.00078
	3.5	6818.9622	0.00114
	4.5	6769.4831	-0.00007
	5.5	6717.8011	-0.00006
	6.5	6663.8885	-0.00022
	7.5	6607.7269	-0.00023
	8.5	6549.3140	0.00013
	10.5	6425.7985	0.00202
	11.5	6360.7579	0.00621
$Q_{2fe}(J)$	0.5	6972.6778	0.00095
	1.5	6967.7871	-0.00113
	2.5	6959.6532	0.00155
	3.5	6948.4046	0.00641
$Q_{1ef}(J)$	1.5	6971.2909	0.00047
	2.5	6965.1937	0.00057
	3.5	6956.3885	0.00050
	4.5	6944.7833	-0.00013
	5.5	6930.3339	-0.00043
	6.5	6913.0241	-0.00099
$R_{1ff}(J)$	1.5	7049.2349	0.00029
	2.5	7075.2315	0.00043
	3.5	7099.0139	0.00139

	4.5	7120.3333	0.00008
	5.5	7138.9909	0.00056
	6.5	7154.8316	-0.00009
	7.5	7167.7454	-0.00040
	8.5	7177.6507	0.00044
	9.5	7184.4799	-0.00269
	10.5	7188.1943	0.00024
	11.5	7188.7309	-0.01473
	12.5	7186.1052	-0.00017
	13.5	7180.2473	0.00050
	14.5	7171.2009	0.05320
	15.5	7158.8017	0.01232
	16.5	7143.2309	0.07482
$R_{2ff}(J)$	0.5	7028.8165	-0.01438
	1.5	7060.6721	0.00150
	2.5	7088.6351	0.00241
	3.5	7112.8750	0.00538
	4.5	7133.5543	0.00160
	5.5	7150.8086	-0.00597
	6.5	7164.7551	0.01357
	7.5	7175.3842	0.00068
	8.5	7182.7593	-0.00658
	9.5	7186.8921	-0.00635
	10.5	7187.7743	-0.00750
	11.5	7185.4071	-0.00405
	12.5	7179.7582	-0.02075
	13.5	7170.8645	-0.01191
	14.5	7158.6884	-0.00612
	15.5	7143.2309	0.00633
$P_{1ee}(J)$	2.5	6887.6215	-0.00119
	3.5	6847.1850	-0.00133

	4.5	6803.6475	0.00027
	5.5	6757.1035	0.00069
	6.5	6707.6815	-0.00050
	7.5	6655.5100	-0.00021
	8.5	6600.6977	-0.00139
	9.5	6543.3460	-0.00045
	10.5	6483.5390	-0.00009
	11.5	6421.3554	-0.00033
	12.5	6356.8691	-0.00021
	13.5	6290.1566	0.00795
	14.5	6221.2594	-0.00019
	15.5	6150.2656	-0.00003
	16.5	6077.2283	-0.00015
	17.5	6002.2082	0.00007
	18.5	5925.2639	0.00064
	19.5	5846.4498	-0.00114
	20.5	5765.8238	-0.00298
	21.5	5683.4409	-0.00386
	22.5	5599.3567	-0.00038
	23.5	5513.6119	-0.00211
	24.5	5426.2626	-0.00102
P _{2ee} (J)	1.5	6911.3124	-0.02040
	2.5	6866.2505	-0.01866
	3.5	6818.8895	0.00310
	4.5	6769.2905	-0.00170
	5.5	6717.4899	-0.00139
	6.5	6663.4585	-0.00079
	7.5	6607.1772	-0.00039
	8.5	6548.6428	-0.00046
	9.5	6487.8690	0.00014
	10.5	6424.8785	-0.00082

	11.5	6359.7088	0.00010
	12.5	6292.3974	-0.00015
	13.5	6222.9913	0.00035
	14.5	6151.5372	0.00019
	15.5	6078.0870	0.00114
	16.5	6002.6897	0.00091
	17.5	5925.3985	0.00083
	18.5	5846.2665	0.00214
	19.5	5765.3412	0.00082
	20.5	5682.6760	-0.00042
	21.5	5598.3229	0.00081
	22.5	5512.3302	0.00469
	23.5	5424.6902	-0.04281
Q _{2ef} (J)	0.5	6972.3910	0.01556
Q _{1fe} (J)	1.5	6971.3932	0.00001
R _{1ee} (J)	1.5	7049.1254	0.00770
	2.5	7075.0416	-0.00266
	3.5	7098.7702	0.00320
	4.5	7120.0473	0.00404
	5.5	7138.6679	-0.00196
	6.5	7154.4951	0.00165
	7.5	7167.3955	-0.00612
	8.5	7177.3112	-0.00009
	9.5	7184.1620	0.00242
	10.5	7187.8997	0.00215
	11.5	7188.4827	-0.00336
	12.5	7185.8999	0.00676
	13.5	7180.1045	0.01221
	14.5	7171.2009	0.13960
	15.5	7158.8017	0.02021

	16.5	7143.4055	0.16838
R _{2ee} (J)	0.5	7028.7619	0.01311
	1.5	7060.6721	-0.00042
	2.5	7088.7196	0.00084
	3.5	7113.0286	-0.00005
	4.5	7133.7623	-0.00814
	5.5	7151.0802	0.00308
	6.5	7165.0230	-0.01316
	7.5	7175.6914	-0.00708
	8.5	7183.0987	0.00860
	9.5	7187.2153	-0.00598
	10.5	7188.1244	0.03159
	11.5	7185.6860	-0.01405
	12.5	7180.0369	0.00137
	13.5	7171.1205	0.03001
	14.5	7158.8017	-0.05423
	15.5	7143.4055	0.08232
P _{1ff} (J)	2.5	6887.4666	-0.00202
	3.5	6846.9068	-0.00380
	4.5	6803.2398	-0.00090
	5.5	6756.5619	-0.00092
	6.5	6707.0079	0.00007
	7.5	6654.7023	0.00105
	8.5	6599.7536	-0.00069
	9.5	6542.2636	-0.00078
	10.5	6482.3185	0.00046
	11.5	6419.9939	0.00003
	12.5	6355.3646	-0.00023
	13.5	6288.5000	0.00018
	14.5	6219.4649	0.00008
	15.5	6148.3243	0.00076

	16.5	6075.1383	0.00047
	17.5	5999.9694	0.00141
	18.5	5922.8728	0.00001
	19.5	5843.9099	0.00034
	20.5	5763.1369	0.00284
	21.5	5680.5999	-0.00052
	22.5	5596.3548	-0.00617
	23.5	5510.4668	0.00072
	24.5	5422.9558	-0.00809
P _{2ff} (J)	1.5	6911.2199	0.00373
	2.5	6866.2505	0.01388
	3.5	6818.9569	-0.00416
	4.5	6769.4824	-0.00077
	5.5	6717.8009	-0.00026
	6.5	6663.8891	0.00038
	7.5	6607.7256	-0.00153
	8.5	6549.3135	-0.00037
	9.5	6488.6593	-0.00263
	10.5	6425.7958	-0.00068
	11.5	6360.7511	-0.00059
	12.5	6293.5680	-0.00011
	13.5	6224.2897	-0.00102
	14.5	6152.9665	-0.00098
	15.5	6079.6478	-0.00054
	16.5	6004.3837	-0.00069
	17.5	5927.2261	-0.00117
	18.5	5848.2274	-0.00125
	19.5	5767.4379	-0.00193
	20.5	5684.9094	-0.00194
	21.5	5600.7044	0.01180
	22.5	5514.8415	0.00990

	23.5	5427.3940	0.01942
Q _{2fe} (J)	0.5	6972.7495	0.07265
Q _{1ef} (J)	1.5	6971.3035	0.01307
	2.5	6965.1937	0.00057

2-1	J	Obs (cm-1)	Obs-Calc
R _{1ff} (J)	1.5	3480.7655	-0.00228
	2.5	3509.7643	-0.00062
	3.5	3537.8653	-0.00045
	4.5	3564.8691	-0.00176
	5.5	3590.6075	0.00529
	6.5	3614.9225	0.00457
	7.5	3637.7172	0.00872
R _{2ff} (J)	0.5	3459.7734	-0.00117
	1.5	3494.1271	-0.00430
	2.5	3526.1999	-0.00050
	3.5	3556.0609	0.00016
	4.5	3583.8330	0.00200
	5.5	3609.6142	0.00337
P _{1ee} (J)	2.5	3322.1410	-0.00099
	3.5	3286.0088	-0.00041
	4.5	3248.1338	-0.00038
	5.5	3208.6391	-0.00075
	6.5	3167.6654	-0.00049
	7.5	3125.3399	0.00011
	8.5	3081.7702	-0.00019
	9.5	3037.0495	-0.00036
	10.5	2991.2571	-0.00051
	11.5	2944.4635	-0.00026
	12.5	2896.7314	-0.00036

	13.5	2848.1191	-0.00110
	14.5	2798.6856	0.00154
	15.5	2748.4748	-0.00066
	16.5	2697.5432	-0.00104
	17.5	2645.9364	-0.00182
$P_{2ee}(J)$	1.5	3344.7833	-0.00043
	2.5	3303.8256	-0.00460
	3.5	3262.0785	-0.00105
	4.5	3219.5847	-0.00107
	5.5	3176.3193	-0.00054
	6.5	3132.2366	-0.00009
	7.5	3087.3032	-0.00077
	8.5	3041.5074	-0.00085
	9.5	2994.8523	-0.00050
	10.5	2947.3525	-0.00097
	11.5	2899.0336	-0.00139
	12.5	2849.9285	0.00039
	13.5	2800.0672	-0.00035
	14.5	2749.4903	-0.00024
	15.5	2698.2323	-0.00350
	16.5	2646.3457	0.00292
	17.5	2593.8583	0.00719
$Q_{2ef}(J)$	0.5	3403.3190	-0.00014
	1.5	3400.7478	-0.00110
	2.5	3396.6831	-0.00551
	3.5	3391.2234	0.00411
	4.5	3384.3909	-0.00104
$Q_{1fe}(J)$	1.5	3402.9216	-0.00048
	2.5	3400.0853	-0.00086
	3.5	3396.0470	-0.00015

	4.5	3390.7582	-0.00050
	5.5	3384.1880	-0.00163
	6.5	3376.3205	-0.00140
R _{1ee} (J)	1.5	3480.6453	-0.00129
	2.5	3509.5623	-0.00126
	3.5	3537.5892	-0.00068
	4.5	3564.5287	-0.00151
	5.5	3590.2116	0.00471
	6.5	3614.4831	0.00576
	7.5	3637.2391	0.00790
R _{2ee} (J)	0.5	3459.6851	-0.00031
	1.5	3494.1271	0.00364
	2.5	3526.2821	0.00230
	3.5	3556.2209	-0.00091
	4.5	3584.0627	-0.00131
	5.5	3609.9073	0.00163
P _{1ff} (J)	2.5	3322.0022	-0.00028
	3.5	3285.7628	-0.00104
	4.5	3247.7776	-0.00075
	5.5	3208.1743	-0.00038
	6.5	3167.0936	-0.00048
	7.5	3124.6624	-0.00153
	8.5	3080.9922	-0.00038
	9.5	3036.1712	-0.00056
	10.5	2990.2801	-0.00047
	11.5	2943.3883	-0.00070
	12.5	2895.5604	-0.00007
	13.5	2846.8527	-0.00091
	14.5	2797.3251	0.00160
	15.5	2747.0184	-0.00401

	16.5	2696.0014	0.00112
	17.5	2644.3058	0.00069
	1.5	3344.6770	0.00004
	2.5	3303.8052	0.00088
	3.5	3262.1543	0.00212
	4.5	3219.7616	0.00013
	5.5	3176.5969	-0.00052
	6.5	3132.6126	-0.00084
	7.5	3087.7769	-0.00035
	8.5	3042.0754	-0.00052
	9.5	2995.5127	-0.00047
	10.5	2948.1046	-0.00056
	11.5	2899.8762	-0.00054
	12.5	2850.8583	-0.00040
	13.5	2801.0859	0.00018
	14.5	2750.5940	-0.00092
	15.5	2699.4267	0.00178
	16.5	2647.6217	0.00670
	18.5	2542.2323	-0.00081
	19.5	2488.7388	-0.00020
$Q_{2fe}(J)$	0.5	3403.6132	-0.00027
	1.5	3401.2389	-0.00027
	2.5	3397.2156	0.00291
	3.5	3391.5846	-0.00674
	4.5	3384.4300	0.00277
$Q_{1ef}(J)$	1.5	3402.8231	-0.00051
	2.5	3399.7266	-0.00039
	3.5	3395.2409	-0.00034
	4.5	3389.3208	-0.00028
	5.5	3381.9455	-0.00070
	6.5	3373.1161	0.00476

	4.5	3248.1307	-0.00348
	5.5	3208.6351	-0.00475
	6.5	3167.6643	-0.00159
	7.5	3125.3368	-0.00299
	8.5	3081.7720	0.00161
	9.5	3037.0512	0.00134
	10.5	2991.2600	0.00239
	12.5	2896.7316	-0.00016
	13.5	2848.1185	-0.00170
	14.5	2798.6831	-0.00096
	15.5	2748.4702	-0.00526
	16.5	2697.5449	0.00066
	17.5	2645.9397	0.00148
	18.5	2593.7037	0.00027
	19.5	2540.8857	0.00152
	20.5	2487.5154	-0.00771
	21.5	2433.6627	0.00150
	22.5	2379.3397	0.00201
	23.5	2324.5878	-0.00222
	24.5	2269.4543	0.00052
	25.5	2213.9441	-0.01844
	27.5	2101.9723	-0.06642
	28.5	2045.6200	-0.04213
P _{2ee} (J)	4.5	3219.5859	0.00013
	7.5	3087.3005	-0.00347
	8.5	3041.5128	0.00455
	9.5	2994.8540	0.00120
	10.5	2947.3524	-0.00107
	11.5	2899.0345	-0.00049
	12.5	2849.9303	0.00219
	13.5	2800.0638	-0.00375

	14.5	2749.4879	-0.00264
	15.5	2698.2348	-0.00100
	16.5	2646.3406	-0.00218
	17.5	2593.8511	-0.00001
	18.5	2540.7994	-0.00074
	20.5	2433.1735	-0.00110
	21.5	2378.6729	-0.00182
P _{1ff} (J)	5.5	3208.1747	0.00002
	6.5	3167.0930	-0.00108
	7.5	3124.6645	0.00057
	8.5	3080.9929	0.00032
	9.5	3036.1734	0.00164
	10.5	2990.2802	-0.00037
	11.5	2943.3894	0.00040
	12.5	2895.5594	-0.00107
	13.5	2846.8532	-0.00041
	14.5	2797.3240	0.00050
	15.5	2747.0239	0.00149
	17.5	2644.3056	0.00049
	18.5	2591.9838	0.00074
	19.5	2539.0763	-0.00226
	20.5	2485.6342	-0.00019
	21.5	2431.6943	0.00269
	22.5	2377.2862	-0.00333
P _{2ff} (J)	5.5	3176.6039	0.00648
	6.5	3132.6126	-0.00084
	7.5	3087.7765	-0.00075
	8.5	3042.0760	0.00008
	9.5	2995.5144	0.00123
	10.5	2948.1065	0.00134
	12.5	2850.8590	0.00030

13.5	2801.0860	0.00028
14.5	2750.5962	0.00128
15.5	2699.4261	0.00118
16.5	2647.6142	-0.00080
19.5	2488.7406	0.00160
20.5	2434.7569	-0.00323
23.5	2270.2757	0.00059
24.5	2214.7062	-0.00385

2-2

R_{2ff}(J)

J	Obs (cm-1)	Obs-Calc
9.5	365.1864	-0.00061
11.5	427.8600	-0.00114
13.5	488.2344	-0.00161
17.5	601.1688	-0.00417
18.5	627.6085	-0.00004
19.5	653.2682	0.00065
20.5	678.1223	-0.00037
21.5	702.1469	-0.00050
22.5	725.3157	-0.00036
23.5	747.6035	-0.00035
24.5	768.9869	0.00014
25.5	789.4418	0.00025
26.5	808.9458	0.00009
27.5	827.4778	0.00053
28.5	845.0148	0.00003
29.5	861.5384	0.00135
30.5	877.0230	-0.00006
31.5	891.4519	0.00026
32.5	904.7981	-0.00313
33.5	917.0455	-0.00404

	34.5	928.1718	-0.00132
	35.5	938.1424	-0.00450
	36.5	946.9451	0.00149
	37.5	954.5353	0.00225
	38.5	960.8804	-0.00092
	39.5	965.9504	0.00058
R _{2ee} (J)	9.5	365.7726	-0.00150
	11.5	428.5537	0.00173
	13.5	489.0126	-0.00093
	17.5	602.0657	-0.00508
	18.5	628.5258	0.00092
	19.5	654.1970	-0.00066
	20.5	679.0623	0.00055
	21.5	703.0909	0.00032
	22.5	726.2587	0.00023
	23.5	748.5411	0.00053
	24.5	769.9132	0.00032
	25.5	790.3531	0.00095
	26.5	809.8355	-0.00035
	27.5	828.3422	0.00018
	29.5	862.3367	0.00050
	30.5	877.7825	0.00052
	31.5	892.1653	-0.00003
	32.5	905.4640	-0.00065
	33.5	917.6570	-0.00057
	34.5	928.7208	0.00023
	35.5	938.6260	-0.00245
	36.5	947.3552	0.00143
	37.5	954.8672	0.00105
	38.5	961.1306	-0.00085
	39.5	966.1101	-0.00068

R _{1ff} (J)	14.5	490.6871	0.00082
	18.5	603.1110	-0.00205
	19.5	629.4600	-0.00165
	21.5	679.8264	0.00011
	22.5	703.7836	-0.00064
	23.5	726.8895	0.00024
	24.5	749.1152	-0.00009
	25.5	770.4372	-0.00010
	26.5	790.8309	-0.00032
	27.5	810.2741	0.00032
	28.5	828.7423	-0.00016
	29.5	846.2152	-0.00006
	30.5	862.6700	-0.00058
	31.5	878.0865	-0.00047
	32.5	892.4428	-0.00011
	33.5	905.7159	-0.00061
	34.5	917.8851	-0.00005
	35.5	928.9255	0.00046
	36.5	938.8108	0.00002
	37.5	947.5149	0.00016
38.5	955.0073	0.00097	
39.5	961.2523	0.00107	
40.5	966.2091	-0.00126	
R _{1ee} (J)	12.5	429.8726	0.00332
	15.5	518.7914	0.00289
	16.5	547.2199	-0.00026
	18.5	602.0535	-0.00039
	20.5	653.9600	-0.00251
	19.5	628.3889	-0.00061
	21.5	678.7435	0.00025
22.5	702.7039	0.00054	

	23.5	725.8159	0.00021
	24.5	748.0538	-0.00040
	25.5	769.3933	-0.00059
	26.5	789.8140	0.00331
	27.5	809.2829	0.00152
	28.5	827.7837	0.00027
	29.5	845.2957	0.00082
	30.5	861.7938	-0.00034
	31.5	877.2608	0.00099
	32.5	891.6703	-0.00013
	33.5	905.0032	-0.00097
	34.5	917.2385	0.00001
	35.5	928.3490	-0.00073
	36.5	938.3114	-0.00125
	37.5	947.0998	0.00004
	38.5	954.6819	0.00118
	39.5	961.0210	-0.00046
	40.5	966.0854	0.00221
Q _{2fe} (J)	0.5	0.1436	0.00006
	1.5	0.2399	-0.00005
Q _{1fe} (J)	1.5	0.0472	0.00003
	2.5	0.1725	0.00000
	3.5	0.3880	-0.00004
	4.5	0.6937	-0.00004
	5.5	1.0845	-0.00003
	6.5	1.5541	-0.00012
R _{1ee} (J)	1.5	77.7717	0.00002
	2.5	109.6499	0.00000
	3.5	141.9307	-0.00008
R _{1ff} (J)	1.5	77.8970	-0.00001

	2.5	109.8654	-0.00004
	3.5	142.2364	-0.00007
R _{2ee} (J)	1.5	93.1241	-0.00014
	2.5	129.3255	0.00014
R _{2ff} (J)	1.5	93.1431	0.00056
	2.5	129.2534	-0.00014
P _{21ee} (J)	1.5	127.4795	-0.00005
P _{21ff} (J)	1.5	127.5759	-0.00003

3-0 J Obs (cm-1) Obs-Calc

R _{1ff} (J)	1.5	10285.4530	-0.02340
	2.5	10307.2063	-0.02874
	3.5	10325.4602	0.01024
	4.5	10339.8591	0.00972
	5.5	10350.2074	-0.01042
	6.5	10356.3981	-0.00062
	7.5	10358.2754	-0.00573
	8.5	10355.7476	-0.03836
	9.5	10348.8333	-0.02240
	10.5	10337.4597	0.01205
	11.5	10321.5387	0.00924
	12.5	10301.0783	0.00193
	13.5	10276.0406	-0.02872
R _{2ff} (J)	0.5	10266.1283	-0.04729
	1.5	10294.0249	0.00137
	2.5	10316.5695	0.06299
	3.5	10333.8426	0.01628
	4.5	10346.1984	0.01180
	5.5	10353.7460	0.00583
	6.5	10356.5943	0.00780

	7.5	10354.8123	0.02733
	8.5	10348.3804	0.01176
	9.5	10337.3388	-0.01556
	10.5	10321.7100	-0.03950
	11.5	10301.5959	0.03972
P _{1ee} (J)	2.5	10126.8184	-0.00358
	3.5	10083.4466	0.00458
	4.5	10035.6848	0.00410
	5.5	9983.5962	0.00601
	6.5	9927.2701	-0.00252
	7.5	9866.8477	0.00740
	8.5	9802.4033	0.00302
	9.5	9734.0503	-0.00048
	10.5	9661.8817	-0.00014
	11.5	9585.9774	0.00028
	12.5	9506.4171	0.00152
	13.5	9423.2733	0.00059
	14.5	9336.6240	0.00253
	15.5	9246.5351	0.00229
	16.5	9153.0795	0.00350
	17.5	9056.3204	0.00166
	18.5	8956.3110	-0.01621
	19.5	8853.1794	0.01348
	20.5	8746.7839	-0.11365
	21.5	8637.5842	0.00151
P _{2ee} (J)	1.5	10151.1073	-0.01736
	2.5	10103.5940	-0.03078
	3.5	10052.2848	0.03697
	4.5	9997.1693	0.00286
	5.5	9938.4400	0.00448
	6.5	9876.0678	0.00403

	7.5	9810.0529	-0.00034
	8.5	9740.4164	0.00198
	9.5	9667.1709	0.00146
	10.5	9590.3504	-0.00060
	11.5	9510.0004	0.00018
	12.5	9426.1656	0.00109
	13.5	9338.8974	0.00158
	14.5	9248.2530	0.00368
	15.5	9154.2868	0.00455
	16.5	9057.0606	0.00748
	17.5	8956.6336	0.01267
	18.5	8853.0349	-0.00968
	19.5	8746.2908	-0.09152
	20.5	8636.6401	-0.05105
	21.5	8523.9806	-0.04578
Q _{2ef} (J)	0.5	10212.1774	0.01010
	1.5	10204.5919	-0.05183
Q _{1fe} (J)	1.5	10210.6119	0.02344
	2.5	10201.1976	-0.61105
R _{1ee} (J)	1.5	10285.3522	-0.02119
	2.5	10307.0878	0.01007
	3.5	10325.2625	0.00813
	4.5	10339.6334	-0.00048
	5.5	10349.9966	-0.00334
	6.5	10356.1912	-0.00345
	7.5	10358.1102	0.00425
	8.5	10355.6530	-0.00103
	9.5	10348.8333	0.05233
	10.5	10337.4597	0.01588
	11.5	10321.5710	-0.03912

	12.5	10301.2157	-0.03933
	13.5	10276.3682	0.00872
R _{2ee} (J)	0.5	10266.1283	0.02389
	1.5	10294.0249	-0.00905
	2.5	10316.5695	-0.02350
	3.5	10333.9861	0.01322
	4.5	10346.3628	-0.01211
	5.5	10353.9517	-0.00108
	6.5	10356.8031	-0.00423
	7.5	10354.9988	-0.00027
	8.5	10348.5459	-0.01589
	9.5	10337.4597	-0.05310
	10.5	10321.8636	0.00384
	11.5	10301.5959	-0.00903
	12.5	10276.7853	0.03746
	13.5	10247.2868	-0.00008
P _{1ff} (J)	2.5	10126.6655	0.00161
	3.5	10083.1552	0.00281
	4.5	10035.2483	0.00362
	5.5	9983.1103	0.11005
	6.5	9926.5280	0.00401
	7.5	9865.9273	-0.00142
	8.5	9801.3250	0.00368
	9.5	9732.8001	0.00038
	10.5	9660.4550	0.00126
	11.5	9584.3687	0.00172
	12.5	9504.6233	0.00489
	13.5	9421.2850	0.00135
	14.5	9334.4349	-0.00092
	15.5	9244.1462	0.00014
	16.5	9150.4837	-0.00016

	17.5	9053.5180	0.00082
	18.5	8953.3072	-0.00518
	19.5	8849.9339	-0.00028
	20.5	8743.4350	-0.01043
	21.5	8633.8945	-0.01237
P _{2ff} (J)	1.5	10151.1073	0.10673
	2.5	10103.5940	0.01267
	3.5	10052.2848	-0.02919
	4.5	9997.3590	0.00201
	5.5	9938.7610	0.00314
	6.5	9876.5253	0.00269
	7.5	9810.6520	-0.00073
	8.5	9741.1583	-0.00055
	9.5	9668.0687	0.00532
	10.5	9591.3993	0.00006
	11.5	9511.2092	0.00160
	12.5	9427.5369	0.00108
	13.5	9340.4361	0.00035
	14.5	9249.9608	-0.00154
	15.5	9156.1733	0.00065
	16.5	9059.1318	0.00688
	17.5	8958.8802	0.00227
	18.5	8855.4987	0.00837
	19.5	8749.0253	0.00515
	20.5	8639.5602	0.03598
Q _{2fe} (J)	1.5	10205.1892	0.05626
Q _{1ef} (J)	1.5	10210.5239	0.03418
	2.5	10201.4463	-0.00252

3-1 J Obs (cm-1) Obs-Calc

R _{1ff} (J)	1.5	6717.0093	-0.00027
	2.5	6741.7689	0.00000
	3.5	6764.3041	0.00090
	4.5	6784.3871	0.00008
	5.5	6801.8298	0.00012
	6.5	6816.4850	0.00004
	7.5	6828.2448	0.00098
	8.5	6837.0248	0.00055
	9.5	6842.7639	0.00082
R _{2ff} (J)	0.5	6697.1203	0.00101
	1.5	6727.4799	-0.00442
	2.5	6754.0747	0.00049
	3.5	6777.0178	0.00036
	4.5	6796.4652	0.00031
	5.5	6812.5367	0.00027
	6.5	6825.3112	-0.00002
	7.5	6834.8380	0.00290
	8.5	6841.1273	-0.00339
9.5	6844.2021	-0.00350	
P _{1ee} (J)	2.5	6561.3411	-0.00018
	3.5	6522.2648	-0.00010
	4.5	6480.1675	-0.00016
	5.5	6435.1274	0.00017
	6.5	6387.2567	0.00020
	7.5	6336.6701	0.00023
	8.5	6283.4722	0.00062
	9.5	6227.7545	0.00031
	10.5	6169.6009	0.00054
11.5	6109.0849	-0.00026	
12.5	6046.2786	0.00057	

	13.5	5981.2458	0.00154
	14.5	5914.0469	0.00095
	15.5	5844.7416	-0.00105
P _{2ee} (J)	1.5	6584.5760	0.00040
	2.5	6541.1883	0.00248
	3.5	6495.4421	0.00111
	4.5	6447.4602	0.00019
	6.5	6344.8413	0.00014
	7.5	6290.1793	-0.00033
	8.5	6233.2793	-0.00012
	9.5	6174.1531	-0.00028
	10.5	6112.8263	0.00115
	11.5	6049.3255	-0.00101
	12.5	5983.6958	0.00074
Q _{2ef} (J)	0.5	6643.1116	0.00060
	1.5	6638.1048	0.00027
	2.5	6630.0119	-0.03814
	3.5	6619.0943	0.00078
Q _{1fe} (J)	1.5	6642.1173	-0.00005
	2.5	6636.3279	-0.00005
	3.5	6628.0511	-0.00003
	4.5	6617.1948	-0.00135
	5.5	6603.7057	-0.00009
	6.5	6587.5493	-0.00007
	7.5	6568.7146	0.00119
R _{1ee} (J)	1.5	6716.9020	-0.00028
	2.5	6741.5968	-0.00023
	3.5	6764.0773	0.00004
	4.5	6784.1210	0.00017
	5.5	6801.5373	0.00032

	6.5	6816.1789	0.00037
	7.5	6827.9355	-0.00003
R _{2ee} (J)	2.5	6754.1549	0.00086
	3.5	6777.1663	0.00026
	4.5	6796.6689	0.00042
	5.5	6812.7816	0.00027
	6.5	6825.5849	0.00017
	7.5	6835.1255	0.00005
	8.5	6841.4286	0.00182
P _{1ff} (J)	2.5	6561.1976	-0.00015
	3.5	6522.0055	-0.00013
	4.5	6479.7825	0.00018
	5.5	6434.6122	0.00007
	6.5	6386.6105	0.00026
	7.5	6335.8915	0.00010
	8.5	6282.5599	0.00029
	9.5	6226.7071	0.00000
	10.5	6168.4168	0.00052
	11.5	6107.7626	0.00048
	12.5	6044.8140	-0.00005
	13.5	5979.6375	0.00006
	14.5	5912.2880	-0.00649
	15.5	5842.8534	0.00847
P _{2ff} (J)	1.5	6584.4609	-0.00047
	2.5	6541.1520	0.00296
	3.5	6495.5079	0.00280
	4.5	6447.6359	0.00062
	5.5	6397.5543	0.00018
	6.5	6345.2478	0.00047
	7.5	6290.7034	0.00055

	8.5	6233.9215	0.00061
	10.5	6113.7101	0.00218
	11.5	6050.3344	0.00176
	13.5	5917.2255	-0.00525
	14.5	5847.5984	0.00861
Q _{2fe} (J)	0.5	6643.3985	0.00062
	1.5	6638.5843	0.00042
	2.5	6630.5655	-0.00012
Q _{1ef} (J)	1.5	6642.0228	-0.00010
	2.5	6635.9826	-0.00008
	3.5	6627.2747	-0.00001
	4.5	6615.8087	0.00024
	5.5	6601.5373	0.00048
	7.5	6564.5243	0.00373
R _{1ff} (J)	1.5	6717.0069	-0.00267
	2.5	6741.7690	0.00010
	3.5	6764.3056	0.00240
	4.5	6784.3902	0.00318
	5.5	6801.8300	0.00032
	6.5	6816.4810	-0.00396
	7.5	6828.2457	0.00188
	8.5	6837.0283	0.00405
	9.5	6842.7624	-0.00068
	10.5	6845.4113	0.00112
	11.5	6844.9250	0.00041
	12.5	6841.2197	-0.05230
	13.5	6834.4107	-0.01241
	14.5	6824.4832	0.13079
R _{2ff} (J)	0.5	6697.0884	-0.03089
	1.5	6727.4883	0.00398

	2.5	6754.0830	0.00879
	3.5	6777.0076	-0.00984
	4.5	6796.4625	-0.00239
	5.5	6812.5358	-0.00063
	6.5	6825.3130	0.00178
	7.5	6834.8238	-0.01130
	8.5	6841.1250	-0.00569
	9.5	6844.2044	-0.00120
	10.5	6844.0543	-0.00388
	11.5	6840.6812	-0.00003
	12.5	6834.0698	0.00540
	13.5	6824.2190	0.02328
P _{1ee} (J)	2.5	6561.3416	0.00032
	3.5	6522.2631	-0.00180
	4.5	6480.1652	-0.00246
	5.5	6435.1213	-0.00593
	6.5	6387.2548	-0.00170
	7.5	6336.6695	-0.00037
	8.5	6283.4706	-0.00098
	9.5	6227.7535	-0.00069
	10.5	6169.6005	0.00014
	11.5	6109.0849	-0.00026
	12.5	6046.2780	-0.00003
	13.5	5981.2441	-0.00016
	14.5	5914.0461	0.00015
	15.5	5844.7439	0.00125
	16.5	5773.3860	-0.00579
	17.5	5700.0453	-0.00353
	18.5	5624.7660	-0.00138
	19.5	5547.5901	-0.00905
	20.5	5468.5904	-0.00348

	21.5	5387.8000	0.00087
$P_{2ee}(J)$	1.5	6584.5748	-0.00080
	2.5	6541.1672	-0.01862
	3.5	6495.4422	0.00121
	4.5	6447.4580	-0.00201
	5.5	6397.2671	0.00304
	6.5	6344.8418	0.00064
	7.5	6290.1566	-0.02303
	8.5	6233.2790	-0.00042
	9.5	6174.1531	-0.00028
	10.5	6112.8253	0.00015
	11.5	6049.3264	-0.00011
	12.5	5983.6948	-0.00026
	13.5	5915.9717	-0.00072
	14.5	5846.2025	-0.00035
	15.5	5774.4344	0.00220
	16.5	5700.6947	-0.01241
	17.5	5625.0748	0.00043
	18.5	5547.5901	0.00974
	19.5	5468.2738	0.00319
	20.5	5387.2692	0.07987
$Q_{2ef}(J)$	0.5	6643.1107	-0.00030
	1.5	6638.0763	-0.02823
	2.5	6630.0876	0.03756
$Q_{1fe}(J)$	1.5	6642.1042	-0.01315
	2.5	6636.3286	0.00065
	3.5	6628.0716	0.02047
	4.5	6617.2068	0.01065
$R_{1ee}(J)$	1.5	6716.9049	0.00262
	2.5	6741.5958	-0.00123

	3.5	6764.0768	-0.00046
	4.5	6784.1244	0.00357
	5.5	6801.5368	-0.00018
	6.5	6816.1764	-0.00213
	7.5	6827.9345	-0.00103
	8.5	6836.6790	-0.04633
	9.5	6842.4815	-0.00288
	10.5	6845.1599	-0.00244
	11.5	6844.7215	0.00335
	12.5	6841.1250	0.00752
	13.5	6834.4107	0.07967
	14.5	6824.4832	0.14988
R _{2ee} (J)	0.5	6697.0884	0.04737
	1.5	6727.4883	0.00341
	2.5	6754.1447	-0.00934
	3.5	6777.1657	-0.00034
	4.5	6796.6694	0.00092
	5.5	6812.7876	0.00627
	6.5	6825.5861	0.00137
	7.5	6835.1242	-0.00125
	8.5	6841.4247	-0.00208
	9.5	6844.4998	0.00305
	10.5	6844.3327	-0.00122
	11.5	6840.9349	0.00368
	12.5	6834.3180	0.03960
	13.5	6824.4832	0.11972
P _{1ff} (J)	2.5	6561.2017	0.00395
	3.5	6522.0038	-0.00183
	4.5	6479.7191	-0.06322
	5.5	6434.6120	-0.00013
	6.5	6386.6101	-0.00014

	7.5	6335.8908	-0.00060
	8.5	6282.5590	-0.00061
	9.5	6226.7072	0.00010
	10.5	6168.4160	-0.00028
	11.5	6107.7620	-0.00012
	12.5	6044.8142	0.00015
	13.5	5979.6377	0.00026
	14.5	5912.2943	-0.00019
	15.5	5842.8459	0.00097
	16.5	5771.3459	-0.00042
	17.5	5697.8533	-0.00100
	18.5	5622.4211	-0.00154
	19.5	5545.0999	-0.00328
	20.5	5465.9456	-0.00016
	21.5	5384.9992	0.00114
P _{2ff} (J)	1.5	6584.4666	0.00523
	2.5	6541.1672	0.01816
	3.5	6495.5045	-0.00060
	4.5	6447.6346	-0.00068
	5.5	6397.5525	-0.00162
	6.5	6345.2468	-0.00053
	7.5	6290.7025	-0.00035
	8.5	6233.9205	-0.00039
	9.5	6174.9112	-0.00343
	10.5	6113.7019	-0.00602
	11.5	6050.3324	-0.00024
	12.5	5984.8266	0.00019
	13.5	5917.2304	-0.00035
	14.5	5847.5898	0.00001
	15.5	5775.9498	0.00057
	16.5	5702.3042	-0.05133

	17.5	5626.8565	0.00119
	18.5	5549.4935	-0.00129
	19.5	5470.3213	0.00197
	20.5	5389.3746	0.00158
Q _{2fe} (J)	0.5	6643.4019	0.00402
	1.5	6638.6203	0.03642
	2.5	6630.5871	0.02148
Q _{1ef} (J)	1.5	6642.0318	0.00890
	2.5	6635.9685	-0.01418
	3.5	6627.2720	-0.00271
	4.5	6615.8061	-0.00236

3-2	J	Obs (cm-1)	Obs-Calc
R _{1ff} (J)	1.5	3314.1375	-0.00130
	2.5	3341.8691	-0.00032
	3.5	3368.6749	0.00098
	4.5	3394.3715	-0.00070
	5.5	3418.7950	-0.00395
	6.5	3441.8116	-0.00780
R _{2ff} (J)	0.5	3293.6577	0.00110
	1.5	3326.4898	-0.00567
	2.5	3357.1250	-0.00235
	3.5	3385.6107	-0.00103
	4.5	3412.0545	0.00610
P _{1ee} (J)	2.5	3161.4266	-0.00102
	3.5	3126.6054	-0.00040
	4.5	3090.1025	-0.00020
	5.5	3052.0218	-0.00032
	6.5	3012.4886	-0.00023
	7.5	2971.6201	-0.00033

	8.5	2929.5192	-0.00025
	9.5	2886.2736	-0.00028
	10.5	2841.9598	-0.00027
	11.5	2796.6454	-0.00022
	12.5	2750.3927	0.00098
	13.5	2703.2525	-0.00228
	14.5	2655.2866	-0.00093
	15.5	2606.5414	0.00158
	16.5	2557.0590	-0.00004
	17.5	2506.8887	-0.00175
P _{2ee} (J)	1.5	3183.5760	-0.00038
	2.5	3144.2260	-0.00538
	3.5	3104.0393	0.00323
	4.5	3063.0564	-0.00094
	5.5	3021.2831	0.00021
	6.5	2978.6801	0.00012
	7.5	2935.2234	0.00012
	8.5	2890.9028	0.00016
	9.5	2845.7222	-0.00006
	10.5	2799.6991	0.00152
	11.5	2752.8506	-0.00153
	12.5	2705.2109	-0.00409
	13.5	2656.8141	-0.00477
	14.5	2607.6959	-0.00288
	15.5	2557.8929	0.00189
	17.5	2456.3656	0.00586
Q _{2ef} (J)	0.5	3239.6493	0.00098
	1.5	3237.1161	0.00043
	2.5	3233.1030	-0.00018
	3.5	3227.6731	-0.01471

Q _{1fe} (J)	1.5	3239.2429	0.00046
	2.5	3236.4135	-0.00079
	3.5	3232.3919	-0.00012
	4.5	3227.1319	0.00071
	5.5	3220.6083	0.00761
R _{1ee} (J)	1.5	3314.0270	-0.00037
	2.5	3341.6828	-0.00057
	3.5	3368.4173	-0.00085
	4.5	3394.0555	-0.00037
	5.5	3418.4325	0.00062
R _{2ee} (J)	0.5	3293.5705	-0.00060
	1.5	3326.4898	0.00413
	2.5	3357.2001	0.00050
	3.5	3385.7608	-0.00032
	4.5	3412.2618	-0.00401
P _{1ff} (J)	5.5	3436.7942	-0.00596
	2.5	3161.2987	0.00043
	3.5	3126.3761	-0.00025
	4.5	3089.7669	-0.00060
	5.5	3051.5810	-0.00041
	6.5	3011.9445	-0.00018
	7.5	2970.9749	-0.00020
	8.5	2928.7747	-0.00015
	9.5	2885.4313	-0.00025
	10.5	2841.0211	-0.00018
	11.5	2795.6112	-0.00032
12.5	2749.2631	-0.00033	
13.5	2702.0302	-0.00324	
14.5	2653.9738	-0.00060	
15.5	2605.1360	-0.00024	

	16.5	2555.5629	-0.00358
	17.5	2505.3110	0.00051
$P_{2ff}(J)$	1.5	3183.4729	0.00039
	2.5	3144.2084	0.00623
	3.5	3104.1052	0.00581
	4.5	3063.2192	0.00041
	5.5	3021.5425	0.00030
	6.5	2979.0350	0.00001
	7.5	2935.6716	-0.00010
	8.5	2891.4426	0.00011
	9.5	2846.3520	0.00006
	10.5	2800.4150	-0.00075
	11.5	2753.6569	-0.00069
	12.5	2706.1060	-0.00056
	13.5	2657.7956	0.00026
	14.5	2608.7595	0.00065
	15.5	2559.0342	0.00092
	16.5	2508.6559	0.00057
	17.5	2457.6620	0.00028
$Q_{2fe}(J)$	0.5	3239.9280	0.00005
	1.5	3237.5872	0.00254
	2.5	3233.6105	-0.00068
	3.5	3228.0491	-0.01114
$Q_{1ef}(J)$	1.5	3239.1508	-0.00133
	2.5	3236.0820	-0.00119
	3.5	3231.6458	0.00037
	4.5	3225.7940	0.00036
	5.5	3218.5038	-0.00229
	6.5	3209.7698	-0.00607
$P_{2ff}(J)$	6.5	2979.0344	-0.00059

	7.5	2935.6670	-0.00470
	10.5	2800.4225	0.00675
	11.5	2753.6602	0.00261
	12.5	2706.1090	0.00244
	13.5	2657.7921	-0.00324
	15.5	2559.0410	0.00772
	18.5	2406.0963	0.00759
	19.5	2353.9665	-0.00528
	20.5	2301.3442	-0.00113
	21.5	2248.2364	-0.00600
	23.5	2140.7442	0.01313
P _{1ff} (J)	5.5	3051.5753	-0.00611
	7.5	2970.9769	0.00180
	8.5	2928.7711	-0.00375
	10.5	2841.0244	0.00312
	12.5	2749.2639	0.00047
	13.5	2702.0330	-0.00044
	14.5	2653.9734	-0.00100
	15.5	2605.1383	0.00206
	18.5	2454.4102	-0.00149
	19.5	2402.9135	0.00193
	20.5	2350.8545	0.00477
P _{1ee} (J)	8.5	2929.5186	-0.00085
	9.5	2886.2790	0.00512
	10.5	2841.9609	0.00083
	13.5	2703.2560	0.00122
	14.5	2655.2848	-0.00273
	18.5	2456.0788	0.00147
	19.5	2404.6613	0.00021
	20.5	2352.6799	-0.00135
	21.5	2300.1825	0.00708

	23.5	2193.7343	0.00810
	24.5	2139.8308	-0.01688
	27.5	1975.8882	-0.04734
P _{2ee} (J)	6.5	2978.6850	0.00502
	10.5	2799.6970	-0.00058
	11.5	2752.8453	-0.00683
	12.5	2705.2123	-0.00269
	14.5	2607.6987	-0.00008
	16.5	2507.4417	0.00932
	19.5	2352.5190	0.00194
	21.5	2246.6349	-0.00765

3-3	J	Obs (cm-1)	Obs-Calc
R _{2ff} (J)	11.5	410.0360	-0.00247
	14.5	495.7066	-0.00065
	15.5	522.9943	-0.00102
	19.5	625.0183	-0.00144
	20.5	648.5990	-0.00044
	21.5	671.3538	0.00111
	22.5	693.2539	0.00129
	23.5	714.2733	0.00043
	24.5	734.3871	-0.00055
	25.5	753.5729	0.00138
	26.5	771.7999	0.00060
	27.5	789.0453	-0.00061
	28.5	805.2858	-0.00032
	29.5	820.4949	0.00060
	30.5	834.6436	-0.00045
	31.5	847.7073	-0.00055
	32.5	859.6551	-0.00144

	33.5	870.4594	0.00065
	34.5	880.0810	0.00081
	35.5	888.4892	0.00637
R _{2ee} (J)	11.5	410.6890	-0.00089
	14.5	496.4723	-0.00102
	15.5	523.7953	0.00442
	18.5	601.4967	-0.00097
	19.5	625.8910	0.00377
	20.5	649.4720	-0.00101
	21.5	672.2266	-0.00084
	22.5	694.1257	0.00210
	23.5	715.1351	0.00001
	24.5	735.2363	0.00025
	25.5	754.4008	-0.00021
	26.5	772.6054	0.00065
	28.5	806.0280	0.00014
	29.5	821.1965	0.00027
	30.5	835.3014	0.00062
	31.5	848.3123	-0.00157
	32.5	860.2065	0.00029
	33.5	870.9459	-0.00037
	34.5	880.5014	0.00184
	35.5	888.8290	0.00116
	37.5	901.6271	-0.00411
	38.5	906.0010	0.00002
R _{1ff} (J)	12.5	412.9386	0.00105
	20.5	626.7479	-0.00408
	21.5	650.2509	-0.00416
	22.5	672.9387	0.00219
	23.5	694.7678	-0.00005
	24.5	715.7209	-0.00054

	25.5	735.7686	-0.00179
	26.5	754.8881	-0.00024
	27.5	773.0495	0.00015
	28.5	790.2270	-0.00068
	29.5	806.3980	0.00051
	30.5	821.5337	0.00106
	31.5	835.6056	-0.00064
	32.5	848.5890	-0.00131
	33.5	860.4567	0.00145
	34.5	871.1689	-0.00033
	35.5	880.6980	0.00049
R _{1ee} (J)	12.5	412.1072	0.00009
	15.5	497.0510	-0.00057
	20.5	625.7452	-0.00185
	21.5	649.2509	0.00056
	22.5	671.9368	-0.00037
	23.5	693.7800	0.00087
	24.5	714.7501	0.00145
	25.5	734.8196	0.00073
	26.5	753.9634	-0.00011
	27.5	772.1573	0.00060
	28.5	789.3732	0.00047
	29.5	805.5851	-0.00078
	30.5	820.7703	0.00023
	31.5	834.8981	-0.00043
	33.5	859.8745	-0.00073
	34.5	870.6640	0.00162
	35.5	880.2730	0.00268
	36.5	888.6600	-0.00078
Q _{1fe} (J)	1.5	0.0432	0.00005
	3.5	0.3586	0.00005

	4.5	0.6437	-0.00011
	6.5	1.4516	-0.00001
R _{1ee} (J)	3.5	136.3848	0.00012
R _{1ff} (J)	3.5	136.6699	-0.00004
R _{2ee} (J)	1.5	89.1300	-0.00005
	2.5	123.8380	-0.00017
R _{2ff} (J)	1.5	89.1506	-0.00015
	2.5	123.7744	-0.00003
P _{1ee} (J)	1.5	128.0721	-0.00002
P _{1ff} (J)	1.5	128.1649	-0.00016

4-4	J	Obs (cm-1)	Obs-Calc
R _{2ff} (J)	23.5	680.6010	0.00042
	24.5	699.3700	-0.00100
	25.5	717.1960	-0.00020
	26.5	734.0490	0.00210
	27.5	749.8820	-0.01120
	29.5	778.4490	0.00094
	30.5	791.0890	-0.00150
R _{2ee} (J)	21.5	641.1360	-0.00422
	22.5	661.7050	-0.00232
	23.5	681.3860	0.00403
	24.5	700.1340	-0.00129
	25.5	717.9450	0.00671
	26.5	734.7580	-0.00362
	27.5	750.5770	0.00166
	29.5	779.0510	0.00195
	30.5	791.6410	-0.00176

R _{1ff} (J)	22.5	641.8590	-0.00429
	23.5	662.3620	-0.00104
	25.5	700.6800	0.00389
	26.5	718.4390	0.00941
	27.5	735.2080	0.00037
	28.5	750.9810	0.00135
	30.5	779.3790	0.00049
	31.5	791.9370	-0.00114
R _{1ee} (J)	22.5	640.9450	-0.00813
	23.5	661.4720	0.00473
	24.5	681.0990	-0.00227
	25.5	699.8230	-0.00226
	26.5	717.6100	0.00061
	27.5	734.4280	0.00435
	28.5	750.2390	0.00147

4-3	J	Obs (cm-1)	Obs-Calc
R _{1ff} (J)	1.5	3148.6104	0.00128
	2.5	3175.0672	0.00012
	3.5	3200.5636	-0.00002
R _{2ff} (J)	0.5	3128.6556	0.00536
	1.5	3159.9629	-0.00636
	2.5	3189.1446	-0.00645
P _{1ee} (J)	2.5	3001.7911	-0.00039
	3.5	2968.2512	-0.00031
	4.5	2933.0833	-0.00055
	5.5	2896.3743	-0.00048
	6.5	2858.2339	-0.00069
	7.5	2818.7702	-0.00073
	8.5	2778.0790	-0.00073

	9.5	2736.2437	-0.00078
	10.5	2693.3372	-0.00098
	11.5	2649.4238	-0.00186
	12.5	2604.5646	-0.00098
	13.5	2558.8113	-0.00060
	14.5	2512.2134	-0.00144
	15.5	2464.8201	-0.00151
	16.5	2416.6755	-0.00131
	17.5	2367.8197	-0.00298
$P_{2ee}(J)$	1.5	3023.4234	0.00019
	2.5	2985.6599	0.00018
	3.5	2946.9897	-0.00051
	4.5	2907.4912	-0.00077
	5.5	2867.1669	-0.00088
	6.5	2825.9955	-0.00112
	7.5	2783.9588	-0.00136
	8.5	2741.0501	-0.00145
	9.5	2697.2759	-0.00006
	10.5	2652.6474	-0.00097
	11.5	2607.1903	-0.00071
	12.5	2560.9308	-0.00029
	13.5	2513.9018	0.00269
	14.5	2466.1261	-0.00146
	15.5	2417.6501	0.00014
$Q_{2ef}(J)$	0.5	3077.0653	-0.00106
	1.5	3074.5594	-0.00133
$Q_{1fe}(J)$	1.5	3076.6597	0.00087
	2.5	3073.8237	-0.00050
	3.5	3069.7973	-0.00070
	4.5	3064.5335	-0.00398

	5.5	3058.0171	0.00560
R _{1ff} (J)	1.5	3148.5084	0.00114
	2.5	3174.8923	-0.00390
	3.5	3200.3286	0.00065
R _{2ee} (J)	0.5	3128.5696	0.00058
	1.5	3159.9629	0.00447
	2.5	3189.2111	-0.00593
P _{1ff} (J)	2.5	3001.6718	-0.00036
	3.5	2968.0376	-0.00037
	4.5	2932.7690	-0.00051
	5.5	2895.9583	-0.00062
	6.5	2857.7179	-0.00073
	7.5	2818.1558	-0.00088
	8.5	2777.3680	-0.00078
	9.5	2735.4372	-0.00089
	10.5	2692.4369	-0.00046
	11.5	2648.4297	-0.00158
	12.5	2603.4786	0.00017
	13.5	2557.6342	0.00144
	14.5	2510.9399	-0.00466
	15.5	2463.4636	0.00250
	16.5	2415.2288	0.00175
	17.5	2366.2860	0.00123
P _{2ee} (J)	1.5	3023.3216	-0.00084
	2.5	2985.6274	0.00012
	3.5	2947.0434	-0.00068
	4.5	2907.6380	-0.00071
	5.5	2867.4071	-0.00097
	6.5	2826.3279	-0.00110
	7.5	2784.3817	-0.00108

	8.5	2741.5615	-0.00126
	9.5	2697.8738	-0.00064
	10.5	2653.3337	0.00063
	11.5	2607.9654	0.00440
	12.5	2561.7859	0.00037
	13.5	2514.8368	-0.00034
	14.5	2467.1452	-0.00308
	15.5	2418.7510	-0.00137
	16.5	2369.6839	0.00076
Q _{2fe} (J)	0.5	3077.3299	-0.00082
	1.5	3075.0089	0.00182
Q _{1ef} (J)	1.5	3076.5748	-0.00162
	2.5	3073.5209	0.00031
	3.5	3069.1102	0.00022
	5.5	3056.0663	0.00052

4-2	J	Obs (cm-1)	Obs-Calc
R _{1ff} (J)	4.5	6451.3739	0.00027
	5.5	6467.5479	0.00034
	6.5	6480.9493	0.00064
	7.5	6491.4696	-0.00016
	8.5	6499.0295	0.00081
	9.5	6503.5600	-0.00088
	10.5	6505.0128	-0.00121
R _{2ff} (J)	0.5	6368.4358	0.00116
	1.5	6397.3144	0.00043
	2.5	6422.5031	-0.00088
	3.5	6444.1123	0.00080
	4.5	6462.2679	-0.00011
	5.5	6477.0813	0.00074

	6.5	6488.6189	-0.00171
	7.5	6496.9273	-0.00191
	8.5	6502.0252	-0.00030
P _{1ee} (J)	2.5	6238.0469	-0.00028
	3.5	6200.2853	0.00032
	4.5	6159.5713	0.00008
	5.5	6115.9657	0.00030
	6.5	6069.5649	0.00022
	7.5	6020.4724	0.00027
	8.5	5968.7842	0.00014
	9.5	5914.5873	0.00007
	10.5	5857.9598	0.00023
	11.5	5798.9722	0.00027
	12.5	5737.6897	0.00006
	13.5	5674.1749	0.00111
	14.5	5608.4749	-0.00713
	15.5	5540.6691	-0.00006
	16.5	5470.7893	0.00189
	17.5	5398.8875	0.00087
	18.5	5325.0127	-0.00153
	19.5	5249.2038	-0.01134
P _{2ee} (J)	1.5	6260.7790	0.00017
	4.5	6128.4362	0.00000
	5.5	6079.7723	0.00004
	6.5	6028.8724	0.00012
	7.5	5975.7311	-0.00023
	8.5	5920.3521	-0.00004
	9.5	5862.7478	0.00016
	10.5	5802.9403	0.00041
	11.5	5740.9592	0.00124
	12.5	5676.8359	-0.00006

	13.5	5610.6132	0.00178
Q _{2ef} (J)	0.5	6316.8513	0.00053
	1.5	6311.9058	0.00036
	2.5	6303.9313	-0.00026
	3.5	6293.0665	-0.00017
	4.5	6279.4101	0.00106
Q _{1fe} (J)	1.5	6315.8585	0.00038
	2.5	6310.0801	0.00021
	3.5	6301.8317	0.00023
	4.5	6291.0251	0.00024
	5.5	6277.6025	0.00038
	6.5	6261.5294	-0.00090
	7.5	6242.7919	-0.00132
	8.5	6221.3809	-0.00405
R _{1ee} (J)	3.5	6432.3617	0.00027
	4.5	6451.1317	-0.00002
	5.5	6467.2836	0.00002
	6.5	6480.6762	0.00073
	7.5	6491.1993	-0.00013
R _{2ee} (J)	0.5	6368.3603	-0.00058
	1.5	6397.3144	0.00035
	2.5	6422.5793	0.00084
	4.5	6462.4577	-0.00042
	5.5	6477.3076	-0.00060
	6.5	6488.8715	-0.00153
	7.5	6497.1955	0.00101
	8.5	6502.2896	-0.00272
	9.5	6504.1722	0.00075
P _{1ff} (J)	2.5	6237.9145	0.00055
	3.5	6200.0420	0.00005

	4.5	6159.2072	0.00024
	5.5	6115.4753	0.00022
	6.5	6068.9463	0.00020
	7.5	6019.7238	0.00009
	8.5	5967.9041	-0.00001
	9.5	5913.5736	-0.00020
	10.5	5856.8110	0.00052
	11.5	5797.6885	0.00364
	12.5	5736.2626	0.00034
	13.5	5672.6039	0.00015
	14.5	5606.7681	0.00102
	15.5	5538.8130	0.00587
	16.5	5468.7744	-0.00184
	17.5	5396.7251	0.00075
	18.5	5322.6974	-0.00159
$P_{2ff}(J)$	1.5	6260.6681	0.00095
	4.5	6128.5960	0.00059
	6.5	6029.2544	-0.00021
	7.5	5976.2276	-0.00015
	8.5	5920.9641	-0.00011
	9.5	5863.4768	-0.00040
	10.5	5803.7889	-0.00007
	11.5	5741.9313	0.00259
	12.5	5677.9287	-0.00186
	13.5	5611.8313	-0.00071
	14.5	5543.6755	0.00291
	15.5	5473.4924	-0.00050
$Q_{2fe}(J)$	0.5	6317.1233	0.00071
	1.5	6312.3629	0.00020
	2.5	6304.4303	0.00062
	3.5	6293.4370	0.00013

Q _{1ef} (J)	4.5	6279.4787	-0.00233
	1.5	6315.7718	0.00011
	2.5	6309.7626	0.00022
	3.5	6301.1146	0.00064
	4.5	6289.7369	-0.00001
	5.5	6275.5822	0.00026
	6.5	6258.6271	-0.00046
	7.5	6238.8669	-0.00198

4-1	J	Obs (cm-1)	Obs-Calc
R _{1ff} (J)	1.5	9790.6506	-0.02457
	2.5	9811.2149	0.00655
	3.5	9828.1936	-0.00327
	4.5	9841.3916	0.00315
	5.5	9850.5752	-0.00309
	6.5	9855.6127	-0.00153
	7.5	9856.3729	-0.01317
	8.5	9852.8115	-0.00195
	9.5	9844.8262	-0.01023
	10.5	9832.4521	0.04309
	11.5	9815.4838	-0.01110
	12.5	9794.0717	0.00701
	13.5	9768.1031	0.00910
	14.5	9737.5448	-0.01737
	15.5	9702.4468	-0.00449
R _{2ff} (J)	0.5	9771.8937	-0.00362
	1.5	9798.3224	0.01957
	2.5	9819.4039	-0.04694
	3.5	9835.5024	-0.01481
	4.5	9846.6916	0.00709

	5.5	9853.1003	0.00782
	6.5	9854.8203	-0.01264
	7.5	9851.9877	0.02734
	8.5	9844.5096	0.00569
	9.5	9832.4521	-0.02462
	10.5	9815.9414	0.05922
	11.5	9794.7177	-0.00019
	12.5	9768.9786	0.00047
	13.5	9738.6314	-0.02395
	14.5	9703.7142	-0.02676
	15.5	9664.2279	0.00211
P _{1ee} (J)	2.5	9637.9502	-0.01065
	3.5	9595.9499	0.00582
	4.5	9549.6353	-0.00088
	5.5	9499.0750	0.00450
	6.5	9444.3342	0.00184
	7.5	9385.5225	0.00093
	8.5	9322.7426	0.00640
	9.5	9256.0725	0.00496
	10.5	9185.6024	0.00253
	11.5	9111.4146	0.00313
	12.5	9033.5784	0.00245
	13.5	8952.1626	-0.00068
	14.5	8867.2500	0.00956
	15.5	8778.8602	-0.01178
	16.5	8687.1261	0.00594
	17.5	8592.0529	0.00789
	18.5	8493.7052	0.00092
	19.5	8392.1530	-0.00021
P _{2ee} (J)	1.5	9661.7792	0.00115
	2.5	9615.9490	-0.02660

	3.5	9566.2972	0.02783
	4.5	9512.8392	0.00033
	5.5	9455.7561	0.00267
	6.5	9395.0363	0.00283
	7.5	9330.6884	0.00072
	8.5	9262.7297	0.00079
	9.5	9191.1819	0.00314
	10.5	9116.0690	0.00153
	11.5	9037.4350	0.00266
	12.5	8955.3145	-0.00154
	13.5	8869.7621	-0.00288
	14.5	8780.8344	0.00637
	15.5	8688.5314	-0.02407
	16.5	8593.0036	0.00551
	17.5	8494.1843	-0.02210
	18.5	8392.2500	0.02006
	19.5	8287.1403	0.02367
Q _{2ef} (J)	0.5	9720.2917	-0.02175
	1.5	9712.8990	0.00470
Q _{1fe} (J)	1.5	9718.6544	-0.07863
	2.5	9710.0038	0.01024
R _{1ee} (J)	2.5	9811.0754	0.00984
	3.5	9828.0236	0.00307
	4.5	9841.1933	-0.00338
	5.5	9850.3796	-0.00908
	6.5	9855.4563	0.01315
	7.5	9856.2598	0.01093
	8.5	9852.7223	-0.00254
	9.5	9844.8262	0.01550
	10.5	9832.4521	-0.00816

	11.5	9815.6602	0.02304
	12.5	9794.3022	-0.00978
	13.5	9768.4665	0.00614
	14.5	9738.0868	0.02510
	15.5	9703.1014	0.00328
R _{2ee} (J)	0.5	9771.8654	0.03459
	1.5	9798.3224	0.00913
	2.5	9819.5145	-0.01840
	3.5	9835.6611	0.00569
	4.5	9846.8711	0.01031
	5.5	9853.2944	0.00502
	6.5	9855.0325	-0.00172
	7.5	9852.1478	-0.00303
	8.5	9844.6880	0.01890
	9.5	9832.5817	-0.02088
	10.5	9815.9414	-0.01349
	11.5	9794.7177	-0.00608
	12.5	9768.9243	0.02072
	13.5	9738.4716	-0.01516
	14.5	9703.5812	0.11643
	15.5	9663.8542	0.02578
P _{1ff} (J)	2.5	9637.8200	0.00657
	3.5	9595.6776	0.00637
	4.5	9549.2215	-0.00028
	5.5	9498.5051	-0.00070
	6.5	9443.6138	0.00213
	7.5	9384.6402	0.00019
	8.5	9321.6902	0.00132
	9.5	9254.8479	-0.00144
	10.5	9184.2099	0.00442
	11.5	9109.8374	0.00194

	12.5	9031.7879	-0.02498
	13.5	8950.2079	0.00015
	14.5	8865.0924	0.00522
	15.5	8776.5102	-0.00562
	16.5	8684.5652	0.00912
	17.5	8589.2384	-0.02976
	18.5	8490.7011	-0.00883
	19.5	8388.9325	-0.00425
$P_{2ff}(J)$	1.5	9661.6646	0.00859
	2.5	9615.9490	0.02193
	3.5	9566.2972	-0.02641
	4.5	9513.0117	-0.00021
	5.5	9456.0493	-0.00459
	6.5	9395.4681	0.00116
	7.5	9331.2617	0.00280
	8.5	9263.4440	0.00138
	9.5	9192.0422	0.00231
	10.5	9117.0836	0.00246
	11.5	9038.6060	0.00224
	12.5	8956.6336	-0.01681
	13.5	8871.2742	0.00679
	14.5	8782.5019	-0.00162
	15.5	8690.4114	0.00255
	16.5	8595.0353	0.00130
	17.5	8496.4290	-0.00030
	18.5	8394.6453	0.00118
	19.5	8289.7205	-0.00572
$Q_{2fe}(J)$	0.5	9720.6028	0.01028
	1.5	9713.3422	-0.01972
$Q_{1ef}(J)$	1.5	9718.6544	0.01193

	2.5	9709.6416	-0.02026
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5-4	J	Obs (cm-1)	Obs-Calc
R _{1ff} (J)	1.5	2983.0726	-0.09354
	2.5	3008.1741	-0.15885
R _{2ff} (J)	0.5	2963.7433	0.00029
P _{1ee} (J)	2.5	2842.2536	-0.00055
	3.5	2809.9684	-0.00073
	4.5	2776.0996	-0.00153
	5.5	2740.7198	-0.00066
	6.5	2703.9228	-0.00072
	7.5	2665.8077	-0.00018
	8.5	2626.4615	-0.00107
	9.5	2585.9650	-0.00117
	10.5	2544.3865	-0.00136
	11.5	2501.7884	-0.00077
	12.5	2458.2237	-0.00200
P _{2ee} (J)	1.5	2863.3369	0.00004
	2.5	2827.1322	0.00077
	3.5	2789.9551	-0.00451
	4.5	2751.9071	0.00015
	5.5	2712.9699	-0.01999
	6.5	2673.1985	-0.00018
	7.5	2632.5229	0.00092
	8.5	2590.9558	-0.00056
	9.5	2548.5076	-0.00039
	10.5	2505.1905	-0.00076
	11.5	2461.0258	-0.00102
Q _{2ef} (J)	0.5	2914.5763	0.00115

Q _{1fe} (J)	1.5	2914.1769	-0.00038
	2.5	2911.3207	0.00299
	3.5	2907.2608	-0.00015
R _{1ee} (J)	1.5	2983.0726	-0.00124
	2.5	3008.1741	-0.00348
R _{2ee} (J)	0.5	2963.6677	0.00104
	1.5	2993.5201	0.00319
P _{1ff} (J)	2.5	2842.1440	-0.00058
	3.5	2809.7707	-0.00051
	4.5	2775.8072	-0.00011
	5.5	2740.3289	-0.00011
	6.5	2703.4351	-0.00002
	7.5	2665.2230	-0.00086
	8.5	2625.7837	-0.00054
	9.5	2585.1939	-0.00073
	10.5	2543.5232	-0.00082
	11.5	2500.8336	-0.00028
	12.5	2457.1819	0.00212
	13.5	2412.6122	-0.00047
	P _{2ff} (J)	1.5	2863.2397
2.5		2827.0957	-0.00050
3.5		2789.9978	-0.00657
4.5		2752.0379	-0.00129
5.5		2713.2106	-0.00063
6.5		2673.5081	-0.00022
7.5		2632.9180	-0.00045
8.5		2591.4374	-0.00081
9.5		2549.0734	-0.00054
10.5		2505.8397	-0.00051
11.5		2461.7585	0.00077

Q _{2fe} (J)	0.5	2914.8200	-0.00347
Q _{1ef} (J)	1.5	2914.1017	-0.00088
	2.5	2911.0405	-0.00064
	3.5	2906.6291	-0.00198

5-3	J	Obs (cm-1)	Obs-Calc
R _{1ff} (J)	4.5	6119.4013	0.00002
	5.5	6134.2277	-0.00015
	6.5	6146.2783	-0.00061
R _{2ff} (J)	0.5	6040.9378	0.00015
	1.5	6068.3060	-0.00017
	2.5	6092.0510	-0.00030
	3.5	6112.2613	0.00084
	4.5	6129.0461	-0.00058
	5.5	6142.5041	0.00003
	6.5	6152.6950	-0.00072
	7.5	6159.6607	0.00375
	8.5	6163.3996	-0.00270
	9.5	6163.9373	0.00531
P _{1ee} (J)	4.5	5840.0448	0.00040
	5.5	5797.7962	-0.00012
	6.5	5752.7753	0.00008
	7.5	5705.0723	-0.00019
	8.5	5654.7755	-0.00042
	9.5	5601.9648	-0.00088
	10.5	5546.7140	-0.00017
	11.5	5489.0863	-0.00080
	12.5	5429.1430	-0.00171
	13.5	5366.9416	-0.00119
	14.5	5302.5343	0.00088

	15.5	5235.9672	0.00174
	16.5	5167.2838	-0.00111
	17.5	5096.5493	0.01424
	18.5	5023.7557	-0.00089
$P_{2ee}(J)$	2.5	5897.9589	-0.00091
	3.5	5855.3417	0.00323
	4.5	5810.3966	0.00029
	5.5	5763.1821	-0.00009
	6.5	5713.7067	-0.00003
	7.5	5661.9718	0.00033
	8.5	5607.9813	-0.00044
	9.5	5551.7503	0.00000
	10.5	5493.2969	-0.00019
	11.5	5432.6474	-0.00040
	12.5	5369.8345	0.00226
	13.5	5304.8817	-0.00123
	14.5	5237.8403	0.00640
	15.5	5168.7212	0.00132
	16.5	5097.5751	-0.00044
	17.5	5024.4205	-0.01444
$Q_{2ef}(J)$	0.5	5991.7698	0.00001
	1.5	5986.8607	-0.00012
	2.5	5978.9260	-0.00089
	3.5	5968.0977	0.00051
	4.5	5954.4695	0.00275
$Q_{1fe}(J)$	1.5	5990.7972	0.00035
	2.5	5984.9972	0.00031
	3.5	5976.7298	0.00033
	4.5	5965.9095	0.00049
	5.5	5952.4767	0.00011

	6.5	5936.3973	0.00064
R _{1ee} (J)	5.5	6133.9943	-0.00022
	6.5	6146.0407	-0.00087
	7.5	6155.2175	-0.00192
	8.5	6161.4414	-0.00296
	9.5	6164.6477	-0.00138
	11.5	6161.7827	0.00046
R _{2ee} (J)	0.5	6040.8675	-0.00161
	1.5	6068.3060	-0.00068
	2.5	6092.1231	0.00173
	3.5	6112.3895	-0.00117
	4.5	6129.2234	-0.00060
	5.5	6142.7147	-0.00034
	6.5	6152.9262	-0.00137
	7.5	6159.9031	0.00544
	8.5	6163.6383	-0.00215
P _{1ff} (J)	3.5	5879.2109	0.00023
	4.5	5839.7011	0.00012
	5.5	5797.3307	0.00026
	6.5	5752.1838	0.00007
	7.5	5704.3531	-0.00003
	8.5	5653.9263	-0.00019
	9.5	5600.9834	-0.00043
	10.5	5545.5975	0.00014
	11.5	5487.8322	-0.00051
	12.5	5427.7503	0.00021
	13.5	5365.4051	-0.00025
	14.5	5300.8516	0.00093
	15.5	5234.1360	0.00089
	16.5	5165.3147	0.00982
	17.5	5094.4034	-0.00012

	18.5	5021.4716	-0.00047
P _{2ff} (J)	3.5	5855.3776	-0.00340
	4.5	5810.5387	-0.00026
	5.5	5763.4310	0.00015
	6.5	5714.0642	-0.00017
	7.5	5662.4391	-0.00108
	8.5	5608.5631	-0.00038
	9.5	5552.4473	0.00014
	10.5	5494.1115	0.00018
	11.5	5433.5803	-0.00143
	12.5	5370.8898	0.00164
	13.5	5306.0624	-0.00064
	14.5	5239.1402	-0.00007
	15.5	5170.1612	0.00686
	16.5	5099.1335	-0.00615
	17.5	5026.1287	-0.00126
Q _{2fe} (J)	0.5	5992.0257	-0.00022
	1.5	5987.2937	-0.00080
	2.5	5979.4056	0.00043
	3.5	5968.4627	-0.00017
	4.5	5954.5581	-0.00147
Q _{1ef} (J)	1.5	5990.7183	0.00004
	2.5	5984.7069	0.00016
	3.5	5976.0708	0.00027
	4.5	5964.7216	0.00060
	5.5	5950.6064	0.00000
	6.5	5933.7014	-0.00025
6-5	J	Obs (cm-1)	Obs-Calc
R _{1ff} (J)	4.5	2884.7935	-0.00271

	5.5	2905.0697	-0.00162
	6.5	2923.9077	-0.00075
	7.5	2941.2085	-0.00121
	8.5	2956.8924	-0.00061
$R_{2ff}(J)$	4.5	2898.4451	0.00032
	5.5	2918.7017	-0.00071
	6.5	2937.0682	-0.00075
	9.5	2980.9147	-0.00059
	10.5	2991.7486	0.00026
	11.5	3000.6566	0.00236
	12.5	3007.6023	-0.00152
$P_{1ee}(J)$	2.5	2681.6186	-0.00042
	3.5	2650.5644	-0.00061
	4.5	2617.9611	-0.00069
	5.5	2583.8648	-0.00044
	6.5	2548.3581	-0.00023
	7.5	2511.5284	-0.00006
	8.5	2473.4578	0.00037
	9.5	2434.2178	-0.00075
	10.5	2393.8761	-0.00076
	11.5	2352.4901	-0.00026
$P_{2ee}(J)$	2.5	2667.4431	-0.00135
	3.5	2631.7501	0.00345
	4.5	2595.1062	-0.00060
	5.5	2557.5525	-0.00076
	6.5	2519.0862	-0.00052
	7.5	2479.7021	-0.00054
	8.5	2439.4010	-0.00001
	9.5	2398.1884	-0.00058
	10.5	2356.0816	0.00129

	11.5	2313.1615	0.06760
R _{1ee} (J)	4.5	2884.5566	0.00007
	5.5	2904.7947	-0.00011
	6.5	2923.6031	-0.00127
	7.5	2940.8859	-0.00109
	8.5	2956.5595	-0.00076
	9.5	2970.5484	-0.00550
	10.5	2982.8046	-0.00180
R _{2ee} (J)	4.5	2898.6202	0.00063
	5.5	2918.9205	-0.00298
	6.5	2937.3262	-0.00100
	7.5	2953.8449	-0.00278
	8.5	2968.4860	-0.00057
P _{1ff} (J)	2.5	2681.5186	-0.00059
	3.5	2650.3812	-0.00173
	4.5	2617.6870	-0.00209
	5.5	2583.4984	-0.00080
	6.5	2547.8981	-0.00070
	7.5	2510.9741	-0.00204
	8.5	2472.8118	-0.00131
	9.5	2433.4827	-0.00015
	10.5	2393.0495	-0.00072
	11.5	2351.5753	0.00222
P _{2ff} (J)	1.5	2702.0302	0.01526
	2.5	2667.4044	-0.00168
	3.5	2631.7808	-0.00064
	4.5	2595.2194	-0.00370
	5.5	2557.7541	0.00033
	6.5	2519.3714	-0.00016
	7.5	2480.0708	-0.00026

8.5	2439.8520	-0.00018
9.5	2398.7218	-0.00041
10.5	2356.6959	0.00080
11.5	2313.7866	-0.00327

6-4

	J	Obs (cm-1)	Obs-Calc
R _{1ff} (J)	1.5	5730.7102	0.00087
	2.5	5751.5854	-0.00086
	3.5	5770.1314	0.00043
	4.5	5786.1678	0.00007
	5.5	5799.5365	0.00009
	6.5	5810.1051	0.00021
	7.5	5817.7694	0.00198
	8.5	5822.4459	0.00716
	9.5	5824.0481	-0.00018
R _{2ff} (J)	1.5	5738.2105	0.00505
	2.5	5760.4382	-0.00128
	3.5	5779.1619	0.00016
	4.5	5794.4677	0.00015
	5.5	5806.4383	0.00052
	6.5	5815.1272	0.00084
	7.5	5820.5626	0.00085
	8.5	5822.7561	0.00346
	9.5	5821.8840	0.19045
P _{1ee} (J)	2.5	5592.8043	-0.00087
	3.5	5557.5251	-0.00046
	4.5	5519.3834	0.00007
	5.5	5478.4060	0.00013
	6.5	5434.6600	0.00011
7.5	5388.2248	0.00015	

	8.5	5339.1788	0.00017
	9.5	5287.5947	0.00017
	10.5	5233.5375	-0.00080
	11.5	5177.0690	-0.00049
	12.5	5118.2424	0.00025
	13.5	5057.1057	0.00017
	15.5	4928.0822	0.00147
	16.5	4860.2736	0.00230
	17.5	4790.3165	0.00611
	18.5	4718.2276	-0.00094
	19.5	4644.0362	-0.01649
P _{2ee} (J)	1.5	5614.4083	-0.00041
	2.5	5575.7925	-0.00020
	3.5	5534.6572	0.00621
	4.5	5491.1224	0.00119
	5.5	5445.2641	0.00074
	6.5	5397.0983	0.00027
	7.5	5346.6326	-0.00024
	8.5	5293.8755	0.00015
	9.5	5238.8383	0.00061
	10.5	5181.5374	0.00030
	12.5	5060.2354	-0.00057
	13.5	4996.2844	-0.00158
	14.5	4930.1717	-0.00015
	15.5	4861.9098	-0.01033
	16.5	4791.5391	-0.01730
	19.5	4567.7657	-0.25786
Q _{2ef} (J)	0.5	5665.6469	-0.00010
	1.5	5660.7440	-0.00005
	2.5	5652.7999	0.00013
	3.5	5641.9366	0.00176

Q _{1fe} (J)	4.5	5628.2434	0.00295
	1.5	5664.7243	-0.00029
	2.5	5658.8608	-0.00010
	3.5	5650.5140	-0.00025
	4.5	5639.6009	-0.00012
	5.5	5626.0608	-0.00007
	6.5	5609.8563	0.00135
R _{1ee} (J)	7.5	5590.9608	0.00107
	1.5	5730.6296	-0.00067
	2.5	5751.4605	0.00072
	3.5	5769.9662	-0.00017
	4.5	5785.9784	0.00033
	5.5	5799.3357	0.00026
	6.5	5809.9064	0.00047
	7.5	5817.5816	-0.00157
	8.5	5822.2813	-0.00015
	9.5	5823.9295	-0.00039
	10.5	5822.5417	0.07386
	11.5	5817.8512	0.00965
R _{2ee} (J)	12.5	5809.7632	-0.23854
	1.5	5738.2044	-0.00389
	2.5	5760.5081	0.00085
	3.5	5779.2845	-0.00078
	4.5	5794.6340	0.00002
	5.5	5806.6338	0.00021
	6.5	5815.3388	0.00029
	7.5	5820.7775	-0.00037
	8.5	5822.9597	-0.00121
	9.5	5821.6938	-0.18868
P _{1ff} (J)	2.5	5592.6920	0.00012

	3.5	5557.3145	0.00009
	4.5	5519.0605	-0.00011
	5.5	5477.9644	0.00010
	6.5	5434.0954	0.00015
	7.5	5387.5338	-0.00005
	8.5	5338.3584	-0.00044
	9.5	5286.6421	-0.00075
	10.5	5232.4509	-0.00076
	11.5	5175.8431	-0.00165
	12.5	5116.8773	0.00118
	13.5	5055.5961	0.00103
	14.5	4992.0443	-0.00240
	15.5	4926.2737	0.00132
	16.5	4858.3094	-0.00046
	17.5	4788.1921	-0.00136
	18.5	4715.9413	-0.01275
P _{2ff} (J)	1.5	5614.3029	0.00054
	2.5	5575.7431	0.00011
	3.5	5534.6748	-0.00688
	4.5	5491.2455	-0.00038
	5.5	5445.4892	0.00006
	6.5	5397.4292	0.00024
	7.5	5347.0721	0.00032
	8.5	5294.4251	0.00020
	9.5	5239.5008	0.00034
	10.5	5182.3160	0.00018
	11.5	5122.8930	0.00050
	12.5	5061.2557	0.00077
	14.5	4931.4426	0.00082
	16.5	4793.0859	-0.00070
	17.5	4720.7569	-0.01094

	18.5	4646.3678	-0.01672
	19.5	4569.9038	-0.05202
Q _{2fe} (J)	0.5	5665.8861	-0.00013
	1.5	5661.1511	-0.00042
	2.5	5653.2538	-0.00030
	3.5	5642.2910	0.00030
	4.5	5628.3479	-0.00022
Q _{1ef} (J)	1.5	5664.6534	-0.00020
	2.5	5658.5975	-0.00007
	3.5	5649.9134	0.00012
	4.5	5638.5136	0.00087
	5.5	5624.3426	0.00125
	6.5	5607.3716	0.00178
	7.5	5587.5871	0.00227

7-5	J	Obs (cm-1)	Obs-Calc
R _{1ff} (J)	1.5	5397.8369	0.00121
	2.5	5417.2946	-0.00081
	3.5	5434.3479	0.00013
	4.5	5448.8294	0.00015
	5.5	5460.5872	0.00018
	6.5	5469.4920	0.00063
	7.5	5475.4341	-0.00119
	10.5	5474.1496	-0.52484
R _{2ff} (J)	0.5	5380.0277	-0.00545
	1.5	5404.2344	0.00385
	2.5	5424.8572	-0.00115
	3.5	5441.9705	0.00024
	4.5	5455.6438	-0.00051
	5.5	5465.9467	-0.00082

	6.5	5472.9226	-0.00071
	8.5	5476.5917	-0.36157
$P_{1ee}(J)$	2.5	5265.9601	-0.00074
	3.5	5231.8422	-0.00053
	4.5	5194.8726	-0.00043
	5.5	5155.0648	-0.00016
	6.5	5112.4700	-0.00018
	7.5	5067.1551	-0.00006
	8.5	5019.1880	0.00002
	9.5	4968.6325	-0.00014
	10.5	4915.5460	-0.00120
	11.5	4859.9827	-0.00085
	12.5	4801.9862	-0.00159
	13.5	4741.6000	-0.00060
	14.5	4678.8569	-0.00064
	15.5	4613.7911	0.00189
	16.5	4546.4201	-0.00110
	17.5	4476.7750	0.00105
	18.5	4404.8639	0.00143
	19.5	4330.6826	-0.01341
$P_{2ee}(J)$	1.5	5286.9041	-0.00031
	2.5	5249.8095	0.00969
	3.5	5210.0852	0.00849
	4.5	5167.8742	-0.00030
	5.5	5123.2622	-0.00023
	6.5	5076.2697	-0.00027
	7.5	5026.9099	-0.00024
	8.5	4975.1916	-0.00057
	9.5	4921.1257	-0.00104
	10.5	4864.7266	-0.00071
	11.5	4806.0100	0.00035

	12.5	4744.9947	0.00379
	13.5	4681.6891	0.00068
	14.5	4616.1271	0.00845
	15.5	4548.2977	0.00149
	16.5	4478.2316	-0.00137
	17.5	4405.9353	-0.00192
	18.5	4331.4011	-0.01182
Q _{2ef} (J)	0.5	5335.7468	-0.00080
	1.5	5330.8124	0.00040
	2.5	5322.7941	0.00119
	3.5	5311.8002	-0.00209
	4.5	5297.9283	0.00145
Q _{1fe} (J)	1.5	5334.9201	-0.00076
	2.5	5328.9386	-0.00054
	3.5	5320.4352	-0.00035
	4.5	5309.3279	0.00015
	5.5	5295.5533	0.00002
	6.5	5279.0674	-0.00170
	7.5	5259.8417	-0.00476
R _{1ee} (J)	1.5	5397.7656	-0.00056
	2.5	5417.1851	0.00023
	3.5	5434.2054	-0.00013
	4.5	5448.6679	-0.00048
	5.5	5460.4213	-0.00021
	6.5	5469.3347	-0.00021
	7.5	5475.3011	0.00002
	8.5	5478.2290	-0.00160
R _{2ee} (J)	0.5	5379.9796	-0.00026
	1.5	5404.2344	-0.00386
	2.5	5424.9271	0.00040

	3.5	5442.0893	-0.00081
	4.5	5455.8026	-0.00021
	5.5	5466.1298	-0.00118
	6.5	5473.1175	-0.00086
	8.5	5476.7840	-0.34957
P _{1ff} (J)	2.5	5265.8566	-0.00070
	3.5	5231.6467	-0.00062
	4.5	5194.5706	-0.00034
	5.5	5154.6472	-0.00028
	6.5	5111.9315	-0.00034
	7.5	5066.4915	-0.00035
	8.5	5018.3956	-0.00043
	9.5	4967.7077	-0.00073
	10.5	4914.4872	0.00023
	11.5	4858.7824	-0.00105
	12.5	4800.6437	-0.00015
	13.5	4740.1042	-0.00460
	14.5	4677.2117	-0.00212
	15.5	4611.9911	0.00161
	16.5	4544.4613	-0.00006
	17.5	4474.6520	0.00212
	18.5	4402.5698	-0.00024
	19.5	4328.2281	-0.00298
P _{2ff} (J)	1.5	5286.8007	0.00022
	3.5	5210.0852	-0.00875
	4.5	5167.9790	0.00011
	5.5	5123.2622	-0.20033
	6.5	5076.5712	0.00010
	7.5	5027.3163	0.00013
	8.5	4975.7066	0.00007
	9.5	4921.7525	-0.00028

	10.5	4865.4685	0.00006
	11.5	4806.8690	-0.00037
	12.5	4745.9704	-0.00237
	13.5	4682.7975	0.00152
	14.5	4617.3548	-0.00067
	15.5	4549.6621	-0.00372
	16.5	4479.7475	0.00863
Q _{2fe} (J)	0.5	5335.9683	-0.00004
	1.5	5331.1899	-0.00006
	2.5	5323.2171	-0.00126
	3.5	5312.1431	0.00095
Q _{1ef} (J)	1.5	5334.8569	-0.00050
	2.5	5328.7022	-0.00040
	3.5	5319.8926	-0.00045
	4.5	5308.3413	0.00038
	5.5	5293.9874	-0.00071
	6.5	5276.8017	0.00163
	7.5	5256.7579	0.00024

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	J	Obs (cm-1)	Obs-Calc
R _{1ff} (J)	1.5	8311.9756	0.00188
	2.5	8328.4712	0.00309
	3.5	8341.2814	0.00215
	4.5	8350.1999	-0.00087
	5.5	8355.0551	0.00298
	7.5	8351.6649	-0.32810
R _{2ff} (J)	1.5	8316.5284	0.01044
	2.5	8333.1992	0.00393
	3.5	8344.8740	0.00350
	5.5	8353.6933	0.01041

P _{1ee} (J)	2.5	8177.1463	-0.00070
	3.5	8138.8044	0.00111
	4.5	8096.2954	0.00083
	5.5	8049.6071	0.00152
	6.5	7998.7723	0.00056
	7.5	7943.8515	0.00015
	8.5	7884.9087	-0.00047
	9.5	7822.0097	0.00107
	10.5	7755.2105	0.00186
	11.5	7684.5598	-0.00288
	12.5	7610.1185	-0.00018
	P _{2ee} (J)	1.5	8199.2086
2.5		8158.1500	0.00194
3.5		8112.9894	0.00835
4.5		8063.8913	0.00239
5.5		8010.9727	0.00017
6.5		7954.2820	0.00072
7.5		7893.8392	-0.00113
8.5		7829.6664	-0.00011
9.5		7761.7770	0.00154
Q _{1fe} (J)	1.5	8249.0639	0.00120
	2.5	8240.1283	0.00301
	3.5	8227.3960	-0.00010
R _{1ee} (J)	1.5	8311.9055	-0.00250
	2.5	8328.3731	0.00208
	3.5	8341.1645	-0.00158
	4.5	8350.0921	0.00218
	5.5	8354.9637	0.00156
R _{2ee} (J)	7.5	8351.8124	-0.18487
	1.5	8316.5284	-0.00995

	2.5	8333.2784	0.00345
	3.5	8344.9949	0.00045
P _{1ff} (J)	2.5	8177.0314	0.00140
	3.5	8138.5790	0.00021
	4.5	8095.9440	0.00154
	5.5	8049.1138	0.00123
	6.5	7998.1296	0.00132
	7.5	7943.0507	0.00114
	8.5	7883.9436	0.00183
	9.5	7820.8678	-0.00063
	10.5	7753.8901	0.00169
	11.5	7683.0545	-0.00061
P _{2ff} (J)	12.5	7608.4098	-0.00664
	1.5	8199.0882	0.00031
	2.5	8158.0810	-0.00052
	3.5	8112.9894	-0.00480
	4.5	8064.0022	0.00054
	5.5	8011.2000	0.00209
	6.5	7954.6279	-0.00060
	7.5	7894.3203	0.00341
	8.5	7830.2794	0.00015
	9.5	7762.5319	0.00086
	10.5	7691.0894	0.00024
	11.5	7615.9705	-0.00150
Q _{2fe} (J)	0.5	8250.6681	-0.00367
Q _{1ef} (J)	1.5	8248.9943	-0.00112
	2.5	8239.8747	-0.00060
	3.5	8226.8280	0.00347

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J

Obs (cm-1)

Obs-Calc

R _{1ff} (J)	1.5	2647.2921	0.00371
	2.5	2669.7488	-0.00342
	3.5	2691.0940	-0.00047
	4.5	2711.1939	-0.00006
	5.5	2729.9265	-0.00040
	6.5	2747.1808	-0.00058
	7.5	2762.8586	-0.00209
	8.5	2776.8819	0.00036
	9.5	2789.1705	-0.00051
R _{2ff} (J)	1.5	2655.5793	-0.00445
	2.5	2680.1816	0.00056
	3.5	2702.7616	-0.00197
	4.5	2723.3658	-0.00061
	5.5	2742.0281	0.00122
	6.5	2758.7700	0.00003
	7.5	2773.6063	0.00138
	8.5	2786.5262	-0.00055
	11.5	2813.6108	0.00117
P _{1ee} (J)	6.5	2390.0520	-0.00141
	7.5	2354.4375	-0.00160
	8.5	2317.5580	-0.00161
	9.5	2279.4826	0.00040
P _{2ee} (J)	4.5	2435.6018	0.00077
	5.5	2399.3602	-0.00288
	6.5	2362.1574	-0.00171
	7.5	2323.9906	-0.00055
R _{1ee} (J)	1.5	2647.2127	-0.00244
	2.5	2669.6290	0.00056
	3.5	2690.9204	-0.00293
	4.5	2710.9829	-0.00008

	5.5	2729.6833	-0.00184
	6.5	2746.9177	-0.00044
	7.5	2762.5837	-0.00132
	8.5	2776.6005	-0.00174
	9.5	2788.8977	0.00105
R _{2ee} (J)	2.5	2680.2393	0.00398
	3.5	2702.8760	0.00016
	4.5	2723.5279	-0.00144
	5.5	2742.2321	0.00047
	6.5	2759.0088	0.00130
	7.5	2773.8645	-0.00196
	8.5	2786.8038	-0.00006
	9.5	2797.8035	-0.00017
	10.5	2806.8412	0.00007
	11.5	2813.8842	-0.00065
	12.5	2818.8948	-0.00350
P _{1ff} (J)	4.5	2456.9360	0.00034
	5.5	2423.9874	0.00005
	6.5	2389.6209	-0.00095
	7.5	2353.9159	-0.00135
	8.5	2316.9481	0.00028
	9.5	2278.7800	-0.00079
P _{2ff} (J)	4.5	2435.7002	-0.00078
	6.5	2362.4162	-0.00156
	7.5	2324.3302	0.00071
	8.5	2285.2788	-0.00121
8-5	J	Obs (cm-1)	Obs-Calc
R _{1ff} (J)	1.5	7808.2688	0.00083
	2.5	7823.1942	-0.00006

	3.5	7834.3223	0.00077
	4.5	7841.3742	-0.07916
	5.5	7844.4132	0.00013
	6.5	7843.0539	0.00042
	7.5	7837.2598	0.00588
R _{2ff} (J)	0.5	7791.4586	-0.01748
	1.5	7811.5592	0.01613
	2.5	7826.4604	-0.00038
	3.5	7836.3205	0.00034
	5.5	7841.2388	-0.01840
	6.5	7836.4517	-0.01459
	7.5	7826.8798	0.00772
P _{1ee} (J)	2.5	7679.5811	-0.00006
	3.5	7642.2887	0.00033
	4.5	7600.8023	0.00066
	5.5	7555.0925	0.00117
	6.5	7505.1763	0.00062
	7.5	7451.0974	0.00061
	8.5	7392.9057	0.00072
	9.5	7330.6505	0.00004
	10.5	7264.3798	0.00048
	11.5	7194.1316	-0.00029
	12.5	7119.9403	-0.00172
	13.5	7041.8371	0.00041
P _{2ee} (J)	1.5	7700.8672	0.00131
	2.5	7661.2642	0.00164
	3.5	7617.4095	-0.00174
	4.5	7569.4979	0.00337
	5.5	7517.6194	0.00015
	6.5	7461.8416	0.00034

	7.5	7402.1884	-0.00052
	8.5	7338.6777	-0.00029
	9.5	7271.3194	0.00017
	10.5	7200.1229	0.00152
	11.5	7125.0936	0.00178
	12.5	7046.2361	0.00015
	13.5	6963.5480	-0.00831
Q _{2ef} (J)	0.5	7749.7111	0.00203
	1.5	7742.2801	0.00535
Q _{1fe} (J)	1.5	7748.5383	0.00080
	2.5	7739.3714	-0.00002
	3.5	7726.3368	0.00241
	4.5	7709.3006	-0.00091
R _{1ee} (J)	1.5	7808.2115	-0.00029
	2.5	7823.1131	-0.00037
	3.5	7834.2321	0.00020
	4.5	7841.2345	-0.13938
	5.5	7844.3633	0.00016
	6.5	7843.0539	0.00198
	7.5	7837.2598	-0.05910
	8.5	7826.8882	-0.17452
	9.5	7811.9428	-0.25263
R _{2ee} (J)	0.5	7791.4586	0.01599
	1.5	7811.5592	-0.01359
	2.5	7826.5464	-0.00033
	3.5	7836.4508	0.00387
	5.5	7841.3818	-0.02796
	6.5	7836.6051	0.00093
P _{1ff} (J)	2.5	7679.4739	-0.00004
	3.5	7642.0794	-0.00020

	4.5	7600.4701	0.00031
	5.5	7554.6217	0.00047
	6.5	7504.5560	0.00005
	7.5	7450.3179	0.00001
	8.5	7391.9587	0.00056
	9.5	7329.5284	0.00134
	10.5	7263.0708	0.00009
	11.5	7192.6306	0.00135
	12.5	7118.2380	0.00164
P _{2ff} (J)	1.5	7700.7505	0.00027
	2.5	7661.1880	0.00046
	3.5	7617.4095	0.00302
	4.5	7569.5801	-0.00122
	5.5	7517.8130	0.00057
	6.5	7462.1524	0.00059
	7.5	7402.6269	0.00104
	8.5	7339.2491	-0.00041
	9.5	7272.0331	-0.00016
	10.5	7200.9842	-0.00161
	11.5	7126.1137	-0.00088
	12.5	7047.6853	0.26025
Q _{2fe} (J)	0.5	7749.9169	-0.00119
Q _{1ef} (J)	1.5	7748.4765	-0.00122
	2.5	7739.1491	0.00087
	3.5	7725.8238	0.00214
	4.5	7708.3673	0.00000

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	J	Obs (cm-1)	Obs-Calc
R _{1ff} (J)	1.5	5057.7256	0.00493
	2.5	5075.6508	-0.00027

	3.5	5091.0678	-0.00043
	4.5	5103.8176	-0.00047
	5.5	5113.7526	-0.00034
	6.5	5120.7416	-0.00189
	7.5	5124.6796	0.00027
R _{2ff} (J)	0.5	5040.4109	-0.00242
	1.5	5062.9034	0.00712
	2.5	5081.7832	-0.00027
	3.5	5097.1133	-0.00017
	4.5	5108.9470	-0.00012
	5.5	5117.3381	0.00154
	6.5	5122.3137	0.00075
	7.5	5123.8856	0.00021
P _{1ee} (J)	2.5	4932.0245	-0.00023
	3.5	4899.0056	-0.00057
	4.5	4863.1152	-0.00103
	5.5	4824.3546	-0.00036
	6.5	4782.7587	-0.00021
	7.5	4738.3805	-0.00023
	8.5	4691.2766	-0.00002
	9.5	4641.5004	0.00039
	10.5	4589.0999	0.00090
	11.5	4534.1159	0.00046
	12.5	4476.5853	0.00051
	13.5	4416.5377	0.00159
P _{2ee} (J)	1.5	4952.2046	-0.00002
	3.5	4878.1985	0.00153
	4.5	4837.2201	-0.00096
	5.5	4793.7195	-0.00040
	6.5	4747.7300	-0.00040

	7.5	4699.2694	-0.00053
	8.5	4648.3475	-0.00078
	9.5	4594.9724	-0.00098
	10.5	4539.1518	-0.00135
	11.5	4480.8977	0.00217
	12.5	4420.2057	-0.00202
Q _{2ef} (J)	0.5	4998.6460	-0.00031
	1.5	4993.6276	-0.00035
	2.5	4985.4497	-0.00042
	3.5	4974.2138	-0.00184
Q _{1fe} (J)	1.5	4997.9864	-0.00008
	2.5	4991.8145	-0.00048
	3.5	4983.0517	-0.00050
	4.5	4971.6159	-0.00021
	5.5	4957.4407	-0.00032
	6.5	4940.4780	-0.00037
	7.5	4920.6915	-0.00101
R _{1ee} (J)	1.5	5057.6654	0.00463
	2.5	5075.5568	-0.00024
	3.5	5090.9498	0.00010
	4.5	5103.6885	0.00002
	5.5	5113.6260	-0.00077
	6.5	5120.6352	0.00006
	7.5	5124.6007	-0.00214
	8.5	5125.4492	0.01485
	9.5	5123.0300	-0.01499
	10.5	5117.2513	-0.10556
R _{2ee} (J)	0.5	5040.3697	-0.00106
	1.5	5062.9034	-0.00812
	2.5	5081.8556	0.00025

	3.5	5097.2319	-0.00077
	4.5	5109.1011	0.00047
	5.5	5117.5107	0.00029
	6.5	5122.4940	0.00068
	7.5	5124.0600	0.00106
	8.5	5122.2001	0.00216
P _{1ff} (J)	2.5	4931.9296	-0.00115
	3.5	4898.8255	-0.00080
	4.5	4862.8344	-0.00010
	5.5	4823.9607	-0.00041
	6.5	4782.2454	-0.00056
	7.5	4737.7431	-0.00019
	8.5	4690.5095	-0.00042
	9.5	4640.5993	-0.00013
	10.5	4588.0597	-0.00014
	11.5	4532.9326	-0.00030
	12.5	4475.2536	-0.00036
	13.5	4415.0512	-0.00073
P _{2ff} (J)	1.5	4952.1030	-0.00043
	3.5	4878.1985	-0.00129
	4.5	4837.2201	-0.08331
	5.5	4793.8924	0.00061
	6.5	4747.9986	0.00012
	7.5	4699.6389	-0.00027
	8.5	4648.8235	0.00051
	9.5	4595.5580	0.00035
	10.5	4539.8508	-0.00024
	11.5	4481.7118	0.00066
	12.5	4421.1470	0.00179
	13.5	4358.1583	-0.00034
Q _{2fe} (J)	0.5	4998.8461	-0.00014

	1.5	4993.9716	-0.00003
	2.5	4985.8387	-0.00080
	3.5	4974.5284	-0.00192
Q _{1ef} (J)	1.5	4997.9297	-0.00071
	2.5	4991.6047	-0.00034
	3.5	4982.5683	-0.00005
	4.5	4970.7321	0.00009
	5.5	4956.0339	0.00042
	6.5	4938.4297	-0.00200
	7.5	4917.9008	0.00073

8-7	J	Obs (cm-1)	Obs-Calc
R _{1ff} (J)	3.5	2514.1855	-0.00088
	4.5	2532.6690	-0.00080
	5.5	2549.7193	-0.00060
	6.5	2565.2269	-0.00088
	7.5	2579.0956	-0.00080
	8.5	2591.2391	-0.00060
	9.5	2601.5802	0.00014
	10.5	2610.0458	0.00009
R _{2ff} (J)	1.5	2480.5567	-0.00104
	2.5	2503.4707	-0.00026
	3.5	2524.3571	-0.00058
	5.5	2560.1366	-0.00043
	6.5	2575.0674	-0.00044
	7.5	2588.0304	-0.00064
	8.5	2599.0132	-0.00034
	9.5	2607.9837	-0.00734
P _{1ee} (J)	2.5	2350.7418	-0.00520
	3.5	2322.2421	0.14718

P _{2ee} (J)	2.5	2338.2532	0.01208
R _{1ee} (J)	1.5	2473.3190	0.00005
	2.5	2494.2795	0.00019
	3.5	2514.0382	-0.00026
	4.5	2532.4885	-0.00027
	5.5	2549.5144	-0.00052
	6.5	2565.0081	-0.00035
	7.5	2578.8720	-0.00030
	8.5	2591.0195	-0.00076
	9.5	2601.3743	-0.00034
	10.5	2609.8629	-0.00076
R _{2ee} (J)	1.5	2480.5567	0.00054
	2.5	2503.5247	-0.00059
	3.5	2524.4645	-0.00046
	6.5	2575.2855	-0.00032
	7.5	2588.2672	-0.00058
	8.5	2599.2585	-0.00167
	9.5	2608.2363	-0.00254
P _{1ff} (J)	2.5	2350.6608	-0.00557
	3.5	2322.0915	0.14705
P _{2ff} (J)	2.5	2338.1872	-0.01051

9-6 J Obs (cm-1) Obs-Calc

R _{1ff} (J)	1.5	7290.3363	0.00010
	2.5	7303.5039	0.00065
	3.5	7312.7016	0.00081
	4.5	7317.7385	-0.00022
	5.5	7318.4393	-0.00162
	6.5	7314.6563	0.00128
	7.5	7306.2519	0.00136

	8.5	7293.1172	0.00408
	9.5	7275.1406	0.00227
R _{2ff} (J)	0.5	7273.9141	-0.00799
	1.5	7292.1041	-0.00073
	2.5	7305.0370	-0.00010
	3.5	7312.7907	-0.00022
	4.5	7315.4509	0.00123
	5.5	7313.0773	0.00046
	6.5	7305.7090	0.00353
P _{1ee} (J)	2.5	7167.9943	-0.00041
	3.5	7131.6353	-0.00016
	4.5	7090.9989	-0.00051
	5.5	7046.0426	-0.00027
	6.5	6996.7654	-0.00047
	7.5	6943.1919	-0.00020
	8.5	6885.3539	-0.00041
	9.5	6823.2854	-0.00025
	10.5	6757.0144	-0.00046
	11.5	6686.5652	0.00131
	12.5	6611.9494	0.00301
P _{2ee} (J)	1.5	7188.3357	0.00149
	2.5	7150.1058	0.00044
	3.5	7107.4216	-0.01400
	4.5	7060.5015	-0.00084
	5.5	7009.4153	-0.00030
	6.5	6954.2349	-0.00049
	7.5	6894.9904	-0.00058
	8.5	6831.6944	-0.00010
	10.5	6692.9487	-0.00079
	11.5	6617.4889	0.00037

Q _{2ef} (J)	0.5	7234.7761	0.00020
	1.5	7227.1627	0.00057
Q _{1fe} (J)	1.5	7233.9535	0.00079
	2.5	7224.4313	0.00078
	3.5	7210.9046	0.00022
	4.5	7193.2490	0.00033
	5.5	7171.3649	0.00323
R _{1ee} (J)	1.5	7290.2905	0.00043
	2.5	7303.4395	-0.00071
	3.5	7312.6374	-0.00021
	4.5	7317.6976	0.00215
	5.5	7318.4393	0.00116
	6.5	7314.7140	0.00116
	7.5	7306.3896	0.00113
R _{2ee} (J)	8.5	7293.3453	-0.00491
	0.5	7273.9141	0.00916
	1.5	7292.1507	0.00054
	2.5	7305.1367	0.00007
	3.5	7312.9279	-0.00047
	4.5	7315.6052	-0.00042
	5.5	7313.2331	0.00164
P _{1ff} (J)	6.5	7305.8410	0.00146
	2.5	7167.8970	0.00002
	3.5	7131.4413	-0.00053
	4.5	7090.6866	-0.00009
	5.5	7045.5934	-0.00027
	6.5	6996.1664	-0.00020
	7.5	6942.4311	-0.00018
	8.5	6884.4216	0.00015
	9.5	6822.1704	-0.00024

	10.5	6755.7072	-0.00048
	11.5	6685.0556	0.00117
	12.5	6610.2231	-0.00131
$P_{2ff}(J)$	1.5	7188.2187	0.00024
	2.5	7150.0190	0.00000
	3.5	7107.4216	0.01326
	4.5	7060.5585	0.00145
	5.5	7009.5694	0.00016
	6.5	6954.5011	0.00007
	7.5	6895.3793	-0.00014
	8.5	6832.2163	0.00079
	9.5	6765.0104	-0.00091
	10.5	6693.7625	-0.00056
	11.5	6618.4605	-0.00135
$Q_{2fe}(J)$	0.5	7234.9611	-0.00017
	1.5	7227.4795	-0.00090
$Q_{1ef}(J)$	1.5	7233.8999	-0.00050
	2.5	7224.2335	-0.00084
	3.5	7210.4510	-0.00053
	4.5	7192.4221	0.00218
	5.5	7170.0422	0.00176

9-7	J	Obs (cm-1)	Obs-Calc
$R_{1ff}(J)$	1.5	4705.9897	-0.00839
	2.5	4722.2405	0.00163
	3.5	4735.8201	0.00116
	4.5	4746.5909	0.00046
	5.5	4754.4088	0.00091
	7.5	4760.6630	-0.00462
	9.5	4753.6999	-0.00168

R _{2ff} (J)	0.5	4689.1227	-0.01385
	2.5	4726.7234	-0.00119
	3.5	4740.0365	0.00137
	4.5	4749.7405	-0.00040
	5.5	4755.8775	0.00020
	6.5	4758.4606	0.00024
	7.5	4757.4862	0.00150
	8.5	4752.9191	-0.00646
	P _{1ee} (J)	2.5	4586.7175
3.5		4554.7244	0.00018
4.5		4519.7994	-0.00029
5.5		4481.9306	-0.00042
6.5		4441.1390	-0.00018
7.5		4397.4616	0.00005
8.5		4350.9402	-0.00002
9.5		4301.6150	-0.00030
10.5		4249.5210	-0.00067
11.5		4194.6877	0.00034
P _{2ee} (J)	12.5	4137.1324	-0.00035
	13.5	4076.8627	-0.00732
	2.5	4571.7771	0.00180
	3.5	4534.6603	-0.00760
	5.5	4452.2323	-0.00005
	6.5	4407.0277	-0.00020
	7.5	4359.1995	-0.00033
	8.5	4308.7566	-0.00014
	9.5	4255.7009	-0.00064
	10.5	4200.0346	0.00085
11.5	4141.7514	0.00161	
12.5	4080.8405	-0.00186	

Q _{2ef} (J)	0.5	4649.9905	0.00013
	1.5	4644.8235	-0.00010
	2.5	4636.3769	0.00066
	3.5	4624.7435	0.00237
Q _{1fe} (J)	1.5	4649.6120	0.00111
	2.5	4643.1526	-0.00019
	3.5	4633.9931	-0.00003
	4.5	4622.0486	-0.00035
	5.5	4607.2504	0.00059
	6.5	4589.5398	0.00014
	7.5	4568.8714	-0.00210
R _{1ee} (J)	1.5	4705.9523	0.00406
	2.5	4722.1621	-0.00039
	4.5	4746.4955	-0.00023
	5.5	4754.3246	-0.00168
	7.5	4760.6630	0.00507
	9.5	4753.8189	-0.00419
R _{2ee} (J)	1.5	4709.7804	-0.01439
	2.5	4726.8064	-0.00017
	3.5	4740.1527	-0.00796
	4.5	4749.8958	-0.00065
	5.5	4756.0494	0.00118
	6.5	4758.6314	-0.00064
	7.5	4757.6465	0.00357
	8.5	4753.0574	0.00088
P _{1ff} (J)	2.5	4586.6313	-0.00130
	3.5	4554.5593	-0.00068
	4.5	4519.5379	-0.00051
	5.5	4481.5607	0.00007
	6.5	4440.6508	-0.00010

	7.5	4396.8481	-0.00025
	8.5	4350.1958	-0.00007
	9.5	4300.7332	-0.00069
	10.5	4248.4961	-0.00122
	11.5	4193.5062	-0.00791
	12.5	4135.8018	-0.00276
	13.5	4075.3819	0.00117
	14.5	4012.2456	-0.00026
$P_{2ff}(J)$	1.5	4605.8797	-0.00023
	2.5	4571.7063	-0.00018
	3.5	4534.6603	0.00774
	5.5	4452.3694	-0.00031
	6.5	4407.2557	-0.00022
	7.5	4359.5248	-0.00029
	8.5	4309.1846	-0.00033
	9.5	4256.2374	-0.00056
	10.5	4200.6808	-0.00276
	11.5	4142.5190	0.00088
$Q_{2fe}(J)$	0.5	4650.1661	0.00062
	1.5	4645.1257	0.00067
	2.5	4636.7183	0.00030
$Q_{1ef}(J)$	1.5	4649.5613	-0.00098
	2.5	4642.9702	0.00025
	3.5	4633.5697	0.00002
	4.5	4621.2714	-0.00025
	6.5	4587.7284	0.00103
9-8	J	Obs (cm-1)	Obs-Calc
$R_{1ff}(J)$	1.5	2292.3816	0.00015
	2.5	2311.8067	0.00011

	3.5	2329.9205	0.00041
	4.5	2346.6166	-0.00009
	5.5	2361.7838	0.00003
	6.5	2375.3130	-0.00027
	7.5	2387.1053	-0.00021
	8.5	2397.0683	-0.00060
	9.5	2405.1179	0.00005
	10.5	2411.1707	0.00033
	11.5	2415.2286	0.08272
	12.5	2416.9686	0.00539
$R_{2ff}(J)$	0.5	2275.1884	0.00160
	1.5	2298.3271	0.00373
	2.5	2319.4125	0.00044
	3.5	2338.4327	0.00000
	4.5	2355.3907	-0.00031
	5.5	2370.2966	0.00001
	6.5	2383.1510	0.00032
	7.5	2393.9411	-0.00062
	8.5	2402.6464	0.00131
	9.5	2409.2244	0.00002
$P_{1ee}(J)$	2.5	2176.2714	0.00005
	3.5	2148.7953	-0.00032
	4.5	2119.7768	0.00348
	5.5	2089.2246	-0.00092
$P_{2ee}(J)$	1.5	2194.5152	-0.00090
	2.5	2164.4406	-0.00017
	3.5	2133.0475	-0.00037
	4.5	2100.4449	0.00855
	5.5	2066.6637	0.00264
$Q_{2ef}(J)$	0.5	2236.0411	0.00048

Q _{1fe} (J)	1.5	2235.9903	-0.00027
	2.5	2232.7071	-0.00006
	3.5	2228.0634	-0.00113
	4.5	2222.0238	0.00122
	5.5	2214.3578	-0.18651
R _{1ee} (J)	1.5	2292.3276	-0.00033
	2.5	2311.7170	0.00014
	3.5	2329.7972	-0.00057
	4.5	2346.4692	-0.00016
	5.5	2361.6201	-0.00068
	6.5	2375.1437	-0.00081
	7.5	2386.9401	-0.00082
	8.5	2396.9180	-0.00031
	9.5	2404.9916	0.00062
	10.5	2411.0796	0.00267
	11.5	2415.0990	0.00342
R _{2ee} (J)	12.5	2416.9686	0.00276
	0.5	2275.1445	-0.00318
	1.5	2298.3271	-0.00494
	2.5	2319.4706	-0.00144
	3.5	2338.5395	-0.00113
	4.5	2355.5388	-0.00083
	5.5	2370.4761	-0.00082
	6.5	2383.3535	0.00023
	7.5	2394.1573	0.00018
	8.5	2402.8634	-0.00063
	9.5	2409.4375	-0.00027
P _{1ff} (J)	2.5	2176.1986	-0.00172
	3.5	2148.6618	0.00067
	4.5	2119.5647	0.00005

	5.5	2088.9340	-0.00252
P _{2ff} (J)	1.5	2194.4361	-0.00090
	2.5	2164.3927	-0.00126
	3.5	2133.0475	-0.00263
	4.5	2100.4965	-0.00188
	5.5	2066.7868	-0.00219
Q _{2fe} (J)	0.5	2236.2070	0.00299
	1.5	2233.6630	0.00072
Q _{1ef} (J)	1.5	2235.9452	-0.00044
	2.5	2232.5382	0.00053
	3.5	2227.6706	-0.00023
	4.5	2221.2987	0.00081
	5.5	2213.3826	-0.00070
	6.5	2203.7537	-0.14762

10-8	J	Obs (cm-1)	Obs-Calc
R _{1ff} (J)	1.5	4337.0654	-0.00056
	2.5	4351.3851	-0.00428
	3.5	4362.8502	0.00305
	4.5	4371.2897	-0.00361
	5.5	4376.5663	-0.01395
	6.5	4378.5716	0.00275
R _{2ff} (J)	0.5	4320.5511	-0.00189
	1.5	4339.1326	0.00051
	2.5	4353.8972	-0.00054
	3.5	4364.8596	0.00148
	4.5	4372.0299	-0.00675
	5.5	4375.4473	-0.00159
P _{1ee} (J)	2.5	4224.5526	-0.00054
	3.5	4193.5062	0.01201

	4.5	4159.3875	-0.00068
	5.5	4122.2107	0.00019
	6.5	4081.9659	0.00040
	7.5	4038.6717	-0.00118
	8.5	3992.3570	-0.00015
	9.5	3943.0430	0.00213
	10.5	3890.7394	-0.00119
P _{2ee} (J)	1.5	4242.6625	0.00396
	2.5	4209.8390	-0.00055
	3.5	4173.9009	0.00369
	4.5	4134.9749	0.01182
	5.5	4093.1202	-0.00009
	6.5	4048.4125	-0.00149
	7.5	4000.8614	-0.00272
	8.5	3950.4765	0.00161
	9.5	3897.2394	-0.00086
	10.5	3841.1458	-0.00055
Q _{1fe} (J)	2.5	4277.3938	0.00213
	3.5	4267.6499	0.00257
	4.5	4254.9413	-0.00834
R _{1ee} (J)	1.5	4337.0281	0.00160
	2.5	4351.3172	-0.01452
	3.5	4362.7792	-0.00356
	4.5	4371.2300	-0.00731
	5.5	4376.5663	0.01719
	6.5	4378.5716	-0.00766
R _{2ee} (J)	0.5	4320.5511	0.00465
	1.5	4339.1812	-0.00018
	2.5	4353.9955	-0.00328
	3.5	4364.9998	-0.00005

	4.5	4372.2060	0.00151
	5.5	4375.6307	0.00367
P _{1ff} (J)	2.5	4224.4748	-0.00351
	3.5	4193.3439	-0.00174
	4.5	4159.1471	-0.00035
	5.5	4121.8635	-0.00008
	6.5	4081.5013	-0.00018
	7.5	4038.0830	0.00028
	8.5	3991.6308	-0.00201
	9.5	3942.1722	-0.00254
	10.5	3889.7292	0.00402
P _{2ff} (J)	1.5	4242.5595	-0.00177
	2.5	4209.7587	-0.00144
	3.5	4173.8613	0.00245
	4.5	4134.9749	-0.00916
	5.5	4093.2147	0.00028
	6.5	4048.5926	0.00072
	7.5	4001.1336	-0.00081
	8.5	3950.8354	-0.00978
	9.5	3897.7190	0.00138
	10.5	3841.7240	-0.01363
Q _{1ef} (J)	2.5	4277.2368	0.00055
	3.5	4267.2853	-0.00039
	4.5	4254.6161	0.33322
10-9	J	Obs (cm-1)	Obs-Calc
R _{1ff} (J)	1.5	2101.1001	0.00038
	2.5	2118.7818	0.00795
	3.5	2134.9956	0.00063
	4.5	2149.6602	-0.00055

	5.5	2162.6596	0.00000
	6.5	2173.8807	-0.00017
	7.5	2183.2189	0.00033
	8.5	2190.5721	0.00076
	9.5	2195.8101	-0.03056
	10.5	2198.9443	0.01589
R _{2ff} (J)	1.5	2105.6412	0.01788
	2.5	2124.6907	0.00151
	3.5	2141.6114	0.00691
	4.5	2156.3499	-0.00930
	5.5	2168.9440	-0.00234
	6.5	2179.3537	0.00258
R _{1ee} (J)	1.5	2101.0618	0.00528
	2.5	2118.6936	-0.00882
	3.5	2134.8956	-0.00398
	4.5	2149.5470	-0.00240
	5.5	2162.5410	-0.00115
	6.5	2173.7709	0.00301
	7.5	2183.1236	0.00269
	8.5	2190.5003	0.00037
	9.5	2195.8101	0.00360
	10.5	2198.9443	0.00165
R _{2ee} (J)	1.5	2105.6412	-0.00600
	2.5	2124.7692	0.00906
	3.5	2141.7160	-0.00258
	4.5	2156.5122	0.00341
	5.5	2169.1266	0.00456
	6.5	2179.5418	-0.00104

11-9 J Obs (cm-1) Obs-Calc

P _{1ee} (J)	2.5	3838.4500	-0.0029
	3.5	3808.2300	0.0168
	4.5	3774.7500	0.0128
	5.5	3737.9900	0.0030
	6.5	3697.9500	0.0029
	7.5	3654.6100	-0.0046
	8.5	3607.9900	-0.0001
	9.5	3558.0700	-0.0019
	P _{2ee} (J)	1.5	3855.0400
2.5		3823.5800	0.0014
3.5		3788.6900	0.0002
4.5		3750.5000	-0.0055
5.5		3709.1200	0.0154
6.5		3664.5600	0.0311
P _{1ff} (J)	2.5	3838.3900	0.0024
	3.5	3808.1000	0.0203
	4.5	3774.5200	0.0047
	5.5	3737.6600	0.0002
P _{2ff} (J)	1.5	3854.9300	-0.0105
	2.5	3823.4500	-0.0083
	3.5	3788.5700	-0.0118
	4.5	3750.4300	0.0003
	5.5	3709.0900	0.0124
	6.5	3664.6000	0.0360

12-8	J	Obs (cm-1)	Obs-Calc
R _{1ff} (J)	1.5	7801.0500	0.0632
	2.5	7803.4700	0.0431
	3.5	7799.4600	0.0604
	4.5	7788.6200	-0.0366

	5.5	7771.0200	0.0677
	6.5	7746.0000	-0.0520
R _{2ff} (J)	0.5	7784.6100	0.0732
	1.5	7792.7500	0.0710
	2.5	7792.9600	0.0397
	3.5	7785.4000	0.0950
	4.5	7769.9800	0.1093
	5.5	7746.6100	-0.0111
P _{1ee} (J)	2.5	7696.8200	-0.0470
P _{2ee} (J)	1.5	7713.0400	0.0440
Q _{2ef} (J)	0.5	7754.5600	0.0394
	1.5	7742.8700	0.0099
Q _{1fe} (J)	1.5	7756.6400	0.0651
	2.5	7741.3800	0.0674
	3.5	7719.7100	0.0251
	4.5	7691.4800	-0.0222
R _{1ee} (J)	1.5	7801.0500	0.0746
	2.5	7803.4700	0.0358
	3.5	7799.5400	0.0854
	4.5	7788.8700	0.0782
	5.5	7771.2500	0.0489
	6.5	7746.4800	0.0325
R _{2ee} (J)	0.5	7784.7000	0.0728
	1.5	7792.9700	0.1121
	2.5	7793.2700	0.1013
	3.5	7785.6700	0.0737
	4.5	7770.3000	0.1248
	5.5	7747.0700	0.1612
P _{1ff} (J)	2.5	7696.7700	-0.0146
	3.5	7657.3100	0.0435
	1.5	7712.8600	0.0131

	0.5	7754.5600	-0.0539
	1.5	7743.0100	-0.0023
Q _{1ef} (J)	1.5	7756.5600	0.0188
	2.5	7741.1600	-0.0252
	3.5	7719.3800	-0.0081
	4.5	7690.9800	0.0254

B²Σ⁺-X²Π

0-7	J	Obs (cm-1)	Obs-Calc
R _{1ee} (J)	5.5	46677.18	-0.0014
R _{2ee} (J)	5.5	46444.74	-0.1019
	7.5	46197.34	-0.0116
	8.5	46048.02	-0.0047
P _{1ee} (J)	1.5	46870.10	-0.0035
	2.5	46817.41	-0.0011
	3.5	46749.39	-0.0047
	4.5	46665.82	-0.0090
	5.5	46566.51	-0.0059
	9.5	46010.64	0.0038
P _{2ee} (J)	2.5	46632.77	0.0028
	3.5	46551.18	-0.0102
	6.5	46199.53	-0.0177
R _{2ff} (J)	0.5	46770.25	-0.0152

	2.5	46723.70	-0.0020
	3.5	46672.21	-0.0117
	4.5	46602.45	0.0084
	5.5	46514.68	-0.0034
R _{1ff} (J)	1.5	46930.92	-0.0183
	2.5	46908.44	-0.0058
	3.5	46870.36	0.0138
	4.5	46816.34	-0.0133
	5.5	46746.21	-0.0070
	6.5	46659.74	0.0015
	7.5	46556.80	-0.0063
P _{2ff} (J)	5.5	46384.53	-0.0263
P _{1ff} (J)	1.5	46880.22	-0.0020
	2.5	46837.58	-0.0030
	3.5	46779.50	-0.0052
	4.5	46705.73	-0.0083
	5.5	46616.08	-0.0119
	6.5	46510.40	-0.0147
	7.5	46388.64	-0.0174
	8.5	46250.78	-0.0180
	9.5	46096.85	-0.0166
Q _{1ef} (J)	6.5	46510.57	-0.0044
	7.5	46388.82	-0.0187
Q _{2ef} (J)	0.5	46739.81	0.0026
	5.5	46384.68	-0.0209
Q _{1fe} (J)	5.5	46677.00	-0.0148
Q _{2fe} (J)	5.5	46444.62	-0.0572
	7.5	46197.15	-0.0036
	8.5	46047.81	0.0082

0-8	J	Obs (cm-1)	Obs-Calc
R _{1ee} (J)	1.5	44487.04	0.0337
	2.5	44457.75	0.0059
	6.5	44197.60	0.0113
	7.5	44095.97	0.0139
	9.5	43848.40	0.0401
R _{2ee} (J)	2.5	44276.18	-0.0172
	4.5	44148.04	-0.0194
	5.5	44059.26	-0.0105
	6.5	43954.47	0.0314
	7.5	43833.86	-0.0058
	8.5	43697.76	-0.0642
P _{1ee} (J)	9.5	43546.58	-0.0009
	1.5	44456.49	0.0089
	2.5	44406.96	-0.0055
	3.5	44343.47	-0.0041
	4.5	44265.80	0.0014
	5.5	44173.81	0.0015
	6.5	44067.43	0.0111
	7.5	43946.62	0.0201
P _{2ee} (J)	8.5	43811.37	0.0014
	2.5	44225.44	0.0094
	3.5	44149.55	-0.0181
	4.5	44057.17	0.0046
	5.5	43948.59	-0.0110
R _{2ff} (J)	6.5	43824.28	0.0112
	0.5	44356.33	0.0124
	1.5	44345.03	-0.0176
	2.5	44316.39	0.0005
	3.5	44270.64	0.0167

	4.5	44208.10	0.0103
	6.5	44033.98	0.0143
	7.5	43922.96	0.0229
	8.5	43796.25	0.0013
R _{1ff} (J)	1.5	44517.35	0.0283
	2.5	44498.02	0.0085
	3.5	44464.45	0.0046
	4.5	44416.38	0.0005
	5.5	44353.61	0.0182
	7.5	44183.26	0.0219
P _{2ff} (J)	1.5	44294.34	0.0088
	2.5	44245.51	-0.0167
	3.5	44179.78	-0.0013
	4.5	44097.47	-0.0038
	5.5	43999.00	0.0224
	6.5	43884.64	-0.0050
	7.5	43754.76	-0.0282
P _{1ff} (J)	3.5	44373.60	-0.0054
	4.5	44305.78	0.0165
	5.5	44223.48	0.0162
	6.5	44126.58	-0.0136
	7.5	44015.11	0.0187
	8.5	43888.99	0.0137
	9.5	43748.34	0.0593
	10.5	43593.14	0.0479
Q _{1ef} (J)	3.5	44373.72	0.0220
	4.5	44305.90	0.0213
	5.5	44223.61	0.0077
	6.5	44126.75	0.0017
	7.5	44015.28	0.0075

	8.5	43889.18	-0.0024
	9.5	43748.50	0.0004
	10.5	43593.34	0.0144
Q _{2ef} (J)	2.5	44245.59	0.0060
	3.5	44179.91	0.0421
	4.5	44097.60	0.0151
	5.5	43999.13	0.0098
	6.5	43884.79	-0.0117
	7.5	43754.95	-0.0255
Q _{1fe} (J)	1.5	44486.95	0.0110
	2.5	44457.66	0.0046
	6.5	44197.43	0.0186
	7.5	44095.78	0.0180
	9.5	43848.10	-0.0314
Q _{2fe} (J)	2.5	44276.06	-0.0486
	4.5	44147.91	-0.0088
	5.5	44059.11	0.0062
	6.5	43954.27	0.0107
	7.5	43833.67	0.0003
	8.5	43697.60	-0.0073
	9.5	43546.35	0.0026

	0-9	J	Obs (cm-1)	Obs-Calc
R _{1ee} (J)		2.5	42225.11	-0.0068
		3.5	42186.50	0.0025
		5.5	42070.46	-0.0030
		7.5	41901.89	0.0058
		8.5	41797.77	0.0087
		3.5	41997.18	-0.0214
		4.5	41932.35	-0.0117

P _{1ee} (J)	5.5	41852.78	0.0165
	1.5	42220.51	-0.0032
	2.5	42174.34	-0.0042
	3.5	42115.59	0.0011
	4.5	42044.11	-0.0027
P _{2ee} (J)	5.5	41959.80	-0.0055
	6.5	41862.61	0.0006
	1.5	42050.79	-0.0170
	2.5	41996.20	0.0080
	3.5	41926.29	-0.0038
R _{2ff} (J)	4.5	41841.48	0.0102
	0.5	42120.22	0.0156
	1.5	42111.55	0.0063
	2.5	42087.22	0.0441
	3.5	42047.35	-0.0157
R _{1ff} (J)	5.5	41922.59	-0.0142
	6.5	41838.23	0.0035
	1.5	42281.37	0.0086
	2.5	42265.39	0.0001
	6.5	42071.23	0.0037
P _{2ff} (J)	2.5	42016.33	0.0159
	3.5	41956.50	-0.0277
	4.5	41881.80	0.0057
P _{1ff} (J)	5.5	41792.47	-0.0051
	3.5	42145.74	-0.0092
	4.5	42084.14	0.0071
	5.5	42009.52	-0.0291
	6.5	41921.91	0.0064
Q _{1ef} (J)	7.5	41821.14	-0.0417
	3.5	42145.85	0.0102

	4.5	42084.26	0.0059
	5.5	42009.68	-0.0036
	6.5	41922.07	0.0057
	7.5	41821.36	-0.0010
Q _{2ef} (J)	0.5	42089.74	-0.0066
	2.5	42016.41	0.0306
	3.5	41956.59	-0.0223
	4.5	41881.92	0.0105
	5.5	41792.62	0.0043
Q _{1fe} (J)	2.5	42225.00	-0.0261
	3.5	42186.39	0.0057
	5.5	42070.31	0.0037
	7.5	41901.68	0.0019
	8.5	41797.52	-0.0224
Q _{2fe} (J)	3.5	41997.07	-0.0203
	4.5	41932.22	0.0009
	5.5	41852.61	0.0092

0-11	J	Obs (cm-1)	Obs-Calc
R _{1ee} (J)	4.5	38272.24	0.0088
P _{1ee} (J)	1.5	38325.71	0.0037
	2.5	38287.04	0.0045
	3.5	38238.93	-0.0051
R _{2ff} (J)	0.5	38226.19	-0.0022
	1.5	38223.26	-0.0109
	2.5	38208.40	0.0054
	3.5	38181.77	0.0101
	4.5	38143.62	0.0008
R _{1ff} (J)	1.5	38386.56	0.0054
	2.5	38378.14	0.0149

	3.5	38360.02	0.0081
Q _{2ef} (J)	0.5	38195.72	-0.0184
Q _{1fe} (J)	4.5	38272.09	-0.0016
0-12	J	Obs (cm-1)	Obs-Calc
R _{1ee} (J)	1.5	36730.42	-0.0152
	2.5	36716.40	-0.0643
	3.5	36694.74	-0.0411
	4.5	36665.22	-0.1248
	5.5	36628.06	-0.0815
	1.5	36699.93	0.0134
P _{1ee} (J)	2.5	36665.72	0.0284
	3.5	36623.86	-0.0085
	4.5	36574.46	0.0071
	5.5	36517.46	-0.0200
	6.5	36453.04	0.0139
P _{2ee} (J)	1.5	36541.34	0.0175
	2.5	36501.62	-0.0432
	3.5	36452.56	-0.0332
R _{2ff} (J)	0.5	36601.89	0.1003
	1.5	36602.31	0.1192
	2.5	36592.80	-0.0203
P _{2ff} (J)	1.5	36551.48	0.0106
	2.5	36522.00	0.0425
	3.5	36483.00	-0.0145
	4.5	36434.94	0.0190
Q _{1ef} (J)	1.5	36710.09	-0.0022
	2.5	36686.00	0.0099
	3.5	36654.18	-0.0425

	4.5	36614.78	0.0104
	5.5	36567.66	0.0172
	6.5	36512.88	-0.0148
Q _{2ef} (J)	0.5	36571.34	0.0042
Q _{2fe} (J)	0.5	36581.48	-0.0057
	1.5	36571.80	0.0236
	2.5	36552.34	-0.0052
	3.5	36523.38	-0.0106
	4.5	36485.18	0.0136
	5.5	36438.00	0.0358

0-13	J	Obs (cm-1)	Obs-Calc
R _{1ee} (J)	1.5	35350.41	-0.0126
	2.5	35341.54	-0.0427
	3.5	35327.19	0.0300
	4.5	35307.20	0.0201
R _{2ee} (J)	3.5	35164.63	-0.0078
	4.5	35137.60	-0.0305
	5.5	35104.14	-0.0366
	6.5	35064.62	-0.0024
P _{1ee} (J)	1.5	35319.90	-0.0034
	2.5	35290.82	0.0139
	3.5	35256.25	0.0066
	4.5	35216.29	0.0080
	5.5	35171.03	-0.0037
	6.5	35120.65	-0.0155
	7.5	35065.37	0.0007
P _{2ee} (J)	1.5	35167.57	0.0091
	2.5	35134.09	-0.0036
	3.5	35093.71	-0.0092

	5.5	34993.51	0.0029
R _{2ff} (J)	0.5	35224.38	-0.0161
	1.5	35228.55	-0.0188
	2.5	35225.44	-0.0199
	3.5	35215.24	-0.0049
R _{1ff} (J)	1.5	35380.76	-0.0018
	2.5	35381.92	-0.0102
	3.5	35377.40	-0.0084
	4.5	35367.21	0.0146
	5.5	35351.34	-0.0093
P _{2ff} (J)	1.5	35177.87	0.0206
	2.5	35154.62	0.0189
	3.5	35124.39	-0.0069
	4.5	35087.53	-0.0114
	6.5	34995.29	0.0506
P _{1ff} (J)	1.5	35330.06	0.0176
	2.5	35311.06	0.0016
	3.5	35286.57	0.0056
	4.5	35256.58	-0.0044
	5.5	35221.22	-0.0041
	6.5	35180.60	-0.0081
	7.5	35134.95	0.0128
Q _{1ef} (J)	1.5	35330.06	-0.0218
	2.5	35311.14	0.0083
	3.5	35286.66	0.0110
	4.5	35256.70	0.0024
	5.5	35221.36	0.0022
	6.5	35180.77	-0.0008
	7.5	35135.11	-0.0125
Q _{2ef} (J)	0.5	35193.95	0.0077

	3.5	35124.49	0.0025
	4.5	35087.66	0.0015
Q _{1fe} (J)	1.5	35350.34	-0.0133
	2.5	35341.44	-0.0540
	3.5	35327.06	0.0162
	4.5	35307.04	0.0046
Q _{2fe} (J)	0.5	35204.04	0.0224
	1.5	35198.05	0.0363
	2.5	35184.83	0.0544
	3.5	35164.50	-0.0147
	4.5	35137.49	0.0010
	5.5	35104.01	0.0021
	6.5	35064.46	0.0178

1-9	J	Obs (cm-1)	Obs-Calc
R _{1ee} (J)	2.5	42872.95	0.0276
	3.5	42826.06	-0.0052
	4.5	42763.96	0.0099
	5.5	42686.13	-0.0024
	6.5	42592.10	0.0078
	7.5	42481.18	-0.0061
R _{2ee} (J)	2.5	42694.78	0.0078
	3.5	42636.73	-0.0351
	6.5	42358.09	0.0554
P _{1ee} (J)	1.5	42880.33	-0.0144
	2.5	42832.19	0.0014
	3.5	42769.46	0.0059
	4.5	42691.92	0.0036
	5.5	42599.37	0.0067
	6.5	42491.54	-0.0089

P _{2ee} (J)	7.5	42368.18	-0.0075
	1.5	42710.61	-0.0222
	2.5	42654.04	-0.0064
	3.5	42580.17	0.0080
	4.5	42489.32	0.0386
R _{2ff} (J)	5.5	42381.67	0.0062
	0.5	42774.10	0.0231
	1.5	42759.40	0.0300
	2.5	42726.79	0.0192
	3.5	42676.34	-0.0134
R _{1ff} (J)	4.5	42608.09	-0.0394
	5.5	42522.02	0.0258
	1.5	42929.21	0.0243
	3.5	42865.57	-0.0089
	P _{2ff} (J)	3.5	42604.39
4.5		42521.36	-0.0242
5.5		42421.46	-0.0029
6.5		42304.62	-0.0019
P _{1ff} (J)		4.5	42723.72
	5.5	42638.53	-0.0009
	6.5	42537.66	0.0313
	7.5	42420.55	-0.0277
	Q _{1ef} (J)	4.5	42723.81
5.5		42638.63	-0.0011
6.5		42537.74	0.0123
7.5		42420.69	0.0060
Q _{2ef} (J)		0.5	42749.57
	3.5	42604.46	0.0401
	4.5	42521.45	-0.0232
	5.5	42421.54	-0.0171

Q _{1fe} (J)	6.5	42304.72	-0.0049
	2.5	42872.86	0.0036
	3.5	42825.97	-0.0102
	4.5	42763.86	0.0121
	5.5	42686.02	-0.0075
	6.5	42592.00	0.0080
Q _{2fe} (J)	7.5	42481.08	-0.0048
	2.5	42694.68	-0.0183
	3.5	42636.67	-0.0082
	6.5	42357.94	0.0097