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Fourier Transform Infrared Emission Spectroscopy of CS

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The vibration–rotation spectrum of CS was observed in emission in the spectral region 1000–1400 cm^{-1} with a Fourier transform spectrometer. The observed spectrum consists of nine $\Delta v = 1$ vibration–rotation bands with $v \leq 9$. The present data combined with previous infrared and microwave measurements provide an improved set of molecular constants. © 1995 Academic Press, Inc.

INTRODUCTION

CS is an important species of atmospheric (*1*) as well as astrophysical interest (*2–8*). CS is formed as intermediate in the photochemical and oxidative reactions of CS_2 (*1*). CS is also one of the most abundant sulfur-containing species in interstellar clouds (*2, 3*). A variety of astronomical objects contain CS, including carbon-rich stars, such as IRC + 10216 (*4, 5*), star-forming regions (*6*), and comets (*7, 8*). Several sulfur-containing linear carbon chain molecules, such as C_2S (*9*) and C_3S (*10*), have also been observed in various extraterrestrial sources. The CS molecule is the first member of the linear C_nS family of molecules.

Because of its relatively long chemical lifetime (*11*), CS and its various isotopomers have been studied extensively in the past decade from the infrared to the vacuum ultraviolet regions. The $A^1\Pi$–$X^1\Sigma^+$ transition has been studied by various workers (*12–14*) over the past several decades. Lagerqvist *et al.* (*13*) observed many perturbations in the excited states and Barrow *et al.* (*14*) identified several triplet states responsible for these perturbations. More recent work is available (*15, 16*), including a definitive deperturbation analysis (*15*). Several additional electronic transitions have been investigated in the visible to the vacuum ultraviolet regions (*17, 18*).

The infrared vibration–rotation spectra of CS have been studied by several authors (*19–23*). Todd (*19*) measured the 2–0 band using a grating spectrometer while Yamada and Hirota (*20*) and Todd and Olson (*21*) measured several $\Delta v = 1$ bands of $^{12}C^{32}S$ and the isotopomers $^{12}C^{34}S$, $^{12}C^{33}S$, and $^{13}C^{32}S$, using a tunable diode laser spectrometer. The infrared bands have also been studied recently with a Fourier transform spectrometer (*22, 23*). The work of Winkel *et al.* (*22*) provided measurements of many $\Delta v = 2$ bands with vibrational levels up to $v = 8$. Although this study provided much-improved molecular parameters, the overtone bands studied do not provide a direct link between the successive vibrational levels. This may result in some uncertainty in the vibrational constants. More recently, Burkholder *et al.* (*23*) have obtained high-resolution measurements of the 1–0 and 2–1 bands of $^{12}C^{32}S$ and the 1–0 bands of the $^{12}C^{33}S$, $^{12}C^{34}S$, and $^{13}C^{32}S$ isotopomers. The observation of vibration–rotation transitions with J up to 41, 28, 32, and 28 for $^{12}C^{32}S$, $^{12}C^{33}S$, $^{12}C^{34}S$, and $^{13}C^{32}S$,

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respectively, provided much-improved rotational and distortion constants for the various isotopomers as well as a precise determination of the band origins.

There are also several microwave and millimeter-wave studies of $^{12}C^{34}S$ and its isotopomers (*24–28*). Mockler and Bird (*24*) first measured the frequencies of the $J = 1–0$ transitions for the $^{12}C^{32}S$, $^{12}C^{33}S$, $^{12}C^{34}S$, and $^{13}C^{32}S$ isotopomers produced in an electrical discharge thorough CS_2. Kewley *et al.* (*25*) have studied the millimeter-wave spectra of $^{12}C^{32}S$ and $^{12}C^{34}S$. In recent work Bogey *et al.* (*27, 28*) have measured the millimeter-wave transitions for different J values for many vibrational levels of CS and its isotopomers, including transitions up to $v = 20$ for $^{12}C^{32}S$. Using these data they determined Dunham coefficients as well as Born–Oppenheimer breakdown parameters.

Using the available vibration–rotation and pure rotation data on this molecule, Coxon and Hajigeorgiou (*29*) recently derived a Born–Oppenheimer potential and the associated radial functions describing the Born–Oppenheimer breakdown in CS. In this study a small number of fitted potential parameters represented the entire data set to within experimental error.

In the present paper we report on the observation of the $\Delta v = 1$ infrared vibration–rotation bands of CS in the region 1000–1400 cm^{-1} at high temperatures. We have measured the rotational structure of nine bands of $^{12}C^{32}S$ from 1–0 to 9–8. Because of the high temperature of the source, the vibration–rotation lines of the strong bands have been observed up to $J = 115$. The direct observation of $\Delta v = 1$ bands with v up to 9 and of high-J transitions provides an improved ground state potential. The present infrared data, when combined with previous infrared and microwave data, provide improved spectroscopic constants and Dunham coefficients for the ground state.

EXPERIMENTAL DETAILS

The vibration–rotation bands of CS were inadvertently observed during a search for NiF emission bands in which a commercial King-type furnace was used. The experiment was intended to produce NiF bands by melting Ni in the carbon furnace in the presence of 75 Torr of CF_4 at a temperature of 2300°C. About 100 Torr of He was also present in the furnace as a buffer gas. The spectra observed in this experiment were very rich, with strong pure rotation and vibration–rotation bands of HF and DF as well as vibration–rotation bands of CO and CS. The carbon required for the formation of CS came from the heating elements and the carbon boat used to hold the sample. The origin of the sulfur impurities necessary to make CS is not completely clear but previous metal sulfide experiments in the furnace as well as a sulfur impurity in the carbon oven parts are possibilities.

The emission from the furnace was observed with the Fourier transform spectrometer associated with the McMath-Pierce solar telescope of the National Solar Observatory at Kitt Peak. The spectrometer was operated with a KCl beam splitter, InAs filters, and Si:As detectors. A total of five scans were coadded in 13 min of integration at a resolution of 0.01 cm^{-1}.

We decided to calibrate our CS spectrum using the vibration–rotation measurements of Burkholder *et al.* (*23*), which were calibrated using the measurements of the $10^00–00^00$ band of N_2O (*30*). The CS measurements of Burkholder *et al.* (*23*) should have an accuracy of ± 0.00022 cm^{-1}.

The strongest CS lines in our spectra are observed with a signal-to-noise ratio of 30 and they have a width of 0.010 cm^{-1}. This limits the precision of measurement of our strong and unblended molecular transitions to about ± 0.0005 cm^{-1}. However,

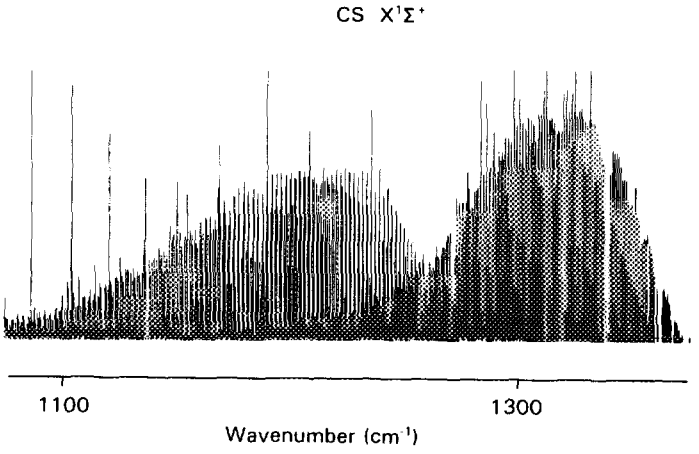

FIG. 1. A compressed view of the vibration–rotation bands of CS.

the intensity of bands involving the higher vibrational levels (with $v > 5$) decreases rapidly and, therefore, the measurements of the high vibrational bands are expected to be accurate to ± 0.002 cm^{-1}.

RESULTS AND DISCUSSION

The line positions were extracted from the spectra using a data reduction program called PC-DECOMP developed by Brault. The peak positions were determined by

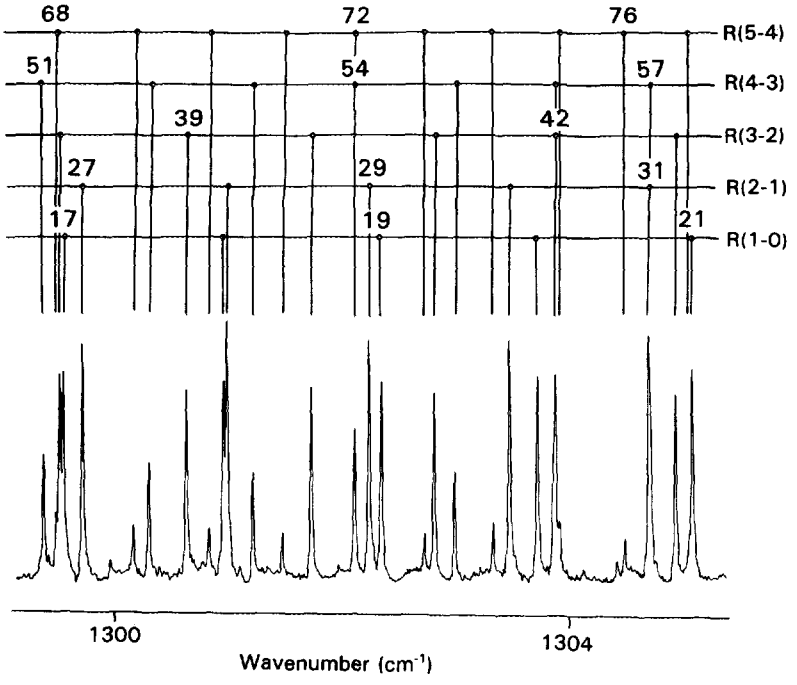

FIG. 2. A portion of the R-branch region of the vibration–rotation bands of CS.

TABLE I

Observed Line Positions (in cm^{-1}) in the Vibration–Rotation Bands of CS

	1-0				2-1				3-2				4-3				5-4			
J	R(J)	O-C	P(J)	O-C	R(J)	O-C	P(J)	O-C	R(J)	O-C	P(J)	O-C	R(J)	O-C	P(J)	O-C	R(J)	O-C	P(J)	O-C
0	1273.7830	-14			1260.8031	10														
1	1275.3946	-2	1270.5276	-3	1262.4011	4	1257.5665	-28	1249.4282	-9										
2	1276.9956	23	1268.8818	-2	1263.9874	-0	1255.9363	11	1251.0033	-6	1243.0082	-28	1238.0432	-5	1230.1105	5				
3	1278.5790	-9	1267.2238	-4	1265.5614	-8	1254.2903	10	1252.5679	11	1241.3739	-30	1239.5942	-5	1228.4873	-4	1226.6442	-9	1215.6222	11
4	1280.1557	11	1265.5564	17	1267.1243	-7	1252.6305	-11	1254.1197	19	1239.7321	11	1241.1350	12	1226.8523	-15	1228.1718	-4	1213.9971	-18
5	1281.7174	2	1263.8744	9	1268.6758	1	1250.9612	-10	1255.6571	4	1238.0735	0	1242.6589	-19	1225.2078	-2	1229.6876	2	1212.3650	-0
6	1283.2669	-9	1262.1809	3	1270.2144	-1	1249.2815	4	1257.1884	49	1236.4052	9	1244.1750	-8	1223.5492	-14	1231.1905	0	1210.7205	10
7	1284.8064	0	1260.4753	-8			1247.5881	-3	1258.6971	-12	1234.7202	-32	1245.6793	7	1221.8811	-4	1232.6821	7	1209.0627	4
8	1286.3357	29	1258.7594	-5	1273.2552	-5	1245.8838	-3	1260.2004	-6	1233.0311	3	1247.1692	-2	1220.1999	-9	1234.1603	-0	1207.3938	5
9	1287.8470	-1	1257.0324	2	1274.7580	0	1244.1712	30	1261.6920	5	1231.3278	11	1248.6490	9	1218.5078	-7	1235.6264	-7	1205.7135	7
10	1289.3516	24	1255.2927	-2	1276.2481	-2	1242.4400	-7	1263.1703	4	1229.6111	1	1250.1145	-0	1216.8057	11	1237.0826	10	1204.0199	-9
11	1290.8398	6	1253.5415	-6	1277.7267	4	1240.7020	4	1264.6356	-4	1227.8838	-0	1251.5686	-2	1215.0888	-4	1238.5236	-3	1202.3185	13
12	1292.3171	2	1251.7804	6	1279.1918	-3	1238.9516	5	1266.0909	10	1226.1446	-5	1253.0106	-2	1213.3628	5	1239.9531	-9		
13	1293.7817	-7	1250.0067	7	1280.6460	3	1237.1892	0	1267.5318	2	1224.3950	1	1254.4401	-4	1211.6242	3	1241.3739	21	1198.8758	4
14	1295.2348	-7	1248.2208	-0	1282.0860	-9	1235.4114	-44	1268.9613	4	1222.6322	-11	1255.8582	3	1209.8745	4	1242.7773	1	1197.1365	-9
15	1296.6754	-10	1246.4243	1	1283.5160	1	1233.6312	2	1270.3785	5	1220.8595	-8	1257.2630	0	1208.1138	9	1244.1712	8	1195.3881	1
16	1298.1048	-1	1244.6170	7	1284.9323	-1	1231.8350	2			1219.0763	4	1258.6555	-1	1206.3411	8	1245.5513	2		
17	1299.5204	-6	1242.7967	-3	1286.3357	-9	1230.0273	0	1273.1737	-11	1217.2805	3	1260.0359	-1	1204.5570	7	1246.9201	7	1191.8552	1
18	1300.9231	-15	1240.9668	4	1287.7281	-2	1228.2082	-3	1274.5539	13	1215.4729	-3	1261.4044	6	1202.7622	11	1248.2743	-10	1190.0726	11
19	1302.3159	1	1239.1252	6	1289.1072	-4	1226.3789	5	1275.9213	-6	1213.6552	3	1262.7593	1	1200.9550	5	1249.6174	-13	1188.2761	-7
20	1303.6948	2	1237.2719	4	1290.4734	-10	1224.5368	-3	1277.2768	1	1211.8259	6	1264.1032	11	1199.1372	5	1250.9502	5	1186.4710	3
21	1305.0606	-1.	1235.4114	42	1291.8290	3	1222.6849	3	1278.6190	-0	1209.9846	0	1265.4328	4	1197.3074	-3	1252.2676	-4	1184.6535	-0
22	1306.4142	-2	1233.5315	-2	1293.1700	-4	1220.8203	-6	1279.9485	-3	1208.1438	112	1266.7508	6	1195.4675	-0	1253.5730	-8	1182.8244	-7
23	1307.7557	2	1231.6449	-2	1294.4994	-1	1218.9464	4	1281.2663	4	1206.2695	-0	1268.0555	1	1193.6169	7	1254.8672	3	1180.9847	-8
24	1309.0840	1	1229.7474	0	1295.8157	-2	1217.0602	2	1282.5708	4	1204.3955	2	1269.3472	-7	1191.7542	4	1256.1473	-1	1179.1346	-1
25	1310.4001	4	1227.8384	-2	1297.1198	0	1215.1634	4	1283.8607	-16	1202.5099	-1	1270.6282	5	1189.8802	-0	1257.4147	-6	1177.2730	1
26	1311.7027	-1	1225.9190	3	1298.4097	-12	1213.2543	-6	1285.1415	1	1200.6122	-14	1271.8956	7	1187.9950	-6	1258.6702	-2	1175.4002	2
27	1312.9932	0	1223.9874	-5	1299.6886	-7	1211.3350	-7	1286.4076	-3	1198.7065	3	1273.1480	-13	1186.0999	-0	1259.9129	1	1173.5169	9
28	1314.2712	4	1222.0455	-5	1300.9544	-5	1209.4058	2	1287.6614	-1	1196.7881	2	1274.3909	1	1184.1935	2	1261.1423	-1	1171.6219	8
29	1315.5357	1	1220.0933	1	1302.2076	-2	1207.4638	-7	1288.9024	-0	1194.8594	9	1275.6202	5	1182.2764	8	1262.3589	-3	1169.7161	9
30	1316.7873	-4	1218.1299	5	1303.4473	-5	1205.5130	5	1290.1305	1	1192.9175	-7	1276.8347	-10	1180.3475	4	1263.5627	-4	1167.8014	31
31	1318.0272	4	1216.1551	3	1304.6757	7	1203.5503	7	1291.3458	3	1190.9673	2	1278.0386	-2	1178.4074	-2	1264.7552	10	1165.8711	6
32	1319.2535	4	1214.1699	6	1305.8893	0	1201.5750	-8	1292.5478	-0	1189.0045	-6	1279.2283	-7	1176.4565	-8	1265.9324	0	1163.9318	-1
33	1320.4663	-2	1212.1725	-5	1307.0901	-5	1199.5912	0	1293.7361	-11			1280.4069	6	1174.4945	-15	1267.0958	-18	1161.9825	1
34	1321.6637	-32	1210.1654	-5	1308.2796	6	1197.5962	4	1294.9136	1	1185.0485	0	1281.5707	1	1172.5244	4	1268.2493	-5	1160.0225	4
35	1322.8545	2	1208.1438	-41	1309.4544	-0	1195.5898	2	1296.0772	3	1183.0541	1	1282.7224	5	1170.5408	-4	1269.3880	-11	1158.0510	0
36	1324.0277	-11	1206.1197	4	1310.6176	8	1193.5725	-1	1297.2276	4	1181.0487	-1	1283.8607	6	1168.5476	-1	1270.5161	9	1156.0693	2
37	1325.1894	-7	1204.0799	-0	1311.7682	21	1191.5452	1	1298.3639	-6	1179.0332	4	1284.9851	-2	1166.5417	-17	1271.6281	-1	1154.0763	-2
38	1326.3381	-3	1202.0296	-3	1312.9022	-2	1189.5069	2	1299.4874	-13	1177.0058	-4	1286.0977	3	1164.5287	3	1272.7283	1	1152.0733	1
39	1327.4732	-4	1199.9688	-4	1314.0257	2	1187.4578	1	1300.6000	3	1174.9677	-12	1287.1959	-5	1162.5015	-13	1273.8148	-2	1150.0597	5
40	1328.5963	7	1197.8986	7	1315.1354	-0	1185.3984	3	1301.6978	2	1172.9210	1			1160.4661	-5	1274.8886	-1	1148.0339	-8
41	1329.7042	-2	1195.8165	5	1316.2324	2	1183.3284	5	1302.7825	2	1170.8628	4	1289.3548	1	1158.4200	3	1275.9476	-15	1145.9993	-1
42	1330.8003	3	1193.7226	-10	1317.3158	1	1181.2467	-5	1303.8529	-8	1168.7935	2	1290.4138	-2	1156.3630	7	1276.9957	-5	1143.9531	-6
43	1331.8825	1	1191.6208	1	1318.3859	-1	1179.1550	-9	1304.9119	0	1166.7138	1	1291.4602	1	1154.2940	-3			1141.8976	3
44	1332.9517	2	1189.5069	-4	1319.4429	-1	1177.0538	-3	1305.9569	1	1164.6238	2	1292.4924	-4	1152.2160	1	1279.0506	-1	1139.8310	6

TABLE I—*Continued*

	1-0				2-1				3-2				4-3				5-4			
J	R(J)	O-C	P(J)	O-C	R(J)	O-C	P(J)	O-C	R(J)	O-C	P(J)	O-C	R(J)	O-C	P(J)	O-C	R(J)	O-C	P(J)	O-C
45	1334.0075	3	1187.3836	3	1320.4871	4	1174.9406	-12	1306.9883	0	1162.5224	-6	1293.5111	-11	1150.1267	-2	1280.0591	12	1137.7517	-14
46	1335.0491	-5	1185.2492	2	1321.5189	19	1172.8193	2	1308.0056	-9	1160.4117	-2	1294.5194	12	1148.0296	21	1281.0523	5	1135.6677	23
47	1336.0786	-1	1183.1040	-2	1322.5338	-1	1170.6858	-2	1309.0104	-8	1158.2908	3	1295.5109	1	1145.9177	0	1282.0320	-1	1133.5668	-4
48	1337.0943	1	1180.9478	-13	1323.5367	-6	1168.5449	24	1310.0028	2	1156.1590	4	1296.4909	9	1143.7979	5	1282.9985	-6	1131.4588	2
49	1338.0962	-2	1178.7836	0	1324.5274	0	1166.3883	-4	1310.9812	8	1154.0164	-0	1297.4557	1	1141.6670	1	1283.9529	4	1129.3394	-1
50	1339.0845	-6	1176.6079	1	1325.5061	22	1164.2250	5	1311.9452	4	1151.8640	1	1298.4078	0	1139.5265	5	1284.8919	-5	1127.2082	-21
51	1340.0595	-7	1174.4215	-2	1326.4661	-8	1162.0506	5	1312.8951	-5	1149.7027	16	1299.3460	-4	1137.3746	-2	1285.8185	-3	1125.0714	7
52	1341.0218	0	1172.2255	1	1327.4160	-3	1159.8657	3	1313.8329	1	1147.5317	37	1300.2709	-6	1135.2130	-3	1286.7319	4	1122.9210	2
53	1341.9698	0	1170.0186	-2	1328.3498	-23	1157.6708	4			1145.3446	-1	1301.1833	4	1133.0419	3	1287.6301	-6	1120.7610	4
54	1342.9041	-0	1167.8014	-6	1329.2743	-0	1155.4656	3	1315.6663	-1	1143.1512	1	1302.0805	-1	1130.8589	-8	1288.5164	2	1118.5914	11
55	1343.8251	3	1165.5757	6	1330.1830	2	1153.2503	3	1316.5623	-5	1140.9480	5	1302.9645	-2	1128.6685	9	1289.3865	-15	1116.4096	-1
56	1344.7312	-7	1163.3382	2	1331.0776	-1	1151.0248	2	1317.4447	-7	1138.7334	-2	1303.8332	-18	1126.4651	-2	1290.2468	8	1114.2192	1
57	1345.6242	-10	1161.0911	2	1331.9586	-1	1148.7890	0	1318.3124	-18			1304.6914	-2	1124.2528	-1	1291.0906	3	1112.0180	-3
58	1346.5050	3	1158.8336	-0	1332.8259	-2	1146.5438	4	1319.1689	-4	1134.2757	1	1305.5348	4	1122.0310	5	1291.9208	0	1109.8080	6
59	1347.3696	-8	1156.5660	-3	1333.6798	2	1144.2875	-2			1132.0306	-9	1306.3632	-2	1119.7976	-4	1292.7370	-4	1107.5861	-3
60	1348.2210	-13	1154.2918	28	1334.5190	-3	1142.0221	1	1320.8380	1	1129.7783	9	1307.1786	1	1117.5550	-4	1293.5391	-11	1105.3550	-3
61	1349.0604	0	1152.0020	3	1335.3453	2	1139.7463	0		0	1127.5130	-2	1307.9790	-7	1115.3041	13	1294.3298	8	1103.1150	7
62	1349.8848	3	1149.7027	-18	1336.1568	-1	1137.4610	4	1322.4510	-1	1125.2391	-0	1308.7671	1	1113.0403	0	1295.1046	7	1100.8621	-12
63	1350.6949	1	1147.3972	-1	1336.9547	-2	1135.1648	-2	1323.2361	-6	1122.9552	1	1309.5400	-3	1110.7675	-3	1295.8640	-8	1098.6038	15
64	1351.4911	1	1145.0805	3	1337.7387	-2	1132.8597	2	1324.0064	-20	1120.6612	1	1310.2999	3	1108.4860	5	1296.6123	6	1096.3314	-1
65	1352.2725	-8	1142.7558	26			1130.5442	1	1324.7662	2	1118.3573	0	1311.0443	-6	1106.1935	3	1297.3448	2	1094.0503	-3
66	1353.0413	-2	1140.4167	3	1339.2642	-6	1128.2189	0			1116.0432	-4			1103.8906	-4	1298.0628	-6	1091.7594	-6
67	1353.7956	-0	1138.0696	-2	1340.0055	-11	1125.8837	-1	1326.2391	1	1113.7206	5			1101.5794	4	1298.7679	-1	1089.4606	11
68	1354.5356	-1	1135.7119	-15	1340.7341	-2	1123.5393	4	1326.9540	-4	1111.3872	4	1313.1960	-1	1099.2571	-1	1299.4592	7	1087.1482	-10
69	1355.2614	-2	1133.3471	-2	1341.4478	-1	1121.1839	-5	1327.6560	4	1109.0438	0	1313.8836	-13	1096.9262	5	1300.1349	0	1084.8288	-3
70	1355.9732	-1	1130.9711	-3	1342.1462	-11	1118.8207	7	1328.3498	73	1106.6886	-24	1314.5595	0	1094.5834	-10	1300.7976	6	1082.5003	11
71	1356.6696	-11	1128.5860	2	1342.8317	-7	1116.4453	-7	1329.0155	2	1104.3282	-2	1315.2201	3	1092.2323	-10	1301.4444	-4	1080.1596	-1
72	1357.3537	-3	1126.1907	1	1343.5032	-1	1114.0654	32	1329.6730	-8	1101.9542	-20	1315.8662	4	1089.8742	16	1302.0806	23	1077.8089	-16
73			1123.7862	5	1344.1597	-2	1111.6679	-10	1330.3179	-0	1099.5729	-14	1316.4978	3	1087.5011	-12	1302.6978	4	1075.4488	-27
74	1358.6775	-2	1121.3712	0	1344.8014	-8	1109.2658	-2	1330.9476	-2	1097.1830	1	1317.1163	14	1085.1229	7	1303.3036	13	1073.0808	-22
75	1359.3167	-13	1118.9479	8	1345.4304	3	1106.8528	-6	1331.5632	0	1094.7815	-3	1317.7182	4	1082.7327	1	1303.8916	-12	1070.7060	12
76	1359.9434	-5	1116.5139	5	1346.0431	-5	1104.4318	5			1092.3710	-1	1318.3061	-3	1080.3324	-10	1304.4700	13	1068.3185	14
77	1360.5556	1	1114.0654	-49	1346.6439	12	1101.9982	-14	1332.7513	5	1089.9508	-1			1077.9236	-11	1305.0301	-1	1065.9199	1
78			1111.6178	2	1347.2268	-5	1099.5571	-13	1333.3233	4	1087.5208	-4			1075.5070	6	1305.5762	-9	1063.5111	-19
79	1361.7347	-4	1109.1572	16	1347.7981	7	1097.1072	-6	1333.8813	8	1085.0821	1			1073.0805	18	1306.1096	-0	1061.0944	-22
80	1362.3020	-12	1106.6886	46	1348.3527	-3	1094.6470	-7	1334.4243	8	1082.6349	16	1320.5150	-5	1070.6417	2	1306.6272	-2		
81			1104.2023	-7	1348.8944	5	1092.1772	-9	1334.9525	5	1080.1706	-46	1321.0323	10	1068.1939	-9	1307.1335	29	1056.2346	-10
82			1101.7130	4			1089.7001	9	1335.4658	0	1077.7088	11			1065.7381	-7	1307.6197	5	1053.7881	-29
83	1363.9202	4	1099.2133	5	1349.9310	-10	1087.2105	-4	1335.9652	3	1075.2324	15	1322.0188	-3	1063.2723	-10			1051.3371	2
84	1364.4302	8	1096.7033	-5	1350.4303	12	1084.7139	6	1336.4483	-10	1072.7482	36	1322.4910	1	1060.7995	10	1308.5522	-1	1048.8734	-1
85	1364.9255	12	1094.1848	-6	1350.9107	-7	1082.2087	24			1070.2485	-6	1322.9479	0	1058.3132	-12			1046.4002	-5
86	1365.4044	0	1091.6574	-3	1351.3797	8	1079.6898	-3	1337.3744	4	1067.7451	8	1323.3904	3	1055.8211	2	1309.4270	8	1043.9177	-10
87	1365.8705	7	1089.1203	-5	1351.8315	-2	1077.1644	-2	1337.8135	-6	1065.2297	-5	1323.8181	5	1053.3166	-16	1309.8417	9	1041.4306	32
88	1366.3206	3	1086.5758	11	1352.2725	29	1074.6296	-3	1338.2378	-15	1062.7070	1	1324.2312	11	1050.8058	-5	1310.2395	-12	1038.9286	18

Table I—*Continued*

	1-0				2-1				3-2				4-3				5-4			
J	R(J)	O-C	P(J)	O-C	R(J)	O-C	P(J)	O-C	R(J)	O-C	P(J)	O-C	R(J)	O-C	P(J)	O-C	R(J)	O-C	P(J)	O-C
89	1366.7561	1	1084.0189	-4	1352.6941	14	1072.0856	-3			1060.1741	-2	1324.6273	-5	1048.2843	-8				
90	1367.1777	9	1081.4545	-3	1353.1000	-9	1069.5330	2			1057.6319	-7	1325.0102	-3	1045.7541	-6				
91	1367.5835	8	1078.8827	15	1353.4943	2	1066.9690	-16			1055.0828	11	1325.3781	-1	1043.2166	14				
92	1367.9732	-5	1076.2977	-7	1353.8713	-10	1064.3986	-6	1339.7914	2	1052.5216	-1	1325.7314	5	1040.6676	11				
93	1368.3485	-11	1073.7066	1	1354.2364	9	1061.8191	4			1049.9470	-56	1326.0672	-14	1038.1103	16				
94			1071.1051	-5	1354.5817	-20	1059.2282	-9			1047.3791	47								
95	1369.0564	0	1068.4972	15			1056.6308	3	1340.7988	14	1044.7852	-19	1326.7001	15						
96	1369.3857	-14	1065.8763	-4	1355.2356	8	1054.0265	36	1341.1030	4	1042.1893	-15	1326.9908	-1						
97			1063.2494	6	1355.5388	12	1051.4126	63	1341.3913	-12	1039.5857	2	1327.2681	1						
98	1370.0057	26	1060.6102	-17	1355.8261	9	1048.7847	40	1341.6676	3	1036.9714	1								
99	1370.2899	16	1057.9677	17	1356.0970	-5	1046.1452	-10					1327.7770	6						
100	1370.5570	-13	1055.3106	-7	1356.3558	13	1043.5061	34	1342.1637	-73			1328.0091	15						
101	1370.8134	5	1052.6453	-23	1356.5990	27	1040.8516	12	1342.3991	-8			1328.2230	-5						
102	1371.0528	5	1049.9743	-9	1356.8232	5			1342.6139	5			1328.4237	-3						
103	1371.2762	-1	1047.2868	-71	1357.0350	12														
104	1371.4873	25	1044.6013	-24	1357.2298	4							1328.7783	-4						
105	1371.6773	-7	1041.9091	42	1357.4092	-4							1328.9314	-14						
106	1371.8550	-6	1039.2019	47	1357.5752	10														
107	1372.0180	2			1357.7232	-1														
108					1357.8564	-5														
109																				
110	1372.4116	8																		
111	1372.5092	-13			1358.1622	-14														
112	1372.5983	38			1358.2315	-30														
113					1358.2882	-13														

TABLE I—*Continued*

	6-5				7-6				8-7				9-8			
J	R(J)	O-C	P(J)	O-C	R(J)	O-C	P(J)	O-C	R(J)	O-C	P(J)	O-C	R(J)	O-C	P(J)	O-C
5	1216.7366	4														
6	1218.2287	13														
7	1219.7063	-2	1196.2645	-7												
8	1221.1751	16	1194.6079	-3							1169.1101	60				
9	1222.6322	40	1192.9374	-21			1180.1853	-26			1167.4616	26				
10	1224.0695	-14	1191.2618	26	1211.0792	-25	1178.5184	-11			1165.8010	-15				
11	1225.4992	-21			1212.5014	12	1176.8388	-6			1164.1315	-27				
12	1226.9184	-10	1187.8685	44	1213.9066	3	1175.1482	3	1200.9159	-1						
13	1228.3253	1	1186.1481	-13	1215.2992	-11	1173.4435	-15	1202.2985	6	1160.7670	37				
14	1229.7160	-28	1184.4235	4	1216.6797	-21	1171.7295	-9	1203.6673	-2	1159.0603	-3				
15	1231.1000	1	1182.6872	17	1218.0504	-7			1205.0250	3						
16	1232.4684	-3			1219.4086	7	1168.2672	-2			1155.6212	2				
17	1233.8257	6	1179.1794	34	1220.7515	-8			1207.7047	28	1153.8849	7				
18	1235.1689	-1	1177.4032	-11	1222.0853	12	1164.7573	-15	1209.0219	1						
19	1236.4995	-9	1175.6218	6	1223.4024	-12	1162.9848	-27	1210.3283	-9	1150.3764	-2				
20	1237.8192	-1	1173.8278	8	1224.7105	0	1161.2069	19	1211.6242	1	1148.6053	-4				
21	1239.1252	-4	1172.0224	9	1226.0060	11	1159.4111	-2	1212.9067	3	1146.8260	22	1199.8301	27		
22	1240.4195	1	1170.2043	-5	1227.2878	11	1157.6066	3			1145.0306	0	1201.0754	-96		
23	1241.6987	-19	1168.3777	8	1228.5549	-9	1155.7892	-10	1215.4326	-6	1143.2241	-20	1202.3185	-116	1130.6801	-18
24	1242.9688	-3	1166.5418	38	1229.8124	1	1153.9636	6	1216.6797	21	1141.4132	26	1203.5504	-121	1128.8781	1
25	1244.2247	-1	1164.6872	-6	1231.0566	6	1152.1272	26	1217.9099	6	1139.5816	-24	1204.7826	5	1127.0627	-4
26	1245.4676	-4	1162.8269	2	1232.2883	12	1150.2762	10	1219.1287	4	1137.7464	2	1205.9881	-9	1125.2391	21
27	1246.6979	-4	1160.9547	3	1233.5041	-13	1148.4166	19	1220.3329	-15			1207.1842	12	1123.4027	27
28	1247.9153	-6	1159.0704	-7	1234.7114	6	1146.5439	7	1221.5303	25	1134.0361	-15	1208.3663	20	1121.5564	45
29	1249.1209	3	1157.1778	8	1235.9032	-3	1144.6613	6			1132.1657	-10	1209.5269	-59	1119.6913	-15
30	1250.3129	5	1155.2728	10	1237.0826	-7			1223.8760	-1	1130.2887	37	1210.6886	2	1117.8175	-53
31	1251.4914	-1	1153.3562	5	1238.2490	-12	1140.8628	-1			1128.3927	4				
32	1252.6564	-11	1151.4287	-1	1239.4053	12	1138.9498	22	1226.1701	-26	1126.4881	-6	1212.9611	3		
33	1253.8104	-2	1149.4905	-5	1240.5462	11	1137.0224	9	1227.3025	10	1124.5753	10	1214.0743	-31	1112.1496	25
34	1254.9532	24	1147.5399	-25	1241.6735	3	1135.0833	-12	1228.4160	-14	1122.6500	10			1110.2370	35
35	1256.0788	9	1145.5829	0			1133.1385	18	1229.5225	23	1120.7117	-12	1216.2700	-18	1108.3117	27
36	1257.1885	-34	1143.6135	8	1243.8904	3	1131.1778	-4	1230.6072	-28	1118.7652	-7	1217.3502	8	1106.3745	7
37	1258.2930	1	1141.6307	-11	1244.9793	4	1129.2108	18	1231.6850	-16					1104.4285	6
38	1259.3809	2	1139.6399	-3	1246.0559	13	1127.2264	-26	1232.7483	-17	1114.8381	-19	1219.4639	-13	1102.4701	-11
39			1137.6375	-3	1247.1148	-23	1125.2391	8	1233.7978	-25	1112.8650	40	1220.5022	-11	1100.5044	6
40	1261.5170	1	1135.6228	-21	1248.1660	-4	1123.2367	-4	1234.8384	9	1110.8742	29	1221.5303	21	1098.5235	-23
41	1262.5648	-3	1133.6013	-1	1249.2047	22	1121.2215	-36	1235.8610	-3	1108.8698	-12	1222.5376	-23	1096.5341	-31
42	1263.6004	3	1131.5692	21	1250.2256	3	1119.2023	-4	1236.8718	-1			1223.5371	-12	1094.5350	-29
43	1264.6236	18	1129.5241	16	1251.2347	-1	1117.1687	-9	1237.8676	-16					1092.5328	47
44	1265.6300	-2	1127.4672	-1	1252.2312	3	1115.1271	11	1238.8536	6	1102.8070	4	1225.4992	43	1090.5091	14
45	1266.6246	-6	1125.4025	9	1253.2140	3	1113.0704	-15	1239.8228	-7	1100.7628	-14	1226.4469	-63	1088.4741	-28
46	1267.6069	1	1123.3256	2	1254.1826	-5	1111.0088	15	1240.7799	-7	1098.7092	-19	1227.3992	12	1086.4361	6
47	1268.5755	5	1121.2355	-33	1255.1392	2	1108.9363	40	1241.7228	-14	1096.6464	-14	1228.3253	-41	1084.3847	10
48	1269.5300	3	1119.1442	24	1256.0788	-27	1106.8478	9	1242.6540	-4			1229.2460	-12		

TABLE I—*Continued*

	6-5				7-6				8-7				9-8			
J	R(J)	O-C	P(J)	O-C	R(J)	O-C	P(J)	O-C	R(J)	O-C	P(J)	O-C	R(J)	O-C	P(J)	O-C
49	1270.4707	-2	1117.0358	13	1257.0072	-32			1243.5708	-2			1230.1525	10	1080.2444	-45
50	1271.3959	-27	1114.9145	-23	1257.9257	-1	1102.6449	-2	1244.4744	3	1090.3902	-49	1231.0407	-16	1078.1703	43
51	1272.3104	-23	1112.7889	1	1258.8269	-7	1100.5296	10	1245.3648	12	1088.2900	-3	1231.9225	30	1076.0747	21
52	1273.2129	-3	1110.6523	18	1259.7168	10	1098.4012	-6	1246.2401	8	1086.1757	7	1232.7820	-9	1073.9698	7
53	1274.0999	-2	1108.5013	-7	1260.5911	8	1096.2657	9	1247.1031	16	1084.0478	-18	1233.6313	-15	1071.8531	-20
54	1274.9734	1	1106.3428	-3	1261.4535	24	1094.1191	15	1247.9481	-20	1081.9154	15	1234.4686	-3	1069.7334	24
55	1275.8322	-6	1104.1724	-18	1262.2982	-1	1091.9621	18	1248.7869	21	1079.7650	-30	1235.2906	-6	1067.5968	1
56	1276.6784	-1	1101.9982	31	1263.1294	-22	1089.7929	3	1249.6052	-5	1077.6130	10	1236.0978	-20	1065.4505	-16
57	1277.5102	-2	1099.8069	11	1263.9534	21	1087.6168	19	1250.4157	29	1075.4448	-9	1236.8970	25	1063.2962	-13
58	1278.3292	6	1097.6071	6	1264.7552	-18	1085.4295	25	1251.2061	-1			1237.6787	33	1061.1327	0
59	1279.1320	-9	1095.3973	2	1265.5481	-7	1083.2331	40	1251.9853	-3	1071.0801	-29	1238.4408	-16	1058.9531	-46
60	1279.9226	-6	1093.1784	9	1266.3268	0	1081.0191	-20	1252.7513	2	1068.8875	10				
61	1280.6987	-10	1090.9467	-14	1267.0908	-0	1078.8028	-3	1253.5026	-2	1066.6816	17				
62	1281.4629	6	1088.7091	5	1267.8429	20	1076.5773	22	1254.2388	-15	1064.4650	16				
63	1282.2093	-15	1086.4597	6	1268.5755	-14					1062.2380	11	1241.3739	33		
64	1282.9450	-4	1084.2025	28	1269.3001	11	1072.0856	-36	1255.6727	-7	1059.9991	-14	1242.0667	-9		
65	1283.6666	8	1081.9291	-14			1069.8288	-26	1256.3718	30	1057.7542		1242.7467	-36		
66	1284.3726	4	1079.6527	13	1270.7005	-3	1067.5652	14			1055.4948	-32	1243.4198	8		
67	1285.0636	-7	1077.3606	-18	1271.3830	26	1065.2835	-27	1257.7193	19	1053.2290	-28				
68	1285.7426	2	1075.0649	13	1272.0480	20	1062.9982	-6	1258.3701	-1	1050.9589	30				
69	1286.4077	15			1272.6976	4	1060.7015	-2	1259.0081	-9	1048.6744	43	1245.3431	35		
70	1287.0572	14	1070.4353	-14	1273.3352	9	1058.3941	-6	1259.6315	-19	1046.3743	-4				
71			1068.1101	15	1273.9572	2	1056.0753	-27					1246.5470	-16		
72			1065.7694	-14			1053.7545	28								
73			1063.4255	22	1275.1598	4	1051.4127	-29					1247.7015	14		
74	1289.5106	-5	1061.0661	-1	1275.7366	-24	1049.0701	3								
75	1290.0899	9	1058.6996	0	1276.3061	18	1046.7140	-5								
76	1290.6531	7	1056.3241	9	1276.8549	-1	1044.3488	-8								
77	1291.2003	-10	1053.9360	-14	1277.3898	-14										
78	1291.7369	13	1051.5462	43	1277.9127	-1										
79	1292.2547	-8	1049.1363	-8	1278.4194	-5										
80	1292.7595	-12	1046.7212	-15	1278.9105	-19										
81			1044.2961	-28												
82			1041.8643	-13	1279.8495	-38										
83	1294.1885	2	1039.4250	20	1280.3038	22										
84	1294.6357	9	1036.9715	5	1280.7354	2										
85	1295.0632	-33														
86	1295.4808	-24														
87	1295.8895	43			1281.9452	-18										
88	1296.2749	26			1282.3246	34										

O-C Observed minus calculated line positions in units of 10-4 cm-1.

TABLE II

Spectroscopic Constants[a] (in cm^{-1}) of the $X^1\Sigma^+$ Vibrational Levels of CS

Constants	v=0	v=1	v=2	v=3	v=4
T_v	0.0	1272.162055(43)	2531.353665(59)	3777.59739(10)	5010.91646(13)
B_v	0.817084141(31)	0.811163722(43)	0.805241221(60)	0.799316671(70)	0.793389601(75)
$10^7 \times D_v$	1.336182(65)	1.337566(63)	1.339021(61)	1.340605(62)	1.342244(61)
$10^{13} \times H_v$	1.974(56)	1.777(53)	1.568(50)	1.383(51)	1.177(49)

Constants	v=5	v=6	v=7	v=8	v=9
T_v	6231.33336(15)	7438.87038(29)	8633.54915(29)	9815.39254(41)	10984.42006(53)
B_v	0.787459946(88)	7.81527353(11)	0.77559205(11)	0.76965316(15)	0.76371073(17)
$10^7 \times D_v$	1.344023(68)	1.345849(80)	1.347867(89)	1.34993(15)	1.351811(22)
$10^{13} \times H_v$	1.024(60)	0.851(83)	0.734(98)	0.61(27)	--

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

fitting a Voigt lineshape function to each spectral feature. The branches in the different bands were sorted using a color Loomis–Wood program running on a PC computer.

The observed spectrum consists of nine vibration–rotation bands including 1–0, 2–1, 3–2, 4–3, 5–4, 6–5, 7–6, 8–7, and 9–8. The intensity of the higher vibrational bands decreases slowly with increasing vibration and it becomes difficult to identify the bands with $v > 9$. A compressed view of the observed bands is presented in Fig. 1.

Carbon and sulfur both have minor isotopes (^{13}C (1.1%), ^{33}S (0.75%), ^{34}S (4.21%), and ^{36}S (0.02%)) so that CS has eight possible isotopic combinations. The $^{12}C^{32}S$ and $^{12}C^{34}S$ isotopomers are the most abundant and they are expected to appear in the intensity ratio of 30:1. In addition to $^{12}C^{32}S$ lines, we observed some very weak lines of the 1–0 and 2–1 bands of the $^{12}C^{34}S$ isotopomer. The very weak intensity of these bands, combined with frequent overlapping due to the strong lines of $^{12}C^{32}S$, prevented

TABLE III

Dunham Constants[a] (in cm^{-1}) of the $X^1\Sigma^+$ State of CS

Y_{01}	0.820043559(42)	$10^7 \times Y_{21}$	-9.83(13)
$10^6 \times Y_{02}$	-1.335514(65)	$10^{11} \times Y_{22}$	-3.81(15)
$10^{13} \times Y_{03}$	2.068(56)	$10^3 \times Y_{30}$	3.8873(94)
Y_{10}	1285.15464(10)	$10^8 \times Y_{31}$	-1.24(12)
$10^3 \times Y_{11}$	-5.918345(49)	$10^{13} \times Y_{32}$	-6.4(12)
$10^9 \times Y_{12}$	-1.3110(76)	$10^6 \times Y_{40}$	-8.53(54)
$10^{14} \times Y_{13}$	-1.969(47)	$10^9 \times Y_{41}$	-1.105(36)
Y_{20}	-6.502605(53)		

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

TABLE IV

Mass-Reduced Dunham Constants and Born–Oppenheimer Breakdown Constants of CS (in cm^{-1})

Constants	Unconstrained	Constrained
U_{10}	3796.06354(407)	3796.08507(446)
U_{20}	-56.736493(468)	-56.736001(546)
$10^{1} \times U_{30}$	1.00187(249)	1.00019(295)
$10^{4} \times U_{40}$	-6.480(423)	-6.193(507)
U_{01}	7.15620308(936)	7.1560789(101)
$10^{1} \times U_{11}$	-1.5253195(107)	-1.52530660(638)
$10^{5} \times U_{21}$	-7.4498(876)	-7.4547(619)
$10^{6} \times U_{31}$	-2.985(246)	-3.192(198)
$10^{7} \times U_{41}$	-7.154(215)	-6.878(189)
$10^{4} \times U_{02}$	-1.0166414(505)	-1.01721669
$10^{7} \times U_{12}$	-2.9696(158)	-3.00217320
$10^{8} \times U_{22}$	-2.5583(910)	-2.35216625
$10^{9} \times U_{32}$	-1.131(243)	-1.37836200
$10^{10} \times U_{03}$	1.3223(382)	1.67035183
$10^{11} \times U_{13}$	-3.7196(911)	-3.27379000
$10^{12} \times U_{23}$		-1.08678460
$10^{13} \times U_{33}$		-1.30687132
$10^{14} \times U_{04}$		-1.32670129
$10^{14} \times U_{14}$		-1.16313796
$10^{16} \times U_{24}$		-1.54832285
$10^{19} \times U_{05}$		-2.41940226
$10^{20} \times U_{15}$		-4.72848064
$10^{21} \times U_{25}$		-5.81678951
$10^{23} \times U_{06}$		-1.06732122
$10^{24} \times U_{16}$		-3.59975351
$10^{28} \times U_{07}$		-3.88434849
$10^{28} \times U_{17}$		-1.30944866
$10^{32} \times U_{08}$		-1.91860182
$10^{37} \times U_{09}$		-8.00597446
Δ_{10}^{C}	0.7477(138)	0.6892(157)
Δ_{01}^{C}	-2.5520(179)	-2.3728(204)
Δ_{10}^{S}	-0.7229(419)	-0.9083(473)
Δ_{01}^{S}	-2.6832(481)	-2.1329(541)

Note. The numbers in parentheses are one standard deviation in units of the last digit.

us from making reliable measurements. We therefore have decided to report data only for the major isotopomer.

A part of the high-resolution spectrum of the R-branch region of the bands is provided in Fig. 2. The R lines of the 1–0, 2–1, 3–2, 4–3, and 5–4 bands are marked in this figure. As expected for a $^1\Sigma^+-^1\Sigma^+$ transition, each band consists of one R- and one P-type branch. The rotational structure of the 1–0, 2–1, 3–2, and 4–3 bands has lines involving J values greater than 100. The wavenumbers of the observed transitions are provided in Table I. The wavenumbers of the CS were fitted to the customary energy level expression:

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

In the final least-squares fit approximate weights for the individual rotational lines were chosen on the basis of signal-to-noise ratio as well as freedom from blending. We have also included the previous Fourier transform infrared (*22, 23*) and microwave measurements (*28*), with appropriate weights in the final fit. The spectroscopic constants for the $X\,^1\Sigma^+$ state obtained from the combined fit are provided in Table II. The molecular constants obtained in this study are in reasonable agreement with values reported earlier (*22, 23*) but are more accurate by an order of magnitude because of the inclusion of pure rotational lines and a more extensive data set. In order to find equilibrium molecular parameters, the rotational lines of $^{12}C^{32}S$ were fit to the Dunham energy level expression (*31*):

$$E(v, J) = \sum Y_{ij}(v+\tfrac{1}{2})^i[J(J+1)]^j. \quad (2)$$

The Dunham Y_{ij} constants for the $X\,^1\Sigma^+$ state of $^{12}C^{32}S$ obtained from this fit are provided in Table III.

The infrared data for the minor isotopomers of CS from Burkholder *et al.* (*23*) and Todd and Olson (*21*) as well as the corresponding pure rotational transitions of Bogey *et al.* (*28*) were combined with our final data set for $^{12}C^{32}S$ to determine a set of mass-reduced Dunham U_{ij} coefficients and Born–Oppenheimer breakdown constants Δ_{ij} (*32, 33*):

$$E(v, J) = \sum U_{ij}\,\mu^{-(i+2j)/2}(v+\tfrac{1}{2})^i[J(J+1)]^j\left(1 + \frac{m_e}{m_C}\Delta_{ij}^C + \frac{m_e}{m_S}\Delta_{ij}^S\right). \quad (3)$$

The U_{ij} and Δ_{ij} constants are reported in Table IV. In this table the set of U's and Δ's labeled as constrained constants were determined by fixing U_{ij}'s with $j > 1$ to values calculated using the U_{i0} and U_{i1} constants (*34*).

CONCLUSION

The infrared vibration–rotation spectrum of CS has been observed at high resolution with a Fourier transform spectrometer. The bands were excited at 2300°C in a carbon tube furnace. The high temperature of the source results in spectra with bands involving high vibrational levels and high-J rotational lines. Our data on the $\Delta v = 1$ sequence bands from 1–0 to 9–8, combined with previously reported infrared and microwave data, provide improved molecular constants. The present work also directly determines the $\Delta G(v+\frac{1}{2})$ vibrational intervals and improves the vibrational constants.

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