Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting information:

High resolution GHz and THz (FTIR) spectroscopy and theory of parity violation and tunneling for 1,2-dithiine ($C_4H_4S_2$) as a candidate for measuring the parity violating energy difference between enantiomers of chiral molecules

S. Albert[a,b], I. Bolotova[a], Z. Chen[a], C. Fábri[a], L. Horný[a], M. Quack*[a], G. Seyfang[a] and D. Zindel[a]

[a] Physical Chemistry, ETH Zurich, CH-8093 Zurich, Switzerland, [b] Swiss Light Source, PSI Villigen, CH-5232 Villigen Switzerland.

* Author for correspondence email address:

martin@quack.ch

Table 11 provide structural parameters along the IRC path. Table 12 gives rotational constants along the reaction path as a function of the $\tau_{C_6S_1S_2C_3}$ coordinate (constrained geometry optimizations with different fixed $\tau_{C_6S_1S_2C_3}$ values were carried out with the Gaussian 09 program package at the MP2/cc-pVTZ level of theory). Projected harmonic wavenumbers along the reaction path ($3N - 7 = 23$ values excluding the ring puckering mode) are given by Tables 13 and 14. Table 15 gives harmonic wavenumbers, electric dipole transition moments and intensities calculated according to the double harmonic approximation (MP2/cc-pVTZ level of theory). The electric dipole transition moment components μ_a, μ_b and μ_c are given in the principal axis frame (see Table 16 for Cartesian coordinates of the equilibrium structure expressed in the principal axis frame). Tables 17, 18, 19, 20, 21, 22, 23, 24, 25 and 26 provide harmonic wavenumbers, intensities corresponding to the double harmonic approximation and equilibrium rotational constants (all of these quantities were calculated with the Gaussian 09 program package, MP2/cc-pVTZ level of theory) for all possible deuterated isotopomers of 1,2-dithiine. Table 27 provides a line list for the rotational transitions of the ground state of dithiine, Tables 28, 29 and 30 line lists for the fundamentals of the ν_{22}, ν_{17} and ν_3 of dithiine.

Table 11: Molecular structural parameters (r in pm, bond (α) and torsional (τ) angles in degrees) along the IRC path for the stereomutation of 1,2-dithiine as calculated with MP2/cc-pVTZ level of theory obtained by the Gaussian 09 program package. The reaction coordinate q_i is given be discrete values numbered from $i = 1$. Internal coordinates are defined as follows: $r_1 = r(S_1C_6)$, $r_2 = r(S_1S_2)$, $r_3 = r(C_5C_6)$, $r_4 = r(C_4C_5)$, $r_5 = r(C_6H_7)$, $r_6 = r(C_5H_{10})$, $\alpha_1 = \alpha(C_6S_1S_2)$, $\alpha_2 = \alpha(S_1C_6C_5)$, $\alpha_3 = \alpha(C_4C_5C_6)$, $\alpha_4 = \alpha(S_1C_6H_7)$, $\alpha_5 = \alpha(C_6C_5H_{10})$, $\tau_1 = \tau(C_6S_1S_2C_3)$, $\tau_2 = \tau(S_2S_1C_6H_7)$, $\tau_3 = \tau(S_2S_1C_6C_5)$ and $\tau_4 = \tau(S_1C_6C_5H_{10})$. The second last column gives the energy with respect to the potential minimum.

r_1	r_2	r_3	r_4	r_5	r_6	α_1	α_2	α_3	α_4	α_5	τ_1	τ_2	τ_3	τ_4	$E/(hc\ \mathrm{cm}^{-1})$	q_i
175.4	212.8	134.2	145.4	108.3	108.1	104.7	129.6	125.7	109.9	116.7	0.0	180.0	0.0	180.0	2899	q_1
175.4	212.8	134.2	145.4	108.3	108.1	104.7	129.6	125.7	109.9	116.7	-1.8	-178.7	1.6	179.7	2892	q_2
175.4	212.7	134.2	145.4	108.3	108.1	104.7	129.5	125.7	109.9	116.7	-3.7	-177.4	3.1	179.5	2875	q_3
175.4	212.7	134.2	145.4	108.3	108.1	104.7	129.5	125.7	110.0	116.7	-5.5	-176.2	4.7	179.2	2846	q_4
175.4	212.6	134.2	145.3	108.3	108.1	104.6	129.4	125.7	110.0	116.7	-7.4	-174.9	6.2	179.0	2804	q_5
175.4	212.5	134.2	145.3	108.3	108.1	104.6	129.3	125.7	110.1	116.7	-9.2	-173.6	7.8	178.7	2754	q_6
175.4	212.4	134.2	145.3	108.3	108.1	104.5	129.2	125.7	110.2	116.7	-11.0	-172.4	9.3	178.5	2690	q_7
175.4	212.3	134.3	145.3	108.3	108.1	104.4	129.0	125.7	110.4	116.7	-12.9	-171.1	10.8	178.3	2618	q_8
175.4	212.2	134.3	145.3	108.3	108.1	104.3	128.9	125.7	110.5	116.7	-14.7	-169.8	12.3	178.1	2534	q_9
175.5	212.0	134.3	145.3	108.3	108.1	104.2	128.7	125.7	110.7	116.7	-16.5	-168.6	13.8	177.9	2444	q_{10}
175.5	211.9	134.3	145.2	108.3	108.1	104.1	128.5	125.7	110.8	116.7	-18.3	-167.3	15.3	177.7	2343	q_{11}
175.5	211.7	134.4	145.2	108.3	108.1	104.0	128.3	125.7	111.0	116.7	-20.1	-166.1	16.7	177.5	2236	q_{12}
175.5	211.5	134.4	145.2	108.3	108.1	103.8	128.0	125.7	111.2	116.8	-21.9	-164.8	18.2	177.3	2120	q_{13}
175.6	211.3	134.4	145.1	108.3	108.1	103.7	127.8	125.6	111.5	116.8	-23.6	-163.6	19.6	177.2	1999	q_{14}
175.6	211.1	134.5	145.1	108.3	108.2	103.5	127.5	125.6	111.7	116.8	-25.4	-162.3	21.0	177.1	1872	q_{15}
175.6	210.8	134.5	145.1	108.3	108.2	103.3	127.3	125.6	111.9	116.8	-27.1	-161.1	22.3	177.0	1742	q_{16}
175.6	210.6	134.5	145.1	108.3	108.2	103.1	127.0	125.6	112.2	116.9	-28.8	-159.9	23.6	176.9	1608	q_{17}
175.7	210.3	134.6	145.0	108.3	108.2	102.9	126.7	125.6	112.4	116.9	-30.5	-158.7	24.9	176.8	1472	q_{18}
175.7	210.1	134.6	145.0	108.3	108.2	102.7	126.4	125.5	112.7	116.9	-32.2	-157.5	26.2	176.7	1334	q_{19}
175.7	209.8	134.7	145.0	108.3	108.2	102.5	126.1	125.5	113.0	117.0	-33.9	-156.3	27.5	176.7	1198	q_{20}
175.8	209.5	134.7	144.9	108.3	108.2	102.2	125.7	125.4	113.2	117.0	-35.6	-155.1	28.7	176.6	1062	q_{21}
175.8	209.3	134.7	144.9	108.3	108.2	102.0	125.4	125.4	113.5	117.0	-37.2	-153.9	29.9	176.6	930	q_{22}
175.8	209.0	134.8	144.9	108.3	108.2	101.7	125.1	125.3	113.8	117.1	-38.8	-152.8	31.1	176.6	801	q_{23}
175.9	208.7	134.8	144.9	108.2	108.2	101.4	124.7	125.2	114.1	117.1	-40.5	-151.6	32.3	176.6	678	q_{24}
175.9	208.4	134.8	144.8	108.2	108.2	101.1	124.4	125.2	114.4	117.2	-42.1	-150.5	33.4	176.6	559	q_{25}
175.9	208.1	134.9	144.8	108.2	108.2	100.8	124.0	125.1	114.6	117.3	-43.6	-149.4	34.5	176.6	449	q_{26}
176.0	207.9	134.9	144.8	108.2	108.2	100.5	123.7	125.0	114.9	117.3	-45.2	-148.3	35.6	176.7	348	q_{27}
176.0	207.6	134.9	144.8	108.2	108.2	100.2	123.3	124.9	115.2	117.4	-46.7	-147.1	36.7	176.7	258	q_{28}
176.0	207.3	135.0	144.8	108.2	108.2	99.8	123.0	124.8	115.5	117.5	-48.2	-146.1	37.7	176.8	179	q_{29}
176.1	207.1	135.0	144.7	108.2	108.2	99.4	122.6	124.7	115.7	117.5	-49.7	-145.0	38.7	176.9	114	q_{30}
176.2	206.2	135.1	144.7	108.2	108.2	98.0	121.4	124.2	116.6	117.9	-55.0	-141.1	42.3	177.2	0	q_{31}

Table 12: Rotational constants (A, B and C, in cm^{-1}) along the reaction path (the reaction coordinate is defined as $\tau_{C_6S_1S_2C_3}$ and given in degrees). Rotational constants were calculated from MP2/cc-pVTZ geometries obtained by setting $\tau_{C_6S_1S_2C_3}$ to a fixed value and optimizing the remaining coordinates. Constrained optimizations were carried out by the Gaussian 09 program package. The values $\tau_{C_6S_1S_2C_3} = 0.0000^\circ$ and $\tau_{C_6S_1S_2C_3} = 54.9891^\circ$ correspond to transition state and equibrium structures. Symmetrically equivalent rotational constant values with $\tau_{C_6S_1S_2C_3} < 0.0000^\circ$ can be readily obtained by reflection to $\tau_{C_6S_1S_2C_3} = 0.0000^\circ$.

$\tau_{C_6S_1S_2C_3}$	A	B	C	$\tau_{C_6S_1S_2C_3}$	A	B	C
0.0000	0.107846	0.100062	0.051904	50.1371	0.110749	0.102956	0.057704
1.6173	0.107851	0.100065	0.051910	51.7545	0.110861	0.103137	0.058096
3.2347	0.107863	0.100076	0.051928	53.3718	0.110965	0.103326	0.058503
4.8520	0.107883	0.100093	0.051958	54.9891	0.111061	0.103524	0.058925
6.4693	0.107912	0.100117	0.052000	56.6064	0.111148	0.103730	0.059362
8.0866	0.107948	0.100148	0.052054	58.2238	0.111224	0.103946	0.059814
9.7040	0.107993	0.100185	0.052119	59.8411	0.111287	0.104174	0.060282
11.3213	0.108045	0.100230	0.052197	61.4584	0.111338	0.104413	0.060766
12.9386	0.108105	0.100280	0.052287	63.0757	0.111374	0.104665	0.061265
14.5559	0.108173	0.100337	0.052388	64.6931	0.111393	0.104932	0.061780
16.1733	0.108247	0.100400	0.052501	66.3104	0.111395	0.105214	0.062310
17.7906	0.108329	0.100470	0.052627	67.9277	0.111379	0.105512	0.062855
19.4079	0.108417	0.100545	0.052764	69.5451	0.111342	0.105829	0.063415
21.0252	0.108512	0.100626	0.052913	71.1624	0.111283	0.106166	0.063989
22.6426	0.108612	0.100712	0.053074	72.7797	0.111202	0.106523	0.064576
24.2599	0.108719	0.100804	0.053247	74.3970	0.111098	0.106901	0.065176
25.8772	0.108830	0.100902	0.053433	76.0144	0.110970	0.107303	0.065787
27.4946	0.108946	0.101004	0.053630	77.6317	0.110817	0.107727	0.066408
29.1119	0.109067	0.101112	0.053839	79.2490	0.110639	0.108176	0.067037
30.7292	0.109192	0.101224	0.054060	80.8663	0.110437	0.108649	0.067673
32.3465	0.109319	0.101341	0.054293	82.4837	0.110212	0.109145	0.068314
33.9639	0.109450	0.101463	0.054539	84.1010	0.109964	0.109666	0.068959
35.5812	0.109582	0.101590	0.054797	85.7183	0.110209	0.109695	0.069606
37.1985	0.109716	0.101721	0.055068	87.3356	0.110773	0.109407	0.070252
38.8158	0.109851	0.101857	0.055351	88.9530	0.111356	0.109103	0.070897
40.4332	0.109985	0.101998	0.055647	90.5703	0.111957	0.108786	0.071539
42.0505	0.110119	0.102144	0.055956	92.1876	0.112572	0.108460	0.072176
43.6678	0.110252	0.102295	0.056278	93.8050	0.113198	0.108129	0.072808
45.2851	0.110382	0.102451	0.056614	95.4223	0.113832	0.107800	0.073434
46.9025	0.110509	0.102613	0.056964	97.0396	0.114468	0.107480	0.074052
48.5198	0.110631	0.102781	0.057327	98.6569	0.115101	0.107178	0.074664

Table 13: Projected harmonic wavenumbers $\widetilde{\omega}$ (in cm^{-1}) along the reaction path (the reaction coordinate is defined as $\tau_{C_6S_1S_2C_3}$ and given in degrees).

$\tau_{C_6S_1S_2C_3}$	$\widetilde{\omega}$																						
0.0000	263.1	313.8	458.1	502.2	512.7	641.9	678.5	729.0	745.6	849.5	925.7	926.6	985.4	1209.1	1213.0	1341.2	1403.0	1627.6	1644.8	3198.4	3202.1	3222.1	3232.7
1.6173	262.9	313.7	458.1	502.4	512.7	641.8	678.6	729.0	745.7	849.5	925.7	926.6	985.4	1209.1	1212.9	1341.2	1403.0	1627.5	1644.8	3198.4	3202.1	3222.0	3232.7
3.2347	262.5	313.7	457.9	502.9	512.7	641.4	678.9	729.0	745.9	849.5	925.8	926.6	985.5	1209.1	1212.9	1341.2	1403.0	1627.4	1644.7	3198.4	3202.1	3222.0	3232.7
4.8520	261.8	313.6	457.7	503.7	512.7	640.8	679.5	729.0	746.3	849.5	925.9	926.7	985.7	1209.0	1212.8	1341.2	1403.0	1627.1	1644.6	3198.3	3202.1	3222.0	3232.6
6.4693	260.9	313.6	457.5	504.9	512.7	639.9	680.2	729.0	746.8	849.5	926.0	926.9	985.9	1208.9	1212.7	1341.2	1402.9	1626.6	1644.4	3198.2	3202.0	3221.9	3232.5
8.0866	259.7	313.4	457.1	506.3	512.7	638.9	681.1	729.0	747.5	849.5	926.2	927.1	986.2	1208.8	1212.5	1341.1	1402.9	1626.1	1644.2	3198.2	3201.9	3221.8	3232.3
9.7040	258.3	313.3	456.8	507.9	512.7	637.7	682.0	729.0	748.3	849.5	926.4	927.3	986.6	1208.7	1212.3	1341.1	1402.9	1625.5	1643.9	3198.1	3201.9	3221.7	3232.2
11.3213	256.6	313.1	456.4	509.6	512.9	636.5	683.1	729.1	749.2	849.5	926.6	927.6	987.0	1208.5	1212.1	1341.0	1402.9	1624.7	1643.6	3198.0	3201.8	3221.5	3232.0
12.9386	254.8	313.0	456.1	511.0	513.7	635.2	684.2	729.1	750.2	849.6	926.9	927.9	987.5	1208.3	1211.8	1341.0	1402.8	1623.9	1643.3	3197.8	3201.7	3221.4	3231.8
14.5559	252.7	312.8	455.7	511.5	515.3	633.8	685.4	729.2	751.4	849.6	927.2	928.2	988.0	1208.0	1211.5	1340.9	1402.8	1622.9	1642.9	3197.7	3201.5	3221.2	3231.5
16.1733	250.5	312.5	455.4	511.7	517.6	632.5	686.5	729.3	752.6	849.7	927.5	928.6	988.5	1207.8	1211.2	1340.9	1402.7	1621.8	1642.4	3197.5	3201.4	3221.0	3231.3
17.7906	248.1	312.3	455.1	511.8	520.1	631.1	687.6	729.4	753.9	849.8	927.8	929.0	989.1	1207.4	1210.8	1340.8	1402.6	1620.7	1641.9	3197.4	3201.3	3220.8	3231.0
19.4079	245.6	312.0	454.8	511.8	522.8	629.8	688.8	729.5	755.3	850.0	928.1	929.4	989.7	1207.1	1210.4	1340.7	1402.5	1619.4	1641.3	3197.2	3201.2	3220.6	3230.7
21.0252	243.0	311.8	454.5	511.8	525.6	628.6	689.8	729.7	756.7	850.1	928.5	929.9	990.4	1206.7	1209.9	1340.5	1402.4	1618.1	1640.7	3197.1	3201.1	3220.4	3230.4
22.6426	240.3	311.5	454.3	511.8	528.4	627.4	690.9	729.9	758.2	850.4	928.8	930.4	991.1	1206.2	1209.4	1340.4	1402.3	1616.7	1640.1	3196.9	3200.9	3220.2	3230.1
24.2599	237.6	311.2	454.1	511.8	531.3	626.4	691.9	730.1	759.7	850.6	929.1	930.9	991.7	1205.7	1208.8	1340.2	1402.1	1615.2	1639.4	3196.7	3200.8	3220.0	3229.7
25.8772	234.9	311.0	453.9	511.9	534.2	625.4	692.8	730.4	761.2	850.9	929.5	931.4	992.4	1205.1	1208.2	1340.1	1401.9	1613.7	1638.6	3196.6	3200.7	3219.7	3229.4
27.4946	232.2	310.7	453.7	512.0	537.1	624.6	693.7	730.7	762.8	851.2	929.8	932.0	993.1	1204.5	1207.5	1339.8	1401.7	1612.0	1637.8	3196.4	3200.6	3219.5	3229.0
29.1119	229.6	310.5	453.5	512.2	539.9	624.0	694.5	731.0	764.3	851.6	930.1	932.5	993.8	1203.8	1206.8	1339.6	1401.5	1610.3	1636.9	3196.3	3200.6	3219.3	3228.6
30.7292	227.1	310.3	453.3	512.4	542.8	623.4	695.3	731.3	765.9	851.9	930.4	933.1	994.4	1203.0	1206.0	1339.3	1401.2	1608.5	1635.9	3196.1	3200.6	3219.1	3228.3
32.3465	224.7	310.2	453.1	512.7	545.5	623.0	696.0	731.7	767.4	852.4	930.6	933.6	995.0	1202.2	1205.1	1339.0	1400.9	1606.6	1634.9	3196.0	3200.5	3218.9	3227.9
33.9639	222.4	310.0	452.9	513.0	548.2	622.8	696.7	732.1	768.9	852.8	930.8	934.2	995.6	1201.2	1204.2	1338.7	1400.6	1604.7	1633.8	3195.9	3200.6	3218.7	3227.6
35.5812	220.3	310.0	452.6	513.4	550.9	622.7	697.3	732.5	770.3	853.3	931.0	934.7	996.2	1200.3	1203.2	1338.3	1400.2	1602.6	1632.7	3195.8	3200.6	3218.6	3227.2
37.1985	218.4	309.9	452.4	513.8	553.4	622.8	697.8	733.0	771.7	853.8	931.2	935.2	996.7	1199.2	1202.1	1337.9	1399.7	1600.5	1631.4	3195.8	3200.7	3218.5	3226.9
38.8158	216.8	310.0	452.1	514.4	555.8	623.0	698.3	733.6	773.0	854.2	931.3	935.7	997.2	1198.0	1201.0	1337.4	1399.2	1598.3	1630.1	3195.8	3200.9	3218.4	3226.6
40.4332	215.4	310.1	451.8	515.0	558.0	623.4	698.8	734.1	774.2	854.7	931.3	936.2	997.6	1196.8	1199.7	1336.9	1398.7	1595.9	1628.6	3195.8	3201.0	3218.4	3226.3
42.0505	214.2	310.2	451.4	515.6	560.2	623.9	699.2	734.7	775.3	855.3	931.3	936.7	997.9	1195.4	1198.4	1336.3	1398.0	1593.4	1627.1	3195.8	3201.3	3218.4	3226.0
43.6678	213.3	310.5	451.0	516.3	562.2	624.6	699.6	735.3	776.4	855.7	931.2	937.1	998.2	1194.0	1197.0	1335.7	1397.3	1590.8	1625.5	3195.8	3201.5	3218.4	3225.8
45.2851	212.7	310.8	450.6	517.1	564.0	625.4	699.9	736.0	777.3	856.2	931.1	937.4	998.4	1192.5	1195.5	1335.0	1396.6	1588.1	1623.7	3195.9	3201.9	3218.5	3225.6
46.9025	212.3	311.3	450.2	517.9	565.7	626.3	700.3	736.6	778.1	856.7	930.9	937.7	998.5	1190.9	1193.9	1334.2	1395.7	1585.2	1621.8	3196.0	3202.2	3218.7	3225.5
48.5198	212.2	311.8	449.8	518.7	567.1	627.3	700.6	737.3	778.8	857.1	930.6	938.0	998.4	1189.2	1192.3	1333.4	1394.8	1582.1	1619.7	3196.1	3202.6	3219.0	3225.4
50.1371	212.4	312.4	449.3	519.6	568.4	628.4	700.9	738.0	779.3	857.5	930.2	938.2	998.3	1187.3	1190.5	1332.5	1393.7	1578.9	1617.5	3196.2	3203.0	3219.3	3225.3

51.7545	212.8	313.2	448.8	520.4	569.6	629.5	701.1	738.7	779.7	857.9	929.8	938.3	998.1	1185.4	1188.6	1331.5	1392.6	1575.4	1615.1	3196.3	3203.5	3219.7	3225.3
53.3718	213.5	314.0	448.3	521.3	570.5	630.8	701.4	739.4	780.0	858.2	929.2	938.3	997.8	1183.4	1186.6	1330.5	1391.4	1571.7	1612.6	3196.5	3204.0	3220.3	3225.4
54.9891	214.4	315.0	447.8	522.1	571.2	632.0	701.7	740.1	780.2	858.5	928.6	938.2	997.3	1181.3	1184.4	1329.3	1390.0	1567.7	1609.8	3196.6	3204.4	3220.9	3225.6
56.6064	215.5	316.1	447.2	522.9	571.8	633.3	702.1	740.7	780.2	858.6	927.9	938.1	996.7	1179.1	1182.2	1328.1	1388.5	1563.5	1606.8	3196.7	3204.9	3221.6	3225.9
58.2238	216.8	317.4	446.7	523.6	572.1	634.6	702.4	741.3	780.1	858.8	927.1	937.8	995.9	1176.8	1179.8	1326.7	1386.9	1558.9	1603.6	3196.7	3205.3	3222.4	3226.3
59.8411	218.3	318.8	446.1	524.1	572.3	635.9	702.8	741.7	779.9	858.8	926.2	937.5	995.0	1174.4	1177.3	1325.3	1385.1	1554.0	1600.2	3196.8	3205.7	3223.4	3226.9
61.4584	219.9	320.3	445.5	524.6	572.2	637.1	703.3	742.1	779.6	858.8	925.2	937.0	993.9	1171.9	1174.7	1323.8	1383.2	1548.8	1596.4	3196.8	3206.1	3224.4	3227.5
63.0757	221.7	321.9	445.0	524.9	572.0	638.3	703.8	742.3	779.3	858.6	924.1	936.3	992.7	1169.3	1171.9	1322.2	1381.2	1543.2	1592.4	3196.8	3206.4	3225.6	3228.3
64.6931	223.5	323.8	444.3	525.1	571.6	639.4	704.3	742.3	778.9	858.4	922.9	935.6	991.2	1166.5	1169.0	1320.4	1378.9	1537.1	1588.1	3196.7	3206.6	3226.8	3229.3
66.3104	225.5	325.7	443.7	525.0	571.0	640.4	705.0	742.1	778.6	858.0	921.6	934.7	989.6	1163.7	1166.0	1318.6	1376.6	1530.6	1583.4	3196.6	3206.7	3228.2	3230.3
67.9277	227.5	327.8	443.0	524.6	570.2	641.3	705.8	741.6	778.3	857.6	920.2	933.7	987.7	1160.8	1162.8	1316.7	1374.0	1523.6	1578.4	3196.5	3206.7	3229.6	3231.5
69.5451	229.6	330.1	442.3	524.0	569.4	642.1	706.6	740.8	778.2	857.0	918.7	932.5	985.7	1157.8	1159.4	1314.6	1371.3	1516.1	1573.0	3196.2	3206.7	3231.1	3232.8
71.1624	231.6	332.5	441.5	523.1	568.3	642.6	707.6	739.5	778.2	856.2	917.1	931.2	983.4	1154.6	1155.9	1312.5	1368.4	1508.0	1567.1	3196.0	3206.5	3232.7	3234.2
72.7797	233.7	335.1	440.6	521.8	567.2	643.0	708.7	737.9	778.4	855.3	915.4	929.7	980.9	1151.4	1152.2	1310.2	1365.2	1499.3	1560.9	3195.6	3206.3	3234.3	3235.7
74.3970	235.7	337.8	439.7	520.1	566.0	643.2	710.0	735.9	778.8	854.3	913.6	928.1	978.2	1148.1	1148.4	1307.8	1361.9	1490.1	1554.2	3195.2	3205.9	3236.0	3237.2
76.0144	237.6	340.6	438.7	518.0	564.7	643.2	711.4	733.4	779.4	853.1	911.8	926.2	975.3	1144.4	1144.7	1305.3	1358.4	1480.1	1547.1	3194.8	3205.5	3237.6	3238.8
77.6317	239.4	343.6	437.6	515.5	563.3	642.9	712.9	730.5	780.2	851.8	909.9	924.2	972.2	1140.2	1141.2	1302.7	1354.7	1469.5	1539.5	3194.2	3205.0	3239.2	3240.3
79.2490	241.0	346.7	436.4	512.5	561.9	642.4	714.6	727.1	781.3	850.2	908.0	922.1	968.9	1135.9	1137.5	1300.0	1350.7	1458.2	1531.5	3193.6	3204.4	3240.8	3241.9
80.8663	242.5	349.9	435.2	509.1	560.4	641.7	716.4	723.4	782.5	848.5	906.1	919.7	965.5	1131.4	1133.8	1297.1	1346.4	1446.3	1522.9	3192.9	3203.7	3242.3	3243.3
82.4837	243.7	353.2	433.9	505.1	559.0	640.7	718.4	719.4	783.9	846.6	904.1	917.2	961.9	1126.7	1129.9	1294.1	1341.7	1433.8	1513.8	3192.1	3202.9	3243.7	3244.7
84.1010	244.7	356.5	432.7	500.7	557.5	639.5	715.0	720.5	785.5	844.4	902.1	914.4	958.3	1121.8	1126.0	1290.9	1336.6	1420.7	1504.3	3191.3	3202.1	3245.0	3246.0
85.7183	245.3	359.9	431.5	495.8	556.0	638.1	710.4	722.6	787.1	842.1	900.1	911.5	954.5	1116.7	1121.9	1287.5	1330.8	1407.3	1494.3	3190.4	3201.1	3246.1	3247.1
87.3356	245.6	363.4	430.4	490.3	554.6	636.4	705.4	724.9	788.9	839.5	898.2	908.4	950.8	1111.4	1117.6	1284.0	1324.2	1393.7	1483.8	3189.4	3200.1	3247.0	3248.0
88.9530	245.4	366.8	429.5	484.1	553.1	634.6	700.3	727.2	790.8	836.6	896.3	905.0	947.0	1105.9	1113.1	1280.2	1316.2	1380.5	1473.0	3188.3	3199.0	3247.7	3248.7
90.5703	244.8	370.1	428.9	477.3	551.7	632.5	695.0	729.6	792.7	833.5	894.4	901.5	943.3	1100.1	1108.5	1276.1	1306.3	1368.1	1461.7	3187.1	3197.9	3248.1	3249.1
92.1876	243.5	373.5	428.5	469.7	550.4	630.3	689.5	731.9	794.6	830.1	892.6	897.8	939.7	1093.9	1103.5	1271.8	1294.1	1357.2	1450.1	3185.9	3196.7	3248.1	3249.2
93.8050	241.5	376.7	428.4	461.4	549.2	628.0	684.1	734.2	796.6	826.4	890.8	894.0	936.0	1087.3	1098.3	1267.0	1279.3	1347.9	1438.2	3184.6	3195.5	3247.8	3248.9
95.4223	238.6	379.8	428.2	452.4	548.1	625.6	678.6	736.3	798.6	822.5	889.1	890.1	932.5	1080.3	1092.5	1261.9	1262.2	1340.1	1426.2	3183.3	3194.2	3247.1	3248.2
97.0396	234.6	382.7	426.4	444.1	547.2	623.2	673.3	738.3	800.5	818.2	886.1	887.4	929.0	1072.6	1086.1	1243.3	1256.3	1333.6	1414.0	3182.0	3192.9	3245.8	3246.9
98.6569	229.1	385.5	418.7	442.3	546.5	621.0	668.1	740.0	802.7	813.7	882.2	885.8	925.7	1064.1	1078.7	1223.7	1250.1	1328.1	1401.8	3180.6	3191.7	3244.0	3245.1

Table 14: Projected harmonic wavenumbers $\widetilde{\omega}$ (in cm^{-1}) along the reaction path (the reaction coordinate is defined as $\tau_{C_6S_1S_2C_3}$ and given in degrees). Since some pairs of the original projected harmonic wavenumbers exhibit avoided crossings along the reaction path, we employed a diabatization algorithm to obtain smoothly crossing harmonic wavenumbers as a function of $\tau_{C_6S_1S_2C_3}$.

$\tau_{C_6S_1S_2C_3}$	$\widetilde{\omega}$																					
0.0000	263.1	313.8	458.1	502.2	512.7	641.9	678.5	729.0	745.6	849.5	925.7	926.6	985.4	1209.1	1213.0	1341.2	1403.0	1627.6	1644.8	3198.4	3202.1	3222.1	3232.7
1.6173	262.9	313.7	458.1	502.4	512.7	641.8	678.6	729.0	745.7	849.5	925.7	926.6	985.4	1209.1	1212.9	1341.2	1403.0	1627.5	1644.8	3198.4	3202.1	3222.0	3232.7
3.2347	262.5	313.7	457.9	502.9	512.7	641.4	678.9	729.0	745.9	849.5	925.8	926.6	985.5	1209.1	1212.9	1341.2	1403.0	1627.4	1644.7	3198.4	3202.1	3222.0	3232.7
4.8520	261.8	313.6	457.7	503.7	512.7	640.8	679.5	729.0	746.3	849.5	925.9	926.7	985.7	1209.0	1212.8	1341.2	1403.0	1627.1	1644.6	3198.3	3202.1	3222.0	3232.6
6.4693	260.9	313.6	457.5	504.9	512.7	639.9	680.2	729.0	746.8	849.5	926.0	926.9	985.9	1208.9	1212.7	1341.2	1402.9	1626.6	1644.4	3198.2	3202.0	3221.9	3232.5
8.0866	259.7	313.4	457.1	506.3	512.7	638.9	681.1	729.0	747.5	849.5	926.2	927.1	986.2	1208.8	1212.5	1341.1	1402.9	1626.1	1644.2	3198.2	3201.9	3221.8	3232.3
9.7040	258.3	313.3	456.8	507.9	512.7	637.7	682.0	729.0	748.3	849.5	926.4	927.3	986.6	1208.7	1212.3	1341.1	1402.9	1625.5	1643.9	3198.1	3201.9	3221.7	3232.2
11.3213	256.6	313.1	456.4	509.6	512.9	636.5	683.1	729.1	749.2	849.5	926.6	927.6	987.0	1208.5	1212.1	1341.0	1402.9	1624.7	1643.6	3198.0	3201.8	3221.5	3232.0
12.9386	254.8	313.0	456.1	513.7	511.0	635.2	684.2	729.1	750.2	849.6	926.9	927.9	987.5	1208.3	1211.8	1341.0	1402.8	1623.9	1643.3	3197.8	3201.7	3221.4	3231.8
14.5559	252.7	312.8	455.7	515.3	511.5	633.8	685.4	729.2	751.4	849.6	927.2	928.2	988.0	1208.0	1211.5	1340.9	1402.8	1622.9	1642.9	3197.7	3201.5	3221.2	3231.5
16.1733	250.5	312.5	455.4	517.6	511.7	632.5	686.5	729.3	752.6	849.7	927.5	928.6	988.5	1207.8	1211.2	1340.9	1402.7	1621.8	1642.4	3197.5	3201.4	3221.0	3231.3
17.7906	248.1	312.3	455.1	520.1	511.8	631.1	687.6	729.4	753.9	849.8	927.8	929.0	989.1	1207.4	1210.8	1340.8	1402.6	1620.7	1641.9	3197.4	3201.3	3220.8	3231.0
19.4079	245.6	312.0	454.8	522.8	511.8	629.8	688.8	729.5	755.3	850.0	928.1	929.4	989.7	1207.1	1210.4	1340.7	1402.5	1619.4	1641.3	3197.2	3201.2	3220.6	3230.7
21.0252	243.0	311.8	454.5	525.6	511.8	628.6	689.8	729.7	756.7	850.1	928.5	929.9	990.4	1206.7	1209.9	1340.5	1402.4	1618.1	1640.7	3197.1	3201.1	3220.4	3230.4
22.6426	240.3	311.5	454.3	528.4	511.8	627.4	690.9	729.9	758.2	850.4	928.8	930.4	991.1	1206.2	1209.4	1340.4	1402.3	1616.7	1640.1	3196.9	3200.9	3220.2	3230.1
24.2599	237.6	311.2	454.1	531.3	511.8	626.4	691.9	730.1	759.7	850.6	929.1	930.9	991.7	1205.7	1208.8	1340.2	1402.1	1615.2	1639.4	3196.7	3200.8	3220.0	3229.7
25.8772	234.9	311.0	453.9	534.2	511.9	625.4	692.8	730.4	761.2	850.9	929.5	931.4	992.4	1205.1	1208.2	1340.1	1401.9	1613.7	1638.6	3196.6	3200.7	3219.7	3229.4
27.4946	232.2	310.7	453.7	537.1	512.0	624.6	693.7	730.7	762.8	851.2	929.8	932.0	993.1	1204.5	1207.5	1339.8	1401.7	1612.0	1637.8	3196.4	3200.6	3219.5	3229.0
29.1119	229.6	310.5	453.5	539.9	512.2	624.0	694.5	731.0	764.3	851.6	930.1	932.5	993.8	1203.8	1206.8	1339.6	1401.5	1610.3	1636.9	3196.3	3200.6	3219.3	3228.6
30.7292	227.1	310.3	453.3	542.8	512.4	623.4	695.3	731.3	765.9	851.9	930.4	933.1	994.4	1203.0	1206.0	1339.3	1401.2	1608.5	1635.9	3196.1	3200.6	3219.1	3228.3
32.3465	224.7	310.2	453.1	545.5	512.7	623.0	696.0	731.7	767.4	852.4	930.6	933.6	995.0	1202.2	1205.1	1339.0	1400.9	1606.6	1634.9	3196.0	3200.5	3218.9	3227.9
33.9639	222.4	310.0	452.9	548.2	513.0	622.8	696.7	732.1	768.9	852.8	930.8	934.2	995.6	1201.2	1204.2	1338.7	1400.6	1604.7	1633.8	3195.9	3200.6	3218.7	3227.6
35.5812	220.3	310.0	452.6	550.9	513.4	622.7	697.3	732.5	770.3	853.3	931.0	934.7	996.2	1200.3	1203.2	1338.3	1400.2	1602.6	1632.7	3195.8	3200.6	3218.6	3227.2
37.1985	218.4	309.9	452.4	553.4	513.8	622.8	697.8	733.0	771.7	853.8	931.2	935.2	996.7	1199.2	1202.1	1337.9	1399.7	1600.5	1631.4	3195.8	3200.7	3218.5	3226.9
38.8158	216.8	310.0	452.1	555.8	514.4	623.0	698.3	733.6	773.0	854.2	931.3	935.7	997.2	1198.0	1201.0	1337.4	1399.2	1598.3	1630.1	3195.8	3200.9	3218.4	3226.6
40.4332	215.4	310.1	451.8	558.0	515.0	623.4	698.8	734.1	774.2	854.7	931.3	936.2	997.6	1196.8	1199.7	1336.9	1398.7	1595.9	1628.6	3195.8	3201.0	3218.4	3226.3
42.0505	214.2	310.2	451.4	560.2	515.6	623.9	699.2	734.7	775.3	855.3	931.3	936.7	997.9	1195.4	1198.4	1336.3	1398.0	1593.4	1627.1	3195.8	3201.3	3218.4	3226.0
43.6678	213.3	310.5	451.0	562.2	516.3	624.6	699.6	735.3	776.4	855.7	931.2	937.1	998.2	1194.0	1197.0	1335.7	1397.3	1590.8	1625.5	3195.8	3201.5	3218.4	3225.8
45.2851	212.7	310.8	450.6	564.0	517.1	625.4	699.9	736.0	777.3	856.2	931.1	937.4	998.4	1192.5	1195.5	1335.0	1396.6	1588.1	1623.7	3195.9	3201.9	3218.5	3225.6
46.9025	212.3	311.3	450.2	565.7	517.9	626.3	700.3	736.6	778.1	856.7	930.9	937.7	998.5	1190.9	1193.9	1334.2	1395.7	1585.2	1621.8	3196.0	3202.2	3218.7	3225.5

48.5198	212.2	311.8	449.8	567.1	518.7	627.3	700.6	737.3	778.8	857.1	930.6	938.0	998.4	1189.2	1192.3	1333.4	1394.8	1582.1	1619.7	3196.1	3202.6	3219.0	3225.4
50.1371	212.4	312.4	449.3	568.4	519.6	628.4	700.9	738.0	779.3	857.5	930.2	938.2	998.3	1187.3	1190.5	1332.5	1393.7	1578.9	1617.5	3196.2	3203.0	3219.3	3225.3
51.7545	212.8	313.2	448.8	569.6	520.4	629.5	701.1	738.7	779.7	857.9	929.8	938.3	998.1	1185.4	1188.6	1331.5	1392.6	1575.4	1615.1	3196.3	3203.5	3219.7	3225.3
53.3718	213.5	314.0	448.3	570.5	521.3	630.8	701.4	739.4	780.0	858.2	929.2	938.3	997.8	1183.4	1186.6	1330.5	1391.4	1571.7	1612.6	3196.5	3204.0	3220.3	3225.4
54.9891	214.4	315.0	447.8	571.2	522.1	632.0	701.7	740.1	780.2	858.5	928.6	938.2	997.3	1181.3	1184.4	1329.3	1390.0	1567.7	1609.8	3196.6	3204.4	3220.9	3225.6
56.6064	215.5	316.1	447.2	571.8	522.9	633.3	702.1	740.7	780.2	858.6	927.9	938.1	996.7	1179.1	1182.2	1328.1	1388.5	1563.5	1606.8	3196.7	3204.9	3221.6	3225.9
58.2238	216.8	317.4	446.7	572.1	523.6	634.6	702.4	741.3	780.1	858.8	927.1	937.8	995.9	1176.8	1179.8	1326.7	1386.9	1558.9	1603.6	3196.7	3205.3	3222.4	3226.3
59.8411	218.3	318.8	446.1	572.3	524.1	635.9	702.8	741.7	779.9	858.8	926.2	937.5	995.0	1174.4	1177.3	1325.3	1385.1	1554.0	1600.2	3196.8	3205.7	3223.4	3226.9
61.4584	219.9	320.3	445.5	572.2	524.6	637.1	703.3	742.1	779.6	858.8	925.2	937.0	993.9	1171.9	1174.7	1323.8	1383.2	1548.8	1596.4	3196.8	3206.1	3224.4	3227.5
63.0757	221.7	321.9	445.0	572.0	524.9	638.3	703.8	742.3	779.3	858.6	924.1	936.3	992.7	1169.3	1171.9	1322.2	1381.2	1543.2	1592.4	3196.8	3206.4	3225.6	3228.3
64.6931	223.5	323.8	444.3	571.6	525.1	639.4	704.3	742.3	778.9	858.4	922.9	935.6	991.2	1166.5	1169.0	1320.4	1378.9	1537.1	1588.1	3196.7	3206.6	3226.8	3229.3
66.3104	225.5	325.7	443.7	571.0	525.0	640.4	705.0	742.1	778.6	858.0	921.6	934.7	989.6	1163.7	1166.0	1318.6	1376.6	1530.6	1583.4	3196.6	3206.7	3228.2	3230.3
67.9277	227.5	327.8	443.0	570.2	524.6	641.3	705.8	741.6	778.3	857.6	920.2	933.7	987.7	1160.8	1162.8	1316.7	1374.0	1523.6	1578.4	3196.5	3206.7	3229.6	3231.5
69.5451	229.6	330.1	442.3	569.4	524.0	642.1	706.6	740.8	778.2	857.0	918.7	932.5	985.7	1157.8	1159.4	1314.6	1371.3	1516.1	1573.0	3196.2	3206.7	3231.1	3232.8
71.1624	231.6	332.5	441.5	568.3	523.1	642.6	707.6	739.5	778.2	856.2	917.1	931.2	983.4	1154.6	1155.9	1312.5	1368.4	1508.0	1567.1	3196.0	3206.5	3232.7	3234.2
72.7797	233.7	335.1	440.6	567.2	521.8	643.0	708.7	737.9	778.4	855.3	915.4	929.7	980.9	1151.4	1152.2	1310.2	1365.2	1499.3	1560.9	3195.6	3206.3	3234.3	3235.7
74.3970	235.7	337.8	439.7	566.0	520.1	643.2	710.0	735.9	778.8	854.3	913.6	928.1	978.2	1148.1	1148.4	1307.8	1361.9	1490.1	1554.2	3195.2	3205.9	3236.0	3237.2
76.0144	237.6	340.6	438.7	564.7	518.0	643.2	711.4	733.4	779.4	853.1	911.8	926.2	975.3	1144.7	1144.4	1305.3	1358.4	1480.1	1547.1	3194.8	3205.5	3237.6	3238.8
77.6317	239.4	343.6	437.6	563.3	515.5	642.9	712.9	730.5	780.2	851.8	909.9	924.2	972.2	1141.2	1140.2	1302.7	1354.7	1469.5	1539.5	3194.2	3205.0	3239.2	3240.3
79.2490	241.0	346.7	436.4	561.9	512.5	642.4	714.6	727.1	781.3	850.2	908.0	922.1	968.9	1137.5	1135.9	1300.0	1350.7	1458.2	1531.5	3193.6	3204.4	3240.8	3241.9
80.8663	242.5	349.9	435.2	560.4	509.1	641.7	716.4	723.4	782.5	848.5	906.1	919.7	965.5	1133.8	1131.4	1297.1	1346.4	1446.3	1522.9	3192.9	3203.7	3242.3	3243.3
82.4837	243.7	353.2	433.9	559.0	505.1	640.7	718.4	719.4	783.9	846.6	904.1	917.2	961.9	1129.9	1126.7	1294.1	1341.7	1433.8	1513.8	3192.1	3202.9	3243.7	3244.7
84.1010	244.7	356.5	432.7	557.5	500.7	639.5	720.5	715.0	785.5	844.4	902.1	914.4	958.3	1126.0	1121.8	1290.9	1336.6	1420.7	1504.3	3191.3	3202.1	3245.0	3246.0
85.7183	245.3	359.9	431.5	556.0	495.8	638.1	722.6	710.4	787.1	842.1	900.1	911.5	954.5	1121.9	1116.7	1287.5	1330.8	1407.3	1494.3	3190.4	3201.1	3246.1	3247.1
87.3356	245.6	363.4	430.4	554.6	490.3	636.4	724.9	705.4	788.9	839.5	898.2	908.4	950.8	1117.6	1111.4	1284.0	1324.2	1393.7	1483.8	3189.4	3200.1	3247.0	3248.0
88.9530	245.4	366.8	429.5	553.1	484.1	634.6	727.2	700.3	790.8	836.6	896.3	905.0	947.0	1113.1	1105.9	1280.2	1316.2	1380.5	1473.0	3188.3	3199.0	3247.7	3248.7
90.5703	244.8	370.1	428.9	551.7	477.3	632.5	729.6	695.0	792.7	833.5	894.4	901.5	943.3	1108.5	1100.1	1276.1	1306.3	1368.1	1461.7	3187.1	3197.9	3248.1	3249.1
92.1876	243.5	373.5	428.5	550.4	469.7	630.3	731.9	689.5	794.6	830.1	892.6	897.8	939.7	1103.5	1093.9	1271.8	1294.1	1357.2	1450.1	3185.9	3196.7	3248.1	3249.2
93.8050	241.5	376.7	428.4	549.2	461.4	628.0	734.2	684.1	796.6	826.4	890.8	894.0	936.0	1098.3	1087.3	1267.0	1279.3	1347.9	1438.2	3184.6	3195.5	3247.8	3248.9
95.4223	238.6	379.8	428.2	548.1	452.4	625.6	736.3	678.6	798.6	822.5	889.1	890.1	932.5	1092.5	1080.3	1261.9	1262.2	1340.1	1426.2	3183.3	3194.2	3247.1	3248.2
97.0396	234.6	382.7	426.4	547.2	444.1	623.2	738.3	673.3	800.5	818.2	887.4	886.1	929.0	1086.1	1072.6	1256.3	1243.3	1333.6	1414.0	3182.0	3192.9	3245.8	3246.9
98.6569	229.1	385.5	418.7	546.5	442.3	621.0	740.0	668.1	802.7	813.7	885.8	882.2	925.7	1078.7	1064.1	1250.1	1223.7	1328.1	1401.8	3180.6	3191.7	3244.0	3245.1

Table 15: Symmetry labels (C_2 point group), calculated harmonic wavenumbers $\widetilde{\omega}_i$ (in cm^{-1}), electric dipole transition moments (μ_a, μ_b, μ_c, in Debye) in the principal axis frame and intensities I (in km/mol), corresponding to the double harmonic approximation. Cartesian coordinates in the principal axis frame are given in Table 16. These data were calculated at the MP2/cc-pVTZ level of theory by the Gaussian 09 program package.

Mode	Symmetry	$\widetilde{\omega}_i$	μ_a	μ_b	μ_c	I
1	A	3226	3.24×10^{-2}	0	0	8.495
2	A	3204	-5.07×10^{-3}	0	0	0.206
3	A	1568	5.31×10^{-2}	0	0	11.063
4	A	1390	-3.58×10^{-2}	0	0	4.468
5	A	1181	5.74×10^{-3}	0	0	0.098
6	A	997	-3.27×10^{-2}	0	0	2.670
7	A	938	1.86×10^{-2}	0	0	0.814
8	A	780	4.20×10^{-2}	0	0	3.451
9	A	740	5.18×10^{-2}	0	0	4.977
10	A	573	-8.35×10^{-3}	0	0	0.100
11	A	523	7.19×10^{-3}	0	0	0.068
12	A	448	1.47×10^{-2}	0	0	0.243
13	A	204	-1.42×10^{-3}	0	0	0.001
14	B	3221	0	-2.31×10^{-2}	1.17×10^{-2}	5.420
15	B	3197	0	-9.64×10^{-3}	4.14×10^{-3}	0.882
16	B	1610	0	-6.25×10^{-3}	-3.60×10^{-3}	0.210
17	B	1329	0	6.28×10^{-2}	-2.24×10^{-2}	14.809
18	B	1184	0	-1.94×10^{-2}	-3.90×10^{-3}	1.162
19	B	929	0	-5.59×10^{-3}	-5.31×10^{-3}	0.139
20	B	858	0	-9.36×10^{-3}	3.42×10^{-2}	2.711
21	B	702	0	1.72×10^{-2}	2.35×10^{-2}	1.495
22	B	632	0	-1.33×10^{-1}	-2.02×10^{-1}	92.517
23	B	315	0	-1.94×10^{-3}	1.01×10^{-2}	0.083
24	B	214	0	1.00×10^{-1}	1.11×10^{-1}	12.041

Table 16: Cartesian coordinates (in bohr) expressed in the principal axis frame. These data were calculated at the MP2/cc-pVTZ level of theory by the Gaussian 09 program package.

atom	a	b	c
S_1	1.8031	1.8364	0.6517
S_2	1.8031	-1.8364	-0.6517
C_3	-1.1220	-2.7816	0.6283
C_4	-3.1653	-1.2539	0.5454
C_5	-3.1653	1.2539	-0.5454
C_6	-1.1220	2.7816	-0.6283
H_7	-1.2229	4.6797	-1.3822
H_8	-1.2229	-4.6797	1.3822
H_9	-4.9295	-1.9765	1.2870
H_{10}	-4.9295	1.9765	-1.2870

Table 17: Calculated harmonic wavenumbers $\widetilde{\omega}_i$ (in cm^{-1}) and IR intensities (in km mol^{-1}) of ($D_7H_8H_9H_{10}$) 1,2-dithiine obtained by the Gaussian 09 program package.

Mode	Symmetry	$\widetilde{\omega}_i$	Intensity
1	A	3224	7.194
2	A	3211	2.778
3	A	3199	1.470
4	A	2375	1.725
5	A	1603	0.292
6	A	1561	11.313
7	A	1371	7.047
8	A	1300	9.380
9	A	1182	0.535
10	A	1050	3.140
11	A	937	0.212
12	A	904	3.158
13	A	873	1.937
14	A	814	2.786
15	A	741	9.090
16	A	706	23.934
17	A	695	0.198
18	A	580	52.109
19	A	573	0.273
20	A	520	0.448
21	A	443	0.285
22	A	312	0.061
23	A	207	5.577
24	A	194	5.718

Table 18: Calculated harmonic wavenumbers $\widetilde{\omega}_i$ (in cm^{-1}) and IR intensities (in km mol^{-1}) of ($H_7H_8H_9D_{10}$) 1,2-dithiine obtained by the Gaussian 09 program package.

Mode	Symmetry	$\widetilde{\omega}_i$	Intensity
1	A	3223	7.280
2	A	3214	3.726
3	A	3201	0.187
4	A	2370	1.508
5	A	1594	0.967
6	A	1564	10.991
7	A	1373	5.682
8	A	1284	11.541
9	A	1183	0.669
10	A	1028	3.952
11	A	941	0.252
12	A	891	0.353
13	A	850	5.577
14	A	840	2.576
15	A	756	10.045
16	A	735	5.787
17	A	681	0.372
18	A	597	50.994
19	A	548	11.351
20	A	501	6.835
21	A	438	1.119
22	A	313	0.150
23	A	214	11.855
24	A	200	0.021

Table 19: Calculated harmonic wavenumbers $\widetilde{\omega}_i$ (in cm^{-1}) and IR intensities (in km mol^{-1}) of ($D_7H_8H_9D_{10}$) 1,2-dithiine obtained by the Gaussian 09 program package.

Mode	Symmetry	$\widetilde{\omega}_i$	Intensity
1	A	3223	7.270
2	A	3201	0.208
3	A	2389	3.137
4	A	2355	0.274
5	A	1589	1.746
6	A	1554	10.422
7	A	1364	8.511
8	A	1193	1.177
9	A	1141	8.539
10	A	941	0.206
11	A	894	0.781
12	A	873	1.058
13	A	802	2.311
14	A	761	6.137
15	A	738	6.773
16	A	694	12.258
17	A	675	0.962
18	A	575	26.693
19	A	546	15.885
20	A	494	10.044
21	A	434	0.765
22	A	310	0.084
23	A	204	6.674
24	A	193	4.409

Table 20: Calculated harmonic wavenumbers $\widetilde{\omega}_i$ (in cm^{-1}) and IR intensities (in km mol^{-1}) of ($D_7H_8D_9H_{10}$) 1,2-dithiine obtained by the Gaussian 09 program package.

Mode	Symmetry	$\widetilde{\omega}_i$	Intensity
1	A	3214	3.637
2	A	3210	3.999
3	A	2375	1.713
4	A	2370	1.517
5	A	1584	0.349
6	A	1559	11.838
7	A	1332	4.628
8	A	1276	9.987
9	A	1065	3.430
10	A	943	0.721
11	A	900	5.110
12	A	846	7.663
13	A	836	1.014
14	A	807	2.732
15	A	726	7.433
16	A	683	0.664
17	A	666	3.415
18	A	576	23.964
19	A	539	22.627
20	A	499	7.131
21	A	433	1.402
22	A	310	0.089
23	A	206	7.043
24	A	192	4.219

Table 21: Calculated harmonic wavenumbers $\widetilde{\omega}_i$ (in cm^{-1}) and IR intensities (in km mol^{-1}) of ($H_7H_8D_9D_{10}$) 1,2-dithiine obtained by the Gaussian 09 program package.

Mode	Symmetry	$\widetilde{\omega}_i$	Intensity
1	A	3214	5.322
2	A	2376	0.746
3	A	1562	11.632
4	A	1337	3.558
5	A	1033	4.579
6	A	858	0.015
7	A	841	0.088
8	A	730	6.839
9	A	713	0.758
10	A	552	0.066
11	A	493	0.139
12	A	430	0.163
13	A	196	0.001
14	B	3214	2.100
15	B	2364	2.182
16	B	1575	1.237
17	B	1256	11.484
18	B	970	0.595
19	B	849	8.549
20	B	827	8.068
21	B	671	0.152
22	B	526	59.237
23	B	312	0.249
24	B	214	11.695

Table 22: Calculated harmonic wavenumbers $\widetilde{\omega}_i$ (in cm^{-1}) and IR intensities (in km mol^{-1}) of ($D_7D_8H_9H_{10}$) 1,2-dithiine obtained by the Gaussian 09 program package.

Mode	Symmetry	$\widetilde{\omega}_i$	Intensity
1	A	3216	3.551
2	A	2374	2.621
3	A	1556	12.013
4	A	1331	5.542
5	A	1080	2.413
6	A	904	0.428
7	A	826	0.020
8	A	725	7.461
9	A	621	0.178
10	A	572	0.074
11	A	517	0.024
12	A	437	0.259
13	A	197	0.001
14	B	3204	4.327
15	B	2375	0.833
16	B	1595	0.023
17	B	1291	8.299
18	B	951	2.280
19	B	866	11.888
20	B	788	3.480
21	B	691	0.569
22	B	567	56.370
23	B	309	0.076
24	B	187	10.464

Table 23: Calculated harmonic wavenumbers $\widetilde{\omega}_i$ (in cm^{-1}) and IR intensities (in km mol^{-1}) of ($D_7H_8D_9D_{10}$) 1,2-dithiine obtained by the Gaussian 09 program package.

Mode	Symmetry	$\widetilde{\omega}_i$	Intensity
1	A	3214	3.712
2	A	2390	2.877
3	A	2371	1.232
4	A	2354	0.720
5	A	1570	2.876
6	A	1554	10.091
7	A	1310	6.375
8	A	1139	8.935
9	A	985	1.729
10	A	872	1.238
11	A	847	6.224
12	A	838	1.040
13	A	796	2.055
14	A	751	0.802
15	A	716	7.165
16	A	672	0.745
17	A	660	0.747
18	A	551	0.274
19	A	513	50.779
20	A	490	0.974
21	A	426	0.217
22	A	308	0.141
23	A	203	8.046
24	A	190	2.993

Table 24: Calculated harmonic wavenumbers $\widetilde{\omega}_i$ (in cm^{-1}) and IR intensities (in km mol^{-1}) of ($D_7D_8H_9D_{10}$) 1,2-dithiine obtained by the Gaussian 09 program package.

Mode	Symmetry	$\widetilde{\omega}_i$	Intensity
1	A	3210	3.920
2	A	2390	3.084
3	A	2375	1.799
4	A	2355	0.255
5	A	1578	0.821
6	A	1552	11.662
7	A	1314	6.583
8	A	1170	7.418
9	A	973	1.660
10	A	903	5.573
11	A	856	1.157
12	A	822	0.180
13	A	782	2.524
14	A	743	0.229
15	A	720	7.123
16	A	674	0.497
17	A	620	0.185
18	A	570	18.951
19	A	537	23.910
20	A	493	9.916
21	A	429	0.968
22	A	308	0.072
23	A	194	0.137
24	A	187	10.236

Table 25: Calculated harmonic wavenumbers $\widetilde{\omega}_i$ (in cm^{-1}) and IR intensities (in km mol^{-1}) of ($D_7D_8D_9D_{10}$) 1,2-dithiine obtained by the Gaussian 09 program package.

Mode	Symmetry	$\widetilde{\omega}_i$	Intensity
1	A	2392	3.214
2	A	2359	0.343
3	A	1551	12.558
4	A	1216	7.846
5	A	845	0.103
6	A	821	0.009
7	A	760	0.052
8	A	707	7.283
9	A	620	0.114
10	A	549	0.025
11	A	487	0.096
12	A	421	0.191
13	A	191	0.001
14	B	2387	2.658
15	B	2351	0.519
16	B	1558	0.578
17	B	1058	6.231
18	B	885	0.226
19	B	777	2.269
20	B	728	0.459
21	B	665	0.042
22	B	505	49.335
23	B	306	0.097
24	B	187	10.271

Table 26: Equilibrium (A_e, B_e and C_e, in cm^{-1}) rotational constants for various deuterated isotopomers of 1,2-dithiine (MP2/cc-pVTZ level of theory) obtained by the Gaussian 09 program package.

isotopomer	A_e	B_e	C_e
($D_7H_8H_9H_{10}$)	0.106700	0.102659	0.057604
($H_7H_8H_9D_{10}$)	0.110264	0.098861	0.057341
($D_7H_8H_9D_{10}$)	0.106404	0.097764	0.056097
($D_7H_8D_9H_{10}$)	0.105423	0.098524	0.056084
($H_7H_8D_9D_{10}$)	0.108814	0.095125	0.055863
($D_7D_8H_9H_{10}$)	0.102388	0.102041	0.056313
($D_7H_8D_9D_{10}$)	0.104422	0.094608	0.054677
($D_7D_8H_9D_{10}$)	0.101846	0.097434	0.054868
($D_7D_8D_9D_{10}$)	0.100140	0.094262	0.053517

Table 27: Rotational transition frequencies ν_{obs} for the *ground state* of dithiine. J'', K_a'' and K_c'' are lower state quantum numbers, J', K_a' and K_c' are upper state quantum numbers, $\nu_{\text{obs.}}$ = observed frequency, $\nu_{\text{cal.}}$ = frequency calculated with the parameters in Table 10. All frequencies are given in MHz.

Table 27: Rotational transitions for the *ground state* of dithiine.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν_{obs} /MHz	$(\nu_{obs} - \nu_{cal})$ /MHz
2	1	2	1	1	1	8370.843	0.004
2	0	2	1	0	1	8568.786	0.002
5	2	3	5	2	4	10104.868	0.004
2	1	1	1	1	0	11064.516	0.003
3	1	3	2	1	2	11979.432	0.006
3	0	3	2	0	2	12003.160	0.003
6	2	4	6	2	5	13048.281	0.000
6	3	4	6	1	5	13053.240	0.012
5	2	4	5	0	5	13074.712	0.000
2	2	0	1	0	1	14454.321	0.002
3	2	2	2	2	1	14576.495	0.008
3	1	2	2	1	1	15121.322	0.001
4	1	4	3	1	3	15501.775	0.002
4	0	4	3	0	3	15503.509	0.003
3	2	1	2	2	0	17149.834	0.006
13	7	7	12	7	6	64606.030	0.003
13	6	7	12	6	6	64610.760	0.007
18	0	18	17	0	17	64666.100	0.000
18	1	18	17	1	17	64666.100	0.000
15	5	11	14	5	10	65770.400	0.001
15	4	11	14	4	10	65770.400	0.001
16	3	13	15	3	12	66370.270	0.006
16	4	13	15	4	12	66370.270	0.006
17	2	15	16	2	14	66972.200	0.006
17	3	15	16	3	14	66972.200	0.006
13	8	6	12	8	5	67549.730	0.003
18	2	17	17	2	16	67574.740	0.001
18	1	17	17	1	16	67574.740	0.001
13	7	6	12	7	5	67638.950	-0.013
14	7	8	13	7	7	68104.560	-0.001
14	6	8	13	6	7	68105.055	0.005
19	1	19	18	1	18	68177.350	0.003
19	0	19	18	0	18	68177.350	0.003
12	10	2	11	10	1	68331.025	0.000
15	6	10	14	6	9	68685.140	0.003
15	5	10	14	5	9	68685.140	0.003
16	5	12	15	5	11	69280.930	0.003
12	9	3	11	9	2	69977.420	0.012
13	9	5	12	9	4	70292.700	-0.002

Continuation, see next page

Continuation of Table 27: *ground state* of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	ν_{obs} /MHz	$(\nu_{obs} - \nu_{cal})$ /MHz
18	3	16	17	3	15	70483.465	0.006
18	2	16	17	2	15	70483.465	0.006
14	8	7	13	8	6	71052.370	0.008
19	1	18	18	1	17	71085.980	0.001
19	2	18	18	2	17	71085.980	0.001
13	12	2	12	12	1	71794.910	-0.004
13	12	1	12	12	0	71905.100	0.004
16	6	11	15	6	10	72194.190	0.010
16	5	11	15	5	10	72194.190	0.010
13	11	3	12	11	2	72407.600	0.008
17	4	13	16	4	12	72791.615	-0.001
17	5	13	16	5	12	72791.615	-0.001
18	3	15	17	3	14	73392.530	0.004
18	4	15	17	4	14	73392.530	0.004
14	9	6	13	9	5	73991.730	-0.004
19	2	17	18	2	16	73994.660	0.003
19	3	17	18	3	16	73994.660	0.003
14	8	6	13	8	5	74179.760	-0.001
15	8	8	14	8	7	74544.350	0.005
15	7	8	14	7	7	74545.780	0.006
20	1	19	19	1	18	74597.140	0.003
20	2	19	19	2	18	74597.140	0.003
13	10	3	12	10	2	75684.940	0.011
17	5	12	16	5	11	75703.813	-0.002
17	6	12	16	6	11	75703.813	-0.002
18	4	14	17	4	13	76302.390	0.002
18	5	14	17	5	13	76302.390	0.002
14	10	5	13	10	4	76590.070	0.004
19	3	16	18	3	15	76903.600	-0.006
19	4	16	18	4	15	76903.600	-0.006
14	13	2	13	13	1	77267.530	0.002
20	2	18	19	2	17	77505.785	0.006
20	3	18	19	3	17	77505.785	0.006
15	9	7	14	9	6	77506.330	0.003
15	8	7	14	8	6	77536.020	0.007
14	9	5	13	9	4	77956.830	-0.006
14	12	3	13	12	2	77993.800	0.008
14	11	4	13	11	3	78027.400	-0.004
21	1	20	20	1	19	78108.210	0.002
21	2	20	20	2	19	78108.210	0.002
17	7	11	16	7	10	78619.850	0.003
17	6	11	16	6	10	78619.850	0.003
14	12	2	13	12	1	78756.550	-0.008
18	5	13	17	5	12	79213.810	-0.003
18	6	13	17	6	12	79213.810	-0.003
19	4	15	18	4	14	79813.195	0.001

Continuation, see next page

Continuation of Table 27: *ground state* of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	ν_{obs} /MHz	$(\nu_{obs} - \nu_{cal})$ /MHz
19	5	15	18	5	14	79813.195	0.001
20	3	17	19	3	16	80414.625	-0.006
20	4	17	19	4	16	80414.625	-0.006
15	10	6	14	10	5	80422.930	0.003
15	9	6	14	9	5	80787.990	-0.010
16	8	8	15	8	7	80995.160	-0.003
21	2	19	20	2	18	81016.825	0.005
21	3	19	20	3	18	81016.825	0.005
14	11	3	13	11	2	81158.460	-0.006
14	10	4	13	10	3	81348.960	0.004
22	1	21	21	1	20	81619.180	-0.008
22	2	21	21	2	20	81619.180	-0.008
18	7	12	17	7	11	82128.165	0.003
18	6	12	17	6	11	82128.165	0.003
23	0	23	22	0	22	82221.450	-0.002
23	1	23	22	1	22	82221.450	-0.002
19	5	14	18	5	13	82724.030	0.000
19	6	14	18	6	13	82724.030	0.000
15	14	2	14	14	1	82732.955	0.002
15	14	1	14	14	0	82767.520	-0.004
15	11	5	14	11	4	82815.530	-0.003
20	4	16	19	4	15	83324.000	0.001
20	5	16	19	5	15	83324.000	0.001
15	13	3	14	13	2	83531.340	0.006
21	3	18	20	3	17	83925.590	0.000
21	4	18	20	4	17	83925.590	0.000
16	10	7	15	10	6	83967.010	0.000
15	13	2	14	13	1	84023.290	0.000
16	9	7	15	9	6	84032.820	0.000
22	2	20	21	2	19	84527.770	-0.004
22	3	20	21	3	19	84527.770	-0.004
15	10	5	14	10	4	84817.880	-0.008
18	8	11	17	8	10	85047.935	0.001
18	7	11	17	7	10	85047.935	0.000
23	1	22	22	1	21	85130.070	-0.002
23	2	22	22	2	21	85130.070	-0.002
41	12	29	41	12	30	85573.999	0.004
41	13	29	41	11	30	85573.999	0.004
40	11	29	40	11	30	85601.695	-0.004
40	12	29	40	10	30	85601.695	-0.004
39	10	29	39	10	30	85627.622	-0.004
39	11	29	39	9	30	85627.622	-0.004
19	6	13	18	6	12	85637.150	-0.003
19	7	13	18	7	12	85637.150	-0.003
38	9	29	38	9	30	85651.869	0.009
38	10	29	38	8	30	85651.869	0.009

Continuation, see next page

Continuation of Table 27: *ground state* of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	ν_{obs} /MHz	$(\nu_{obs} - \nu_{cal})$ /MHz
37	8	29	37	8	30	85674.477	-0.006
37	9	29	37	7	30	85674.477	-0.006
36	7	29	36	7	30	85695.565	-0.008
36	8	29	36	6	30	85695.565	-0.008
35	6	29	35	6	30	85715.200	-0.006
35	7	29	35	5	30	85715.200	-0.006
24	0	24	23	0	23	85732.235	0.000
24	1	24	23	1	23	85732.235	0.000
34	5	29	34	5	30	85733.448	-0.008
34	6	29	34	4	30	85733.448	-0.008
20	5	15	19	5	14	86234.375	-0.001
20	6	15	19	6	14	86234.375	-0.001
15	12	3	14	12	2	86439.510	-0.002
16	11	6	15	11	5	86830.990	-0.005
21	4	17	20	4	16	86834.775	-0.003
21	5	17	20	5	16	86834.775	-0.003
22	3	19	21	3	18	87436.470	-0.005
22	4	19	21	4	18	87436.470	-0.005
17	10	8	16	10	7	87446.750	-0.007
17	9	8	16	9	7	87456.150	0.003
16	10	6	15	10	5	87486.720	-0.001
15	11	4	14	11	3	87570.070	-0.009
23	2	21	22	2	20	88038.635	-0.001
23	3	21	22	3	20	88038.635	-0.001
16	15	2	15	15	1	88194.400	-0.004
16	15	1	15	15	0	88213.270	0.000
41	11	30	41	11	31	88510.601	0.001
41	12	30	41	10	31	88510.601	0.001
40	10	30	40	10	31	88536.227	-0.006
40	11	30	40	9	31	88536.227	-0.006
19	8	12	18	8	11	88554.380	-0.002
19	7	12	18	7	11	88554.380	-0.002
39	9	30	39	9	31	88560.242	-0.005
39	10	30	39	8	31	88560.242	-0.005
38	8	30	38	8	31	88582.707	-0.011
38	9	30	38	7	31	88582.707	-0.011
37	7	30	37	7	31	88603.713	-0.006
37	8	30	37	6	31	88603.713	-0.006
36	6	30	36	6	31	88623.316	-0.004
36	7	30	36	5	31	88623.316	-0.004
24	1	23	23	1	22	88640.850	-0.005
24	2	23	23	2	22	88640.850	-0.005
35	5	30	35	5	31	88641.592	0.001
35	6	30	35	4	31	88641.592	0.001
34	4	30	34	4	31	88658.593	-0.005
34	5	30	34	3	31	88658.593	-0.005

Continuation, see next page

Continuation of Table 27: *ground state* of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	ν_{obs} /MHz	$(\nu_{obs} - \nu_{cal})$ /MHz
33	3	30	33	3	31	88674.407	0.002
33	4	30	33	2	31	88674.407	0.002
32	2	30	32	2	31	88689.075	-0.001
32	3	30	32	1	31	88689.075	-0.001
31	1	30	31	1	31	88702.672	0.002
31	2	30	31	0	31	88702.672	0.002
16	12	5	15	12	4	88954.570	-0.007
16	14	3	15	14	2	89033.730	-0.005
20	6	14	19	6	13	89146.570	-0.006
20	7	14	19	7	13	89146.570	-0.006
25	0	25	24	0	24	89242.910	-0.002
25	1	25	24	1	24	89242.910	-0.002
16	14	2	15	14	1	89339.030	-0.003
16	13	4	15	13	3	89593.125	0.004
21	5	16	20	5	15	89744.790	0.001
21	6	16	20	6	15	89744.790	0.001
22	4	18	21	4	17	90345.510	-0.002
22	5	18	21	5	17	90345.510	-0.002
17	11	7	16	11	6	90431.440	-0.007
17	10	7	16	10	6	90567.480	-0.001
18	10	9	17	10	8	90927.660	-0.005
18	9	9	17	9	8	90928.800	-0.005
23	3	20	22	3	19	90947.280	0.003
23	4	20	22	4	19	90947.280	0.003
42	11	31	42	11	32	91419.219	-0.005
42	12	31	42	10	32	91419.219	-0.005
41	10	31	41	10	32	91444.612	-0.002
41	11	31	41	9	32	91444.612	-0.002
40	9	31	40	9	32	91468.451	-0.002
40	10	31	40	8	32	91468.451	-0.002
19	9	11	18	9	10	91479.040	0.000
19	8	11	18	8	10	91479.040	-0.003
39	8	31	39	8	32	91490.808	-0.004
39	9	31	39	7	32	91490.808	-0.004
38	7	31	38	7	32	91511.750	-0.008
38	8	31	38	6	32	91511.750	-0.008
37	6	31	37	6	32	91531.350	-0.006
37	7	31	37	5	32	91531.350	-0.006
35	4	31	35	4	32	91566.766	-0.001
35	5	31	35	3	32	91566.766	-0.001
34	3	31	34	3	32	91582.700	-0.001
34	4	31	34	2	32	91582.700	-0.001
33	2	31	33	2	32	91597.537	0.004
33	3	31	33	1	32	91597.537	0.004
16	13	3	15	13	2	91598.780	-0.003
16	11	5	15	11	4	91651.860	-0.004

Continuation, see next page

Continuation of Table 27: *ground state* of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	ν_{obs} /MHz	$(\nu_{obs} - \nu_{cal})$ /MHz
20	7	13	19	7	12	92061.970	0.004
20	8	13	19	8	12	92061.970	0.004
25	1	24	24	1	23	92151.530	-0.003
25	2	24	24	2	23	92151.530	-0.003
21	7	15	20	7	14	92656.275	0.000
21	6	15	20	6	14	92656.275	0.000
26	0	26	25	0	25	92753.480	0.001
26	1	26	25	1	25	92753.480	0.001
17	12	6	16	12	5	93200.525	0.001
22	5	17	21	5	16	93255.230	0.004
22	6	17	21	6	16	93255.230	0.004
16	12	4	15	12	3	93530.430	0.003
17	16	2	16	16	1	93653.810	0.009
17	16	1	16	16	0	93663.950	-0.006
23	4	19	22	4	18	93856.190	0.003
23	5	19	22	5	18	93856.190	0.003
18	11	8	17	11	7	93911.340	0.000
18	10	8	17	10	7	93932.930	0.000
17	11	6	16	11	5	94290.870	-0.004
44	12	32	44	12	33	94300.842	-0.003
44	13	32	44	11	33	94300.842	-0.003
43	11	32	43	11	33	94327.595	0.001
43	12	32	43	10	33	94327.595	0.001
42	10	32	42	10	33	94352.787	-0.001
42	11	32	42	9	33	94352.787	-0.001
41	9	32	41	9	33	94376.481	-0.013
41	10	32	41	8	33	94376.481	-0.013
13	9	4	12	7	5	94397.640	0.001
40	8	32	40	8	33	94398.771	-0.005
40	9	32	40	7	33	94398.771	-0.005
39	7	32	39	7	33	94419.689	-0.008
39	8	32	39	6	33	94419.689	-0.008
38	6	32	38	6	33	94439.319	-0.001
38	7	32	38	5	33	94439.319	-0.001
36	4	32	36	4	33	94474.905	0.001
36	5	32	36	3	33	94474.905	0.001
35	3	32	35	3	33	94490.988	0.007
35	4	32	35	2	33	94490.988	0.007
34	2	32	34	2	33	94505.987	0.000
34	3	32	34	1	33	94505.987	0.000
17	15	3	16	15	2	94512.320	0.006
17	15	2	16	15	1	94696.060	-0.001
20	9	12	19	9	11	94982.940	0.003
20	8	12	19	8	11	94982.940	0.003
17	13	5	16	13	4	94996.725	-0.003
25	2	23	24	2	22	95060.065	0.004

Continuation, see next page

Continuation of Table 27: *ground state* of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	ν_{obs} /MHz	$(\nu_{obs} - \nu_{cal})$ /MHz
25	3	23	24	3	22	95060.065	0.004
17	14	4	16	14	3	95248.210	-0.001
21	7	14	20	7	13	95570.290	-0.002
21	8	14	20	8	13	95570.290	-0.002
26	1	25	25	1	24	95662.100	-0.001
26	2	25	25	2	24	95662.100	-0.001
22	6	16	21	6	15	96166.150	0.004
22	7	16	21	7	15	96166.150	0.004
27	0	27	26	0	26	96263.930	0.000
27	1	27	26	1	26	96263.930	0.000
17	14	3	16	14	2	96715.516	0.004
23	5	18	22	5	17	96765.656	0.001
23	6	18	22	6	17	96765.656	0.001
50	17	33	50	17	34	97051.842	0.037
49	16	33	49	16	34	97086.856	0.051
48	15	33	48	15	34	97120.006	0.032
18	11	7	17	11	6	97157.364	-0.004
42	10	33	42	8	34	97284.380	-0.001
42	9	33	42	9	34	97284.380	-0.001
41	9	33	41	7	34	97306.610	-0.009
41	8	33	41	8	34	97306.610	-0.009
40	8	33	40	6	34	97327.540	-0.004
40	7	33	40	7	34	97327.540	-0.004
14	12	2	13	10	3	97328.415	-0.010
39	7	33	39	5	34	97347.210	-0.004
39	6	33	39	6	34	97347.210	-0.004
38	6	33	38	4	34	97365.690	0.005
38	5	33	38	5	34	97365.690	0.005
24	4	20	23	4	19	97366.794	0.004
24	5	20	23	5	19	97366.794	0.004
19	11	9	18	11	8	97381.872	-0.003
37	5	33	37	3	34	97383.011	0.000
37	4	33	37	4	34	97383.011	0.000
19	10	9	18	10	8	97384.740	-0.004
36	4	33	36	2	34	97399.254	0.009
36	3	33	36	3	34	97399.254	0.009
35	3	33	35	1	34	97414.450	0.012
35	2	33	35	2	34	97414.450	0.012
34	1	33	34	1	34	97428.660	0.020
34	2	33	34	0	34	97428.660	0.020
20	9	11	19	9	10	97913.842	-0.004
20	10	11	19	10	10	97913.842	0.008
25	3	22	24	3	21	97968.603	-0.001
25	4	22	24	4	21	97968.603	-0.001
17	12	5	16	12	4	98368.181	-0.003
21	8	13	20	8	12	98488.619	0.002

Continuation, see next page

Continuation of Table 27: *ground state* of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	ν_{obs} /MHz	$(\nu_{obs} - \nu_{cal})$ /MHz
21	9	13	20	9	12	98488.619	0.002
26	2	24	25	2	23	98570.616	0.001
26	3	24	25	3	23	98570.616	0.001
13	8	5	12	6	6	98648.750	-0.005
22	7	15	21	7	14	99079.105	-0.004
22	8	15	21	8	14	99079.105	-0.004
18	17	1	17	17	0	99117.615	-0.003
27	1	26	26	1	25	99172.558	0.003
27	2	26	26	2	25	99172.558	0.003
17	13	4	16	13	3	99218.588	-0.002
23	6	17	22	6	16	99676.122	0.004
23	7	17	22	7	16	99676.122	0.004
28	0	28	27	0	27	99774.262	0.000
28	1	28	27	1	27	99774.262	0.000
18	16	3	17	16	2	99975.782	0.000
14	10	4	13	8	5	100009.863	0.005
18	16	2	17	16	1	100083.681	0.001
44	10	34	44	10	35	100168.579	0.002
44	11	34	44	9	35	100168.579	0.002
43	9	34	43	9	35	100192.123	-0.002
43	10	34	43	8	35	100192.123	-0.002
42	9	34	42	7	35	100214.349	0.000
42	8	34	42	8	35	100214.349	0.000
41	8	34	41	6	35	100235.303	-0.002
41	7	34	41	7	35	100235.303	-0.002
40	7	34	40	5	35	100255.043	-0.002
40	6	34	40	6	35	100255.043	-0.002
39	6	34	39	4	35	100273.618	-0.006
39	5	34	39	5	35	100273.618	-0.006
24	5	19	23	5	18	100276.054	0.002
24	6	19	23	6	18	100276.054	0.002
38	5	34	38	3	35	100291.098	0.007
38	4	34	38	4	35	100291.098	0.007
37	4	34	37	2	35	100307.500	0.005
37	3	34	37	3	35	100307.500	0.005
36	3	34	36	1	35	100322.905	0.017
36	2	34	36	2	35	100322.905	0.017
19	12	8	18	12	7	100385.063	-0.002
19	11	8	18	11	7	100431.723	0.010
18	15	4	17	15	3	100835.468	0.010
20	11	10	19	11	9	100862.918	-0.008
20	10	10	19	10	9	100863.271	0.011
25	4	21	24	4	20	100877.316	0.005
25	5	21	24	5	20	100877.316	0.005
18	14	5	17	14	4	100936.732	-0.002
18	12	6	17	12	5	101191.832	-0.001

Continuation, see next page

Continuation of Table 27: *ground state* of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	ν_{obs} /MHz	$(\nu_{obs} - \nu_{cal})$ /MHz
21	10	12	20	10	11	101414.340	0.003
21	9	12	20	9	11	101414.340	0.002
21	9	12	20	9	11	101414.340	0.002
21	10	12	20	10	11	101414.340	0.003
26	3	23	25	3	22	101479.121	0.003
26	4	23	25	4	22	101479.121	0.003
18	15	3	17	15	2	101852.378	-0.002
14	12	3	13	10	4	101950.483	-0.006
13	7	6	12	5	7	101951.694	0.008
22	8	14	21	8	13	101995.472	0.000
22	9	14	21	9	13	101995.472	0.000
27	3	25	26	3	24	102081.057	0.000
27	2	25	26	2	24	102081.057	0.000
15	12	3	14	10	4	102418.974	-0.007
23	7	16	22	7	15	102588.253	0.001
23	8	16	22	8	15	102588.253	0.001
14	11	4	13	9	5	102606.822	0.010
28	2	27	27	2	26	102682.889	-0.001
28	1	27	27	1	26	102682.889	-0.001
40	6	35	40	4	36	103181.522	0.001
40	5	35	40	5	36	103181.522	0.001
24	6	18	23	6	17	103186.141	0.001
24	7	18	23	7	17	103186.141	0.001
39	5	35	39	3	36	103199.148	0.004
39	4	35	39	4	36	103199.148	0.004
38	4	35	38	2	36	103215.742	0.008
38	3	35	38	3	36	103215.742	0.008
36	1	35	36	1	36	103246.013	0.019
36	2	35	36	0	36	103246.013	0.019
29	0	29	28	0	28	103284.469	-0.001
29	1	29	28	1	28	103284.469	-0.001
25	5	20	24	5	19	103786.400	0.004
25	6	20	24	6	19	103786.400	0.004
19	12	7	18	12	6	103824.530	-0.003
20	12	9	19	12	8	103845.125	-0.005
20	11	9	19	11	8	103851.910	-0.003
26	4	22	25	4	21	104387.740	-0.002
26	5	22	25	5	21	104387.740	-0.002
19	18	2	18	18	1	104570.210	0.008
19	18	1	18	18	0	104573.040	-0.006
18	14	4	17	14	3	104648.140	-0.005
18	13	5	17	13	4	104886.175	-0.004
22	10	13	21	10	12	104917.500	-0.006
22	9	13	21	9	12	104917.500	-0.006
27	3	24	26	3	23	104989.520	-0.004
27	4	24	26	4	23	104989.520	-0.004

Continuation, see next page

Continuation of Table 27: *ground state* of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	ν_{obs} /MHz	$(\nu_{obs} - \nu_{cal})$ /MHz
19	17	3	18	17	2	105430.350	0.003
19	17	2	18	17	1	105492.430	-0.007
23	8	15	22	8	14	105503.120	0.001
23	9	15	22	9	14	105503.120	0.001
28	2	26	27	2	25	105591.380	-0.002
28	3	26	27	3	25	105591.380	-0.002
49	13	36	49	13	37	105905.218	0.005
49	14	36	49	12	37	105905.218	0.005
48	12	36	48	12	37	105932.751	-0.001
48	13	36	48	11	37	105932.751	-0.001
47	11	36	47	11	37	105958.888	-0.010
47	12	36	47	10	37	105958.888	-0.010
46	10	36	46	10	37	105983.700	-0.004
46	11	36	46	9	37	105983.700	-0.004
44	8	36	44	8	37	106029.486	-0.013
44	9	36	44	7	37	106029.486	-0.013
43	7	36	43	7	37	106050.577	-0.009
43	8	36	43	6	37	106050.577	-0.009
42	6	36	42	6	37	106070.528	-0.002
42	7	36	42	5	37	106070.528	-0.002
41	5	36	41	5	37	106089.373	-0.004
41	6	36	41	4	37	106089.373	-0.004
24	7	17	23	7	16	106097.610	0.002
24	8	17	23	8	16	106097.610	0.002
40	4	36	40	4	37	106107.175	0.002
40	5	36	40	3	37	106107.175	0.002
39	3	36	39	3	37	106123.967	0.006
39	4	36	39	2	37	106123.967	0.006
38	2	36	38	2	37	106139.793	0.009
38	3	36	38	1	37	106139.793	0.009
37	1	36	37	1	37	106154.698	0.014
37	2	36	37	0	37	106154.698	0.014
29	1	28	28	1	27	106193.100	-0.002
29	2	28	28	2	27	106193.100	-0.002
19	16	4	18	16	3	106369.540	0.006
25	6	19	24	6	18	106696.170	-0.002
25	7	19	24	7	18	106696.170	-0.002
19	15	5	18	15	4	106775.020	-0.008
30	0	30	29	0	29	106794.550	0.001
30	1	30	29	1	29	106794.550	0.001
19	16	3	18	16	2	107042.640	0.000
26	5	21	25	5	20	107296.680	0.005
26	6	21	25	6	20	107296.680	0.005
21	12	10	20	12	9	107315.350	-0.004
21	11	10	20	11	9	107316.210	0.001
22	11	12	21	11	11	107849.150	0.003

Continuation, see next page

Continuation of Table 27: *ground state* of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	ν_{obs} /MHz	$(\nu_{obs} - \nu_{cal})$ /MHz
22	10	12	21	10	11	107849.150	0.000
27	4	23	26	4	22	107898.075	0.001
27	5	23	26	5	22	107898.075	0.001
19	13	6	18	13	5	108144.225	-0.001
23	10	14	22	10	13	108422.440	0.002
23	9	14	22	9	13	108422.440	0.002
28	3	25	27	3	24	108499.815	-0.001
28	4	25	27	4	24	108499.815	-0.001
50	13	37	50	13	38	108812.734	0.005
50	14	37	50	12	38	108812.734	0.005
49	12	37	49	12	38	108840.167	0.003
49	13	37	49	11	38	108840.167	0.003
48	11	37	48	11	38	108866.248	-0.005
48	12	37	48	10	38	108866.248	-0.005
47	10	37	47	10	38	108891.040	-0.005
47	11	37	47	9	38	108891.040	-0.005
46	9	37	46	9	38	108914.579	-0.010
46	10	37	46	8	38	108914.579	-0.010
45	8	37	45	8	38	108936.923	-0.007
45	9	37	45	7	38	108936.923	-0.007
44	7	37	44	7	38	108958.119	0.003
44	8	37	44	6	38	108958.119	0.003
43	6	37	43	6	38	108978.188	-0.002
43	7	37	43	5	38	108978.188	-0.002
42	5	37	42	5	38	108997.189	-0.008
42	6	37	42	4	38	108997.189	-0.008
24	8	16	23	8	15	109011.310	0.003
24	8	16	23	8	15	109011.310	0.003
29	2	27	28	2	26	109101.590	0.006
29	3	27	28	3	26	109101.590	0.006
30	1	29	29	1	28	109703.185	-0.002
30	2	29	29	2	28	109703.185	-0.002
19	15	4	18	15	3	109865.900	0.003
20	19	2	19	19	1	110028.025	0.014
20	19	1	19	19	0	110029.480	-0.015
26	6	20	25	6	19	110206.183	-0.002
26	7	20	25	7	19	110206.183	-0.002
21	13	9	20	13	8	110318.440	0.000
21	12	9	20	12	8	110333.600	0.004
15	14	1	14	12	2	110526.900	0.008
20	13	7	19	13	6	110591.770	0.003
27	5	22	26	5	21	110806.880	0.005
27	6	22	26	6	21	110806.880	0.005
20	18	3	19	18	2	110880.140	0.000
20	18	2	19	18	1	110915.265	-0.003
19	14	5	18	14	4	111148.615	-0.014

Continuation, see next page

Continuation of Table 27: *ground state* of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	ν_{obs} /MHz	$(\nu_{obs} - \nu_{cal})$ /MHz
23	11	13	22	11	12	111349.080	0.008
23	10	13	22	10	12	111349.080	0.008
15	14	2	14	12	3	111370.330	-0.003
28	4	24	27	4	23	111408.305	0.004
28	5	24	27	5	23	111408.305	0.004
15	11	5	14	9	6	111430.620	0.008
46	8	38	46	8	39	111844.260	-0.013
46	9	38	46	7	39	111844.260	-0.013
20	17	4	19	17	3	111864.430	-0.001
45	7	38	45	7	39	111865.558	-0.020
45	8	38	45	6	39	111865.558	-0.020
44	6	38	44	6	39	111885.800	0.000
44	7	38	44	5	39	111885.800	0.000
43	5	38	43	5	39	111904.980	-0.002
43	6	38	43	4	39	111904.980	-0.002
20	15	6	19	15	5	111908.900	-0.007
42	4	38	42	4	39	111923.180	0.016
42	5	38	42	3	38	111923.180	0.016
24	9	15	23	9	14	111928.570	0.002
24	10	15	23	10	14	111928.570	0.002
41	3	38	41	3	39	111940.400	0.016
41	4	38	41	2	39	111940.400	0.016
40	2	38	40	2	39	111956.710	0.028
40	3	38	40	1	39	111956.710	0.028
29	3	26	28	3	25	112009.990	0.000
29	4	26	28	4	25	112009.990	0.000
20	17	3	19	17	2	112293.550	-0.006
20	16	5	19	16	4	112517.490	-0.006
30	2	28	29	2	27	112611.660	-0.001
30	3	28	29	3	27	112611.660	-0.001
26	7	19	25	7	18	113116.660	-0.001
26	8	19	25	8	18	113116.660	-0.001
31	1	30	30	1	29	113213.140	0.001
31	2	30	30	2	29	113213.140	0.001
21	14	8	20	14	7	113352.110	0.000
21	13	8	20	13	7	113536.240	-0.004
27	6	21	26	6	20	113716.160	0.002
27	7	21	26	7	20	113716.160	0.002
22	13	10	21	13	9	113775.930	-0.011
22	12	10	21	12	9	113778.010	0.004
32	0	32	31	0	31	113814.300	-0.005
32	1	32	31	1	31	113814.300	-0.005
23	12	12	22	12	11	114288.000	0.008
28	5	23	27	5	22	114316.990	0.005
28	6	23	27	6	22	114316.990	0.005
48	9	39	48	9	40	114728.980	-0.016

Continuation, see next page

Continuation of Table 27: *ground state* of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	ν_{obs} /MHz	$(\nu_{obs} - \nu_{cal})$ /MHz
48	10	39	48	8	40	114728.980	-0.016
47	8	39	47	8	40	114751.510	-0.022
47	9	39	47	7	40	114751.510	-0.022
46	7	39	46	7	40	114772.960	-0.014
46	8	39	46	6	40	114772.960	-0.014
45	6	39	45	6	40	114793.350	-0.012
45	7	39	45	5	40	114793.350	-0.012
44	5	39	44	5	40	114812.730	-0.004
44	6	39	44	4	40	114812.730	-0.004
43	4	39	43	4	40	114831.125	-0.004
43	5	39	43	3	40	114831.125	-0.004
29	4	25	28	4	24	114918.420	0.003
29	5	25	28	5	24	114918.420	0.003
25	9	16	24	9	15	115435.530	0.002
25	10	16	24	10	15	115435.530	0.002
30	3	27	29	3	26	115520.040	0.000
30	4	27	29	4	26	115520.040	0.000
26	8	18	25	8	17	116028.675	0.004
26	9	18	25	9	17	116028.675	0.004
31	2	29	30	2	28	116121.605	-0.002
31	3	29	30	3	28	116121.605	-0.002
27	7	20	26	7	19	116626.250	-0.005
27	8	20	26	8	19	116626.250	-0.005
22	14	9	21	14	8	116802.325	-0.006
22	13	9	21	13	8	116834.485	-0.004
28	6	22	27	6	21	117226.075	0.003
28	7	22	27	7	21	117226.075	0.003
33	0	33	32	0	32	117323.970	-0.003
33	0	33	32	0	32	117323.970	-0.003
21	18	4	20	18	3	117332.265	-0.002

Table 28: Rovibrational transition wavenumbers $\tilde{\nu}_{obs}$ for the fundamental $\nu_{22} \leftarrow gs$ of dithiine. J'', K_a'' and K_c'' are lower state quantum numbers, J', K_a' and K_c' are upper state quantum numbers, $\tilde{\nu}_{\text{obs.}}$ = observed wavenumber, $\tilde{\nu}_{\text{cal.}}$ = wavenumber calculated with the parameters in Table 10. All wavenumbers are given in cm^{-1}.

Table 28: Rovibrational transitions of $\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
76	35	41	77	36	41	606.164080	0.000191

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
76	36	41	77	37	41	606.164080	0.000191
76	40	36	77	41	36	606.164080	0.000159
76	41	36	77	42	36	606.164080	0.000159
72	69	3	73	70	3	606.369110	-0.000313
72	69	4	73	70	4	606.369110	-0.000313
72	69	3	73	70	4	606.369110	-0.000313
72	69	4	73	70	3	606.369110	-0.000313
75	35	41	76	36	41	606.385340	-0.000128
75	34	41	76	35	41	606.385340	-0.000128
71	68	3	72	69	3	606.605960	-0.000153
71	68	4	72	69	4	606.605960	-0.000153
74	34	40	75	35	40	606.605960	-0.000147
74	35	40	75	36	40	606.605960	-0.000147
71	68	3	72	69	4	606.605960	-0.000153
71	68	4	72	69	3	606.605960	-0.000153
70	69	1	71	70	1	606.731570	0.000061
70	69	2	71	70	2	606.731570	0.000061
70	69	1	71	70	2	606.731570	0.000061
70	69	2	71	70	1	606.731570	0.000061
73	37	36	74	38	36	606.826790	0.000351
73	38	36	74	39	36	606.826790	0.000351
73	34	39	74	35	39	606.826790	0.000005
73	35	39	74	36	39	606.826790	0.000005
70	67	3	71	68	3	606.842640	-0.000086
70	67	4	71	68	4	606.842640	-0.000086
70	67	3	71	68	4	606.842640	-0.000086
70	67	4	71	68	3	606.842640	-0.000086
69	68	1	70	69	1	606.968910	0.000117
69	68	2	70	69	2	606.968910	0.000117
69	68	1	70	69	2	606.968910	0.000117
69	68	2	70	69	1	606.968910	0.000117
69	67	3	70	68	3	607.023830	-0.000159
69	67	3	70	68	2	607.023830	-0.000159
69	67	2	70	68	3	607.023830	-0.000159
72	37	35	73	38	35	607.047840	0.000089
72	38	35	73	39	35	607.047840	0.000089
69	66	3	70	67	3	607.078790	-0.000453
69	66	4	70	67	4	607.078790	-0.000453
69	66	3	70	67	4	607.078790	-0.000453
69	66	4	70	67	3	607.078790	-0.000453
68	67	1	69	68	1	607.206350	0.000357
68	67	2	69	68	2	607.206350	0.000357
68	67	1	69	68	2	607.206350	0.000357
68	67	2	69	68	1	607.206350	0.000357
69	63	6	70	64	6	607.244930	-0.000601
69	63	7	70	64	7	607.244930	-0.000601

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
69	63	6	70	64	7	607.244930	-0.000601
69	63	7	70	64	6	607.244930	-0.000601
68	66	3	69	67	3	607.260940	0.000137
68	66	3	69	67	2	607.260940	0.000137
68	66	2	69	67	3	607.260940	0.000137
71	34	37	72	35	37	607.268560	0.000267
71	35	37	72	36	37	607.268560	0.000267
71	37	35	72	38	35	607.268560	0.000094
71	36	35	72	37	35	607.268560	0.000094
71	33	38	72	34	38	607.268560	-0.000167
71	34	38	72	35	38	607.268560	-0.000167
68	65	3	69	66	3	607.315720	0.000042
68	65	4	69	66	4	607.315720	0.000042
68	65	3	69	66	4	607.315720	0.000042
68	65	4	69	66	3	607.315720	0.000042
67	66	1	68	67	1	607.442830	-0.000280
67	66	2	68	67	2	607.442830	-0.000280
67	66	1	68	67	2	607.442830	-0.000280
67	66	2	68	67	1	607.442830	-0.000280
68	62	6	69	63	6	607.481160	0.000294
68	62	7	69	63	7	607.481160	0.000294
68	62	6	69	63	7	607.481160	0.000294
68	62	7	69	63	6	607.481160	0.000294
70	35	36	71	36	36	607.489180	0.000013
70	34	36	71	35	36	607.489180	0.000013
70	36	35	71	37	35	607.489180	-0.000081
70	35	35	71	36	35	607.489180	-0.000081
70	34	37	71	35	37	607.489180	-0.000249
70	33	37	71	34	37	607.489180	-0.000249
67	65	3	68	66	3	607.497270	-0.000260
67	65	3	68	66	2	607.497270	-0.000260
67	65	2	68	66	3	607.497270	-0.000260
67	64	3	68	65	3	607.551790	-0.000228
67	64	4	68	65	4	607.551790	-0.000228
67	64	3	68	65	4	607.551790	-0.000228
67	64	4	68	65	3	607.551790	-0.000228
67	62	5	68	63	5	607.661040	-0.000227
67	62	6	68	63	6	607.661040	-0.000227
67	62	5	68	63	6	607.661040	-0.000227
67	62	6	68	63	5	607.661040	-0.000227
66	65	1	67	66	1	607.680520	0.000377
66	65	2	67	66	2	607.680520	0.000377
66	65	1	67	66	2	607.680520	0.000377
66	65	2	67	66	1	607.680520	0.000377
69	34	35	70	35	35	607.709970	-0.000153
69	35	35	70	36	35	607.709970	-0.000153

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
69	34	36	70	35	36	607.709970	-0.000234
69	33	36	70	34	36	607.709970	-0.000234
67	61	6	68	62	6	607.716000	-0.000106
67	61	7	68	62	7	607.716000	-0.000106
67	61	6	68	62	7	607.716000	-0.000106
67	61	7	68	62	6	607.716000	-0.000106
66	64	3	67	65	3	607.734950	0.000776
66	64	3	67	65	2	607.734950	0.000776
66	64	2	67	65	3	607.734950	0.000776
66	63	3	67	64	3	607.788520	0.000247
66	63	4	67	64	4	607.788520	0.000247
66	63	3	67	64	4	607.788520	0.000247
66	63	4	67	64	3	607.788520	0.000247
66	61	5	67	62	5	607.896640	-0.000131
66	61	6	67	62	6	607.896640	-0.000131
66	61	5	67	62	6	607.896640	-0.000131
66	61	6	67	62	5	607.896640	-0.000131
65	64	1	66	65	1	607.916990	-0.000085
65	64	2	66	65	2	607.916990	-0.000085
65	64	1	66	65	2	607.916990	-0.000085
65	64	2	66	65	1	607.916990	-0.000085
68	33	35	69	34	35	607.931040	-0.000033
68	34	35	69	35	35	607.931040	-0.000033
68	34	34	69	35	34	607.931040	-0.000141
68	35	34	69	36	34	607.931040	-0.000141
66	60	6	67	61	6	607.951410	0.000155
66	60	7	67	61	7	607.951410	0.000155
66	60	6	67	61	7	607.951410	0.000155
66	60	7	67	61	6	607.951410	0.000155
65	62	3	66	63	3	608.024220	-0.000220
65	62	4	66	63	4	608.024220	-0.000220
65	62	3	66	63	4	608.024220	-0.000220
65	62	4	66	63	3	608.024220	-0.000220
65	60	5	66	61	5	608.131700	-0.000497
65	60	6	66	61	6	608.131700	-0.000497
65	60	5	66	61	6	608.131700	-0.000497
65	60	6	66	61	5	608.131700	-0.000497
67	33	34	68	34	34	608.152280	0.000225
67	34	34	68	35	34	608.152280	0.000225
67	32	35	68	33	35	608.152280	0.000151
67	33	35	68	34	35	608.152280	0.000151
67	34	33	68	35	33	608.152280	-0.000082
67	35	33	68	36	33	608.152280	-0.000082
64	63	1	65	64	1	608.154020	0.000096
64	63	2	65	64	2	608.154020	0.000096
64	63	1	65	64	2	608.154020	0.000096

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
64	63	2	65	64	1	608.154020	0.000096
65	59	6	66	60	6	608.186230	-0.000086
65	59	7	66	60	7	608.186230	-0.000086
65	59	6	66	60	7	608.186230	-0.000086
65	59	7	66	60	6	608.186230	-0.000086
64	62	3	65	63	3	608.207350	0.000157
64	62	3	65	63	2	608.207350	0.000157
64	62	2	65	63	3	608.207350	0.000157
64	61	3	65	62	3	608.259650	-0.000874
64	61	4	65	62	4	608.259650	-0.000874
64	61	3	65	62	4	608.259650	-0.000874
64	61	4	65	62	3	608.259650	-0.000874
64	59	5	65	60	5	608.367020	-0.000498
64	59	6	65	60	6	608.367020	-0.000498
64	59	5	65	60	6	608.367020	-0.000498
64	59	6	65	60	5	608.367020	-0.000498
66	33	34	67	34	34	608.372970	-0.000066
66	32	34	67	33	34	608.372970	-0.000066
66	34	33	67	35	33	608.372970	-0.000180
66	33	33	67	34	33	608.372970	-0.000180
63	62	1	64	63	1	608.390990	0.000305
63	62	2	64	63	2	608.390990	0.000305
63	62	1	64	63	2	608.390990	0.000305
63	62	2	64	63	1	608.390990	0.000305
64	58	6	65	59	6	608.420940	-0.000357
64	58	7	65	59	7	608.420940	-0.000357
64	58	6	65	59	7	608.420940	-0.000357
64	58	7	65	59	6	608.420940	-0.000357
63	61	3	64	62	3	608.443540	-0.000023
63	61	3	64	62	2	608.443540	-0.000023
63	61	2	64	62	3	608.443540	-0.000023
64	57	7	65	58	7	608.475070	-0.000295
64	57	8	65	58	8	608.475070	-0.000295
64	57	7	65	58	8	608.475070	-0.000295
64	57	8	65	58	7	608.475070	-0.000295
63	60	3	64	61	3	608.496620	0.000106
63	60	4	64	61	4	608.496620	0.000106
63	60	3	64	61	4	608.496620	0.000106
63	60	4	64	61	3	608.496620	0.000106
65	32	33	66	33	33	608.594280	0.000209
65	33	33	66	34	33	608.594280	0.000209
65	31	34	66	32	34	608.594280	0.000134
65	32	34	66	33	34	608.594280	0.000134
65	33	32	66	34	32	608.594280	-0.000105
65	34	32	66	35	32	608.594280	-0.000105
63	58	5	64	59	5	608.603010	0.000247

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
63	58	6	64	59	6	608.603010	0.000247
63	58	5	64	59	6	608.603010	0.000247
63	58	6	64	59	5	608.603010	0.000247
62	61	1	63	62	1	608.627490	0.000147
62	61	2	63	62	2	608.627490	0.000147
62	61	1	63	62	2	608.627490	0.000147
62	61	2	63	62	1	608.627490	0.000147
63	57	6	64	58	6	608.656230	0.000053
63	57	7	64	58	7	608.656230	0.000053
63	57	6	64	58	7	608.656230	0.000053
63	57	7	64	58	6	608.656230	0.000053
62	60	3	63	61	3	608.679920	0.000085
62	60	3	63	61	2	608.679920	0.000085
62	60	2	63	61	3	608.679920	0.000085
63	56	7	64	57	7	608.710160	0.000244
63	56	8	64	57	8	608.710160	0.000244
63	56	7	64	57	8	608.710160	0.000244
63	56	8	64	57	7	608.710160	0.000244
62	59	3	63	60	3	608.732450	0.000044
62	59	4	63	60	4	608.732450	0.000044
62	59	3	63	60	4	608.732450	0.000044
62	59	4	63	60	3	608.732450	0.000044
64	31	33	65	32	33	608.815360	0.000238
64	32	33	65	33	33	608.815360	0.000238
64	32	32	65	33	32	608.815360	0.000123
64	33	32	65	34	32	608.815360	0.000123
64	30	34	65	31	34	608.815360	-0.000023
64	31	34	65	32	34	608.815360	-0.000023
62	57	5	63	58	5	608.838150	0.000237
62	57	6	63	58	6	608.838150	0.000237
62	57	5	63	58	6	608.838150	0.000237
62	57	6	63	58	5	608.838150	0.000237
61	60	1	62	61	1	608.864070	0.000159
61	60	2	62	61	2	608.864070	0.000159
61	60	1	62	61	2	608.864070	0.000159
61	60	2	62	61	1	608.864070	0.000159
62	56	6	63	57	6	608.890990	0.000008
62	56	7	63	57	7	608.890990	0.000008
62	56	6	63	57	7	608.890990	0.000008
62	56	7	63	57	6	608.890990	0.000008
61	59	3	62	60	3	608.916120	0.000104
61	59	3	62	60	2	608.916120	0.000104
61	59	2	62	60	3	608.916120	0.000104
62	55	7	63	56	7	608.944450	0.000064
62	55	8	63	56	8	608.944450	0.000064
62	55	7	63	56	8	608.944450	0.000064

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
62	55	8	63	56	7	608.944450	0.000064
61	58	3	62	59	3	608.968320	0.000108
61	58	4	62	59	4	608.968320	0.000108
61	58	3	62	59	4	608.968320	0.000108
61	58	4	62	59	3	608.968320	0.000108
63	32	32	64	33	32	609.036250	0.000021
63	31	32	64	32	32	609.036250	0.000021
63	31	33	64	32	33	609.036250	-0.000060
63	30	33	64	31	33	609.036250	-0.000060
61	56	5	62	57	5	609.073220	0.000241
61	56	6	62	57	6	609.073220	0.000241
61	56	5	62	57	6	609.073220	0.000241
61	56	6	62	57	5	609.073220	0.000241
60	59	1	61	60	1	609.100160	-0.000211
60	59	2	61	60	2	609.100160	-0.000211
60	59	1	61	60	2	609.100160	-0.000211
60	59	2	61	60	1	609.100160	-0.000211
61	55	6	62	56	6	609.125630	-0.000065
61	55	7	62	56	7	609.125630	-0.000065
61	55	6	62	56	7	609.125630	-0.000065
61	55	7	62	56	6	609.125630	-0.000065
60	58	3	61	59	3	609.152960	0.000860
60	58	3	61	59	2	609.152960	0.000860
60	58	2	61	59	3	609.152960	0.000860
61	54	7	62	55	7	609.178550	-0.000221
61	54	8	62	55	8	609.178550	-0.000221
61	54	7	62	55	8	609.178550	-0.000221
61	54	8	62	55	7	609.178550	-0.000221
60	57	3	61	58	3	609.203800	-0.000116
60	57	4	61	58	4	609.203800	-0.000116
60	57	3	61	58	4	609.203800	-0.000116
60	57	4	61	58	3	609.203800	-0.000116
62	31	32	63	32	32	609.257470	0.000096
62	30	32	63	31	32	609.257470	0.000096
62	31	31	63	32	31	609.257470	-0.000014
62	32	31	63	33	31	609.257470	-0.000014
62	29	33	63	30	33	609.257470	-0.000175
62	30	33	63	31	33	609.257470	-0.000175
60	55	5	61	56	5	609.308020	0.000070
60	55	6	61	56	6	609.308020	0.000070
60	55	5	61	56	6	609.308020	0.000070
60	55	6	61	56	5	609.308020	0.000070
59	58	1	60	59	1	609.336580	-0.000148
59	58	2	60	59	2	609.336580	-0.000148
59	58	1	60	59	2	609.336580	-0.000148
59	58	2	60	59	1	609.336580	-0.000148

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
60	54	6	61	55	6	609.360210	-0.000105
60	54	7	61	55	7	609.360210	-0.000105
60	54	6	61	55	7	609.360210	-0.000105
60	54	7	61	55	6	609.360210	-0.000105
59	57	3	60	58	3	609.388070	-0.000015
59	57	3	60	58	2	609.388070	-0.000015
59	57	2	60	58	3	609.388070	-0.000015
59	56	3	60	57	3	609.439750	0.000228
59	56	4	60	57	4	609.439750	0.000228
59	56	3	60	57	4	609.439750	0.000228
59	56	4	60	57	3	609.439750	0.000228
61	31	31	62	32	31	609.478920	0.000336
61	30	31	62	31	31	609.478920	0.000336
61	29	32	62	30	32	609.478920	0.000245
61	30	32	62	31	32	609.478920	0.000245
61	31	30	62	32	30	609.478920	0.000021
61	32	30	62	33	30	609.478920	0.000021
61	29	33	62	30	33	609.478920	-0.000213
61	28	33	62	29	33	609.478920	-0.000213
59	55	4	60	56	4	609.491300	0.000210
59	55	5	60	56	5	609.491300	0.000210
59	55	4	60	56	5	609.491300	0.000210
59	55	5	60	56	4	609.491300	0.000210
59	54	5	60	55	5	609.542430	-0.000402
59	54	6	60	55	6	609.542430	-0.000402
59	54	5	60	55	6	609.542430	-0.000402
59	54	6	60	55	5	609.542430	-0.000402
58	57	1	59	58	1	609.573100	0.000127
58	57	2	59	58	2	609.573100	0.000127
58	57	1	59	58	2	609.573100	0.000127
58	57	2	59	58	1	609.573100	0.000127
59	53	6	60	54	6	609.594800	-0.000052
59	53	7	60	54	7	609.594800	-0.000052
59	53	6	60	54	7	609.594800	-0.000052
59	53	7	60	54	6	609.594800	-0.000052
58	56	3	59	57	3	609.623880	-0.000081
58	56	3	59	57	2	609.623880	-0.000081
58	56	2	59	57	3	609.623880	-0.000081
59	52	7	60	53	7	609.647830	0.000538
59	52	8	60	53	8	609.647830	0.000538
59	52	7	60	53	8	609.647830	0.000538
59	52	8	60	53	7	609.647830	0.000538
58	55	3	59	56	3	609.675020	-0.000006
58	55	4	59	56	4	609.675020	-0.000006
58	55	3	59	56	4	609.675020	-0.000006
58	55	4	59	56	3	609.675020	-0.000006

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
60	30	30	61	31	30	609.700270	0.000338
60	31	30	61	32	30	609.700270	0.000338
60	28	32	61	29	32	609.700270	0.000156
60	29	32	61	30	32	609.700270	0.000156
60	31	29	61	32	29	609.700270	-0.000197
60	32	29	61	33	29	609.700270	-0.000197
58	54	4	59	55	4	609.726220	-0.000013
58	54	5	59	55	5	609.726220	-0.000013
58	54	4	59	55	5	609.726220	-0.000013
58	54	5	59	55	4	609.726220	-0.000013
58	53	5	59	54	5	609.777790	0.000166
58	53	6	59	54	6	609.777790	0.000166
58	53	5	59	54	6	609.777790	0.000166
58	53	6	59	54	5	609.777790	0.000166
57	56	1	58	57	1	609.809070	-0.000038
57	56	2	58	57	2	609.809070	-0.000038
57	56	1	58	57	2	609.809070	-0.000038
57	56	2	58	57	1	609.809070	-0.000038
58	52	6	59	53	6	609.829820	0.000517
58	52	7	59	53	7	609.829820	0.000517
58	52	6	59	53	7	609.829820	0.000517
58	52	7	59	53	6	609.829820	0.000517
57	55	3	58	56	3	609.860260	0.000529
57	55	3	58	56	2	609.860260	0.000529
57	55	2	58	56	3	609.860260	0.000529
58	51	7	59	52	7	609.881930	0.000500
58	51	8	59	52	8	609.881930	0.000500
58	51	7	59	52	8	609.881930	0.000500
58	51	8	59	52	7	609.881930	0.000500
57	54	3	58	55	3	609.910390	-0.000047
57	54	4	58	55	4	609.910390	-0.000047
57	54	3	58	55	4	609.910390	-0.000047
57	54	4	58	55	3	609.910390	-0.000047
59	30	30	60	31	30	609.921500	0.000358
59	29	30	60	30	30	609.921500	0.000358
59	29	31	60	30	31	609.921500	0.000256
59	28	31	60	29	31	609.921500	0.000256
59	30	29	60	31	29	609.921500	0.000046
59	31	29	60	32	29	609.921500	0.000046
59	28	32	60	29	32	609.921500	-0.000219
59	27	32	60	28	32	609.921500	-0.000219
57	53	4	58	54	4	609.961240	-0.000033
57	53	5	58	54	5	609.961240	-0.000033
57	53	4	58	54	5	609.961240	-0.000033
57	53	5	58	54	4	609.961240	-0.000033
57	52	5	58	53	5	610.012220	-0.000093

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
57	52	6	58	53	6	610.012220	-0.000093
57	52	5	58	53	6	610.012220	-0.000093
57	52	6	58	53	5	610.012220	-0.000093
56	55	1	57	56	1	610.044950	-0.000184
56	55	2	57	56	2	610.044950	-0.000184
56	55	1	57	56	2	610.044950	-0.000184
56	55	2	57	56	1	610.044950	-0.000184
57	51	6	58	52	6	610.063600	-0.000068
57	51	7	58	52	7	610.063600	-0.000068
57	51	6	58	52	7	610.063600	-0.000068
57	51	7	58	52	6	610.063600	-0.000068
56	54	3	57	55	3	610.095310	-0.000080
56	54	3	57	55	2	610.095310	-0.000080
56	54	2	57	55	3	610.095310	-0.000080
57	50	7	58	51	7	610.115180	-0.000315
57	50	8	58	51	8	610.115180	-0.000315
57	50	7	58	51	8	610.115180	-0.000316
57	50	8	58	51	7	610.115180	-0.000315
58	28	30	59	29	30	610.142660	0.000158
58	29	30	59	30	30	610.142660	0.000158
58	29	29	59	30	29	610.142660	0.000062
58	30	29	59	31	29	610.142660	0.000062
58	27	31	59	28	31	610.142660	-0.000143
58	28	31	59	29	31	610.142660	-0.000143
56	53	3	57	54	3	610.145660	-0.000068
56	53	4	57	54	4	610.145660	-0.000068
56	53	3	57	54	4	610.145660	-0.000068
56	53	4	57	54	3	610.145660	-0.000068
56	52	4	57	53	4	610.196230	0.000025
56	52	5	57	53	5	610.196230	0.000025
56	52	4	57	53	5	610.196230	0.000025
56	52	5	57	53	4	610.196230	0.000025
56	51	5	57	52	5	610.246850	-0.000056
56	51	6	57	52	6	610.246850	-0.000056
56	51	5	57	52	6	610.246850	-0.000056
56	51	6	57	52	5	610.246850	-0.000056
55	54	1	56	55	1	610.280970	-0.000064
55	54	2	56	55	2	610.280970	-0.000064
55	54	1	56	55	2	610.280970	-0.000064
55	54	2	56	55	1	610.280970	-0.000064
56	50	6	57	51	6	610.298000	0.000072
56	50	7	57	51	7	610.298000	0.000072
56	50	6	57	51	7	610.298000	0.000072
56	50	7	57	51	6	610.298000	0.000072
55	53	3	56	54	3	610.330840	-0.000091
55	53	3	56	54	2	610.330840	-0.000091

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
55	53	2	56	54	3	610.330840	-0.000091
56	49	7	57	50	7	610.349560	0.000101
56	49	8	57	50	8	610.349560	0.000101
56	49	7	57	50	8	610.349560	0.000101
56	49	8	57	50	7	610.349560	0.000102
57	29	28	58	30	28	610.364350	0.000133
57	30	28	58	31	28	610.364350	0.000133
57	27	31	58	28	31	610.364350	-0.000165
57	26	31	58	27	31	610.364350	-0.000165
55	52	3	56	53	3	610.380860	-0.000047
55	52	4	56	53	4	610.380860	-0.000047
55	52	3	56	53	4	610.380860	-0.000047
55	52	4	56	53	3	610.380860	-0.000047
55	51	4	56	52	4	610.430980	-0.000063
55	51	5	56	52	5	610.430980	-0.000063
55	51	4	56	52	5	610.430980	-0.000063
55	51	5	56	52	4	610.430980	-0.000063
55	50	5	56	51	5	610.481390	-0.000009
55	50	6	56	51	6	610.481390	-0.000009
55	50	5	56	51	6	610.481390	-0.000009
55	50	6	56	51	5	610.481390	-0.000009
54	53	1	55	54	1	610.516570	-0.000242
54	53	2	55	54	2	610.516570	-0.000242
54	53	1	55	54	2	610.516570	-0.000242
54	53	2	55	54	1	610.516570	-0.000242
55	49	6	56	50	6	610.532150	0.000042
55	49	7	56	50	7	610.532150	0.000042
55	49	6	56	50	7	610.532150	0.000042
55	49	7	56	50	6	610.532150	0.000042
54	52	3	55	53	3	610.566340	-0.000013
54	52	3	55	53	2	610.566340	-0.000013
54	52	2	55	53	3	610.566340	-0.000013
55	48	7	56	49	7	610.583310	-0.000041
55	48	8	56	49	8	610.583310	-0.000040
55	48	7	56	49	8	610.583310	-0.000041
55	48	8	56	49	7	610.583310	-0.000039
56	28	29	57	29	29	610.585640	0.000263
56	27	29	57	28	29	610.585640	0.000263
56	28	28	57	29	28	610.585640	0.000174
56	29	28	57	30	28	610.585640	0.000174
56	27	30	57	28	30	610.585640	-0.000054
56	26	30	57	27	30	610.585640	-0.000054
54	51	3	55	52	3	610.615060	-0.000923
54	51	4	55	52	4	610.615060	-0.000923
54	51	3	55	52	4	610.615060	-0.000923
54	51	4	55	52	3	610.615060	-0.000923

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
54	50	4	55	51	4	610.665520	-0.000245
54	50	5	55	51	5	610.665520	-0.000245
54	50	4	55	51	5	610.665520	-0.000245
54	50	5	55	51	4	610.665520	-0.000245
54	49	5	55	50	5	610.715500	-0.000292
54	49	6	55	50	6	610.715500	-0.000292
54	49	5	55	50	6	610.715500	-0.000292
54	49	6	55	50	5	610.715500	-0.000292
53	52	1	54	53	1	610.752370	-0.000100
53	52	2	54	53	2	610.752370	-0.000100
53	52	1	54	53	2	610.752370	-0.000100
53	52	2	54	53	1	610.752370	-0.000100
54	48	6	55	49	6	610.765900	-0.000288
54	48	7	55	49	7	610.765900	-0.000288
54	48	6	55	49	7	610.765900	-0.000288
54	48	7	55	49	6	610.765900	-0.000288
53	51	3	54	52	3	610.801380	-0.000273
53	51	3	54	52	2	610.801380	-0.000273
53	51	2	54	52	3	610.801380	-0.000273
55	28	28	56	29	28	610.807150	0.000258
55	27	28	56	28	28	610.807150	0.000258
55	26	29	56	27	29	610.807150	0.000133
55	27	29	56	28	29	610.807150	0.000133
55	28	27	56	29	27	610.807150	-0.000050
55	29	27	56	30	27	610.807150	-0.000050
54	47	7	55	48	7	610.817280	0.000117
54	47	8	55	48	8	610.817280	0.000118
54	47	7	55	48	8	610.817280	0.000115
54	47	8	55	48	7	610.817280	0.000120
53	50	3	54	51	3	610.850360	-0.000582
53	50	4	54	51	4	610.850360	-0.000582
53	50	3	54	51	4	610.850360	-0.000582
53	50	4	54	51	3	610.850360	-0.000582
53	49	4	54	50	4	610.900360	-0.000020
53	49	5	54	50	5	610.900360	-0.000020
53	49	4	54	50	5	610.900360	-0.000020
53	49	5	54	50	4	610.900360	-0.000020
53	48	5	54	49	5	610.949950	-0.000122
53	48	6	54	49	6	610.949950	-0.000122
53	48	5	54	49	6	610.949950	-0.000122
53	48	6	54	49	5	610.949950	-0.000122
52	51	1	53	52	1	610.987800	-0.000181
52	51	2	53	52	2	610.987800	-0.000181
52	51	1	53	52	2	610.987800	-0.000181
52	51	2	53	52	1	610.987800	-0.000181
53	47	6	54	48	6	611.000230	0.000061

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
53	47	7	54	48	7	611.000230	0.000061
53	47	6	54	48	7	611.000230	0.000061
53	47	7	54	48	6	611.000230	0.000061
54	26	28	55	27	28	611.028860	0.000386
54	27	28	55	28	28	611.028860	0.000386
54	27	27	55	28	27	611.028860	0.000303
54	28	27	55	29	27	611.028860	0.000303
54	25	29	55	26	29	611.028860	0.000056
54	26	29	55	27	29	611.028860	0.000056
54	28	26	55	29	26	611.028860	-0.000244
54	29	26	55	30	26	611.028860	-0.000244
52	50	3	53	51	3	611.037310	0.000480
52	50	3	53	51	2	611.037310	0.000480
52	50	2	53	51	3	611.037310	0.000480
53	46	7	54	47	7	611.051600	0.000717
53	46	8	54	47	8	611.051600	0.000720
53	46	7	54	47	8	611.051600	0.000714
53	46	8	54	47	7	611.051600	0.000722
52	49	3	53	50	3	611.085670	-0.000098
52	49	4	53	50	4	611.085670	-0.000098
52	49	3	53	50	4	611.085670	-0.000098
52	49	4	53	50	3	611.085670	-0.000098
52	48	4	53	49	4	611.134800	-0.000077
52	48	5	53	49	5	611.134800	-0.000077
52	48	4	53	49	5	611.134800	-0.000077
52	48	5	53	49	4	611.134800	-0.000077
52	47	5	53	48	5	611.184410	0.000160
52	47	6	53	48	6	611.184410	0.000160
52	47	5	53	48	6	611.184410	0.000160
52	47	6	53	48	5	611.184410	0.000160
51	50	1	52	51	1	611.222770	-0.000593
51	50	2	52	51	2	611.222770	-0.000593
51	50	1	52	51	2	611.222770	-0.000593
51	50	2	52	51	1	611.222770	-0.000593
53	26	28	54	27	28	611.250580	0.000371
53	25	28	54	26	28	611.250580	0.000371
53	28	26	54	29	26	611.250580	0.000194
53	27	26	54	28	26	611.250580	0.000194
53	25	29	54	26	29	611.250580	-0.000158
53	24	29	54	25	29	611.250580	-0.000158
52	45	7	53	46	7	611.284530	0.000004
52	45	8	53	46	8	611.284530	0.000009
52	45	7	53	46	8	611.284530	-0.000001
52	45	8	53	46	7	611.284530	0.000014
51	48	3	52	49	3	611.320230	-0.000246
51	48	4	52	49	4	611.320230	-0.000246

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
51	48	3	52	49	4	611.320230	-0.000246
51	48	4	52	49	3	611.320230	-0.000246
51	47	4	52	48	4	611.369260	0.000005
51	47	5	52	48	5	611.369260	0.000005
51	47	4	52	48	5	611.369260	0.000005
51	47	5	52	48	4	611.369260	0.000005
51	46	5	52	47	5	611.417990	-0.000327
51	46	6	52	47	6	611.417990	-0.000327
51	46	5	52	47	6	611.417990	-0.000327
51	46	6	52	47	5	611.417990	-0.000327
50	49	1	51	50	1	611.458600	-0.000006
50	49	2	51	50	2	611.458600	-0.000006
50	49	1	51	50	2	611.458600	-0.000006
50	49	2	51	50	1	611.458600	-0.000006
51	45	6	52	46	6	611.467280	-0.000554
51	45	7	52	46	7	611.467280	-0.000554
51	45	6	52	46	7	611.467280	-0.000555
51	45	7	52	46	6	611.467280	-0.000553
52	25	27	53	26	27	611.472130	0.000387
52	26	27	53	27	27	611.472130	0.000387
52	27	26	53	28	26	611.472130	0.000306
52	26	26	53	27	26	611.472130	0.000306
52	24	28	53	25	28	611.472130	0.000046
52	25	28	53	26	28	611.472130	0.000046
52	27	25	53	28	25	611.472130	-0.000252
52	28	25	53	29	25	611.472130	-0.000252
50	48	3	51	49	3	611.506470	-0.000312
50	48	3	51	49	2	611.506470	-0.000312
50	48	2	51	49	3	611.506470	-0.000312
51	44	7	52	45	7	611.518160	0.000085
51	44	8	52	45	8	611.518160	0.000094
51	44	7	52	45	8	611.518160	0.000076
51	44	8	52	45	7	611.518160	0.000103
50	47	3	51	48	3	611.554920	-0.000137
50	47	4	51	48	4	611.554920	-0.000137
50	47	3	51	48	4	611.554920	-0.000137
50	47	4	51	48	3	611.554920	-0.000137
50	46	4	51	47	4	611.603210	-0.000308
50	46	5	51	47	5	611.603210	-0.000308
50	46	4	51	47	5	611.603210	-0.000308
50	46	5	51	47	4	611.603210	-0.000308
50	45	5	51	46	5	611.652190	-0.000082
50	45	6	51	46	6	611.652190	-0.000082
50	45	5	51	46	6	611.652190	-0.000082
50	45	6	51	46	5	611.652190	-0.000082
49	48	1	50	49	1	611.693610	-0.000091

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
49	48	2	50	49	2	611.693610	-0.000091
51	25	26	52	26	26	611.693610	0.000184
51	26	26	52	27	26	611.693610	0.000184
51	24	27	52	25	27	611.693610	0.000046
51	25	27	52	26	27	611.693610	0.000046
51	26	25	52	27	25	611.693610	-0.000131
51	27	25	52	28	25	611.693610	-0.000131
49	48	1	50	49	2	611.693610	-0.000091
49	48	2	50	49	1	611.693610	-0.000091
50	44	6	51	45	6	611.701430	-0.000082
50	44	7	51	45	7	611.701430	-0.000081
50	44	6	51	45	7	611.701430	-0.000083
50	44	7	51	45	6	611.701430	-0.000080
49	47	3	50	48	3	611.741330	-0.000218
49	47	3	50	48	2	611.741330	-0.000218
49	47	2	50	48	3	611.741330	-0.000218
50	43	7	51	44	7	611.751630	0.000086
50	43	8	51	44	8	611.751630	0.000102
50	43	7	51	44	8	611.751630	0.000069
50	43	8	51	44	7	611.751630	0.000119
49	46	3	50	47	3	611.789300	-0.000201
49	46	4	50	47	4	611.789300	-0.000201
49	46	3	50	47	4	611.789300	-0.000201
49	46	4	50	47	3	611.789300	-0.000201
49	45	4	50	46	4	611.837470	-0.000180
49	45	5	50	46	5	611.837470	-0.000180
49	45	4	50	46	5	611.837470	-0.000180
49	45	5	50	46	4	611.837470	-0.000180
49	44	5	50	45	5	611.886100	-0.000009
49	44	6	50	45	6	611.886100	-0.000008
49	44	5	50	45	6	611.886100	-0.000009
49	44	6	50	45	5	611.886100	-0.000008
50	25	26	51	26	26	611.915500	0.000326
50	24	26	51	25	26	611.915500	0.000326
50	25	25	51	26	25	611.915500	0.000244
50	26	25	51	27	25	611.915500	0.000244
50	24	27	51	25	27	611.915500	-0.000023
50	23	27	51	24	27	611.915500	-0.000023
48	47	1	49	48	1	611.928370	-0.000274
48	47	2	49	48	2	611.928370	-0.000274
48	47	1	49	48	2	611.928370	-0.000274
48	47	2	49	48	1	611.928370	-0.000274
49	43	6	50	44	6	611.935970	0.000878
49	43	7	50	44	7	611.935970	0.000880
49	43	6	50	44	7	611.935970	0.000876
49	43	7	50	44	6	611.935970	0.000882

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
48	46	3	49	47	3	611.976190	0.000023
48	46	3	49	47	2	611.976190	0.000023
48	46	2	49	47	3	611.976190	0.000023
49	42	7	50	43	7	611.984630	-0.000309
49	42	8	50	43	8	611.984630	-0.000281
49	42	7	50	43	8	611.984630	-0.000339
49	42	8	50	43	7	611.984630	-0.000251
48	45	3	49	46	3	612.024300	0.000492
48	45	4	49	46	4	612.024300	0.000492
48	45	3	49	46	4	612.024300	0.000492
48	45	4	49	46	3	612.024300	0.000492
48	44	4	49	45	4	612.071490	-0.000156
48	44	5	49	45	5	612.071490	-0.000156
48	44	4	49	45	5	612.071490	-0.000156
48	44	5	49	45	4	612.071490	-0.000156
48	43	5	49	44	5	612.119890	0.000065
48	43	6	49	44	6	612.119890	0.000065
48	43	5	49	44	6	612.119890	0.000065
48	43	6	49	44	5	612.119890	0.000065
49	25	25	50	26	25	612.137200	0.000274
49	24	25	50	25	25	612.137200	0.000274
49	23	26	50	24	26	612.137200	0.000135
49	24	26	50	25	26	612.137200	0.000135
49	25	24	50	26	24	612.137200	-0.000051
49	26	24	50	27	24	612.137200	-0.000051
47	46	1	48	47	1	612.163000	-0.000439
47	46	2	48	47	2	612.163000	-0.000439
47	46	1	48	47	2	612.163000	-0.000439
47	46	2	48	47	1	612.163000	-0.000439
48	42	6	49	43	6	612.168640	0.000083
48	42	7	49	43	7	612.168640	0.000086
48	42	6	49	43	7	612.168640	0.000079
48	42	7	49	43	6	612.168640	0.000090
47	45	3	48	46	3	612.210620	-0.000030
47	45	3	48	46	2	612.210620	-0.000030
47	45	2	48	46	3	612.210620	-0.000030
48	41	7	49	42	7	612.218270	0.000025
48	41	8	49	42	8	612.218270	0.000074
48	41	7	49	42	8	612.218270	-0.000028
48	41	8	49	42	7	612.218270	0.000127
47	43	4	48	44	4	612.305470	-0.000047
47	43	5	48	44	5	612.305470	-0.000047
47	43	4	48	44	5	612.305470	-0.000047
47	43	5	48	44	4	612.305470	-0.000047
47	42	5	48	43	5	612.353280	-0.000139
47	42	6	48	43	6	612.353280	-0.000139

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
47	42	5	48	43	6	612.353280	-0.000139
47	42	6	48	43	5	612.353280	-0.000138
48	23	25	49	24	25	612.358590	-0.000136
48	24	25	49	25	25	612.358590	-0.000136
48	24	24	49	25	24	612.358590	-0.000225
48	25	24	49	26	24	612.358590	-0.000225
46	45	1	47	46	1	612.397830	-0.000230
46	45	2	47	46	2	612.397830	-0.000230
46	45	1	47	46	2	612.397830	-0.000230
46	45	2	47	46	1	612.397830	-0.000230
47	41	6	48	42	6	612.401910	-0.000012
47	41	7	48	42	7	612.401910	-0.000006
47	41	6	48	42	7	612.401910	-0.000018
47	41	7	48	42	6	612.401910	0.000000
46	44	3	47	45	3	612.444610	-0.000361
46	44	3	47	45	2	612.444610	-0.000361
46	44	2	47	45	3	612.444610	-0.000361
47	40	7	48	41	7	612.451340	-0.000135
47	40	8	48	41	8	612.451340	-0.000051
47	40	7	48	41	8	612.451340	-0.000229
47	40	8	48	41	7	612.451340	0.000043
46	43	3	47	44	3	612.491870	-0.000122
46	43	4	47	44	4	612.491870	-0.000122
46	43	3	47	44	4	612.491870	-0.000122
46	43	4	47	44	3	612.491870	-0.000122
46	42	4	47	43	4	612.539270	0.000030
46	42	5	47	43	5	612.539270	0.000030
46	42	4	47	43	5	612.539270	0.000030
46	42	5	47	43	4	612.539270	0.000030
47	23	24	48	24	24	612.580830	0.000313
47	24	24	48	25	24	612.580830	0.000313
47	22	25	48	23	25	612.580830	0.000177
47	23	25	48	24	25	612.580830	0.000177
47	25	23	48	26	23	612.580830	-0.000028
47	24	23	48	25	23	612.580830	-0.000028
45	45	0	46	46	0	612.585450	-0.000526
45	45	1	46	46	1	612.585450	-0.000526
45	45	0	46	46	1	612.585450	-0.000526
45	45	1	46	46	0	612.585450	-0.000526
46	41	5	47	42	5	612.586710	-0.000173
46	41	6	47	42	6	612.586710	-0.000172
46	41	5	47	42	6	612.586710	-0.000174
46	41	6	47	42	5	612.586710	-0.000172
45	44	1	46	45	1	612.632330	-0.000197
45	44	2	46	45	2	612.632330	-0.000197
45	44	1	46	45	2	612.632330	-0.000197

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
45	44	2	46	45	1	612.632330	-0.000197
46	40	6	47	41	6	612.634490	-0.000676
46	40	7	47	41	7	612.634490	-0.000665
46	40	6	47	41	7	612.634490	-0.000687
46	40	7	47	41	6	612.634490	-0.000653
45	43	3	46	44	3	612.679230	0.000105
45	43	3	46	44	2	612.679230	0.000105
45	43	2	46	44	3	612.679230	0.000105
46	39	7	47	40	7	612.684330	-0.000310
46	39	8	47	40	8	612.684330	-0.000165
46	39	7	47	40	8	612.684330	-0.000475
46	39	8	47	40	7	612.684330	0.000000
45	42	3	46	43	3	612.725140	-0.000715
45	42	4	46	43	4	612.725140	-0.000715
45	42	3	46	43	4	612.725140	-0.000715
45	42	4	46	43	3	612.725140	-0.000715
45	41	4	46	42	4	612.772610	-0.000218
45	41	5	46	42	5	612.772610	-0.000218
45	41	4	46	42	5	612.772610	-0.000218
45	41	5	46	42	4	612.772610	-0.000218
46	22	24	47	23	24	612.802650	0.000311
46	23	23	47	24	23	612.802650	0.000209
46	24	23	47	25	23	612.802650	0.000209
46	21	25	47	22	25	612.802650	-0.000041
46	22	25	47	23	25	612.802650	-0.000041
44	44	0	45	45	0	612.820270	-0.000287
44	44	1	45	45	1	612.820270	-0.000287
45	40	5	46	41	5	612.820270	0.000060
45	40	6	46	41	6	612.820270	0.000061
44	44	0	45	45	1	612.820270	-0.000287
44	44	1	45	45	0	612.820270	-0.000287
45	40	5	46	41	6	612.820270	0.000058
45	40	6	46	41	5	612.820270	0.000062
44	43	1	45	44	1	612.866750	-0.000061
44	43	2	45	44	2	612.866750	-0.000061
44	43	1	45	44	2	612.866750	-0.000061
44	43	2	45	44	1	612.866750	-0.000061
45	39	6	46	40	6	612.868260	-0.000049
45	39	7	46	40	7	612.868260	-0.000029
45	39	6	46	40	7	612.868260	-0.000070
45	39	7	46	40	6	612.868260	-0.000008
44	42	3	45	43	3	612.913190	0.000063
44	42	3	45	43	2	612.913190	0.000063
44	42	2	45	43	3	612.913190	0.000063
45	38	7	46	39	7	612.917720	-0.000019
45	38	8	46	39	8	612.917720	0.000226

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
45	38	7	46	39	8	612.917720	-0.000306
45	38	8	46	39	7	612.917720	0.000514
44	41	3	45	42	3	612.959490	-0.000080
44	41	4	45	42	4	612.959490	-0.000080
44	41	3	45	42	4	612.959490	-0.000080
44	41	4	45	42	3	612.959490	-0.000080
44	40	4	45	41	4	613.006130	-0.000135
44	40	5	45	41	5	613.006130	-0.000135
44	40	4	45	41	5	613.006130	-0.000135
44	40	5	45	41	4	613.006130	-0.000135
45	29	17	46	30	17	613.037750	0.000024
44	39	5	45	40	5	613.053580	0.000166
44	39	6	45	40	6	613.053580	0.000168
44	39	5	45	40	6	613.053580	0.000164
44	39	6	45	40	5	613.053580	0.000170
43	42	1	44	43	1	613.101340	0.000417
43	42	2	44	43	2	613.101340	0.000417
44	38	6	45	39	6	613.101340	0.000006
44	38	7	45	39	7	613.101340	0.000040
43	42	1	44	43	2	613.101340	0.000417
43	42	2	44	43	1	613.101340	0.000417
44	38	6	45	39	7	613.101340	-0.000032
44	38	7	45	39	6	613.101340	0.000078
43	41	3	44	42	3	613.146790	-0.000161
43	41	3	44	42	2	613.146790	-0.000161
43	41	2	44	42	3	613.146790	-0.000161
44	37	7	45	38	7	613.150460	-0.000349
44	37	8	45	38	8	613.150460	0.000063
43	40	3	44	41	3	613.193120	-0.000003
43	40	4	44	41	4	613.193120	-0.000003
43	40	3	44	41	4	613.193120	-0.000003
43	40	4	44	41	3	613.193120	-0.000003
43	39	4	44	40	4	613.239520	-0.000038
43	39	5	44	40	5	613.239520	-0.000038
43	39	4	44	40	5	613.239520	-0.000039
43	39	5	44	40	4	613.239520	-0.000038
44	22	23	45	23	23	613.245950	-0.000024
44	21	23	45	22	23	613.245950	-0.000024
44	23	22	45	24	22	613.245950	-0.000145
44	22	22	45	23	22	613.245950	-0.000145
44	21	24	45	22	24	613.245950	-0.000369
44	20	24	45	21	24	613.245950	-0.000369
44	28	17	45	29	17	613.257100	-0.000198
43	38	5	44	39	5	613.287030	0.000557
43	38	6	44	39	6	613.287030	0.000560
43	38	5	44	39	6	613.287030	0.000552

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
43	38	6	44	39	5	613.287030	0.000565
42	42	0	43	43	0	613.289070	-0.000093
42	42	1	43	43	1	613.289070	-0.000093
42	42	0	43	43	1	613.289070	-0.000093
42	42	1	43	43	0	613.289070	-0.000093
42	41	1	43	42	1	613.334540	-0.000319
42	41	2	43	42	2	613.334540	-0.000319
43	37	6	44	38	6	613.334540	0.000282
43	37	7	44	38	7	613.334540	0.000342
42	41	1	43	42	2	613.334540	-0.000319
42	41	2	43	42	1	613.334540	-0.000319
43	37	6	44	38	7	613.334540	0.000215
43	37	7	44	38	6	613.334540	0.000409
42	40	3	43	41	3	613.380700	0.000092
42	40	3	43	41	2	613.380700	0.000092
42	40	2	43	41	3	613.380700	0.000092
43	36	7	44	37	7	613.383500	-0.000364
43	36	8	44	37	8	613.383500	0.000321
42	39	3	43	40	3	613.426390	-0.000117
42	39	4	43	40	4	613.426390	-0.000117
42	39	3	43	40	4	613.426390	-0.000117
42	39	4	43	40	3	613.426390	-0.000117
43	21	22	44	22	22	613.467670	-0.000111
43	22	22	44	23	22	613.467670	-0.000111
43	20	23	44	21	23	613.467670	-0.000223
43	21	23	44	22	23	613.467670	-0.000223
42	38	4	43	39	4	613.473250	0.000560
42	38	5	43	39	5	613.473250	0.000560
42	38	4	43	39	5	613.473250	0.000559
42	38	5	43	39	4	613.473250	0.000560
43	27	17	44	28	17	613.476710	-0.000400
42	37	5	43	38	5	613.519100	-0.000294
42	37	6	43	38	6	613.519100	-0.000287
42	37	5	43	38	6	613.519100	-0.000302
42	37	6	43	38	5	613.519100	-0.000280
41	41	0	42	42	0	613.523120	-0.000064
41	41	1	42	42	1	613.523120	-0.000064
41	41	0	42	42	1	613.523120	-0.000064
41	41	1	42	42	0	613.523120	-0.000064
41	40	1	42	41	1	613.568350	-0.000257
41	40	2	42	41	2	613.568350	-0.000257
41	40	1	42	41	2	613.568350	-0.000257
41	40	2	42	41	1	613.568350	-0.000257
41	39	3	42	40	3	613.614030	-0.000048
41	39	3	42	40	2	613.614030	-0.000048
41	39	2	42	40	3	613.614030	-0.000048

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
42	35	8	43	36	8	613.615870	0.000050
41	38	3	42	39	3	613.659820	0.000107
41	38	4	42	39	4	613.659820	0.000107
41	38	3	42	39	4	613.659820	0.000107
41	38	4	42	39	3	613.659820	0.000107
42	20	22	43	21	22	613.689630	0.000066
42	21	22	43	22	22	613.689630	0.000066
42	22	21	43	23	21	613.689630	-0.000080
42	21	21	43	22	21	613.689630	-0.000080
42	19	23	43	20	23	613.689630	-0.000266
42	20	23	43	21	23	613.689630	-0.000266
42	26	17	43	27	17	613.696910	-0.000234
41	37	4	42	38	4	613.705590	-0.000073
41	37	5	42	38	5	613.705590	-0.000072
41	37	4	42	38	5	613.705590	-0.000074
41	37	5	42	38	4	613.705590	-0.000072
41	36	5	42	37	5	613.752410	0.000235
41	36	6	42	37	6	613.752410	0.000248
41	36	5	42	37	6	613.752410	0.000221
41	36	6	42	37	5	613.752410	0.000262
40	40	0	41	41	0	613.756980	-0.000022
40	40	1	41	41	1	613.756980	-0.000022
40	40	0	41	41	1	613.756980	-0.000022
40	40	1	41	41	0	613.756980	-0.000022
41	35	6	42	36	6	613.799610	-0.000180
41	35	7	42	36	7	613.799610	0.000000
41	35	6	42	36	7	613.799610	-0.000391
41	35	7	42	36	6	613.799610	0.000211
40	39	1	41	40	1	613.801990	-0.000169
40	39	2	41	40	2	613.801990	-0.000169
40	39	1	41	40	2	613.801990	-0.000169
40	39	2	41	40	1	613.801990	-0.000169
40	38	3	41	39	3	613.847340	-0.000036
40	38	3	41	39	2	613.847340	-0.000036
40	38	2	41	39	3	613.847340	-0.000036
41	34	8	42	35	8	613.848520	0.000223
40	37	3	41	38	3	613.892510	-0.000246
40	37	4	41	38	4	613.892510	-0.000246
40	37	3	41	38	4	613.892510	-0.000246
40	37	4	41	38	3	613.892510	-0.000246
41	21	21	42	22	21	613.911510	0.000166
41	19	22	42	20	22	613.911510	0.000076
41	22	20	42	23	20	613.911510	-0.000268
41	18	23	42	19	23	613.911510	-0.000465
41	25	17	42	26	17	613.917350	-0.000013
40	36	4	41	37	4	613.937960	-0.000507

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
40	36	5	41	37	5	613.937960	-0.000505
40	36	4	41	37	5	613.937960	-0.000508
40	36	5	41	37	4	613.937960	-0.000504
40	35	5	41	36	5	613.984870	0.000060
40	35	6	41	36	6	613.984870	0.000083
40	35	5	41	36	6	613.984870	0.000034
40	35	6	41	36	5	613.984870	0.000108
39	39	0	40	40	0	613.990740	0.000122
39	39	1	40	40	1	613.990740	0.000122
39	39	0	40	40	1	613.990740	0.000122
39	39	1	40	40	0	613.990740	0.000122
40	34	6	41	35	6	614.032440	0.000019
40	34	7	41	35	7	614.032440	0.000325
40	34	6	41	35	7	614.032440	-0.000351
39	38	1	40	39	1	614.035650	0.000135
39	38	2	40	39	2	614.035650	0.000135
39	38	1	40	39	2	614.035650	0.000135
39	38	2	40	39	1	614.035650	0.000135
39	37	3	40	38	3	614.080850	0.000381
39	37	3	40	38	2	614.080850	0.000381
39	37	2	40	38	3	614.080850	0.000381
39	36	3	40	37	3	614.125680	0.000070
39	36	4	40	37	4	614.125680	0.000070
39	36	3	40	37	4	614.125680	0.000070
39	36	4	40	37	3	614.125680	0.000070
40	21	20	41	22	20	614.133790	0.000565
40	19	22	41	20	22	614.133790	0.000431
40	21	19	41	22	19	614.133790	-0.000194
40	24	17	41	25	17	614.137640	-0.000124
40	26	15	41	27	15	614.145860	-0.000174
39	35	4	40	36	4	614.170960	-0.000146
39	35	5	40	36	5	614.170960	-0.000143
39	35	4	40	36	5	614.170960	-0.000148
39	35	5	40	36	4	614.170960	-0.000141
39	34	5	40	35	5	614.216890	-0.000407
39	34	6	40	35	6	614.216890	-0.000366
39	34	5	40	35	6	614.216890	-0.000453
39	34	6	40	35	5	614.216890	-0.000320
38	38	0	39	39	0	614.224250	0.000237
38	38	1	39	39	1	614.224250	0.000237
38	38	0	39	39	1	614.224250	0.000237
38	38	1	39	39	0	614.224250	0.000237
39	33	6	40	34	6	614.265030	0.000030
39	33	7	40	34	7	614.265030	0.000546
38	37	1	39	38	1	614.268520	-0.000140
38	37	2	39	38	2	614.268520	-0.000140

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
38	37	1	39	38	2	614.268520	-0.000140
38	37	2	39	38	1	614.268520	-0.000140
38	36	3	39	37	3	614.313230	-0.000149
38	36	3	39	37	2	614.313230	-0.000149
38	36	2	39	37	3	614.313230	-0.000149
39	20	20	40	21	20	614.354870	0.000103
39	19	20	40	20	20	614.354870	0.000103
39	19	21	40	20	21	614.354870	0.000042
39	18	21	40	19	21	614.354870	0.000042
38	35	3	39	36	3	614.357800	-0.000484
38	35	4	39	36	4	614.357800	-0.000484
39	23	17	40	24	17	614.357800	-0.000502
38	35	3	39	36	4	614.357800	-0.000484
38	35	4	39	36	3	614.357800	-0.000484
39	25	15	40	26	15	614.365630	0.000152
38	34	4	39	35	4	614.403320	-0.000258
38	34	5	39	35	5	614.403320	-0.000254
38	34	4	39	35	5	614.403320	-0.000263
38	34	5	39	35	4	614.403320	-0.000249
38	33	5	39	34	5	614.449140	-0.000510
38	33	6	39	34	6	614.449140	-0.000437
38	33	5	39	34	6	614.449140	-0.000592
38	33	6	39	34	5	614.449140	-0.000355
37	37	0	38	38	0	614.457460	0.000261
37	37	1	38	38	1	614.457460	0.000261
37	37	0	38	38	1	614.457460	0.000261
37	37	1	38	38	0	614.457460	0.000261
38	32	6	39	33	6	614.496780	-0.000762
38	32	7	39	33	7	614.496780	0.000100
37	36	1	38	37	1	614.502290	0.000677
37	36	2	38	37	2	614.502290	0.000677
37	36	1	38	37	2	614.502290	0.000677
37	36	2	38	37	1	614.502290	0.000677
37	35	3	38	36	3	614.546070	-0.000016
37	35	3	38	36	2	614.546070	-0.000016
37	35	2	38	36	3	614.546070	-0.000016
38	19	20	39	20	20	614.576290	-0.000081
38	18	20	39	19	20	614.576290	-0.000081
38	20	19	39	21	19	614.576290	-0.000301
38	19	19	39	20	19	614.576290	-0.000301
38	24	15	39	25	15	614.585140	0.000004
37	34	3	38	35	3	614.590680	-0.000085
37	34	4	38	35	4	614.590680	-0.000085
37	34	3	38	35	4	614.590680	-0.000086
37	34	4	38	35	3	614.590680	-0.000084
37	33	4	38	34	4	614.635810	-0.000061

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
37	33	5	38	34	5	614.635810	-0.000053
37	33	4	38	34	5	614.635810	-0.000070
37	33	5	38	34	4	614.635810	-0.000045
37	32	5	38	33	5	614.681460	-0.000404
37	32	6	38	33	6	614.681460	-0.000277
37	32	5	38	33	6	614.681460	-0.000552
37	32	6	38	33	5	614.681460	-0.000129
36	36	0	37	37	0	614.690280	0.000111
36	36	1	37	37	1	614.690280	0.000111
36	36	0	37	37	1	614.690280	0.000111
36	36	1	37	37	0	614.690280	0.000111
37	31	7	38	32	7	614.728720	0.000034
36	35	1	37	36	1	614.734430	0.000088
36	35	2	37	36	2	614.734430	0.000088
36	35	1	37	36	2	614.734430	0.000088
36	35	2	37	36	1	614.734430	0.000088
36	34	3	37	35	3	614.778630	0.000040
36	34	3	37	35	2	614.778630	0.000040
36	34	2	37	35	3	614.778630	0.000040
37	20	18	38	21	18	614.797960	-0.000576
37	19	19	38	20	19	614.797960	-0.000039
37	18	20	38	19	20	614.797960	-0.000063
37	17	21	38	18	21	614.797960	-0.000564
37	23	15	38	24	15	614.804790	-0.000181
36	33	3	37	34	3	614.823230	0.000179
36	33	4	37	34	4	614.823230	0.000180
36	33	3	37	34	4	614.823230	0.000179
36	33	4	37	34	3	614.823230	0.000181
36	32	4	37	33	4	614.867670	-0.000317
36	32	5	37	33	5	614.867670	-0.000302
36	32	4	37	33	5	614.867670	-0.000333
36	32	5	37	33	4	614.867670	-0.000287
36	31	5	37	32	5	614.913950	0.000003
36	31	6	37	32	6	614.913950	0.000223
36	31	5	37	32	6	614.913950	-0.000260
35	35	0	36	36	0	614.923470	0.000562
35	35	1	36	36	1	614.923470	0.000562
35	35	0	36	36	1	614.923470	0.000562
35	35	1	36	36	0	614.923470	0.000562
36	30	7	37	31	7	614.960420	-0.000035
35	34	1	36	35	1	614.967320	0.000471
35	34	2	36	35	2	614.967320	0.000471
35	34	1	36	35	2	614.967320	0.000471
35	34	2	36	35	1	614.967320	0.000471
35	33	3	36	34	3	615.010890	0.000013
35	33	3	36	34	2	615.010890	0.000013

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
35	33	2	36	34	3	615.010890	0.000013
36	20	17	37	21	17	615.020280	-0.000341
36	16	21	37	17	21	615.020280	-0.000129
36	22	15	37	23	15	615.024860	-0.000109
35	32	3	36	33	3	615.055280	0.000138
35	32	4	36	33	4	615.055280	0.000139
35	32	3	36	33	4	615.055280	0.000136
35	32	4	36	33	3	615.055280	0.000140
35	31	4	36	32	4	615.099850	-0.000081
35	31	5	36	32	5	615.099850	-0.000055
35	31	4	36	32	5	615.099850	-0.000110
35	31	5	36	32	4	615.099850	-0.000026
35	30	5	36	31	5	615.145640	-0.000275
35	30	6	36	31	6	615.145640	0.000102
34	34	0	35	35	0	615.155690	0.000266
34	34	1	35	35	1	615.155690	0.000266
34	34	0	35	35	1	615.155690	0.000266
34	34	1	35	35	0	615.155690	0.000266
34	33	1	35	34	1	615.199310	0.000170
34	33	2	35	34	2	615.199310	0.000170
34	33	1	35	34	2	615.199310	0.000170
34	33	2	35	34	1	615.199310	0.000170
35	19	17	36	20	17	615.241100	-0.000459
35	18	18	36	19	18	615.241100	0.000145
35	17	19	36	18	19	615.241100	0.000164
35	16	20	36	17	20	615.241100	-0.000308
34	32	3	35	33	3	615.242910	-0.000041
34	32	3	35	33	2	615.242910	-0.000041
34	32	2	35	33	3	615.242910	-0.000041
34	31	3	35	32	3	615.287100	0.000074
34	31	4	35	32	4	615.287100	0.000077
34	31	3	35	32	4	615.287100	0.000072
34	31	4	35	32	3	615.287100	0.000079
34	30	4	35	31	4	615.331800	0.000115
34	30	5	35	31	5	615.331800	0.000163
34	30	4	35	31	5	615.331800	0.000062
34	30	5	35	31	4	615.331800	0.000216
34	29	5	35	30	5	615.377840	0.000041
33	33	0	34	34	0	615.387720	0.000020
33	33	1	34	34	1	615.387720	0.000020
33	33	0	34	34	1	615.387720	0.000020
33	33	1	34	34	0	615.387720	0.000020
33	32	1	34	33	1	615.431370	0.000161
33	32	2	34	33	2	615.431370	0.000161
33	32	1	34	33	2	615.431370	0.000161
33	32	2	34	33	1	615.431370	0.000161

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
34	18	17	35	19	17	615.462300	-0.000253
34	17	18	35	18	18	615.462300	0.000075
34	16	19	35	17	19	615.462300	-0.000141
33	31	3	34	32	3	615.474830	0.000015
33	31	3	34	32	2	615.474830	0.000015
33	31	2	34	32	3	615.474830	0.000014
33	30	3	34	31	3	615.518550	-0.000153
33	30	4	34	31	4	615.518550	-0.000148
33	30	3	34	31	4	615.518550	-0.000157
33	30	4	34	31	3	615.518550	-0.000143
33	29	4	34	30	4	615.563230	-0.000040
33	29	5	34	30	5	615.563230	0.000045
33	29	4	34	30	5	615.563230	-0.000138
33	29	5	34	30	4	615.563230	0.000142
33	28	5	34	29	5	615.609420	-0.000212
32	32	0	33	33	0	615.619820	0.000089
32	32	1	33	33	1	615.619820	0.000089
32	32	0	33	33	1	615.619820	0.000089
32	32	1	33	33	0	615.619820	0.000089
32	31	1	33	32	1	615.663050	0.000020
32	31	2	33	32	2	615.663050	0.000020
32	31	1	33	32	2	615.663050	0.000020
32	31	2	33	32	1	615.663050	0.000020
33	18	16	34	19	16	615.684050	-0.000214
33	17	17	34	18	17	615.684050	0.000467
33	16	18	34	17	18	615.684050	0.000537
33	15	19	34	16	19	615.684050	0.000101
32	30	3	33	31	3	615.706880	0.000441
32	30	3	33	31	2	615.706880	0.000442
32	30	2	33	31	3	615.706880	0.000441
32	29	3	33	30	3	615.749960	-0.000206
32	29	4	33	30	4	615.749960	-0.000198
32	29	3	33	30	4	615.749960	-0.000215
32	29	4	33	30	3	615.749960	-0.000189
31	31	0	32	32	0	615.851580	0.000068
31	31	1	32	32	1	615.851580	0.000068
31	31	0	32	32	1	615.851580	0.000068
31	31	1	32	32	0	615.851580	0.000068
31	30	1	32	31	1	615.894270	-0.000347
31	30	2	32	31	2	615.894270	-0.000347
31	30	1	32	31	2	615.894270	-0.000347
31	30	2	32	31	1	615.894270	-0.000347
32	17	16	33	18	16	615.904890	-0.000124
32	16	17	33	17	17	615.904890	0.000271
32	15	18	33	16	18	615.904890	0.000100
32	14	19	33	15	19	615.904890	-0.000542

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
31	29	3	32	30	3	615.938070	0.000223
31	29	3	32	30	2	615.938070	0.000224
31	29	2	32	30	3	615.938070	0.000222
31	28	3	32	29	3	615.980800	-0.000621
31	28	4	32	29	4	615.980800	-0.000605
31	28	3	32	29	4	615.980800	-0.000638
31	28	4	32	29	3	615.980800	-0.000588
31	27	4	32	28	4	616.026360	0.000438
31	27	5	32	28	5	616.026360	0.000700
30	30	0	31	31	0	616.083120	0.000074
30	30	1	31	31	1	616.083120	0.000074
30	30	0	31	31	1	616.083120	0.000074
30	30	1	31	31	0	616.083120	0.000074
30	29	1	31	30	1	616.126100	0.000138
30	29	2	31	30	2	616.126100	0.000139
31	16	16	32	17	16	616.126100	0.000314
31	15	17	32	16	17	616.126100	0.000442
31	14	18	32	15	18	616.126100	0.000047
30	29	1	31	30	2	616.126100	0.000138
30	29	2	31	30	1	616.126100	0.000139
30	28	3	31	29	3	616.169020	0.000010
30	28	3	31	29	2	616.169020	0.000011
30	28	2	31	29	3	616.169020	0.000008
30	27	3	31	28	3	616.212780	0.000321
30	27	4	31	28	4	616.212780	0.000350
30	27	3	31	28	4	616.212780	0.000289
30	27	4	31	28	3	616.212780	0.000382
29	29	0	30	30	0	616.314760	0.000429
29	29	1	30	30	1	616.314760	0.000429
29	29	0	30	30	1	616.314760	0.000429
29	29	1	30	30	0	616.314760	0.000429
29	28	1	30	29	1	616.357340	0.000281
29	28	2	30	29	2	616.357340	0.000281
29	28	1	30	29	2	616.357340	0.000281
29	28	2	30	29	1	616.357340	0.000281
29	27	3	30	28	3	616.400090	0.000148
29	27	3	30	28	2	616.400090	0.000151
29	27	2	30	28	3	616.400090	0.000144
28	28	0	29	29	0	616.545320	-0.000023
28	28	1	29	29	1	616.545320	-0.000023
28	28	0	29	29	1	616.545320	-0.000023
28	28	1	29	29	0	616.545320	-0.000023
28	27	1	29	28	1	616.587990	0.000088
28	27	2	29	28	2	616.587990	0.000088
28	27	1	29	28	2	616.587990	0.000088
28	27	2	29	28	1	616.587990	0.000089

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
28	26	3	29	27	3	616.629800	-0.000823
28	26	3	29	27	2	616.629800	-0.000819
28	26	2	29	27	3	616.629800	-0.000832
27	27	0	28	28	0	616.775970	-0.000130
27	27	1	28	28	1	616.775970	-0.000130
27	27	0	28	28	1	616.775970	-0.000130
27	27	1	28	28	0	616.775970	-0.000130
27	26	1	28	27	1	616.818420	-0.000067
27	26	2	28	27	2	616.818420	-0.000067
27	26	1	28	27	2	616.818420	-0.000067
27	26	2	28	27	1	616.818420	-0.000067
27	25	3	28	26	3	616.861360	0.000303
27	25	3	28	26	2	616.861360	0.000312
27	25	2	28	26	3	616.861360	0.000286
26	26	0	27	27	0	617.007200	0.000616
26	26	1	27	27	1	617.007200	0.000616
26	26	0	27	27	1	617.007200	0.000616
26	26	1	27	27	0	617.007200	0.000617
26	25	1	27	26	1	617.048950	0.000144
26	25	2	27	26	2	617.048950	0.000144
26	25	1	27	26	2	617.048950	0.000143
26	25	2	27	26	1	617.048950	0.000145
26	24	3	27	25	3	617.091770	0.000528
26	24	3	27	25	2	617.091770	0.000544
26	24	2	27	25	3	617.091770	0.000495
25	25	0	26	26	0	617.237130	0.000347
25	25	1	26	26	1	617.237130	0.000347
25	25	0	26	26	1	617.237130	0.000347
25	25	1	26	26	0	617.237130	0.000347
25	24	1	26	25	1	617.279080	0.000219
25	24	2	26	25	2	617.279080	0.000219
25	24	1	26	25	2	617.279080	0.000218
25	24	2	26	25	1	617.279080	0.000220
25	23	3	26	24	3	617.321210	0.000050
25	23	3	26	24	2	617.321210	0.000082
25	23	2	26	24	3	617.321210	-0.000011
24	24	0	25	25	0	617.466910	0.000193
24	24	1	25	25	1	617.466910	0.000193
24	24	0	25	25	1	617.466910	0.000193
24	24	1	25	25	0	617.466910	0.000193
24	23	1	25	24	1	617.508660	0.000015
24	23	2	25	24	2	617.508660	0.000017
24	23	1	25	24	2	617.508660	0.000013
24	23	2	25	24	1	617.508660	0.000018
24	22	3	25	23	3	617.550970	0.000149
24	22	3	25	23	2	617.550970	0.000209

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
24	22	2	25	23	3	617.550970	0.000035
23	23	0	24	24	0	617.696440	0.000077
23	23	1	24	24	1	617.696440	0.000077
23	23	0	24	24	1	617.696440	0.000077
23	23	1	24	24	0	617.696440	0.000077
23	22	1	24	23	1	617.738090	-0.000062
23	22	2	24	23	2	617.738090	-0.000058
23	22	1	24	23	2	617.738090	-0.000065
23	22	2	24	23	1	617.738090	-0.000055
23	21	3	24	22	3	617.780360	0.000147
23	21	3	24	22	2	617.780360	0.000259
23	21	2	24	22	3	617.780360	-0.000065
22	22	0	23	23	0	617.925810	0.000097
22	22	1	23	23	1	617.925810	0.000097
22	22	0	23	23	1	617.925810	0.000097
22	22	1	23	23	0	617.925810	0.000097
22	21	1	23	22	1	617.967410	0.000034
22	21	2	23	22	2	617.967410	0.000041
22	21	1	23	22	2	617.967410	0.000027
22	21	2	23	22	1	617.967410	0.000048
22	20	3	23	21	3	618.008870	-0.000454
22	20	3	23	21	2	618.008870	-0.000244
22	20	2	23	21	3	618.008870	-0.000844
21	21	0	22	22	0	618.154840	0.000060
21	21	1	22	22	1	618.154840	0.000061
21	21	0	22	22	1	618.154840	0.000060
21	21	1	22	22	0	618.154840	0.000061
21	20	1	22	21	1	618.196460	0.000130
21	20	2	22	21	2	618.196460	0.000143
21	20	1	22	21	2	618.196460	0.000116
21	20	2	22	21	1	618.196460	0.000156
20	20	0	21	21	0	618.383340	-0.000212
20	20	1	21	21	1	618.383340	-0.000212
20	20	0	21	21	1	618.383340	-0.000213
20	20	1	21	21	0	618.383340	-0.000211
20	19	1	21	20	1	618.424960	-0.000031
20	19	2	21	20	2	618.424960	-0.000006
20	19	1	21	20	2	618.424960	-0.000057
20	19	2	21	20	1	618.424960	0.000021
19	19	0	20	20	0	618.611820	-0.000198
19	19	1	20	20	1	618.611820	-0.000197
19	19	0	20	20	1	618.611820	-0.000199
19	19	1	20	20	0	618.611820	-0.000196
19	18	1	20	19	1	618.653440	0.000073
19	18	2	20	19	2	618.653440	0.000120
19	18	1	20	19	2	618.653440	0.000021

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
19	18	2	20	19	1	618.653440	0.000172
18	17	1	19	18	1	618.881090	-0.000368
18	17	2	19	18	2	618.881090	-0.000277
18	17	1	19	18	2	618.881090	-0.000466
18	17	2	19	18	1	618.881090	-0.000179
16	16	0	17	17	0	619.295250	-0.000340
16	16	1	17	17	1	619.295250	-0.000333
16	16	0	17	17	1	619.295250	-0.000347
16	16	1	17	17	0	619.295250	-0.000325
15	15	0	16	16	0	619.522710	-0.000122
15	15	1	16	16	1	619.522710	-0.000107
15	15	0	16	16	1	619.522710	-0.000137
15	15	1	16	16	0	619.522710	-0.000092
14	14	0	15	15	0	619.749520	-0.000237
14	14	1	15	15	1	619.749520	-0.000207
14	14	0	15	15	1	619.749520	-0.000266
14	14	1	15	15	0	619.749520	-0.000177
13	13	0	14	14	0	619.976050	-0.000320
13	13	1	14	14	1	619.976050	-0.000262
13	13	0	14	14	1	619.976050	-0.000380
13	13	1	14	14	0	619.976050	-0.000203
14	2	12	13	1	12	626.067840	-0.000152
14	3	12	13	2	12	626.067840	-0.000152
14	14	0	13	13	0	626.144570	-0.000463
14	14	1	13	13	1	626.144570	-0.000520
14	14	0	13	13	1	626.144570	-0.000580
14	14	1	13	13	0	626.144570	-0.000403
15	3	12	14	2	12	626.276640	-0.000185
15	4	12	14	3	12	626.276640	-0.000185
15	15	0	14	14	0	626.361570	-0.000284
15	15	1	14	14	1	626.361570	-0.000313
15	15	0	14	14	1	626.361570	-0.000343
15	15	1	14	14	0	626.361570	-0.000254
16	4	12	15	3	12	626.484650	-0.000622
16	5	12	15	4	12	626.484650	-0.000622
16	2	14	15	1	14	626.490150	-0.000130
16	3	14	15	2	14	626.490150	-0.000130
71	31	40	71	30	41	626.537920	-0.000640
16	16	0	15	15	0	626.577710	-0.000628
16	16	1	15	15	1	626.577710	-0.000643
16	16	0	15	15	1	626.577710	-0.000658
16	16	1	15	15	0	626.577710	-0.000613
17	3	14	16	2	14	626.698590	0.000044
17	4	14	16	3	14	626.698590	0.000044
62	21	41	62	20	42	626.745070	0.000070
17	16	1	16	15	1	626.756370	0.000611

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
17	16	2	16	15	2	626.756370	0.000307
17	16	1	16	15	2	626.756370	-0.000048
17	16	2	16	15	1	626.756370	0.000966
17	17	0	16	16	0	626.794360	-0.000135
17	17	1	16	16	1	626.794360	-0.000143
17	17	0	16	16	1	626.794360	-0.000150
17	17	1	16	16	0	626.794360	-0.000128
18	4	14	17	3	14	626.906340	-0.000111
18	5	14	17	4	14	626.906340	-0.000111
53	11	42	53	10	43	626.952490	0.000550
18	17	1	17	16	1	626.972000	0.000201
18	17	2	17	16	2	626.972000	0.000036
18	17	1	17	16	2	626.972000	-0.000152
18	17	2	17	16	1	626.972000	0.000390
18	18	0	17	17	0	627.009900	-0.000416
18	18	1	17	17	1	627.009900	-0.000419
18	18	0	17	17	1	627.009900	-0.000423
18	18	1	17	17	0	627.009900	-0.000412
28	9	20	27	8	19	627.101880	-0.000066
19	7	12	18	6	12	627.107680	-0.000647
19	8	12	18	7	12	627.107680	-0.000647
19	5	14	18	4	14	627.113640	-0.000368
19	6	14	18	5	14	627.113640	-0.000368
19	17	2	18	16	2	627.147580	0.000124
19	17	3	18	16	3	627.147580	-0.001560
31	6	26	30	5	25	627.155090	-0.000448
79	32	47	79	31	48	627.158980	-0.000580
19	18	1	18	17	1	627.186690	-0.000796
19	18	2	18	17	2	627.186690	-0.000885
19	18	1	18	17	2	627.186690	-0.000984
19	18	2	18	17	1	627.186690	-0.000697
19	19	0	18	18	0	627.225650	-0.000164
19	19	1	18	18	1	627.225650	-0.000166
19	19	0	18	18	1	627.225650	-0.000168
19	19	1	18	18	0	627.225650	-0.000162
29	10	20	28	9	19	627.308210	0.000321
20	8	12	19	7	12	627.315070	-0.000194
20	9	12	19	8	12	627.315070	-0.000194
20	6	14	19	5	14	627.320620	-0.000602
20	7	14	19	6	14	627.320620	-0.000602
20	6	15	19	5	15	627.324160	0.000040
20	5	15	19	4	15	627.324160	0.000040
32	7	26	31	6	25	627.360350	-0.000332
79	30	49	79	29	50	627.364980	-0.000217
20	19	1	19	18	1	627.402940	0.000124
20	19	2	19	18	2	627.402940	0.000077

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
20	19	1	19	18	2	627.402940	0.000025
20	19	2	19	18	1	627.402940	0.000176
20	20	0	19	19	0	627.440490	-0.000500
20	20	1	19	19	1	627.440490	-0.000501
20	20	0	19	19	1	627.440490	-0.000502
20	20	1	19	19	0	627.440490	-0.000499
30	11	20	29	10	19	627.514150	0.000461
21	9	12	20	8	12	627.521580	-0.000226
21	10	12	20	9	12	627.521580	-0.000226
21	7	14	20	6	14	627.528150	0.000072
21	8	14	20	7	14	627.528150	0.000072
21	7	15	20	6	15	627.530990	-0.000097
21	6	15	20	5	15	627.530990	-0.000097
33	8	26	32	7	25	627.565150	-0.000544
79	29	51	79	28	52	627.571780	0.000751
21	19	2	20	18	2	627.579050	0.000163
21	19	3	20	18	3	627.579050	-0.000396
21	20	1	20	19	1	627.618190	0.000360
21	20	2	20	19	2	627.618190	0.000336
21	20	1	20	19	2	627.618190	0.000309
21	20	2	20	19	1	627.618190	0.000387
31	12	20	30	11	19	627.719940	0.000583
22	11	11	21	10	11	627.724200	-0.000061
22	12	11	21	11	11	627.724200	-0.000061
22	10	12	21	9	12	627.728140	0.000149
22	11	12	21	10	12	627.728140	0.000149
22	8	14	21	7	14	627.734560	-0.000040
22	9	14	21	8	14	627.734560	-0.000040
22	8	15	21	7	15	627.737910	0.000179
22	7	15	21	6	15	627.737910	0.000179
34	9	26	33	8	25	627.770040	-0.000531
22	20	2	21	19	2	627.794420	0.000491
22	20	3	21	19	3	627.794420	0.000177
22	20	2	21	19	3	627.794420	-0.000213
22	20	3	21	19	2	627.794420	0.000882
22	21	1	21	20	1	627.832380	-0.000130
22	21	2	21	20	2	627.832380	-0.000143
22	21	1	21	20	2	627.832380	-0.000157
22	21	2	21	20	1	627.832380	-0.000117
32	13	20	31	12	19	627.925270	0.000355
23	12	11	22	11	11	627.929690	-0.000088
23	13	11	22	12	11	627.929690	-0.000088
23	11	12	22	10	12	627.933770	-0.000020
23	12	12	22	11	12	627.933770	-0.000020
23	9	14	22	8	14	627.941120	0.000331
23	10	14	22	9	14	627.941120	0.000331

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
35	10	26	34	9	25	627.975530	0.000195
23	21	2	22	20	2	628.008930	0.000344
23	21	3	22	20	3	628.008930	0.000169
23	21	2	22	20	3	628.008930	-0.000043
23	21	3	22	20	2	628.008930	0.000556
23	22	1	22	21	1	628.047460	0.000579
23	22	2	22	21	2	628.047460	0.000572
23	22	1	22	21	2	628.047460	0.000565
23	22	2	22	21	1	628.047460	0.000586
33	14	20	32	13	19	628.129780	-0.000584
24	13	11	23	12	11	628.134740	-0.000147
24	14	11	23	13	11	628.134740	-0.000149
24	10	14	23	9	14	628.146850	0.000213
24	11	14	23	10	14	628.146850	0.000213
24	10	15	23	9	15	628.150150	0.000126
24	9	15	23	8	15	628.150150	0.000126
24	9	16	23	8	16	628.153340	0.000013
24	8	16	23	7	16	628.153340	0.000013
24	8	17	23	7	17	628.156780	0.000176
24	7	17	23	6	17	628.156780	0.000176
24	23	1	23	22	1	628.261240	0.000290
24	23	2	23	22	2	628.261240	0.000287
24	23	1	23	22	2	628.261240	0.000283
24	23	2	23	22	1	628.261240	0.000294
24	24	0	23	23	0	628.298720	0.000193
24	24	1	23	23	1	628.298720	0.000193
24	24	0	23	23	1	628.298720	0.000193
24	24	1	23	23	0	628.298720	0.000193
25	14	11	24	13	11	628.339860	0.000267
25	15	11	24	14	11	628.339860	0.000263
25	11	14	24	10	14	628.352700	0.000541
25	12	14	24	11	14	628.352700	0.000541
25	11	15	24	10	15	628.355920	0.000221
25	10	15	24	9	15	628.355920	0.000221
25	10	16	24	9	16	628.359120	-0.000005
25	9	16	24	8	16	628.359120	-0.000005
25	9	17	24	8	17	628.362670	0.000181
25	8	17	24	7	17	628.362670	0.000181
25	22	3	24	21	3	628.397900	0.000213
25	22	4	24	21	4	628.397900	-0.000653
25	23	2	24	22	2	628.436890	0.000005
25	23	3	24	22	3	628.436890	-0.000047
25	23	2	24	22	3	628.436890	-0.000108
25	23	3	24	22	2	628.436890	0.000066
25	24	1	24	23	1	628.475230	0.000514
25	24	2	24	23	2	628.475230	0.000513

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
25	24	1	24	23	2	628.475230	0.000511
25	24	2	24	23	1	628.475230	0.000516
25	25	0	24	24	0	628.512310	0.000170
25	25	1	24	24	1	628.512310	0.000170
25	25	0	24	24	1	628.512310	0.000170
25	25	1	24	24	0	628.512310	0.000170
26	15	11	25	14	11	628.543820	-0.000072
26	16	11	25	15	11	628.543820	-0.000081
26	13	13	25	12	13	628.553320	-0.000056
26	14	13	25	13	13	628.553320	-0.000056
26	12	14	25	11	14	628.557480	0.000129
26	13	14	25	12	14	628.557480	0.000129
26	12	15	25	11	15	628.561220	0.000156
26	11	15	25	10	15	628.561220	0.000156
26	11	16	25	10	16	628.564820	0.000207
26	10	16	25	9	16	628.564820	0.000207
26	10	17	25	9	17	628.568480	0.000398
26	9	17	25	8	17	628.568480	0.000398
26	4	23	25	3	23	628.589040	-0.000347
26	3	23	25	2	23	628.589040	-0.000347
26	23	3	25	22	3	628.612020	0.000154
26	23	4	25	22	4	628.612020	-0.000345
26	24	2	25	23	2	628.650800	0.000245
26	24	3	25	23	3	628.650800	0.000217
26	24	2	25	23	3	628.650800	0.000185
26	24	3	25	23	2	628.650800	0.000277
26	25	1	25	24	1	628.688300	0.000132
26	25	2	25	24	2	628.688300	0.000131
26	25	1	25	24	2	628.688300	0.000130
26	25	2	25	24	1	628.688300	0.000133
26	26	0	25	25	0	628.725520	0.000075
26	26	1	25	25	1	628.725520	0.000075
26	26	0	25	25	1	628.725520	0.000075
26	26	1	25	25	0	628.725520	0.000075
27	16	11	26	15	11	628.747720	-0.000054
27	17	11	26	16	11	628.747720	-0.000074
27	14	13	26	13	13	628.758160	0.000143
27	15	13	26	14	13	628.758160	0.000143
27	13	14	26	12	14	628.762620	0.000392
27	14	14	26	13	14	628.762620	0.000392
27	13	15	26	12	15	628.766060	-0.000062
27	12	15	26	11	15	628.766060	-0.000062
27	12	16	26	11	16	628.770020	0.000203
27	11	16	26	10	16	628.770020	0.000203
27	11	17	26	10	17	628.773370	-0.000022
27	10	17	26	9	17	628.773370	-0.000022

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
27	9	19	26	8	19	628.780760	0.000314
27	8	19	26	7	19	628.780760	0.000314
27	5	23	26	4	23	628.795040	0.000023
27	4	23	26	3	23	628.795040	0.000023
27	24	3	26	23	3	628.826080	0.000431
27	24	4	26	23	4	628.826080	0.000147
27	24	3	26	23	4	628.826080	-0.000224
27	24	4	26	23	3	628.826080	0.000802
27	25	2	26	24	2	628.864110	0.000190
27	25	3	26	24	3	628.864110	0.000176
27	25	2	26	24	3	628.864110	0.000159
27	25	3	26	24	2	628.864110	0.000207
27	26	1	26	25	1	628.901030	-0.000314
27	26	2	26	25	2	628.901030	-0.000314
27	26	1	26	25	2	628.901030	-0.000315
27	26	2	26	25	1	628.901030	-0.000313
27	27	0	26	26	0	628.938360	-0.000093
27	27	1	26	26	1	628.938360	-0.000093
27	27	0	26	26	1	628.938360	-0.000093
27	27	1	26	26	0	628.938360	-0.000093
28	17	11	27	16	11	628.951160	-0.000083
28	18	11	27	17	11	628.951160	-0.000126
28	15	13	27	14	13	628.962370	0.000047
28	16	13	27	15	13	628.962370	0.000046
28	14	15	27	13	15	628.971220	0.000346
28	13	15	27	12	15	628.971220	0.000346
28	13	16	27	12	16	628.974900	0.000175
28	12	16	27	11	16	628.974900	0.000175
28	12	17	27	11	17	628.978630	0.000202
28	11	17	27	10	17	628.978630	0.000202
28	10	19	27	9	19	628.985840	0.000182
28	9	19	27	8	19	628.985840	0.000182
28	6	23	27	5	23	629.000750	0.000346
28	5	23	27	4	23	629.000750	0.000346
28	25	3	27	24	3	629.039350	0.000287
28	25	4	27	24	4	629.039350	0.000127
28	25	3	27	24	4	629.039350	-0.000077
28	25	4	27	24	3	629.039350	0.000492
28	26	2	27	25	2	629.077290	0.000291
28	26	3	27	25	3	629.077290	0.000283
28	26	2	27	25	3	629.077290	0.000274
28	26	3	27	25	2	629.077290	0.000300
28	27	1	27	26	1	629.114380	0.000170
28	27	2	27	26	2	629.114380	0.000170
28	27	1	27	26	2	629.114380	0.000170
28	27	2	27	26	1	629.114380	0.000171

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
28	28	0	27	27	0	629.151310	0.000140
28	28	1	27	27	1	629.151310	0.000140
28	28	0	27	27	1	629.151310	0.000140
28	28	1	27	27	0	629.151310	0.000140
29	18	11	28	17	11	629.154220	-0.000058
29	19	11	28	18	11	629.154220	-0.000147
29	16	13	28	15	13	629.166120	-0.000172
29	17	13	28	16	13	629.166120	-0.000172
29	14	16	28	13	16	629.179540	0.000181
29	13	16	28	12	16	629.179540	0.000181
29	13	17	28	12	17	629.183360	0.000163
29	12	17	28	11	17	629.183360	0.000163
29	11	19	28	10	19	629.190740	0.000129
29	10	19	28	9	19	629.190740	0.000129
29	7	23	28	6	23	629.205830	0.000295
29	6	23	28	5	23	629.205830	0.000295
29	25	4	28	24	4	629.213270	0.000519
29	25	5	28	24	5	629.213270	-0.000693
29	26	3	28	25	3	629.252230	0.000074
29	26	4	28	25	4	629.252230	-0.000014
29	26	3	28	25	4	629.252230	-0.000126
29	26	4	28	25	3	629.252230	0.000186
29	27	2	28	26	2	629.289980	0.000200
29	27	3	28	26	3	629.289980	0.000196
29	27	2	28	26	3	629.289980	0.000191
29	27	3	28	26	2	629.289980	0.000205
29	28	1	28	27	1	629.327040	0.000235
29	28	2	28	27	2	629.327040	0.000235
29	28	1	28	27	2	629.327040	0.000235
29	28	2	28	27	1	629.327040	0.000235
29	29	0	28	28	0	629.363670	0.000080
29	29	1	28	28	1	629.363670	0.000080
29	29	0	28	28	1	629.363670	0.000080
29	29	1	28	28	0	629.363670	0.000080
30	17	13	29	16	13	629.369540	-0.000404
30	18	13	29	17	13	629.369540	-0.000404
30	16	15	29	15	15	629.379750	0.000232
30	15	15	29	14	15	629.379750	0.000232
30	14	17	29	13	17	629.387610	-0.000078
30	13	17	29	12	17	629.387610	-0.000078
30	12	19	29	11	19	629.395770	0.000463
30	11	19	29	10	19	629.395770	0.000463
30	8	23	29	7	23	629.410680	0.000237
30	7	23	29	6	23	629.410680	0.000237
30	26	4	29	25	4	629.426690	0.000487
30	26	5	29	25	5	629.426690	-0.000227

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
30	27	3	29	26	3	629.465410	0.000463
30	27	4	29	26	4	629.465410	0.000415
30	27	3	29	26	4	629.465410	0.000354
30	27	4	29	26	3	629.465410	0.000524
30	28	2	29	27	2	629.502420	0.000133
30	28	3	29	27	3	629.502420	0.000130
30	28	2	29	27	3	629.502420	0.000128
30	28	3	29	27	2	629.502420	0.000135
30	29	1	29	28	1	629.539450	0.000341
30	29	2	29	28	2	629.539450	0.000341
30	29	1	29	28	2	629.539450	0.000341
30	29	2	29	28	1	629.539450	0.000341
31	18	13	30	17	13	629.573170	-0.000086
31	19	13	30	18	13	629.573170	-0.000088
30	30	0	29	29	0	629.575760	0.000034
30	30	1	29	29	1	629.575760	0.000034
30	30	0	29	29	1	629.575760	0.000034
30	30	1	29	29	0	629.575760	0.000034
31	17	15	30	16	15	629.583930	0.000512
31	16	15	30	15	15	629.583930	0.000512
31	16	16	30	15	16	629.588070	0.000260
31	15	16	30	14	16	629.588070	0.000260
31	15	17	30	14	17	629.592030	0.000098
31	14	17	30	13	17	629.592030	0.000098
31	13	19	30	12	19	629.599700	-0.000071
31	12	19	30	11	19	629.599700	-0.000071
31	11	21	30	10	21	629.607390	-0.000019
31	10	21	30	9	21	629.607390	-0.000019
31	9	23	30	8	23	629.615470	0.000334
31	8	23	30	7	23	629.615470	0.000334
31	27	4	30	26	4	629.639510	0.000273
31	27	5	30	26	5	629.639510	-0.000142
31	28	3	30	27	3	629.677510	0.000062
31	28	4	30	27	4	629.677510	0.000035
31	28	3	30	27	4	629.677510	0.000002
31	28	4	30	27	3	629.677510	0.000094
31	29	2	30	28	2	629.714610	0.000092
31	29	3	30	28	3	629.714610	0.000091
31	29	2	30	28	3	629.714610	0.000090
31	29	3	30	28	2	629.714610	0.000094
31	30	1	30	29	1	629.751450	0.000311
31	30	2	30	29	2	629.751450	0.000311
31	30	1	30	29	2	629.751450	0.000311
31	30	2	30	29	1	629.751450	0.000311
32	19	13	31	18	13	629.776390	0.000145
32	20	13	31	19	13	629.776390	0.000141

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
31	31	0	30	30	0	629.787590	0.000007
31	31	1	30	30	1	629.787590	0.000007
32	18	15	31	17	15	629.787590	0.000544
32	17	15	31	16	15	629.787590	0.000544
31	31	0	30	30	1	629.787590	0.000007
31	31	1	30	30	0	629.787590	0.000007
32	17	16	31	16	16	629.791730	0.000092
32	16	16	31	15	16	629.791730	0.000092
32	16	17	31	15	17	629.795800	-0.000126
32	15	17	31	14	17	629.795800	-0.000126
32	14	19	31	13	19	629.804000	0.000002
32	13	19	31	12	19	629.804000	0.000002
32	12	20	31	11	20	629.808040	0.000136
32	13	20	31	12	20	629.808040	0.000136
32	12	21	31	11	21	629.812030	0.000245
32	11	21	31	10	21	629.812030	0.000245
32	28	4	31	27	4	629.852270	0.000353
32	28	5	31	27	5	629.852270	0.000115
32	28	4	31	27	5	629.852270	-0.000212
32	29	3	31	28	3	629.889660	-0.000001
32	29	4	31	28	4	629.889660	-0.000016
32	29	3	31	28	4	629.889660	-0.000033
32	29	4	31	28	3	629.889660	0.000016
32	30	2	31	29	2	629.926560	0.000086
32	30	3	31	29	3	629.926560	0.000086
32	30	2	31	29	3	629.926560	0.000085
32	30	3	31	29	2	629.926560	0.000087
32	31	1	31	30	1	629.962980	0.000086
32	31	2	31	30	2	629.962980	0.000086
32	31	1	31	30	2	629.962980	0.000086
32	31	2	31	30	1	629.962980	0.000086
33	20	13	32	19	13	629.978600	-0.000322
33	21	13	32	20	13	629.978600	-0.000330
33	19	15	32	18	15	629.990440	0.000035
33	18	15	32	17	15	629.990440	0.000035
33	18	16	32	17	16	629.995220	0.000000
33	17	16	32	16	16	629.995220	0.000000
32	32	0	31	31	0	629.999400	0.000241
32	32	1	31	31	1	629.999400	0.000241
33	17	17	32	16	17	629.999400	-0.000290
33	16	17	32	15	17	629.999400	-0.000290
32	32	0	31	31	1	629.999400	0.000241
32	32	1	31	31	0	629.999400	0.000241
33	15	19	32	14	19	630.008070	0.000068
33	14	19	32	13	19	630.008070	0.000068
33	13	20	32	12	20	630.012240	0.000242

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
33	14	20	32	13	20	630.012240	0.000242
33	12	22	32	11	22	630.019850	-0.000046
33	11	22	32	10	22	630.019850	-0.000046
33	11	23	32	10	23	630.023980	0.000114
33	10	23	32	9	23	630.023980	0.000114
33	29	4	32	28	4	630.064400	0.000148
33	29	5	32	28	5	630.064400	0.000013
33	29	4	32	28	5	630.064400	-0.000170
33	29	5	32	28	4	630.064400	0.000330
33	30	3	32	29	3	630.101770	0.000163
33	30	4	32	29	4	630.101770	0.000155
33	30	3	32	29	4	630.101770	0.000146
33	30	4	32	29	3	630.101770	0.000172
33	31	2	32	30	2	630.138390	0.000227
33	31	3	32	30	3	630.138390	0.000227
33	31	2	32	30	3	630.138390	0.000227
33	31	3	32	30	2	630.138390	0.000228
33	32	1	32	31	1	630.174530	0.000149
33	32	2	32	31	2	630.174530	0.000149
33	32	1	32	31	2	630.174530	0.000149
33	32	2	32	31	1	630.174530	0.000149
34	21	13	33	20	13	630.180970	-0.000294
34	22	13	33	21	13	630.180970	-0.000312
34	20	15	33	19	15	630.193460	-0.000032
34	19	15	33	18	15	630.193460	-0.000032
34	19	16	33	18	16	630.198450	-0.000106
34	18	16	33	17	16	630.198450	-0.000106
34	18	17	33	17	17	630.203160	-0.000044
34	17	17	33	16	17	630.203160	-0.000044
33	33	0	32	32	0	630.210520	0.000071
33	33	1	32	32	1	630.210520	0.000071
33	33	0	32	32	1	630.210520	0.000071
33	33	1	32	32	0	630.210520	0.000071
34	16	19	33	15	19	630.212380	0.000596
34	15	19	33	14	19	630.212380	0.000596
34	14	20	33	13	20	630.216110	0.000236
34	15	20	33	14	20	630.216110	0.000236
34	14	21	33	13	21	630.219860	-0.000050
34	13	21	33	12	21	630.219860	-0.000050
34	13	22	33	12	22	630.223790	-0.000121
34	12	22	33	11	22	630.223790	-0.000121
34	10	25	33	9	25	630.236040	-0.000049
34	9	25	33	8	25	630.236040	-0.000049
34	30	4	33	29	4	630.276550	0.000248
34	30	5	33	29	5	630.276550	0.000173
34	30	4	33	29	5	630.276550	0.000072

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
34	30	5	33	29	4	630.276550	0.000350
34	31	3	33	30	3	630.313460	0.000169
34	31	4	33	30	4	630.313460	0.000165
34	31	3	33	30	4	630.313460	0.000160
34	31	4	33	30	3	630.313460	0.000174
34	32	2	33	31	2	630.349480	-0.000120
34	32	3	33	31	3	630.349480	-0.000120
34	32	2	33	31	3	630.349480	-0.000121
34	32	3	33	31	2	630.349480	-0.000120
35	22	13	34	21	13	630.383230	-0.000059
35	23	13	34	22	13	630.383230	-0.000095
34	33	1	33	32	1	630.385570	-0.000024
34	33	2	33	32	2	630.385570	-0.000024
34	33	1	33	32	2	630.385570	-0.000024
34	33	2	33	32	1	630.385570	-0.000024
35	21	15	34	20	15	630.396160	-0.000169
35	20	15	34	19	15	630.396160	-0.000169
35	20	16	34	19	16	630.401180	-0.000465
35	19	16	34	18	16	630.401180	-0.000465
35	19	17	34	18	17	630.406600	0.000096
35	18	17	34	17	17	630.406600	0.000096
35	15	20	34	14	20	630.419660	0.000100
35	16	20	34	15	20	630.419660	0.000100
34	34	0	33	33	0	630.421630	0.000150
34	34	1	33	33	1	630.421630	0.000150
34	34	0	33	33	1	630.421630	0.000150
34	34	1	33	33	0	630.421630	0.000150
35	15	21	34	14	21	630.423270	-0.000397
35	14	21	34	13	21	630.423270	-0.000397
35	14	22	34	13	22	630.427690	-0.000054
35	13	22	34	12	22	630.427690	-0.000054
35	11	25	34	10	25	630.439960	-0.000083
35	10	25	34	9	25	630.439960	-0.000083
35	30	5	34	29	5	630.450270	0.000235
35	30	6	34	29	6	630.450270	-0.000328
35	31	4	34	30	4	630.488170	0.000108
35	31	5	34	30	5	630.488170	0.000066
35	31	4	34	30	5	630.488170	0.000011
35	31	5	34	30	4	630.488170	0.000164
35	32	3	34	31	3	630.524830	0.000111
35	32	4	34	31	4	630.524830	0.000109
35	32	3	34	31	4	630.524830	0.000106
35	32	4	34	31	3	630.524830	0.000114
35	33	2	34	32	2	630.561030	0.000257
35	33	3	34	32	3	630.561030	0.000257
35	33	2	34	32	3	630.561030	0.000257

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
35	33	3	34	32	2	630.561030	0.000257
36	23	13	35	22	13	630.584860	-0.000115
36	24	13	35	23	13	630.584860	-0.000186
35	34	1	34	33	1	630.596440	-0.000119
35	34	2	34	33	2	630.596440	-0.000119
35	34	1	34	33	2	630.596440	-0.000119
35	34	2	34	33	1	630.596440	-0.000119
36	22	15	35	21	15	630.598760	-0.000162
36	21	15	35	20	15	630.598760	-0.000162
36	21	16	35	20	16	630.604410	-0.000107
36	20	16	35	19	16	630.604410	-0.000107
36	20	17	35	19	17	630.609490	-0.000091
36	19	17	35	18	17	630.609490	-0.000091
36	18	19	35	17	19	630.618540	-0.000211
36	17	19	35	16	19	630.618540	-0.000211
36	16	20	35	15	20	630.623090	0.000042
36	17	20	35	16	20	630.623090	0.000042
36	16	21	35	15	21	630.627270	0.000023
36	15	21	35	14	21	630.627270	0.000023
35	35	0	34	34	0	630.632250	0.000010
35	35	1	34	34	1	630.632250	0.000010
35	35	0	34	34	1	630.632250	0.000010
35	35	1	34	34	0	630.632250	0.000010
36	12	25	35	11	25	630.644150	0.000338
36	11	25	35	10	25	630.644150	0.000338
36	31	5	35	30	5	630.662210	0.000120
36	31	6	35	30	6	630.662210	-0.000209
36	32	4	35	31	4	630.699480	-0.000089
36	32	5	35	31	5	630.699480	-0.000112
36	32	4	35	31	5	630.699480	-0.000142
36	32	5	35	31	4	630.699480	-0.000058
36	33	3	35	32	3	630.735940	0.000055
36	33	4	35	32	4	630.735940	0.000054
36	33	3	35	32	4	630.735940	0.000053
36	33	4	35	32	3	630.735940	0.000056
36	34	2	35	33	2	630.771910	0.000217
36	34	3	35	33	3	630.771910	0.000217
36	34	2	35	33	3	630.771910	0.000217
36	34	3	35	33	2	630.771910	0.000217
37	24	13	36	23	13	630.786390	0.000075
37	25	13	36	24	13	630.786390	-0.000062
37	23	15	36	22	15	630.801090	-0.000174
37	22	15	36	21	15	630.801090	-0.000173
36	35	1	35	34	1	630.807400	0.000148
36	35	2	35	34	2	630.807400	0.000148
36	35	1	35	34	2	630.807400	0.000148

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
36	35	2	35	34	1	630.807400	0.000148
37	21	17	36	20	17	630.812330	-0.000122
37	20	17	36	19	17	630.812330	-0.000122
37	17	20	36	16	20	630.826340	-0.000016
37	18	20	36	17	20	630.826340	-0.000016
37	17	21	36	16	21	630.830030	-0.000611
37	16	21	36	15	21	630.830030	-0.000611
37	16	22	36	15	22	630.834470	-0.000390
37	15	22	36	14	22	630.834470	-0.000390
36	36	0	35	35	0	630.843070	0.000338
36	36	1	35	35	1	630.843070	0.000338
36	36	0	35	35	1	630.843070	0.000338
36	36	1	35	35	0	630.843070	0.000338
37	13	25	36	12	25	630.847560	0.000129
37	12	25	36	11	25	630.847560	0.000129
37	10	28	36	9	28	630.860490	0.000106
37	9	28	36	8	28	630.860490	0.000106
37	33	4	36	32	4	630.910690	-0.000117
37	33	5	36	32	5	630.910690	-0.000130
37	33	4	36	32	5	630.910690	-0.000147
37	33	5	36	32	4	630.910690	-0.000101
37	34	3	36	33	3	630.946410	-0.000412
37	34	4	36	33	4	630.946410	-0.000412
37	34	3	36	33	4	630.946410	-0.000413
37	34	4	36	33	3	630.946410	-0.000411
37	35	2	36	34	2	630.982090	-0.000275
37	35	3	36	34	3	630.982090	-0.000275
37	35	2	36	34	3	630.982090	-0.000275
37	35	3	36	34	2	630.982090	-0.000275
38	24	15	37	23	15	631.003060	-0.000304
38	23	15	37	22	15	631.003060	-0.000303
38	23	16	37	22	16	631.009100	-0.000473
38	22	16	37	21	16	631.009100	-0.000473
38	22	17	37	21	17	631.015040	-0.000071
38	21	17	37	20	17	631.015040	-0.000071
37	36	1	36	35	1	631.017780	0.000077
37	36	2	36	35	2	631.017780	0.000077
37	36	1	36	35	2	631.017780	0.000077
37	36	2	36	35	1	631.017780	0.000077
38	18	20	37	17	20	631.029260	-0.000223
38	19	20	37	18	20	631.029260	-0.000223
38	18	21	37	17	21	631.033870	0.000004
38	17	21	37	16	21	631.033870	0.000004
38	17	22	37	16	22	631.038210	0.000044
38	16	22	37	15	22	631.038210	0.000044
38	16	23	37	15	23	631.043000	0.000591

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
38	15	23	37	14	23	631.043000	0.000591
38	14	25	37	13	25	631.050570	-0.000307
38	13	25	37	12	25	631.050570	-0.000307
37	37	0	36	36	0	631.053220	0.000251
37	37	1	36	36	1	631.053220	0.000251
37	37	0	36	36	1	631.053220	0.000251
37	37	1	36	36	0	631.053220	0.000251
38	11	28	37	10	28	631.064220	0.000322
38	10	28	37	9	28	631.064220	0.000322
38	33	5	37	32	5	631.085420	0.000146
38	33	6	37	32	6	631.085420	0.000038
38	33	5	37	32	6	631.085420	-0.000117
38	33	6	37	32	5	631.085420	0.000301
38	34	4	37	33	4	631.121600	-0.000207
38	34	5	37	33	5	631.121600	-0.000214
38	34	4	37	33	5	631.121600	-0.000223
38	34	5	37	33	4	631.121600	-0.000198
38	35	3	37	34	3	631.157350	-0.000157
38	35	4	37	34	4	631.157350	-0.000157
38	35	3	37	34	4	631.157350	-0.000158
38	35	4	37	34	3	631.157350	-0.000157
38	36	2	37	35	2	631.192590	-0.000205
38	36	3	37	35	3	631.192590	-0.000205
38	36	2	37	35	3	631.192590	-0.000205
38	36	3	37	35	2	631.192590	-0.000205
39	25	15	38	24	15	631.204770	-0.000455
39	24	15	38	23	15	631.204770	-0.000452
39	24	16	38	23	16	631.211560	-0.000221
39	23	16	38	22	16	631.211560	-0.000221
38	37	1	37	36	1	631.227740	-0.000162
38	37	2	37	36	2	631.227740	-0.000162
39	21	19	38	20	19	631.227740	-0.000040
39	20	19	38	19	19	631.227740	-0.000040
38	37	1	37	36	2	631.227740	-0.000162
38	37	2	37	36	1	631.227740	-0.000162
39	19	21	38	18	21	631.236570	-0.000370
39	18	21	38	17	21	631.236570	-0.000370
39	18	22	38	17	22	631.241930	0.000621
39	17	22	38	16	22	631.241930	0.000621
39	17	23	38	16	23	631.246480	0.000853
39	16	23	38	15	23	631.246480	0.000853
39	15	25	38	14	25	631.254110	-0.000081
39	14	25	38	13	25	631.254110	-0.000081
39	33	6	38	32	6	631.259020	0.000322
39	33	7	38	32	7	631.259020	-0.000406
38	38	0	37	37	0	631.262900	-0.000059

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
38	38	1	37	37	1	631.262900	-0.000059
39	13	27	38	12	27	631.262900	0.000046
39	12	27	38	11	27	631.262900	0.000046
38	38	0	37	37	1	631.262900	-0.000059
38	38	1	37	37	0	631.262900	-0.000059
39	34	5	38	33	5	631.296490	0.000051
39	34	6	38	33	6	631.296490	-0.000010
39	34	5	38	33	6	631.296490	-0.000097
39	34	6	38	33	5	631.296490	0.000138
39	35	4	38	34	4	631.332480	-0.000083
39	35	5	38	34	5	631.332480	-0.000087
39	35	4	38	34	5	631.332480	-0.000092
39	35	5	38	34	4	631.332480	-0.000079
39	36	3	38	35	3	631.367940	-0.000014
39	36	4	38	35	4	631.367940	-0.000015
39	36	3	38	35	4	631.367940	-0.000015
39	36	4	38	35	3	631.367940	-0.000014
39	37	2	38	36	2	631.402840	-0.000151
39	37	3	38	36	3	631.402840	-0.000151
39	37	2	38	36	3	631.402840	-0.000151
39	37	3	38	36	2	631.402840	-0.000151
40	26	15	39	25	15	631.406700	-0.000158
40	25	15	39	24	15	631.406700	-0.000151
40	25	16	39	24	16	631.413630	-0.000152
40	24	16	39	23	16	631.413630	-0.000151
40	22	19	39	21	19	631.430450	0.000000
40	21	19	39	20	19	631.430450	0.000000
40	20	20	39	19	20	631.435120	-0.000129
40	21	20	39	20	20	631.435120	-0.000129
39	38	1	38	37	1	631.438080	0.000215
39	38	2	38	37	2	631.438080	0.000215
39	38	1	38	37	2	631.438080	0.000215
39	38	2	38	37	1	631.438080	0.000215
40	20	21	39	19	21	631.439990	0.000143
40	19	21	39	18	21	631.439990	0.000143
40	19	22	39	18	22	631.443960	-0.000357
40	18	22	39	17	22	631.443960	-0.000357
40	18	23	39	17	23	631.448960	0.000263
40	17	23	39	16	23	631.448960	0.000263
40	16	25	39	15	25	631.457170	-0.000194
40	15	25	39	14	25	631.457170	-0.000194
40	14	27	39	13	27	631.466140	0.000052
40	13	27	39	12	27	631.466140	0.000052
40	34	6	39	33	6	631.470420	0.000123
40	34	7	39	33	7	631.470420	-0.000307
40	13	28	39	12	28	631.470420	-0.000098

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
40	12	28	39	11	28	631.470420	-0.000098
39	39	0	38	38	0	631.472850	0.000157
39	39	1	38	38	1	631.472850	0.000157
39	39	0	38	38	1	631.472850	0.000157
39	39	1	38	38	0	631.472850	0.000157
40	11	30	39	10	30	631.479330	-0.000270
40	10	30	39	9	30	631.479330	-0.000270
40	35	5	39	34	5	631.507300	-0.000055
40	35	6	39	34	6	631.507300	-0.000089
40	35	5	39	34	6	631.507300	-0.000137
40	35	6	39	34	5	631.507300	-0.000007
40	36	4	39	35	4	631.543080	-0.000011
40	36	5	39	35	5	631.543080	-0.000013
40	36	4	39	35	5	631.543080	-0.000015
40	36	5	39	35	4	631.543080	-0.000008
40	37	3	39	36	3	631.578130	-0.000050
40	37	4	39	36	4	631.578130	-0.000051
40	37	3	39	36	4	631.578130	-0.000051
40	37	4	39	36	3	631.578130	-0.000050
41	27	15	40	26	15	631.608490	0.000226
41	26	15	40	25	15	631.608490	0.000240
40	38	2	39	37	2	631.612890	-0.000066
40	38	3	39	37	3	631.612890	-0.000066
40	38	2	39	37	3	631.612890	-0.000066
40	38	3	39	37	2	631.612890	-0.000066
41	26	16	40	25	16	631.615390	-0.000190
41	25	16	40	24	16	631.615390	-0.000189
41	23	19	40	22	19	631.632780	-0.000179
41	22	19	40	21	19	631.632780	-0.000179
41	21	20	40	20	20	631.637690	-0.000217
41	22	20	40	21	20	631.637690	-0.000217
41	21	21	40	20	21	631.641870	-0.000748
41	20	21	40	19	21	631.641870	-0.000748
40	39	1	39	38	1	631.647220	-0.000361
40	39	2	39	38	2	631.647220	-0.000361
41	20	22	40	19	22	631.647220	0.000037
41	19	22	40	18	22	631.647220	0.000037
40	39	1	39	38	2	631.647220	-0.000361
40	39	2	39	38	1	631.647220	-0.000361
41	19	23	40	18	23	631.651580	-0.000059
41	18	23	40	17	23	631.651580	-0.000059
41	17	25	40	16	25	631.660410	-0.000002
41	16	25	40	15	25	631.660410	-0.000002
41	16	26	40	15	26	631.664760	-0.000028
41	15	26	40	14	26	631.664760	-0.000028
41	15	27	40	14	27	631.669030	-0.000158

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
41	14	27	40	13	27	631.669030	-0.000158
41	14	28	40	13	28	631.673700	0.000063
41	13	28	40	12	28	631.673700	0.000063
41	13	29	40	12	29	631.678090	-0.000060
41	12	29	40	11	29	631.678090	-0.000060
40	40	0	39	39	0	631.682270	0.000089
40	40	1	39	39	1	631.682270	0.000089
41	12	30	40	11	30	631.682270	-0.000462
41	11	30	40	10	30	631.682270	-0.000462
40	40	0	39	39	1	631.682270	0.000089
40	40	1	39	39	0	631.682270	0.000089
41	36	5	40	35	5	631.718060	0.000023
41	36	6	40	35	6	631.718060	0.000004
41	36	5	40	35	6	631.718060	-0.000023
41	36	6	40	35	5	631.718060	0.000049
41	37	4	40	36	4	631.753270	-0.000115
41	37	5	40	36	5	631.753270	-0.000116
41	37	4	40	36	5	631.753270	-0.000117
41	37	5	40	36	4	631.753270	-0.000113
41	38	3	40	37	3	631.788740	0.000556
41	38	4	40	37	4	631.788740	0.000556
41	38	3	40	37	4	631.788740	0.000556
41	38	4	40	37	3	631.788740	0.000556
42	28	15	41	27	15	631.809500	0.000056
42	27	15	41	26	15	631.809500	0.000082
42	27	16	41	26	16	631.816860	-0.000325
42	26	16	41	25	16	631.816860	-0.000323
41	39	2	40	38	2	631.822810	0.000129
41	39	3	40	38	3	631.822810	0.000129
41	39	2	40	38	3	631.822810	0.000129
41	39	3	40	38	2	631.822810	0.000129
42	24	19	41	23	19	631.835130	-0.000194
42	23	19	41	22	19	631.835130	-0.000194
42	22	20	41	21	20	631.840390	-0.000029
42	23	20	41	22	20	631.840390	-0.000029
42	22	21	41	21	21	631.845030	-0.000229
42	21	21	41	20	21	631.845030	-0.000229
42	21	22	41	20	22	631.849650	-0.000265
42	20	22	41	19	22	631.849650	-0.000265
42	20	23	41	19	23	631.854180	-0.000274
42	19	23	41	18	23	631.854180	-0.000274
42	17	26	41	16	26	631.868000	0.000248
42	16	26	41	15	26	631.868000	0.000248
42	16	27	41	15	27	631.872130	-0.000059
42	15	27	41	14	27	631.872130	-0.000059
42	15	28	41	14	28	631.876630	-0.000019

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
42	14	28	41	13	28	631.876630	-0.000019
42	14	29	41	13	29	631.881190	0.000015
42	13	29	41	12	29	631.881190	0.000015
42	13	30	41	12	30	631.885950	0.000190
42	12	30	41	11	30	631.885950	0.000190
41	41	0	40	40	0	631.891630	0.000196
41	41	1	40	40	1	631.891630	0.000196
41	41	0	40	40	1	631.891630	0.000196
41	41	1	40	40	0	631.891630	0.000196
42	36	6	41	35	6	631.892740	0.000208
42	36	7	41	35	7	631.892740	0.000062
42	36	6	41	35	7	631.892740	-0.000162
42	36	7	41	35	6	631.892740	0.000431
42	37	5	41	36	5	631.928670	0.000185
42	37	6	41	36	6	631.928670	0.000175
42	37	5	41	36	6	631.928670	0.000160
42	37	6	41	36	5	631.928670	0.000200
42	38	4	41	37	4	631.963070	-0.000397
42	38	5	41	37	5	631.963070	-0.000397
42	38	4	41	37	5	631.963070	-0.000398
42	38	5	41	37	4	631.963070	-0.000396
42	39	3	41	38	3	631.998020	0.000058
42	39	4	41	38	4	631.998020	0.000058
42	39	3	41	38	4	631.998020	0.000058
42	39	4	41	38	3	631.998020	0.000058
43	29	15	42	28	15	632.010260	-0.000139
43	28	15	42	27	15	632.010260	-0.000087
43	28	16	42	27	16	632.018340	-0.000262
43	27	16	42	26	16	632.018340	-0.000258
42	40	2	41	39	2	632.031950	-0.000239
42	40	3	41	39	3	632.031950	-0.000239
42	40	2	41	39	3	632.031950	-0.000239
42	40	3	41	39	2	632.031950	-0.000239
43	25	19	42	24	19	632.037320	-0.000217
43	24	19	42	23	19	632.037320	-0.000217
43	23	20	42	22	20	632.042820	0.000024
43	24	20	42	23	20	632.042820	0.000024
43	22	22	42	21	22	632.052250	-0.000275
43	21	22	42	20	22	632.052250	-0.000275
43	21	23	42	20	23	632.056820	-0.000330
43	20	23	42	19	23	632.056820	-0.000330
42	41	1	41	40	1	632.066100	-0.000213
42	41	2	41	40	2	632.066100	-0.000213
43	19	25	42	18	25	632.066100	-0.000052
43	18	25	42	17	25	632.066100	-0.000052
42	41	1	41	40	2	632.066100	-0.000213

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
42	41	2	41	40	1	632.066100	-0.000213
43	18	26	42	17	26	632.070530	-0.000083
43	17	26	42	16	26	632.070530	-0.000083
43	17	27	42	16	27	632.074570	-0.000507
43	16	27	42	15	27	632.074570	-0.000507
43	16	28	42	15	28	632.079620	0.000055
43	15	28	42	14	28	632.079620	0.000055
43	15	29	42	14	29	632.083770	-0.000325
43	14	29	42	13	29	632.083770	-0.000325
43	14	30	42	13	30	632.088280	-0.000415
43	13	30	42	12	30	632.088280	-0.000415
42	42	0	41	41	0	632.100410	-0.000031
42	42	1	41	41	1	632.100410	-0.000031
42	42	0	41	41	1	632.100410	-0.000031
42	42	1	41	41	0	632.100410	-0.000031
43	37	6	42	36	6	632.103100	-0.000139
43	37	7	42	36	7	632.103100	-0.000223
43	37	6	42	36	7	632.103100	-0.000350
43	37	7	42	36	6	632.103100	-0.000012
43	38	5	42	37	5	632.138880	0.000172
43	38	6	42	37	6	632.138880	0.000167
43	38	5	42	37	6	632.138880	0.000159
43	38	6	42	37	5	632.138880	0.000180
43	39	4	42	38	4	632.173020	-0.000320
43	39	5	42	38	5	632.173020	-0.000320
43	39	4	42	38	5	632.173020	-0.000321
43	39	5	42	38	4	632.173020	-0.000320
43	40	3	42	39	3	632.207100	-0.000421
43	40	4	42	39	4	632.207100	-0.000421
43	40	3	42	39	4	632.207100	-0.000421
43	40	4	42	39	3	632.207100	-0.000421
44	30	15	43	29	15	632.211230	0.000104
44	29	15	43	28	15	632.211230	0.000201
44	29	16	43	28	16	632.219700	-0.000122
44	28	16	43	27	16	632.219700	-0.000114
44	26	19	43	25	19	632.239830	0.000205
44	25	19	43	24	19	632.239830	0.000205
43	41	2	42	40	2	632.241300	-0.000171
43	41	3	42	40	3	632.241300	-0.000171
43	41	2	42	40	3	632.241300	-0.000171
43	41	3	42	40	2	632.241300	-0.000171
44	24	20	43	23	20	632.244940	-0.000113
44	25	20	43	24	20	632.244940	-0.000113
44	24	21	43	23	21	632.249310	-0.000843
44	23	21	43	22	21	632.249310	-0.000843
44	23	22	43	22	22	632.254880	-0.000144

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
44	22	22	43	21	22	632.254880	-0.000144
44	22	23	43	21	23	632.259620	-0.000114
44	21	23	43	20	23	632.259620	-0.000114
44	20	25	43	19	25	632.268970	0.000096
44	19	25	43	18	25	632.268970	0.000096
44	19	26	43	18	26	632.273780	0.000408
44	18	26	43	17	26	632.273780	0.000408
43	42	1	42	41	1	632.275400	0.000057
43	42	2	42	41	2	632.275400	0.000057
43	42	1	42	41	2	632.275400	0.000057
43	42	2	42	41	1	632.275400	0.000057
44	18	27	43	17	27	632.277730	-0.000133
44	17	27	43	16	27	632.277730	-0.000133
44	17	28	43	16	28	632.282120	-0.000257
44	16	28	43	15	28	632.282120	-0.000257
44	16	29	43	15	29	632.286710	-0.000221
44	15	29	43	14	29	632.286710	-0.000221
43	43	0	42	42	0	632.309200	-0.000025
43	43	1	42	42	1	632.309200	-0.000025
43	43	0	42	42	1	632.309200	-0.000025
43	43	1	42	42	0	632.309200	-0.000025
44	38	6	43	37	6	632.313340	-0.000365
44	38	7	43	37	7	632.313340	-0.000412
44	38	6	43	37	7	632.313340	-0.000484
44	38	7	43	37	6	632.313340	-0.000293
44	39	5	43	38	5	632.348820	0.000106
44	39	6	43	38	6	632.348820	0.000102
44	39	5	43	38	6	632.348820	0.000098
44	39	6	43	38	5	632.348820	0.000110
44	40	4	43	39	4	632.383100	0.000102
44	40	5	43	39	5	632.383100	0.000102
44	40	4	43	39	5	632.383100	0.000102
44	40	5	43	39	4	632.383100	0.000102
45	31	15	44	30	15	632.411250	-0.000392
45	30	15	44	29	15	632.411250	-0.000214
45	30	16	44	29	16	632.420870	0.000006
45	29	16	44	28	16	632.420870	0.000022
45	27	19	44	26	19	632.441650	0.000078
45	26	19	44	25	19	632.441650	0.000078
45	25	20	44	24	20	632.447000	-0.000183
45	26	20	44	25	20	632.447000	-0.000183
44	42	2	43	41	2	632.450460	-0.000079
44	42	3	43	41	3	632.450460	-0.000079
44	42	2	43	41	3	632.450460	-0.000079
44	42	3	43	41	2	632.450460	-0.000079
45	25	21	44	24	21	632.451950	-0.000479

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
45	24	21	44	23	21	632.451950	-0.000479
45	24	22	44	23	22	632.457330	-0.000086
45	23	22	44	22	22	632.457330	-0.000086
45	23	23	44	22	23	632.462230	0.000004
45	22	23	44	21	23	632.462230	0.000004
45	21	25	44	20	25	632.471230	-0.000263
45	20	25	44	19	25	632.471230	-0.000263
45	20	26	44	19	26	632.475930	-0.000111
45	19	26	44	18	26	632.475930	-0.000111
45	19	27	44	18	27	632.480120	-0.000451
45	18	27	44	17	27	632.480120	-0.000451
44	43	1	43	42	1	632.484520	0.000370
44	43	2	43	42	2	632.484520	0.000370
44	43	1	43	42	2	632.484520	0.000370
44	43	2	43	42	1	632.484520	0.000370
45	17	29	44	16	29	632.489100	-0.000571
45	16	29	44	15	29	632.489100	-0.000571
45	16	30	44	15	30	632.494000	-0.000285
45	15	30	44	14	30	632.494000	-0.000285
44	44	0	43	43	0	632.517870	0.000086
44	44	1	43	43	1	632.517870	0.000086
44	44	0	43	43	1	632.517870	0.000086
44	44	1	43	43	0	632.517870	0.000086
45	39	6	44	38	6	632.523780	-0.000165
45	39	7	44	38	7	632.523780	-0.000192
45	39	6	44	38	7	632.523780	-0.000232
45	39	7	44	38	6	632.523780	-0.000125
45	40	5	44	39	5	632.558650	0.000125
45	40	6	44	39	6	632.558650	0.000124
45	40	5	44	39	6	632.558650	0.000121
45	40	6	44	39	5	632.558650	0.000128
45	41	4	44	40	4	632.592550	0.000103
45	41	5	44	40	5	632.592550	0.000103
45	41	4	44	40	5	632.592550	0.000103
45	41	5	44	40	4	632.592550	0.000103
46	32	15	45	31	15	632.611920	-0.000032
46	31	15	45	30	15	632.611920	0.000290
46	31	16	45	30	16	632.621310	-0.000403
46	30	16	45	29	16	632.621310	-0.000372
45	42	3	44	41	3	632.625690	-0.000325
45	42	4	44	41	4	632.625690	-0.000325
45	42	3	44	41	4	632.625690	-0.000325
45	42	4	44	41	3	632.625690	-0.000325
46	28	19	45	27	19	632.643220	-0.000190
46	27	19	45	26	19	632.643220	-0.000190
46	26	20	45	25	20	632.649250	0.000046

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
46	27	20	45	26	20	632.649250	0.000046
46	26	21	45	25	21	632.654410	-0.000192
46	25	21	45	24	21	632.654410	-0.000192
45	43	2	44	42	2	632.659490	0.000091
45	43	3	44	42	3	632.659490	0.000091
46	25	22	45	24	22	632.659490	-0.000224
46	24	22	45	23	22	632.659490	-0.000224
45	43	2	44	42	3	632.659490	0.000091
45	43	3	44	42	2	632.659490	0.000091
46	24	23	45	23	23	632.664500	-0.000114
46	23	23	45	22	23	632.664500	-0.000114
46	22	25	45	21	25	632.673750	-0.000274
46	21	25	45	20	25	632.673750	-0.000274
46	21	26	45	20	26	632.678400	-0.000228
46	20	26	45	19	26	632.678400	-0.000228
46	20	27	45	19	27	632.683500	0.000310
46	19	27	45	18	27	632.683500	0.000310
46	19	28	45	18	28	632.687910	0.000147
46	18	28	45	17	28	632.687910	0.000147
45	44	1	44	43	1	632.692380	-0.000356
45	44	2	44	43	2	632.692380	-0.000356
46	18	29	45	17	29	632.692380	0.000035
46	17	29	45	16	29	632.692380	0.000035
45	44	1	44	43	2	632.692380	-0.000356
45	44	2	44	43	1	632.692380	-0.000356
46	17	30	45	16	30	632.696640	-0.000329
46	16	30	45	15	30	632.696640	-0.000329
46	39	7	45	38	7	632.698880	0.000156
46	39	8	45	38	8	632.698880	-0.000032
46	15	32	45	14	32	632.706340	-0.000056
46	14	32	45	13	32	632.706340	-0.000056
45	45	0	44	44	0	632.726240	0.000125
45	45	1	44	44	1	632.726240	0.000125
45	45	0	44	44	1	632.726240	0.000125
45	45	1	44	44	0	632.726240	0.000125
46	40	6	45	39	6	632.733990	0.000019
46	40	7	45	39	7	632.733990	0.000004
46	40	6	45	39	7	632.733990	-0.000018
46	40	7	45	39	6	632.733990	0.000042
46	41	5	45	40	5	632.768040	-0.000088
46	41	6	45	40	6	632.768040	-0.000089
46	41	5	45	40	6	632.768040	-0.000090
46	41	6	45	40	5	632.768040	-0.000087
46	42	4	45	41	4	632.801650	-0.000042
46	42	5	45	41	5	632.801650	-0.000042
46	42	4	45	41	5	632.801650	-0.000042

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
46	42	5	45	41	4	632.801650	-0.000042
47	33	15	46	32	15	632.811730	-0.000319
47	32	15	46	31	15	632.811730	0.000247
47	32	16	46	31	16	632.822450	0.000065
47	31	16	46	30	16	632.822450	0.000124
46	43	3	45	42	3	632.834820	-0.000134
46	43	4	45	42	4	632.834820	-0.000134
46	43	3	45	42	4	632.834820	-0.000134
46	43	4	45	42	3	632.834820	-0.000134
47	29	19	46	28	19	632.845470	0.000348
47	28	19	46	27	19	632.845470	0.000348
47	27	20	46	26	20	632.850970	-0.000154
47	28	20	46	27	20	632.850970	-0.000154
47	27	21	46	26	21	632.856620	-0.000064
47	26	21	46	25	21	632.856620	-0.000064
47	26	22	46	25	22	632.861710	-0.000213
47	25	22	46	24	22	632.861710	-0.000213
47	25	23	46	24	23	632.866970	0.000048
47	24	23	46	23	23	632.866970	0.000048
46	44	2	45	43	2	632.868130	0.000077
46	44	3	45	43	3	632.868130	0.000077
46	44	2	45	43	3	632.868130	0.000077
46	44	3	45	43	2	632.868130	0.000077
47	23	25	46	22	25	632.876380	-0.000101
47	22	25	46	21	25	632.876380	-0.000101
47	22	26	46	21	26	632.881010	-0.000120
47	21	26	46	20	26	632.881010	-0.000120
47	21	27	46	20	27	632.885530	-0.000211
47	20	27	46	19	27	632.885530	-0.000211
47	19	29	46	18	29	632.894930	-0.000023
47	18	29	46	17	29	632.894930	-0.000023
47	18	30	46	17	30	632.899280	-0.000311
47	17	30	46	16	30	632.899280	-0.000311
46	45	1	45	44	1	632.900950	-0.000167
46	45	2	45	44	2	632.900950	-0.000167
46	45	1	45	44	2	632.900950	-0.000167
46	45	2	45	44	1	632.900950	-0.000167
47	40	7	46	39	7	632.909180	0.000091
47	40	8	46	39	8	632.909180	-0.000018
47	16	32	46	15	32	632.909180	0.000165
47	15	32	46	14	32	632.909180	0.000165
46	46	0	45	45	0	632.934290	0.000065
46	46	1	45	45	1	632.934290	0.000065
46	46	0	45	45	1	632.934290	0.000065
46	46	1	45	45	0	632.934290	0.000065
47	41	6	46	40	6	632.944030	0.000249

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
47	41	7	46	40	7	632.944030	0.000241
47	41	6	46	40	7	632.944030	0.000229
47	41	7	46	40	6	632.944030	0.000262
47	42	5	46	41	5	632.977460	-0.000065
47	42	6	46	41	6	632.977460	-0.000065
47	42	5	46	41	6	632.977460	-0.000066
47	42	6	46	41	5	632.977460	-0.000064
47	43	4	46	42	4	633.010760	0.000004
47	43	5	46	42	5	633.010760	0.000004
47	43	4	46	42	5	633.010760	0.000004
47	43	5	46	42	4	633.010760	0.000004
48	34	15	47	33	15	633.012270	0.000302
48	33	16	47	32	16	633.022770	-0.000114
48	32	16	47	31	16	633.022770	-0.000006
47	44	3	46	43	3	633.043360	-0.000332
47	44	4	46	43	4	633.043360	-0.000332
47	44	3	46	43	4	633.043360	-0.000332
47	44	4	46	43	3	633.043360	-0.000332
48	30	19	47	29	19	633.046410	-0.000320
48	29	19	47	28	19	633.046410	-0.000320
48	28	20	47	27	20	633.053300	0.000362
48	29	20	47	28	20	633.053300	0.000362
48	28	21	47	27	21	633.058130	-0.000540
48	27	21	47	26	21	633.058130	-0.000540
48	27	22	47	26	22	633.063950	-0.000087
48	26	22	47	25	22	633.063950	-0.000087
48	26	23	47	25	23	633.069060	-0.000092
48	25	23	47	24	23	633.069060	-0.000092
47	45	2	46	44	2	633.076170	-0.000331
47	45	3	46	44	3	633.076170	-0.000331
47	45	2	46	44	3	633.076170	-0.000331
47	45	3	46	44	2	633.076170	-0.000331
48	24	25	47	23	25	633.079070	0.000203
48	23	25	47	22	25	633.079070	0.000203
48	23	26	47	22	26	633.083270	-0.000306
48	22	26	47	21	26	633.083270	-0.000306
48	22	27	47	21	27	633.088480	0.000255
48	21	27	47	20	27	633.088480	0.000255
48	21	28	47	20	28	633.093010	0.000148
48	20	28	47	19	28	633.093010	0.000148
48	20	29	47	19	29	633.097250	-0.000238
48	19	29	47	18	29	633.097250	-0.000238
48	19	30	47	18	30	633.102220	0.000080
48	18	30	47	17	30	633.102220	0.000080
47	46	1	46	45	1	633.109200	-0.000079
47	46	2	46	45	2	633.109200	-0.000079

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
47	46	1	46	45	2	633.109200	-0.000079
47	46	2	46	45	1	633.109200	-0.000079
48	17	32	47	16	32	633.111660	0.000074
48	16	32	47	15	32	633.111660	0.000074
47	47	0	46	46	0	633.141940	-0.000185
47	47	1	46	46	1	633.141940	-0.000185
47	47	0	46	46	1	633.141940	-0.000185
47	47	1	46	46	0	633.141940	-0.000185
48	42	6	47	41	6	633.153190	-0.000209
48	42	7	47	41	7	633.153190	-0.000213
48	42	6	47	41	7	633.153190	-0.000220
48	42	7	47	41	6	633.153190	-0.000202
48	43	5	47	42	5	633.186680	-0.000063
48	43	6	47	42	6	633.186680	-0.000063
48	43	5	47	42	6	633.186680	-0.000063
48	43	6	47	42	5	633.186680	-0.000062
49	35	15	48	34	15	633.211850	0.000136
48	44	4	47	43	4	633.219590	-0.000026
48	44	5	47	43	5	633.219590	-0.000026
48	44	4	47	43	5	633.219590	-0.000026
48	44	5	47	43	4	633.219590	-0.000026
49	34	16	48	33	16	633.223540	0.000344
49	33	16	48	32	16	633.223540	0.000539
49	31	19	48	30	19	633.247990	-0.000231
49	30	19	48	29	19	633.247990	-0.000231
48	45	3	47	44	3	633.251900	-0.000341
48	45	4	47	44	4	633.251900	-0.000341
48	45	3	47	44	4	633.251900	-0.000341
48	45	4	47	44	3	633.251900	-0.000341
49	29	20	48	28	20	633.254550	-0.000115
49	30	20	48	29	20	633.254550	-0.000115
49	29	21	48	28	21	633.260300	-0.000260
49	28	21	48	27	21	633.260300	-0.000260
49	28	22	48	27	22	633.265980	-0.000101
49	27	22	48	26	22	633.265980	-0.000101
49	27	23	48	26	23	633.271170	-0.000130
49	26	23	48	25	23	633.271170	-0.000130
49	25	25	48	24	25	633.281070	-0.000123
49	24	25	48	23	25	633.281070	-0.000123
48	46	2	47	45	2	633.284630	-0.000112
48	46	3	47	45	3	633.284630	-0.000112
48	46	2	47	45	3	633.284630	-0.000112
48	46	3	47	45	2	633.284630	-0.000112
49	24	26	48	23	26	633.286530	0.000571
49	23	26	48	22	26	633.286530	0.000571
49	23	27	48	22	27	633.290800	0.000148

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
49	22	27	48	21	27	633.290800	0.000148
49	22	28	48	21	28	633.294930	-0.000396
49	21	28	48	20	28	633.294930	-0.000396
49	21	29	48	20	29	633.300240	0.000265
49	20	29	48	19	29	633.300240	0.000265
49	20	30	48	19	30	633.304750	0.000096
49	19	30	48	18	30	633.304750	0.000096
49	19	31	48	18	31	633.309000	-0.000348
49	18	31	48	17	31	633.309000	-0.000348
49	18	32	48	17	32	633.313910	-0.000189
49	17	32	48	16	32	633.313910	-0.000189
48	47	1	47	46	1	633.317360	0.000117
48	47	2	47	46	2	633.317360	0.000117
48	47	1	47	46	2	633.317360	0.000117
48	47	2	47	46	1	633.317360	0.000117
49	42	7	48	41	7	633.328850	-0.000289
49	42	8	48	41	8	633.328850	-0.000325
49	42	7	48	41	8	633.328850	-0.000383
49	42	8	48	41	7	633.328850	-0.000231
48	48	0	47	47	0	633.349220	-0.000593
48	48	1	47	47	1	633.349220	-0.000593
48	48	0	47	47	1	633.349220	-0.000593
48	48	1	47	47	0	633.349220	-0.000593
49	43	6	48	42	6	633.362850	0.000034
49	43	7	48	42	7	633.362850	0.000032
49	43	6	48	42	7	633.362850	0.000028
49	43	7	48	42	6	633.362850	0.000038
49	44	5	48	43	5	633.395590	-0.000173
49	44	6	48	43	6	633.395590	-0.000173
49	44	5	48	43	6	633.395590	-0.000174
49	44	6	48	43	5	633.395590	-0.000173
50	36	15	49	35	15	633.411740	0.000393
50	35	16	49	34	16	633.424040	0.000696
49	45	4	48	44	4	633.428230	-0.000059
49	45	5	48	44	5	633.428230	-0.000059
49	45	4	48	44	5	633.428230	-0.000059
49	45	5	48	44	4	633.428230	-0.000059
50	32	19	49	31	19	633.449740	0.000124
50	31	19	49	30	19	633.449740	0.000124
50	30	20	49	29	20	633.456230	-0.000067
50	31	20	49	30	20	633.456230	-0.000067
49	46	3	48	45	3	633.460590	-0.000005
49	46	4	48	45	4	633.460590	-0.000005
49	46	3	48	45	4	633.460590	-0.000005
49	46	4	48	45	3	633.460590	-0.000005
50	30	21	49	29	21	633.462210	-0.000173

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
50	29	21	49	28	21	633.462210	-0.000173
50	29	22	49	28	22	633.467510	-0.000539
50	28	22	49	27	22	633.467510	-0.000539
50	28	23	49	27	23	633.473570	0.000176
50	27	23	49	26	23	633.473570	0.000176
50	26	25	49	25	25	633.483960	0.000507
50	25	25	49	24	25	633.483960	0.000507
50	25	26	49	24	26	633.488390	0.000107
50	24	26	49	23	26	633.488390	0.000107
49	47	2	48	46	2	633.492840	0.000041
49	47	3	48	46	3	633.492840	0.000041
50	24	27	49	23	27	633.492840	-0.000187
50	23	27	49	22	27	633.492840	-0.000187
49	47	2	48	46	3	633.492840	0.000041
49	47	3	48	46	2	633.492840	0.000041
50	23	28	49	22	28	633.498250	0.000513
50	22	28	49	21	28	633.498250	0.000513
50	22	29	49	21	29	633.502490	0.000075
50	21	29	49	20	29	633.502490	0.000075
50	21	30	49	20	30	633.506530	-0.000576
50	20	30	49	19	30	633.506530	-0.000576
50	20	31	49	19	31	633.511740	-0.000083
50	19	31	49	18	31	633.511740	-0.000083
50	19	32	49	18	32	633.516600	0.000023
50	18	32	49	17	32	633.516600	0.000023
49	48	1	48	47	1	633.525050	0.000039
49	48	2	48	47	2	633.525050	0.000039
49	48	1	48	47	2	633.525050	0.000039
49	48	2	48	47	1	633.525050	0.000039
50	43	7	49	42	7	633.538950	0.000105
50	43	8	49	42	8	633.538950	0.000085
50	43	7	49	42	8	633.538950	0.000052
50	43	8	49	42	7	633.538950	0.000138
49	49	0	48	48	0	633.557060	-0.000231
49	49	1	48	48	1	633.557060	-0.000231
49	49	0	48	48	1	633.557060	-0.000231
49	49	1	48	48	0	633.557060	-0.000231
50	44	6	49	43	6	633.572110	0.000055
50	44	7	49	43	7	633.572110	0.000053
50	44	6	49	43	7	633.572110	0.000051
50	44	7	49	43	6	633.572110	0.000057
50	45	5	49	44	5	633.604740	0.000130
50	45	6	49	44	6	633.604740	0.000130
50	45	5	49	44	6	633.604740	0.000130
50	45	6	49	44	5	633.604740	0.000130
51	37	15	50	36	15	633.611200	0.000285

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
51	36	16	50	35	16	633.623600	0.000276
50	46	4	49	45	4	633.636580	-0.000205
50	46	5	49	45	5	633.636580	-0.000205
50	46	4	49	45	5	633.636580	-0.000205
50	46	5	49	45	4	633.636580	-0.000205
51	33	19	50	32	19	633.650670	-0.000246
51	32	19	50	31	19	633.650670	-0.000245
51	31	20	50	30	20	633.657840	0.000002
51	32	20	50	31	20	633.657840	0.000002
51	31	21	50	30	21	633.664530	0.000402
51	30	21	50	29	21	633.664530	0.000402
50	47	3	49	46	3	633.668440	-0.000320
50	47	4	49	46	4	633.668440	-0.000320
50	47	3	49	46	4	633.668440	-0.000320
50	47	4	49	46	3	633.668440	-0.000320
51	30	22	50	29	22	633.669760	-0.000179
51	29	22	50	28	22	633.669760	-0.000179
51	29	23	50	28	23	633.675120	-0.000296
51	28	23	50	27	23	633.675120	-0.000296
51	27	25	50	26	25	633.685730	0.000069
51	26	25	50	25	25	633.685730	0.000069
51	26	26	50	25	26	633.690810	0.000261
51	25	26	50	24	26	633.690810	0.000261
51	25	27	50	24	27	633.695410	0.000056
51	24	27	50	23	27	633.695410	0.000056
50	48	2	49	47	2	633.700340	-0.000324
50	48	3	49	47	3	633.700340	-0.000324
51	24	28	50	23	28	633.700340	0.000240
51	23	28	50	22	28	633.700340	0.000240
50	48	2	49	47	3	633.700340	-0.000324
50	48	3	49	47	2	633.700340	-0.000324
51	23	29	50	22	29	633.704660	-0.000153
51	22	29	50	21	29	633.704660	-0.000153
51	22	30	50	21	30	633.709750	0.000218
51	21	30	50	20	30	633.709750	0.000218
51	21	31	50	20	31	633.714490	0.000235
51	20	31	50	19	31	633.714490	0.000235
51	43	8	50	42	8	633.715000	0.000448
51	43	9	50	42	9	633.715000	0.000310
51	20	32	50	19	32	633.718950	-0.000062
51	19	32	50	18	32	633.718950	-0.000062
51	19	33	50	18	33	633.724050	0.000225
51	18	33	50	17	33	633.724050	0.000225
50	49	1	49	48	1	633.732540	-0.000033
50	49	2	49	48	2	633.732540	-0.000033
50	49	1	49	48	2	633.732540	-0.000033

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
50	49	2	49	48	1	633.732540	-0.000033
51	44	7	50	43	7	633.748550	0.000200
51	44	8	50	43	8	633.748550	0.000189
51	44	7	50	43	8	633.748550	0.000170
51	44	8	50	43	7	633.748550	0.000219
50	50	0	49	49	0	633.764330	-0.000244
50	50	1	49	49	1	633.764330	-0.000244
50	50	0	49	49	1	633.764330	-0.000244
50	50	1	49	49	0	633.764330	-0.000244
51	45	6	50	44	6	633.781270	0.000167
51	45	7	50	44	7	633.781270	0.000167
51	45	6	50	44	7	633.781270	0.000165
51	45	7	50	44	6	633.781270	0.000168
52	38	15	51	37	15	633.810860	0.000361
51	46	5	50	45	5	633.813100	-0.000170
51	46	6	50	45	6	633.813100	-0.000170
51	46	5	50	45	6	633.813100	-0.000170
51	46	6	50	45	5	633.813100	-0.000170
52	37	16	51	36	16	633.823500	0.000357
51	47	4	50	46	4	633.844970	-0.000127
51	47	5	50	46	5	633.844970	-0.000127
51	47	4	50	46	5	633.844970	-0.000127
51	47	5	50	46	4	633.844970	-0.000127
52	34	19	51	33	19	633.852110	0.000001
52	33	19	51	32	19	633.852110	0.000001
52	32	20	51	31	20	633.859220	-0.000077
52	33	20	51	32	20	633.859220	-0.000077
52	32	21	51	31	21	633.866240	0.000450
52	31	21	51	30	21	633.866240	0.000450
52	31	22	51	30	22	633.871610	-0.000165
52	30	22	51	29	22	633.871610	-0.000165
51	48	3	50	47	3	633.876860	0.000109
51	48	4	50	47	4	633.876860	0.000109
51	48	3	50	47	4	633.876860	0.000109
51	48	4	50	47	3	633.876860	0.000109
52	28	25	51	27	25	633.887910	0.000094
52	27	25	51	26	25	633.887910	0.000094
52	27	26	51	26	26	633.893220	0.000434
52	26	26	51	25	26	633.893220	0.000434
52	26	27	51	25	27	633.897970	0.000329
52	25	27	51	24	27	633.897970	0.000329
52	25	28	51	24	28	633.902380	-0.000045
52	24	28	51	23	28	633.902380	-0.000045
51	49	2	50	48	2	633.908240	-0.000097
51	49	3	50	48	3	633.908240	-0.000097
51	49	2	50	48	3	633.908240	-0.000097

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
51	49	3	50	48	2	633.908240	-0.000097
52	23	30	51	22	30	633.911790	-0.000118
52	22	30	51	21	30	633.911790	-0.000118
52	22	31	51	21	31	633.916370	-0.000281
52	21	31	51	20	31	633.916370	-0.000281
52	21	32	51	20	32	633.921640	0.000219
52	20	32	51	19	32	633.921640	0.000219
52	20	33	51	19	33	633.926480	0.000245
52	19	33	51	18	33	633.926480	0.000245
51	50	1	50	49	1	633.940470	0.000517
51	50	2	50	49	2	633.940470	0.000517
51	50	1	50	49	2	633.940470	0.000517
51	50	2	50	49	1	633.940470	0.000517
52	45	7	51	44	7	633.957860	0.000185
52	45	8	51	44	8	633.957860	0.000179
52	45	7	51	44	8	633.957860	0.000168
52	45	8	51	44	7	633.957860	0.000195
51	51	0	50	50	0	633.971760	0.000096
51	51	1	50	50	1	633.971760	0.000096
51	51	0	50	50	1	633.971760	0.000096
51	51	1	50	50	0	633.971760	0.000096
52	46	6	51	45	6	633.990120	0.000135
52	46	7	51	45	7	633.990120	0.000135
52	46	6	51	45	7	633.990120	0.000134
52	46	7	51	45	6	633.990120	0.000136
53	39	15	52	38	15	634.010230	0.000026
52	47	5	51	46	5	634.021680	-0.000084
52	47	6	51	46	6	634.021680	-0.000084
52	47	5	51	46	6	634.021680	-0.000085
52	47	6	51	46	5	634.021680	-0.000084
52	48	4	51	47	4	634.053250	0.000016
52	48	5	51	47	5	634.053250	0.000016
53	35	19	52	34	19	634.053250	0.000039
53	34	19	52	33	19	634.053250	0.000041
52	48	4	51	47	5	634.053250	0.000016
52	48	5	51	47	4	634.053250	0.000016
53	33	20	52	32	20	634.060650	-0.000038
53	34	20	52	33	20	634.060650	-0.000038
53	33	21	52	32	21	634.067450	0.000050
53	32	21	52	31	21	634.067450	0.000050
53	32	22	52	31	22	634.073460	-0.000087
53	31	22	52	30	22	634.073460	-0.000087
53	31	23	52	30	23	634.079160	-0.000134
53	30	23	52	29	23	634.079160	-0.000134
52	49	3	51	48	3	634.084700	0.000140
52	49	4	51	48	4	634.084700	0.000140

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
52	49	3	51	48	4	634.084700	0.000140
52	49	4	51	48	3	634.084700	0.000140
53	28	26	52	27	26	634.095010	0.000036
53	27	26	52	26	26	634.095010	0.000036
53	27	27	52	26	27	634.099800	-0.000084
53	26	27	52	25	27	634.099800	-0.000084
53	26	28	52	25	28	634.105160	0.000443
53	25	28	52	24	28	634.105160	0.000443
53	25	29	52	24	29	634.109580	0.000078
53	24	29	52	23	29	634.109580	0.000078
53	24	30	52	23	30	634.114280	0.000018
53	23	30	52	22	30	634.114280	0.000018
52	50	2	51	49	2	634.115710	-0.000121
52	50	3	51	49	3	634.115710	-0.000121
52	50	2	51	49	3	634.115710	-0.000121
52	50	3	51	49	2	634.115710	-0.000121
53	23	31	52	22	31	634.119200	0.000174
53	22	31	52	21	31	634.119200	0.000174
53	22	32	52	21	32	634.123990	0.000180
53	21	32	52	20	32	634.123990	0.000180
53	21	33	52	20	33	634.128650	0.000034
53	20	33	52	19	33	634.128650	0.000034
53	45	8	52	44	8	634.134090	-0.000027
53	45	9	52	44	9	634.134090	-0.000073
53	45	8	52	44	9	634.134090	-0.000153
53	45	9	52	44	8	634.134090	0.000054
52	51	1	51	50	1	634.147150	0.000013
52	51	2	51	50	2	634.147150	0.000013
52	51	1	51	50	2	634.147150	0.000013
52	51	2	51	50	1	634.147150	0.000013
53	46	7	52	45	7	634.167030	0.000220
53	46	8	52	45	8	634.167030	0.000217
53	46	7	52	45	8	634.167030	0.000211
53	46	8	52	45	7	634.167030	0.000226
52	52	0	51	51	0	634.178490	-0.000070
52	52	1	51	51	1	634.178490	-0.000070
52	52	0	51	51	1	634.178490	-0.000070
52	52	1	51	51	0	634.178490	-0.000070
53	47	6	52	46	6	634.198890	0.000211
53	47	7	52	46	7	634.198890	0.000211
53	47	6	52	46	7	634.198890	0.000210
53	47	7	52	46	6	634.198890	0.000211
54	40	15	53	39	15	634.209730	-0.000419
53	48	5	52	47	5	634.230090	0.000009
53	48	6	52	47	6	634.230090	0.000009
53	48	5	52	47	6	634.230090	0.000009

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
53	48	6	52	47	5	634.230090	0.000009
54	36	19	53	35	19	634.254310	0.000091
54	35	19	53	34	19	634.254310	0.000094
53	49	4	52	48	4	634.261040	-0.000156
53	49	5	52	48	5	634.261040	-0.000156
53	49	4	52	48	5	634.261040	-0.000156
53	49	5	52	48	4	634.261040	-0.000156
54	34	20	53	33	20	634.262210	0.000219
54	35	20	53	34	20	634.262210	0.000219
54	34	21	53	33	21	634.269090	0.000161
54	33	21	53	32	21	634.269090	0.000161
54	33	22	53	32	22	634.275440	0.000176
54	32	22	53	31	22	634.275440	0.000176
54	32	23	53	31	23	634.281410	0.000258
54	31	23	53	30	23	634.281410	0.000258
53	50	3	52	49	3	634.292310	0.000119
53	50	4	52	49	4	634.292310	0.000119
54	30	25	53	29	25	634.292310	0.000302
54	29	25	53	28	25	634.292310	0.000302
53	50	3	52	49	4	634.292310	0.000119
53	50	4	52	49	3	634.292310	0.000119
54	29	26	53	28	26	634.296880	-0.000236
54	28	26	53	27	26	634.296880	-0.000236
54	28	27	53	27	27	634.302810	0.000713
54	27	27	53	26	27	634.302810	0.000713
54	27	28	53	26	28	634.307440	0.000457
54	26	28	53	25	28	634.307440	0.000457
54	26	29	53	25	29	634.311860	0.000057
54	25	29	53	24	29	634.311860	0.000057
54	25	30	53	24	30	634.316770	0.000171
54	24	30	53	23	30	634.316770	0.000171
54	24	31	53	23	31	634.321640	0.000260
54	23	31	53	22	31	634.321640	0.000260
53	51	2	52	50	2	634.323100	-0.000040
53	51	3	52	50	3	634.323100	-0.000040
53	51	2	52	50	3	634.323100	-0.000040
53	51	3	52	50	2	634.323100	-0.000040
54	23	32	53	22	32	634.326460	0.000293
54	22	32	53	21	32	634.326460	0.000293
54	22	33	53	21	33	634.331220	0.000235
54	21	33	53	20	33	634.331220	0.000235
54	46	8	53	45	8	634.343600	0.000009
54	46	9	53	45	9	634.343600	-0.000018
54	46	8	53	45	9	634.343600	-0.000064
54	46	9	53	45	8	634.343600	0.000055
53	52	1	52	51	1	634.354110	-0.000031

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
53	52	2	52	51	2	634.354110	-0.000031
53	52	1	52	51	2	634.354110	-0.000031
53	52	2	52	51	1	634.354110	-0.000031
54	47	7	53	46	7	634.375910	0.000149
54	47	8	53	46	8	634.375910	0.000147
54	47	7	53	46	8	634.375910	0.000143
54	47	8	53	46	7	634.375910	0.000152
53	53	0	52	52	0	634.385090	-0.000169
53	53	1	52	52	1	634.385090	-0.000169
53	53	0	52	52	1	634.385090	-0.000169
53	53	1	52	52	0	634.385090	-0.000169
54	48	6	53	47	6	634.407500	0.000284
54	48	7	53	47	7	634.407500	0.000284
54	48	6	53	47	7	634.407500	0.000284
54	48	7	53	47	6	634.407500	0.000284
54	49	5	53	48	5	634.438140	-0.000087
54	49	6	53	48	6	634.438140	-0.000087
54	49	5	53	48	6	634.438140	-0.000087
54	49	6	53	48	5	634.438140	-0.000087
55	37	19	54	36	19	634.455310	0.000181
55	36	19	54	35	19	634.455310	0.000188
55	35	20	54	34	20	634.463250	0.000036
55	36	20	54	35	20	634.463250	0.000035
54	50	4	53	49	4	634.468960	-0.000030
54	50	5	53	49	5	634.468960	-0.000030
54	50	4	53	49	5	634.468960	-0.000030
54	50	5	53	49	4	634.468960	-0.000030
55	35	21	54	34	21	634.470400	0.000005
55	34	21	54	33	21	634.470400	0.000005
55	34	22	54	33	22	634.476950	0.000027
55	33	22	54	32	22	634.476950	0.000027
55	33	23	54	32	23	634.483100	0.000137
55	32	23	54	31	23	634.483100	0.000137
55	31	25	54	30	25	634.494700	0.000663
55	30	25	54	29	25	634.494700	0.000663
55	30	26	54	29	26	634.499270	0.000033
55	29	26	54	28	26	634.499270	0.000033
55	29	27	54	28	27	634.504240	-0.000038
55	28	27	54	27	27	634.504240	-0.000038
55	28	28	54	27	28	634.509380	0.000163
55	27	28	54	26	28	634.509380	0.000163
55	27	29	54	26	29	634.514350	0.000271
55	26	29	54	25	29	634.514350	0.000271
55	26	30	54	25	30	634.519040	0.000134
55	25	30	54	24	30	634.519040	0.000134
55	25	31	54	24	31	634.524010	0.000308

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
55	24	31	54	23	31	634.524010	0.000308
55	24	32	54	23	32	634.528680	0.000170
55	23	32	54	22	32	634.528680	0.000170
54	52	2	53	51	2	634.530110	-0.000164
54	52	3	53	51	3	634.530110	-0.000164
54	52	2	53	51	3	634.530110	-0.000164
54	52	3	53	51	2	634.530110	-0.000164
55	23	33	54	22	33	634.533610	0.000270
55	22	33	54	21	33	634.533610	0.000270
55	47	8	54	46	8	634.553290	0.000418
55	47	9	54	46	9	634.553290	0.000403
55	47	8	54	46	9	634.553290	0.000376
55	47	9	54	46	8	634.553290	0.000444
54	53	1	53	52	1	634.560970	0.000003
54	53	2	53	52	2	634.560970	0.000003
54	53	1	53	52	2	634.560970	0.000003
54	53	2	53	52	1	634.560970	0.000003
55	48	7	54	47	7	634.583970	-0.000576
55	48	8	54	47	8	634.583970	-0.000578
55	48	7	54	47	8	634.583970	-0.000579
55	48	8	54	47	7	634.583970	-0.000575
54	54	0	53	53	0	634.591670	-0.000107
54	54	1	53	53	1	634.591670	-0.000107
54	54	0	53	53	1	634.591670	-0.000107
54	54	1	53	53	0	634.591670	-0.000107
55	49	6	54	48	6	634.615420	-0.000153
55	49	7	54	48	7	634.615420	-0.000153
55	49	6	54	48	7	634.615420	-0.000153
55	49	7	54	48	6	634.615420	-0.000153
55	50	5	54	49	5	634.646370	0.000165
55	50	6	54	49	6	634.646370	0.000165
55	50	5	54	49	6	634.646370	0.000165
55	50	6	54	49	5	634.646370	0.000165
56	38	19	55	37	19	634.656180	0.000250
56	37	19	55	36	19	634.656180	0.000262
56	36	20	55	35	20	634.664400	0.000045
56	37	20	55	36	20	634.664400	0.000044
56	36	21	55	35	21	634.671780	-0.000024
56	35	21	55	34	21	634.671780	-0.000024
55	51	4	54	50	4	634.676740	0.000118
55	51	5	54	50	5	634.676740	0.000118
55	51	4	54	50	5	634.676740	0.000118
55	51	5	54	50	4	634.676740	0.000118
56	35	22	55	34	22	634.678780	0.000253
56	34	22	55	33	22	634.678780	0.000253
56	34	23	55	33	23	634.684830	0.000102

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
56	33	23	55	32	23	634.684830	0.000102
56	32	25	55	31	25	634.696140	0.000107
56	31	25	55	30	25	634.696140	0.000107
56	31	26	55	30	26	634.701510	0.000192
56	30	26	55	29	26	634.701510	0.000192
55	52	3	54	51	3	634.706790	-0.000148
55	52	4	54	51	4	634.706790	-0.000148
56	30	27	55	29	27	634.706790	0.000357
56	29	27	55	28	27	634.706790	0.000357
55	52	3	54	51	4	634.706790	-0.000148
55	52	4	54	51	3	634.706790	-0.000148
56	29	28	55	28	28	634.711420	0.000000
56	28	28	55	27	28	634.711420	0.000000
56	28	29	55	27	29	634.716680	0.000352
56	27	29	55	26	29	634.716680	0.000352
56	27	30	55	26	30	634.720910	-0.000276
56	26	30	55	25	30	634.720910	-0.000276
56	26	31	55	25	31	634.726240	0.000225
56	25	31	55	24	31	634.726240	0.000225
56	25	32	55	24	32	634.730800	-0.000041
56	24	32	55	23	32	634.730800	-0.000041
56	24	33	55	23	33	634.736020	0.000350
56	23	33	55	22	33	634.736020	0.000350
55	53	2	54	52	2	634.737290	0.000050
55	53	3	54	52	3	634.737290	0.000050
55	53	2	54	52	3	634.737290	0.000050
55	53	3	54	52	2	634.737290	0.000050
56	48	8	55	47	8	634.762300	0.000338
56	48	9	55	47	9	634.762300	0.000330
56	48	8	55	47	9	634.762300	0.000315
56	48	9	55	47	8	634.762300	0.000353
55	54	1	54	53	1	634.768000	0.000382
55	54	2	54	53	2	634.768000	0.000382
55	54	1	54	53	2	634.768000	0.000382
55	54	2	54	53	1	634.768000	0.000382
56	49	7	55	48	7	634.793160	-0.000006
56	49	8	55	48	8	634.793160	-0.000007
56	49	7	55	48	8	634.793160	-0.000008
56	49	8	55	48	7	634.793160	-0.000005
55	55	0	54	54	0	634.797980	-0.000133
55	55	1	54	54	1	634.797980	-0.000133
55	55	0	54	54	1	634.797980	-0.000133
55	55	1	54	54	0	634.797980	-0.000133
56	50	6	55	49	6	634.824010	0.000234
56	50	7	55	49	7	634.824010	0.000234
56	50	6	55	49	7	634.824010	0.000234

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
56	50	7	55	49	6	634.824010	0.000234
56	51	5	55	50	5	634.854140	0.000114
56	51	6	55	50	6	634.854140	0.000114
56	51	5	55	50	6	634.854140	0.000114
56	51	6	55	50	5	634.854140	0.000114
57	39	19	56	38	19	634.856600	-0.000027
57	38	19	56	37	19	634.856600	-0.000004
57	37	20	56	36	20	634.865730	0.000315
57	38	20	56	37	20	634.865730	0.000313
57	37	21	56	36	21	634.873130	-0.000004
57	36	21	56	35	21	634.873130	-0.000004
56	52	4	55	51	4	634.883970	-0.000106
56	52	5	55	51	5	634.883970	-0.000106
56	52	4	55	51	5	634.883970	-0.000106
56	52	5	55	51	4	634.883970	-0.000106
57	35	23	56	34	23	634.886580	0.000138
57	34	23	56	33	23	634.886580	0.000138
57	33	25	56	32	25	634.898070	0.000070
57	32	25	56	31	25	634.898070	0.000070
57	32	26	56	31	26	634.903670	0.000305
57	31	26	56	30	26	634.903670	0.000305
57	31	27	56	30	27	634.908750	0.000201
57	30	27	56	29	27	634.908750	0.000201
56	53	3	55	52	3	634.914030	-0.000027
56	53	4	55	52	4	634.914030	-0.000027
57	30	28	56	29	28	634.914030	0.000424
57	29	28	56	28	28	634.914030	0.000424
56	53	3	55	52	4	634.914030	-0.000027
56	53	4	55	52	3	634.914030	-0.000027
57	29	29	56	28	29	634.918590	0.000026
57	28	29	56	27	29	634.918590	0.000026
57	28	30	56	27	30	634.923340	-0.000112
57	27	30	56	26	30	634.923340	-0.000112
57	27	31	56	26	31	634.928070	-0.000242
57	26	31	56	25	31	634.928070	-0.000242
57	26	32	56	25	32	634.933410	0.000259
57	25	32	56	24	32	634.933410	0.000259
57	25	33	56	24	33	634.938270	0.000270
57	24	33	56	23	33	634.938270	0.000270
56	54	2	55	53	2	634.944150	0.000112
56	54	3	55	53	3	634.944150	0.000112
56	54	2	55	53	3	634.944150	0.000112
56	54	3	55	53	2	634.944150	0.000112
57	20	37	56	19	37	634.957720	-0.000044
57	21	37	56	20	37	634.957720	-0.000044
57	49	8	56	48	8	634.970970	0.000091

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
57	49	9	56	48	9	634.970970	0.000086
57	49	8	56	48	9	634.970970	0.000078
57	49	9	56	48	8	634.970970	0.000099
56	55	1	55	54	1	634.974340	0.000255
56	55	2	55	54	2	634.974340	0.000255
56	55	1	55	54	2	634.974340	0.000255
56	55	2	55	54	1	634.974340	0.000255
57	50	7	56	49	7	635.002120	0.000516
57	50	8	56	49	8	635.002120	0.000516
57	50	7	56	49	8	635.002120	0.000515
57	50	8	56	49	7	635.002120	0.000516
56	56	0	55	55	0	635.004360	0.000085
56	56	1	55	55	1	635.004360	0.000085
56	56	0	55	55	1	635.004360	0.000085
56	56	1	55	55	0	635.004360	0.000085
57	51	6	56	50	6	635.031850	0.000048
57	51	7	56	50	7	635.031850	0.000048
57	51	6	56	50	7	635.031850	0.000048
57	51	7	56	50	6	635.031850	0.000048
58	40	19	57	39	19	635.057460	0.000243
58	39	19	57	38	19	635.057460	0.000285
57	52	5	56	51	5	635.061860	0.000179
57	52	6	56	51	6	635.061860	0.000179
57	52	5	56	51	6	635.061860	0.000179
57	52	6	56	51	5	635.061860	0.000179
58	38	20	57	37	20	635.066630	0.000236
58	39	20	57	38	20	635.066630	0.000232
58	38	21	57	37	21	635.074780	0.000381
58	37	21	57	36	21	635.074780	0.000381
58	37	22	57	36	22	635.081420	-0.000145
58	36	22	57	35	22	635.081420	-0.000145
58	36	23	57	35	23	635.088020	-0.000091
58	35	23	57	34	23	635.088020	-0.000091
57	53	4	56	52	4	635.091530	0.000149
57	53	5	56	52	5	635.091530	0.000149
57	53	4	56	52	5	635.091530	0.000149
57	53	5	56	52	4	635.091530	0.000149
58	34	25	57	33	25	635.099830	-0.000091
58	33	25	57	32	25	635.099830	-0.000091
58	33	26	57	32	26	635.105490	0.000107
58	32	26	57	31	26	635.105490	0.000107
58	32	27	57	31	27	635.110830	0.000179
58	31	27	57	30	27	635.110830	0.000179
58	48	10	57	47	10	635.116200	0.000135
58	48	11	57	47	11	635.116200	-0.000202
58	31	28	57	30	28	635.116200	0.000440

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
58	30	28	57	29	28	635.116200	0.000440
57	54	3	56	53	3	635.121000	-0.000014
57	54	4	56	53	4	635.121000	-0.000014
58	30	29	57	29	29	635.121000	0.000231
58	29	29	57	28	29	635.121000	0.000231
57	54	3	56	53	4	635.121000	-0.000014
57	54	4	56	53	3	635.121000	-0.000014
58	29	30	57	28	30	635.126030	0.000335
58	28	30	57	27	30	635.126030	0.000335
58	28	31	57	27	31	635.130850	0.000266
58	27	31	57	26	31	635.130850	0.000266
58	27	32	57	26	32	635.135420	-0.000031
58	26	32	57	25	32	635.135420	-0.000031
58	26	33	57	25	33	635.140600	0.000287
58	25	33	57	24	33	635.140600	0.000287
58	49	9	57	48	9	635.148800	0.000247
58	49	10	57	48	10	635.148800	0.000214
58	49	9	57	48	10	635.148800	0.000151
58	49	10	57	48	9	635.148800	0.000310
57	55	2	56	54	2	635.150700	0.000038
57	55	3	56	54	3	635.150700	0.000038
57	55	2	56	54	3	635.150700	0.000038
57	55	3	56	54	2	635.150700	0.000038
58	21	37	57	20	37	635.159490	-0.000577
58	22	37	57	21	37	635.159490	-0.000577
57	56	1	56	55	1	635.179960	-0.000424
57	56	2	56	55	2	635.179960	-0.000424
58	50	8	57	49	8	635.179960	0.000348
58	50	9	57	49	9	635.179960	0.000345
57	56	1	56	55	2	635.179960	-0.000424
57	56	2	56	55	1	635.179960	-0.000424
58	50	8	57	49	9	635.179960	0.000341
58	50	9	57	49	8	635.179960	0.000353
57	57	0	56	56	0	635.210030	-0.000232
57	57	1	56	56	1	635.210030	-0.000232
58	51	7	57	50	7	635.210030	0.000136
58	51	8	57	50	8	635.210030	0.000136
57	57	0	56	56	1	635.210030	-0.000232
57	57	1	56	56	0	635.210030	-0.000232
58	51	7	57	50	8	635.210030	0.000135
58	51	8	57	50	7	635.210030	0.000136
58	52	6	57	51	6	635.239830	0.000146
58	52	7	57	51	7	635.239830	0.000146
58	52	6	57	51	7	635.239830	0.000146
58	52	7	57	51	6	635.239830	0.000146
59	41	19	58	40	19	635.258020	0.000324

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
59	40	19	58	39	19	635.258020	0.000399
59	39	20	58	38	20	635.267560	0.000294
59	40	20	58	39	20	635.267560	0.000287
58	53	5	57	52	5	635.269190	0.000016
58	53	6	57	52	6	635.269190	0.000016
58	53	5	57	52	6	635.269190	0.000016
58	53	6	57	52	5	635.269190	0.000016
59	39	21	58	38	21	635.275530	-0.000059
59	38	21	58	37	21	635.275530	-0.000058
59	38	22	58	37	22	635.283050	0.000055
59	37	22	58	36	22	635.283050	0.000055
59	37	23	58	36	23	635.289810	0.000078
59	36	23	58	35	23	635.289810	0.000078
58	54	4	57	53	4	635.298810	0.000293
58	54	5	57	53	5	635.298810	0.000293
58	54	4	57	53	5	635.298810	0.000293
58	54	5	57	53	4	635.298810	0.000293
59	35	25	58	34	25	635.301940	0.000133
59	34	25	58	33	25	635.301940	0.000133
59	34	26	58	33	26	635.307310	-0.000058
59	33	26	58	32	26	635.307310	-0.000058
59	33	27	58	32	27	635.312650	-0.000066
59	32	27	58	31	27	635.312650	-0.000066
59	32	28	58	31	28	635.318190	0.000294
59	31	28	58	30	28	635.318190	0.000294
59	31	29	58	30	29	635.323090	0.000132
59	30	29	58	29	29	635.323090	0.000132
59	49	10	58	48	10	635.326320	0.000444
59	49	11	58	48	11	635.326320	0.000242
59	49	10	58	48	11	635.326320	-0.000169
58	55	3	57	54	3	635.327800	-0.000012
58	55	4	57	54	4	635.327800	-0.000012
59	30	30	58	29	30	635.327800	-0.000133
59	29	30	58	28	30	635.327800	-0.000133
58	55	3	57	54	4	635.327800	-0.000012
58	55	4	57	54	3	635.327800	-0.000012
59	29	31	58	28	31	635.333190	0.000344
59	28	31	58	27	31	635.333190	0.000344
59	28	32	58	27	32	635.338050	0.000315
59	27	32	58	26	32	635.338050	0.000315
59	27	33	58	26	33	635.342670	0.000055
59	26	33	58	25	33	635.342670	0.000055
58	56	2	57	55	2	635.357500	0.000383
58	56	3	57	55	3	635.357500	0.000383
59	50	9	58	49	9	635.357500	-0.000136
59	50	10	58	49	10	635.357500	-0.000155

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
58	56	2	57	55	3	635.357500	0.000383
58	56	3	57	55	2	635.357500	0.000383
59	50	9	58	49	10	635.357500	-0.000191
59	50	10	58	49	9	635.357500	-0.000100
59	22	37	58	21	37	635.362100	-0.000283
59	23	37	58	22	37	635.362100	-0.000283
58	57	1	57	56	1	635.386520	-0.000006
58	57	2	57	56	2	635.386520	-0.000006
58	57	1	57	56	2	635.386520	-0.000006
58	57	2	57	56	1	635.386520	-0.000006
59	51	8	58	50	8	635.388440	0.000257
59	51	9	58	50	9	635.388440	0.000255
59	51	8	58	50	9	635.388440	0.000253
59	51	9	58	50	8	635.388440	0.000259
58	58	0	57	57	0	635.416180	0.000108
58	58	1	57	57	1	635.416180	0.000108
58	58	0	57	57	1	635.416180	0.000108
58	58	1	57	57	0	635.416180	0.000108
59	52	7	58	51	7	635.418250	0.000236
59	52	8	58	51	8	635.418250	0.000235
59	52	7	58	51	8	635.418250	0.000235
59	52	8	58	51	7	635.418250	0.000236
59	53	6	58	52	6	635.447870	0.000469
59	53	7	58	52	7	635.447870	0.000469
59	53	6	58	52	7	635.447870	0.000468
59	53	7	58	52	6	635.447870	0.000469
60	42	19	59	41	19	635.458340	0.000296
60	41	19	59	40	19	635.458340	0.000428
60	40	20	59	39	20	635.468210	0.000164
60	41	20	59	40	20	635.468210	0.000150
59	54	5	58	53	5	635.476800	0.000281
59	54	6	58	53	6	635.476800	0.000281
60	40	21	59	39	21	635.476800	0.000093
60	39	21	59	38	21	635.476800	0.000094
59	54	5	58	53	6	635.476800	0.000281
59	54	6	58	53	5	635.476800	0.000281
60	39	22	59	38	22	635.484400	0.000043
60	38	22	59	37	22	635.484400	0.000043
60	38	23	59	37	23	635.491180	-0.000113
60	37	23	59	36	23	635.491180	-0.000113
60	36	25	59	35	25	635.503670	0.000018
60	35	25	59	34	25	635.503670	0.000018
59	55	4	58	54	4	635.505520	0.000022
59	55	5	58	54	5	635.505520	0.000022
59	55	4	58	54	5	635.505520	0.000022
59	55	5	58	54	4	635.505520	0.000022

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
60	35	26	59	34	26	635.509500	0.000174
60	34	26	59	33	26	635.509500	0.000174
60	34	27	59	33	27	635.514980	0.000226
60	33	27	59	32	27	635.514980	0.000226
60	33	28	59	32	28	635.519930	-0.000075
60	32	28	59	31	28	635.519930	-0.000075
60	32	29	59	31	29	635.524970	-0.000151
60	31	29	59	30	29	635.524970	-0.000151
60	31	30	59	30	30	635.530260	0.000118
60	30	30	59	29	30	635.530260	0.000118
60	50	10	59	49	10	635.535550	0.000128
60	50	11	59	49	11	635.535550	0.000008
60	30	31	59	29	31	635.535550	0.000458
60	29	31	59	28	31	635.535550	0.000458
60	50	10	59	49	11	635.535550	-0.000235
60	29	32	59	28	32	635.540150	0.000145
60	28	32	59	27	32	635.540150	0.000145
60	28	33	59	27	33	635.545200	0.000290
60	27	33	59	26	33	635.545200	0.000290
59	57	2	58	56	2	635.563490	0.000066
59	57	3	58	56	3	635.563490	0.000066
59	57	2	58	56	3	635.563490	0.000066
59	57	3	58	56	2	635.563490	0.000066
60	51	9	59	50	9	635.566950	0.000416
60	51	10	59	50	10	635.566950	0.000405
60	51	9	59	50	10	635.566950	0.000384
60	51	10	59	50	9	635.566950	0.000436
60	19	41	59	18	41	635.585340	-0.000037
60	20	41	59	19	41	635.585340	-0.000037
59	58	1	58	57	1	635.592470	-0.000019
59	58	2	58	57	2	635.592470	-0.000019
59	58	1	58	57	2	635.592470	-0.000019
59	58	2	58	57	1	635.592470	-0.000019
60	52	8	59	51	8	635.596530	-0.000051
60	52	9	59	51	9	635.596530	-0.000051
60	52	8	59	51	9	635.596530	-0.000053
60	52	9	59	51	8	635.596530	-0.000049
59	59	0	58	58	0	635.621560	-0.000158
59	59	1	58	58	1	635.621560	-0.000158
59	59	0	58	58	1	635.621560	-0.000158
59	59	1	58	58	0	635.621560	-0.000158
60	53	7	59	52	7	635.626130	0.000160
60	53	8	59	52	8	635.626130	0.000160
60	53	7	59	52	8	635.626130	0.000160
60	53	8	59	52	7	635.626130	0.000160
60	54	6	59	53	6	635.655220	0.000262

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
60	54	7	59	53	7	635.655220	0.000262
60	54	6	59	53	7	635.655220	0.000262
60	54	7	59	53	6	635.655220	0.000262
61	43	19	60	42	19	635.658260	0.000005
61	42	19	60	41	19	635.658260	0.000233
61	41	20	60	40	20	635.668890	0.000170
61	42	20	60	41	20	635.668890	0.000146
61	41	21	60	40	21	635.677860	0.000120
61	40	21	60	39	21	635.677860	0.000122
60	55	5	59	54	5	635.683840	0.000138
60	55	6	59	54	6	635.683840	0.000138
60	55	5	59	54	6	635.683840	0.000138
60	55	6	59	54	5	635.683840	0.000138
61	40	22	60	39	22	635.685500	-0.000155
61	39	22	60	38	22	635.685500	-0.000155
61	39	23	60	38	23	635.692820	0.000023
61	38	23	60	37	23	635.692820	0.000023
61	37	25	60	36	25	635.705560	0.000098
61	36	25	60	35	25	635.705560	0.000098
61	36	26	60	35	26	635.711360	0.000124
61	35	26	60	34	26	635.711360	0.000124
60	56	4	59	55	4	635.712530	0.000200
60	56	5	59	55	5	635.712530	0.000200
60	56	4	59	55	5	635.712530	0.000200
60	56	5	59	55	4	635.712530	0.000200
61	35	27	60	34	27	635.716860	0.000108
61	34	27	60	33	27	635.716860	0.000108
61	34	28	60	33	28	635.721970	-0.000103
61	33	28	60	32	28	635.721970	-0.000103
61	33	29	60	32	29	635.727230	-0.000025
61	32	29	60	31	29	635.727230	-0.000025
61	32	30	60	31	30	635.731940	-0.000386
61	31	30	60	30	30	635.731940	-0.000386
61	31	31	60	30	31	635.737410	0.000096
61	30	31	60	29	31	635.737410	0.000096
60	57	3	59	56	3	635.741000	0.000078
60	57	4	59	56	4	635.741000	0.000078
60	57	3	59	56	4	635.741000	0.000078
60	57	4	59	56	3	635.741000	0.000078
61	30	32	60	29	32	635.742440	0.000177
61	29	32	60	28	32	635.742440	0.000177
61	51	10	60	50	10	635.745300	0.000557
61	51	11	60	50	11	635.745300	0.000487
61	51	10	60	50	11	635.745300	0.000344
61	51	11	60	50	10	635.745300	0.000700
61	29	33	60	28	33	635.747070	-0.000118

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
61	28	33	60	27	33	635.747070	-0.000118
61	24	37	60	23	37	635.766500	-0.000496
61	25	37	60	24	37	635.766500	-0.000496
60	58	2	59	57	2	635.769730	0.000174
60	58	3	59	57	3	635.769730	0.000174
60	58	2	59	57	3	635.769730	0.000174
60	58	3	59	57	2	635.769730	0.000174
61	52	9	60	51	9	635.775330	0.000081
61	52	10	60	51	10	635.775330	0.000075
61	52	9	60	51	10	635.775330	0.000063
61	52	10	60	51	9	635.775330	0.000093
61	20	41	60	19	41	635.787530	-0.000087
61	21	41	60	20	41	635.787530	-0.000087
60	59	1	59	58	1	635.798330	0.000033
60	59	2	59	58	2	635.798330	0.000033
60	59	1	59	58	2	635.798330	0.000033
60	59	2	59	58	1	635.798330	0.000033
61	53	8	60	52	8	635.804830	0.000026
61	53	9	60	52	9	635.804830	0.000025
61	53	8	60	52	9	635.804830	0.000024
61	53	9	60	52	8	635.804830	0.000026
60	60	0	59	59	0	635.827020	-0.000189
60	60	1	59	59	1	635.827020	-0.000189
60	60	0	59	59	1	635.827020	-0.000189
60	60	1	59	59	0	635.827020	-0.000189
61	54	7	60	53	7	635.833390	-0.000372
61	54	8	60	53	8	635.833390	-0.000372
61	54	7	60	53	8	635.833390	-0.000373
61	54	8	60	53	7	635.833390	-0.000372
61	55	6	60	54	6	635.862660	0.000301
61	55	7	60	54	7	635.862660	0.000301
61	55	6	60	54	7	635.862660	0.000301
61	55	7	60	54	6	635.862660	0.000301
62	42	20	61	41	20	635.869230	-0.000024
62	43	20	61	42	20	635.869230	-0.000068
62	42	21	61	41	21	635.878590	-0.000084
62	41	21	61	40	21	635.878590	-0.000079
62	41	22	61	40	22	635.886460	-0.000419
62	40	22	61	39	22	635.886460	-0.000419
61	56	5	60	55	5	635.890990	0.000252
61	56	6	60	55	6	635.890990	0.000252
61	56	5	60	55	6	635.890990	0.000252
61	56	6	60	55	5	635.890990	0.000252
62	40	23	61	39	23	635.893970	-0.000259
62	39	23	61	38	23	635.893970	-0.000259
62	38	25	61	37	25	635.906990	-0.000226

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
62	37	25	61	36	25	635.906990	-0.000226
62	37	26	61	36	26	635.912950	-0.000156
62	36	26	61	35	26	635.912950	-0.000156
61	57	4	60	56	4	635.918980	-0.000017
61	57	5	60	56	5	635.918980	-0.000017
62	36	27	61	35	27	635.918980	0.000263
62	35	27	61	34	27	635.918980	0.000263
61	57	4	60	56	5	635.918980	-0.000017
61	57	5	60	56	4	635.918980	-0.000017
62	35	28	61	34	28	635.923930	-0.000186
62	34	28	61	33	28	635.923930	-0.000186
62	34	29	61	33	29	635.928980	-0.000379
62	33	29	61	32	29	635.928980	-0.000379
62	33	30	61	32	30	635.934510	0.000023
62	32	30	61	31	30	635.934510	0.000023
62	32	31	61	31	31	635.939370	-0.000154
62	31	31	61	30	31	635.939370	-0.000154
62	31	32	61	30	32	635.944570	0.000073
62	30	32	61	29	32	635.944570	0.000073
61	58	3	60	57	3	635.947210	-0.000039
61	58	4	60	57	4	635.947210	-0.000039
61	58	3	60	57	4	635.947210	-0.000039
61	58	4	60	57	3	635.947210	-0.000039
62	30	33	61	29	33	635.949350	-0.000096
62	29	33	61	28	33	635.949350	-0.000096
62	52	10	61	51	10	635.954110	0.000268
62	52	11	61	51	11	635.954110	0.000227
62	52	10	61	51	11	635.954110	0.000143
62	52	11	61	51	10	635.954110	0.000352
62	25	37	61	24	37	635.969480	0.000190
62	26	37	61	25	37	635.969480	0.000190
61	59	2	60	58	2	635.975710	0.000169
61	59	3	60	58	3	635.975710	0.000169
61	59	2	60	58	3	635.975710	0.000169
61	59	3	60	58	2	635.975710	0.000169
62	53	9	61	52	9	635.984110	0.000327
62	53	10	61	52	10	635.984110	0.000324
62	53	9	61	52	10	635.984110	0.000317
62	53	10	61	52	9	635.984110	0.000334
62	21	41	61	20	41	635.989910	0.000044
62	22	41	61	21	41	635.989910	0.000044
61	60	1	60	59	1	636.003910	-0.000042
61	60	2	60	59	2	636.003910	-0.000042
61	60	1	60	59	2	636.003910	-0.000042
61	60	2	60	59	1	636.003910	-0.000042
62	54	8	61	53	8	636.013360	0.000501

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
62	54	9	61	53	9	636.013360	0.000501
62	54	8	61	53	9	636.013360	0.000500
62	54	9	61	53	8	636.013360	0.000501
61	61	0	60	60	0	636.032350	-0.000180
61	61	1	60	60	1	636.032350	-0.000180
61	61	0	60	60	1	636.032350	-0.000180
61	61	1	60	60	0	636.032350	-0.000180
62	55	7	61	54	7	636.041440	0.000040
62	55	8	61	54	8	636.041440	0.000040
62	55	7	61	54	8	636.041440	0.000040
62	55	8	61	54	7	636.041440	0.000040
62	56	6	61	55	6	636.069580	-0.000026
62	56	7	61	55	7	636.069580	-0.000026
63	43	20	62	42	20	636.069580	-0.000070
63	44	20	62	43	20	636.069580	-0.000149
62	56	6	61	55	7	636.069580	-0.000026
62	56	7	61	55	6	636.069580	-0.000026
63	43	21	62	42	21	636.079330	-0.000169
63	42	21	62	41	21	636.079330	-0.000161
63	42	22	62	41	22	636.087880	-0.000130
63	41	22	62	40	22	636.087880	-0.000130
63	41	23	62	40	23	636.095370	-0.000229
63	40	23	62	39	23	636.095370	-0.000229
62	57	5	61	56	5	636.097590	-0.000023
62	57	6	61	56	6	636.097590	-0.000023
62	57	5	61	56	6	636.097590	-0.000023
62	57	6	61	56	5	636.097590	-0.000023
63	39	25	62	38	25	636.108990	0.000073
63	38	25	62	37	25	636.108990	0.000073
63	38	26	62	37	26	636.114780	-0.000151
63	37	26	62	36	26	636.114780	-0.000151
63	37	27	62	36	27	636.120290	-0.000345
63	36	27	62	35	27	636.120290	-0.000345
62	58	4	61	57	4	636.126020	0.000507
62	58	5	61	57	5	636.126020	0.000507
63	36	28	62	35	28	636.126020	-0.000100
63	35	28	62	34	28	636.126020	-0.000100
62	58	4	61	57	5	636.126020	0.000507
62	58	5	61	57	4	636.126020	0.000507
63	34	30	62	33	30	636.136310	-0.000301
63	33	30	62	32	30	636.136310	-0.000301
63	33	31	62	32	31	636.141670	-0.000021
63	32	31	62	31	31	636.141670	-0.000021
63	32	32	62	31	32	636.146690	-0.000027
63	31	32	62	30	32	636.146690	-0.000027
63	31	33	62	30	33	636.151680	-0.000011

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
63	30	33	62	29	33	636.151680	-0.000011
62	59	3	61	58	3	636.153470	0.000060
62	59	4	61	58	4	636.153470	0.000060
62	59	3	61	58	4	636.153470	0.000060
62	59	4	61	58	3	636.153470	0.000060
63	53	10	62	52	10	636.162920	0.000181
63	53	11	62	52	11	636.162920	0.000157
63	53	10	62	52	11	636.162920	0.000109
63	53	11	62	52	10	636.162920	0.000230
63	26	37	62	25	37	636.171780	0.000197
63	27	37	62	26	37	636.171780	0.000197
62	60	2	61	59	2	636.181600	0.000235
62	60	3	61	59	3	636.181600	0.000235
62	60	2	61	59	3	636.181600	0.000235
62	60	3	61	59	2	636.181600	0.000235
63	54	9	62	53	9	636.192070	-0.000065
63	54	10	62	53	10	636.192070	-0.000067
63	22	41	62	21	41	636.192070	-0.000050
63	23	41	62	22	41	636.192070	-0.000050
63	54	9	62	53	10	636.192070	-0.000070
63	54	10	62	53	9	636.192070	-0.000061
62	61	1	61	60	1	636.209420	-0.000028
62	61	2	61	60	2	636.209420	-0.000028
62	61	1	61	60	2	636.209420	-0.000028
62	61	2	61	60	1	636.209420	-0.000028
63	55	8	62	54	8	636.220660	-0.000094
63	55	9	62	54	9	636.220660	-0.000094
63	55	8	62	54	9	636.220660	-0.000094
63	55	9	62	54	8	636.220660	-0.000094
62	62	0	61	61	0	636.237600	-0.000097
62	62	1	61	61	1	636.237600	-0.000097
62	62	0	61	61	1	636.237600	-0.000097
62	62	1	61	61	0	636.237600	-0.000097
63	56	7	62	55	7	636.248820	-0.000064
63	56	8	62	55	8	636.248820	-0.000064
63	56	7	62	55	8	636.248820	-0.000064
63	56	8	62	55	7	636.248820	-0.000064
64	44	20	63	43	20	636.269900	0.000026
64	45	20	63	44	20	636.269900	-0.000110
63	57	6	62	56	6	636.276840	0.000143
63	57	7	62	56	7	636.276840	0.000143
63	57	6	62	56	7	636.276840	0.000143
63	57	7	62	56	6	636.276840	0.000143
64	44	21	63	43	21	636.280110	-0.000108
64	43	21	63	42	21	636.280110	-0.000094
64	43	22	63	42	22	636.288510	-0.000536

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
64	42	22	63	41	22	636.288510	-0.000535
64	42	23	63	41	23	636.296820	-0.000067
64	41	23	63	40	23	636.296820	-0.000066
63	58	5	62	57	5	636.304260	-0.000069
63	58	6	62	57	6	636.304260	-0.000069
63	58	5	62	57	6	636.304260	-0.000069
63	58	6	62	57	5	636.304260	-0.000069
64	40	25	63	39	25	636.310190	-0.000364
64	39	25	63	38	25	636.310190	-0.000364
64	39	26	63	38	26	636.316820	0.000128
64	38	26	63	37	26	636.316820	0.000128
64	38	27	63	37	27	636.322500	-0.000007
64	37	27	63	36	27	636.322500	-0.000007
64	37	28	63	36	28	636.327490	-0.000589
64	36	28	63	35	28	636.327490	-0.000589
63	59	4	62	58	4	636.332180	0.000294
63	59	5	62	58	5	636.332180	0.000294
63	59	4	62	58	5	636.332180	0.000294
63	59	5	62	58	4	636.332180	0.000294
64	36	29	63	35	29	636.333410	-0.000052
64	35	29	63	34	29	636.333410	-0.000052
64	35	30	63	34	30	636.338400	-0.000297
64	34	30	63	33	30	636.338400	-0.000297
64	34	31	63	33	31	636.343610	-0.000226
64	33	31	63	32	31	636.343610	-0.000226
64	33	32	63	32	32	636.348290	-0.000605
64	32	32	63	31	32	636.348290	-0.000605
64	32	33	63	31	33	636.353800	-0.000100
64	31	33	63	30	33	636.353800	-0.000100
63	60	3	62	59	3	636.359550	0.000123
63	60	4	62	59	4	636.359550	0.000123
63	60	3	62	59	4	636.359550	0.000123
63	60	4	62	59	3	636.359550	0.000123
64	54	10	63	53	10	636.371310	-0.000114
64	54	11	63	53	11	636.371310	-0.000128
64	54	10	63	53	11	636.371310	-0.000156
64	54	11	63	53	10	636.371310	-0.000086
64	27	37	63	26	37	636.373880	0.000030
64	28	37	63	27	37	636.373880	0.000030
63	61	2	62	60	2	636.387180	0.000135
63	61	3	62	60	3	636.387180	0.000135
63	61	2	62	60	3	636.387180	0.000135
63	61	3	62	60	2	636.387180	0.000135
64	23	41	63	22	41	636.394500	0.000131
64	24	41	63	23	41	636.394500	0.000131
64	56	8	63	55	8	636.428450	-0.000029

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
64	56	9	63	55	9	636.428450	-0.000029
64	56	8	63	55	9	636.428450	-0.000029
64	56	9	63	55	8	636.428450	-0.000029
63	63	0	62	62	0	636.442820	0.000116
63	63	1	62	62	1	636.442820	0.000116
63	63	0	62	62	1	636.442820	0.000116
63	63	1	62	62	0	636.442820	0.000116
64	57	7	63	56	7	636.456320	0.000117
64	57	8	63	56	8	636.456320	0.000117
64	57	7	63	56	8	636.456320	0.000117
64	57	8	63	56	7	636.456320	0.000117
65	45	20	64	44	20	636.470110	0.000197
65	46	20	64	45	20	636.470110	-0.000037
64	58	6	63	57	6	636.483460	-0.000175
64	58	7	63	57	7	636.483460	-0.000175
64	58	6	63	57	7	636.483460	-0.000175
64	58	7	63	57	6	636.483460	-0.000175
65	44	22	64	43	22	636.489820	-0.000154
65	43	22	64	42	22	636.489820	-0.000152
64	59	5	63	58	5	636.511730	0.000834
64	59	6	63	58	6	636.511730	0.000834
65	41	25	64	40	25	636.511730	-0.000380
65	40	25	64	39	25	636.511730	-0.000380
64	59	5	63	58	6	636.511730	0.000834
64	59	6	63	58	5	636.511730	0.000834
65	40	26	64	39	26	636.517820	-0.000568
65	39	26	64	38	26	636.517820	-0.000568
65	39	27	64	38	27	636.524080	-0.000240
65	38	27	64	37	27	636.524080	-0.000240
65	38	28	64	37	28	636.529850	-0.000129
65	37	28	64	36	28	636.529850	-0.000129
65	37	29	64	36	29	636.535420	-0.000027
65	36	29	64	35	29	636.535420	-0.000027
64	60	4	63	59	4	636.538000	-0.000092
64	60	5	63	59	5	636.538000	-0.000092
64	60	4	63	59	5	636.538000	-0.000092
64	60	5	63	59	4	636.538000	-0.000092
65	36	30	64	35	30	636.540600	-0.000147
65	35	30	64	34	30	636.540600	-0.000147
65	35	31	64	34	31	636.545920	-0.000017
65	34	31	64	33	31	636.545920	-0.000017
65	34	32	64	33	32	636.550650	-0.000385
65	33	32	64	32	32	636.550650	-0.000385
65	33	33	64	32	33	636.556060	-0.000021
65	32	33	64	31	33	636.556060	-0.000021
64	61	3	63	60	3	636.565640	0.000346

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
64	61	4	63	60	4	636.565640	0.000346
64	61	3	63	60	4	636.565640	0.000346
64	61	4	63	60	3	636.565640	0.000346
65	28	37	64	27	37	636.576200	0.000097
65	29	37	64	28	37	636.576200	0.000097
65	55	10	64	54	10	636.579770	-0.000136
65	55	11	64	54	11	636.579770	-0.000144
65	55	10	64	54	11	636.579770	-0.000160
65	55	11	64	54	10	636.579770	-0.000120
64	62	2	63	61	2	636.592510	-0.000056
64	62	3	63	61	3	636.592510	-0.000056
64	62	2	63	61	3	636.592510	-0.000056
64	62	3	63	61	2	636.592510	-0.000056
65	24	41	64	23	41	636.596420	-0.000185
65	25	41	64	24	41	636.596420	-0.000185
65	56	9	64	55	9	636.608430	0.000130
65	56	10	64	55	10	636.608430	0.000129
65	56	9	64	55	10	636.608430	0.000128
65	56	10	64	55	9	636.608430	0.000131
64	63	1	63	62	1	636.620180	0.000205
64	63	2	63	62	2	636.620180	0.000205
64	63	1	63	62	2	636.620180	0.000205
64	63	2	63	62	1	636.620180	0.000205
65	57	8	64	56	8	636.636020	-0.000023
65	57	9	64	56	9	636.636020	-0.000023
65	57	8	64	56	9	636.636020	-0.000023
65	57	9	64	56	8	636.636020	-0.000023
64	64	0	63	63	0	636.647870	0.000315
64	64	1	63	63	1	636.647870	0.000315
64	64	0	63	63	1	636.647870	0.000315
64	64	1	63	63	0	636.647870	0.000315
65	58	7	64	57	7	636.663290	-0.000070
65	58	8	64	57	8	636.663290	-0.000070
65	58	7	64	57	8	636.663290	-0.000070
65	58	8	64	57	7	636.663290	-0.000070
65	59	6	64	58	6	636.690520	0.000104
65	59	7	64	58	7	636.690520	0.000104
66	45	22	65	44	22	636.690520	-0.000259
66	44	22	65	43	22	636.690520	-0.000254
65	59	6	64	58	7	636.690520	0.000104
65	59	7	64	58	6	636.690520	0.000104
66	42	25	65	41	25	636.712890	-0.000698
66	41	25	65	40	25	636.712890	-0.000698
65	60	5	64	59	5	636.717380	0.000064
65	60	6	64	59	6	636.717380	0.000064
65	60	5	64	59	6	636.717380	0.000064

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
65	60	6	64	59	5	636.717380	0.000064
66	41	26	65	40	26	636.719700	-0.000307
66	40	26	65	39	26	636.719700	-0.000307
66	40	27	65	39	27	636.725510	-0.000546
66	39	27	65	38	27	636.725510	-0.000546
66	39	28	65	38	28	636.731670	-0.000150
66	38	28	65	37	28	636.731670	-0.000150
66	38	29	65	37	29	636.737280	-0.000081
66	37	29	65	36	29	636.737280	-0.000081
65	61	4	64	60	4	636.744230	0.000078
65	61	5	64	60	5	636.744230	0.000078
65	61	4	64	60	5	636.744230	0.000078
65	61	5	64	60	4	636.744230	0.000078
66	36	31	65	35	31	636.747800	-0.000181
66	35	31	65	34	31	636.747800	-0.000181
66	35	32	65	34	32	636.753460	0.000328
66	34	32	65	33	32	636.753460	0.000328
66	34	33	65	33	33	636.758360	0.000144
66	33	33	65	32	33	636.758360	0.000144
65	62	3	64	61	3	636.771320	0.000308
65	62	4	64	61	4	636.771320	0.000308
65	62	3	64	61	4	636.771320	0.000308
65	62	4	64	61	3	636.771320	0.000308
66	29	37	65	28	37	636.778220	-0.000118
66	30	37	65	29	37	636.778220	-0.000118
66	56	10	65	55	10	636.788300	0.000105
66	56	11	65	55	11	636.788300	0.000100
66	56	10	65	55	11	636.788300	0.000091
66	56	11	65	55	10	636.788300	0.000114
65	63	2	64	62	2	636.798220	0.000276
65	63	3	64	62	3	636.798220	0.000276
66	25	41	65	24	41	636.798220	-0.000619
66	26	41	65	25	41	636.798220	-0.000619
65	63	2	64	62	3	636.798220	0.000276
65	63	3	64	62	2	636.798220	0.000276
66	57	9	65	56	9	636.816090	-0.000017
66	57	10	65	56	10	636.816090	-0.000018
66	57	9	65	56	10	636.816090	-0.000018
66	57	10	65	56	9	636.816090	-0.000017
65	64	1	64	63	1	636.825320	0.000316
65	64	2	64	63	2	636.825320	0.000316
65	64	1	64	63	2	636.825320	0.000316
65	64	2	64	63	1	636.825320	0.000316
66	58	8	65	57	8	636.843080	-0.000345
66	58	9	65	57	9	636.843080	-0.000345
66	58	8	65	57	9	636.843080	-0.000345

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
66	58	9	65	57	8	636.843080	-0.000345
65	65	0	64	64	0	636.852280	0.000019
65	65	1	64	64	1	636.852280	0.000019
65	65	0	64	64	1	636.852280	0.000019
65	65	1	64	64	0	636.852280	0.000019
66	59	7	65	58	7	636.870030	-0.000326
66	59	8	65	58	8	636.870030	-0.000326
66	59	7	65	58	8	636.870030	-0.000326
66	59	8	65	58	7	636.870030	-0.000326
67	46	22	66	45	22	636.890960	-0.000478
67	45	22	66	44	22	636.890960	-0.000469
66	60	6	65	59	6	636.897590	0.000550
66	60	7	65	59	7	636.897590	0.000550
66	60	6	65	59	7	636.897590	0.000550
66	60	7	65	59	6	636.897590	0.000550
67	43	25	66	42	25	636.914760	-0.000209
67	42	25	66	41	25	636.914760	-0.000209
67	42	26	66	41	26	636.921220	-0.000322
67	41	26	66	40	26	636.921220	-0.000322
66	61	5	65	60	5	636.923660	0.000080
66	61	6	65	60	6	636.923660	0.000080
66	61	5	65	60	6	636.923660	0.000080
66	61	6	65	60	5	636.923660	0.000080
67	41	27	66	40	27	636.927550	-0.000165
67	40	27	66	39	27	636.927550	-0.000165
67	40	28	66	39	28	636.933500	-0.000088
67	39	28	66	38	28	636.933500	-0.000088
67	39	29	66	38	29	636.938860	-0.000358
67	38	29	66	37	29	636.938860	-0.000358
67	38	30	66	37	30	636.943890	-0.000769
67	37	30	66	36	30	636.943890	-0.000769
66	62	4	65	61	4	636.950010	-0.000055
66	62	5	65	61	5	636.950010	-0.000055
67	37	31	66	36	31	636.950010	0.000041
67	36	31	66	35	31	636.950010	0.000041
66	62	4	65	61	5	636.950010	-0.000055
66	62	5	65	61	4	636.950010	-0.000055
67	36	32	66	35	32	636.955120	-0.000055
67	35	32	66	34	32	636.955120	-0.000055
67	35	33	66	34	33	636.960120	-0.000181
67	34	33	66	33	33	636.960120	-0.000181
66	63	3	65	62	3	636.976770	0.000197
66	63	4	65	62	4	636.976770	0.000197
66	63	3	65	62	4	636.976770	0.000197
66	63	4	65	62	3	636.976770	0.000197
67	30	37	66	29	37	636.980380	-0.000139

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
67	31	37	66	30	37	636.980380	-0.000139
67	57	10	66	56	10	636.995990	-0.000283
67	57	11	66	56	11	636.995990	-0.000285
67	57	10	66	56	11	636.995990	-0.000290
67	57	11	66	56	10	636.995990	-0.000277
67	26	41	66	25	41	637.000820	-0.000214
67	27	41	66	26	41	637.000820	-0.000214
66	64	2	65	63	2	637.003520	0.000355
66	64	3	65	63	3	637.003520	0.000355
66	64	2	65	63	3	637.003520	0.000355
66	64	3	65	63	2	637.003520	0.000355
67	58	9	66	57	9	637.023530	-0.000205
67	58	10	66	57	10	637.023530	-0.000206
67	58	9	66	57	10	637.023530	-0.000206
67	58	10	66	57	9	637.023530	-0.000205
66	65	1	65	64	1	637.030080	0.000189
66	65	2	65	64	2	637.030080	0.000189
66	65	1	65	64	2	637.030080	0.000189
66	65	2	65	64	1	637.030080	0.000189
67	59	8	66	58	8	637.050430	-0.000217
67	59	9	66	58	9	637.050430	-0.000217
67	59	8	66	58	9	637.050430	-0.000217
67	59	9	66	58	8	637.050430	-0.000217
67	60	7	66	59	7	637.077030	-0.000158
67	60	8	66	59	8	637.077030	-0.000158
67	60	7	66	59	8	637.077030	-0.000158
67	60	8	66	59	7	637.077030	-0.000158
67	61	6	66	60	6	637.103440	-0.000058
67	61	7	66	60	7	637.103440	-0.000058
67	61	6	66	60	7	637.103440	-0.000058
67	61	7	66	60	6	637.103440	-0.000058
68	44	25	67	43	25	637.116120	-0.000123
68	43	25	67	42	25	637.116120	-0.000123
68	43	26	67	42	26	637.122910	-0.000061
68	42	26	67	41	26	637.122910	-0.000061
68	42	27	67	41	27	637.129060	-0.000222
68	41	27	67	40	27	637.129060	-0.000222
68	41	28	67	40	28	637.134990	-0.000273
68	40	28	67	39	28	637.134990	-0.000273
68	39	30	67	38	30	637.146160	-0.000349
68	38	30	67	37	30	637.146160	-0.000349
68	38	31	67	37	31	637.151540	-0.000338
68	37	31	67	36	31	637.151540	-0.000338
67	63	4	66	62	4	637.155890	0.000070
67	63	5	66	62	5	637.155890	0.000070
67	63	4	66	62	5	637.155890	0.000070

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
67	63	5	66	62	4	637.155890	0.000070
68	36	33	67	35	33	637.162240	-0.000080
68	35	33	67	34	33	637.162240	-0.000080
67	64	3	66	63	3	637.182260	0.000275
67	64	4	66	63	4	637.182260	0.000275
68	31	37	67	30	37	637.182260	-0.000398
68	32	37	67	31	37	637.182260	-0.000398
67	64	3	66	63	4	637.182260	0.000275
67	64	4	66	63	3	637.182260	0.000275
68	27	41	67	26	41	637.203170	-0.000033
68	28	41	67	27	41	637.203170	-0.000033
67	65	2	66	64	2	637.208340	0.000104
67	65	3	66	64	3	637.208340	0.000104
67	65	2	66	64	3	637.208340	0.000104
67	65	3	66	64	2	637.208340	0.000104
68	59	9	67	58	9	637.231130	-0.000048
68	59	10	67	58	10	637.231130	-0.000048
68	59	9	67	58	10	637.231130	-0.000048
68	59	10	67	58	9	637.231130	-0.000048
67	66	1	66	65	1	637.234920	0.000286
67	66	2	66	65	2	637.234920	0.000286
67	66	1	66	65	2	637.234920	0.000286
67	66	2	66	65	1	637.234920	0.000286
68	60	8	67	59	8	637.257580	-0.000110
68	60	9	67	59	9	637.257580	-0.000110
68	60	8	67	59	9	637.257580	-0.000110
68	60	9	67	59	8	637.257580	-0.000110
68	61	7	67	60	7	637.283620	-0.000236
68	61	8	67	60	8	637.283620	-0.000236
68	61	7	67	60	8	637.283620	-0.000236
68	61	8	67	60	7	637.283620	-0.000236
68	62	6	67	61	6	637.309450	-0.000353
68	62	7	67	61	7	637.309450	-0.000353
68	62	6	67	61	7	637.309450	-0.000353
68	62	7	67	61	6	637.309450	-0.000353
69	45	25	68	44	25	637.317480	0.000095
69	44	25	68	43	25	637.317480	0.000095
69	43	27	68	42	27	637.330470	-0.000264
69	42	27	68	41	27	637.330470	-0.000264
68	63	5	67	62	5	637.335650	0.000022
68	63	6	67	62	6	637.335650	0.000022
68	63	5	67	62	6	637.335650	0.000022
68	63	6	67	62	5	637.335650	0.000022
69	42	28	68	41	28	637.337250	0.000419
69	41	28	68	40	28	637.337250	0.000419
69	40	30	68	39	30	637.347620	-0.000643

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
69	39	30	68	38	30	637.347620	-0.000643
69	39	31	68	38	31	637.354370	0.000662
69	38	31	68	37	31	637.354370	0.000662
69	38	32	68	37	32	637.358070	-0.000965
69	37	32	68	36	32	637.358070	-0.000965
68	64	4	67	63	4	637.361530	0.000099
68	64	5	67	63	5	637.361530	0.000099
68	64	4	67	63	5	637.361530	0.000099
68	64	5	67	63	4	637.361530	0.000099
69	37	33	68	36	33	637.364160	-0.000103
69	36	33	68	35	33	637.364160	-0.000103
69	32	37	68	31	37	637.384440	-0.000293
69	33	37	68	32	37	637.384440	-0.000293
68	65	3	67	64	3	637.387290	0.000046
68	65	4	67	64	4	637.387290	0.000046
68	65	3	67	64	4	637.387290	0.000046
68	65	4	67	64	3	637.387290	0.000046
69	28	41	68	27	41	637.405250	-0.000081
69	29	41	68	28	41	637.405250	-0.000081
68	66	2	67	65	2	637.413260	0.000098
68	66	3	67	65	3	637.413260	0.000098
68	66	2	67	65	3	637.413260	0.000098
68	66	3	67	65	2	637.413260	0.000098
69	60	9	68	59	9	637.438000	-0.000440
69	60	10	68	59	10	637.438000	-0.000440
69	60	9	68	59	10	637.438000	-0.000440
69	60	10	68	59	9	637.438000	-0.000440
68	67	1	67	66	1	637.439290	0.000073
68	67	2	67	66	2	637.439290	0.000073
68	67	1	67	66	2	637.439290	0.000073
68	67	2	67	66	1	637.439290	0.000073
69	61	8	68	60	8	637.464340	-0.000212
69	61	9	68	60	9	637.464340	-0.000212
69	61	8	68	60	9	637.464340	-0.000212
69	61	9	68	60	8	637.464340	-0.000212
69	62	7	68	61	7	637.490360	0.000014
69	62	8	68	61	8	637.490360	0.000014
69	62	7	68	61	8	637.490360	0.000014
69	62	8	68	61	7	637.490360	0.000014
69	63	6	68	62	6	637.515960	0.000018
69	63	7	68	62	7	637.515960	0.000018
69	63	6	68	62	7	637.515960	0.000018
69	63	7	68	62	6	637.515960	0.000018
70	46	25	69	45	25	637.518110	-0.000260
70	45	25	69	44	25	637.518110	-0.000260
70	45	26	69	44	26	637.525070	-0.000391

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
70	44	26	69	43	26	637.525070	-0.000391
70	44	27	69	43	27	637.531850	-0.000208
70	43	27	69	42	27	637.531850	-0.000208
70	43	28	69	42	28	637.538300	0.000027
70	42	28	69	41	28	637.538300	0.000027
69	64	5	68	63	5	637.541470	0.000045
69	64	6	68	63	6	637.541470	0.000045
69	64	5	68	63	6	637.541470	0.000045
69	64	6	68	63	5	637.541470	0.000045
70	41	30	69	40	30	637.549730	-0.000178
70	40	30	69	39	30	637.549730	-0.000178
70	40	31	69	39	31	637.555450	0.000019
70	39	31	69	38	31	637.555450	0.000019
70	39	32	69	38	32	637.560620	-0.000198
70	38	32	69	37	32	637.560620	-0.000198
69	65	4	68	64	4	637.566780	-0.000100
69	65	5	68	64	5	637.566780	-0.000100
69	65	4	68	64	5	637.566780	-0.000100
69	65	5	68	64	4	637.566780	-0.000100
70	33	37	69	32	37	637.586660	-0.000084
70	34	37	69	33	37	637.586660	-0.000084
69	66	3	68	65	3	637.592380	0.000021
69	66	4	68	65	4	637.592380	0.000021
69	66	3	68	65	4	637.592380	0.000021
69	66	4	68	65	3	637.592380	0.000021
70	29	41	69	28	41	637.607230	-0.000167
70	30	41	69	29	41	637.607230	-0.000167
69	67	2	68	66	2	637.618150	0.000212
69	67	3	68	66	3	637.618150	0.000212
69	67	2	68	66	3	637.618150	0.000212
69	67	3	68	66	2	637.618150	0.000212
69	68	1	68	67	1	637.643900	0.000237
69	68	2	68	67	2	637.643900	0.000237
69	68	1	68	67	2	637.643900	0.000237
69	68	2	68	67	1	637.643900	0.000237
70	61	9	69	60	9	637.645300	-0.000207
70	61	10	69	60	10	637.645300	-0.000207
70	61	9	69	60	10	637.645300	-0.000207
70	61	10	69	60	9	637.645300	-0.000207
70	62	8	69	61	8	637.670970	-0.000277
70	62	9	69	61	9	637.670970	-0.000277
70	62	8	69	61	9	637.670970	-0.000277
70	62	9	69	61	8	637.670970	-0.000277
70	63	7	69	62	7	637.696650	-0.000023
70	63	8	69	62	8	637.696650	-0.000023
70	63	7	69	62	8	637.696650	-0.000023

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
70	63	8	69	62	7	637.696650	-0.000023
71	47	25	70	46	25	637.719380	0.000185
71	46	25	70	45	25	637.719380	0.000185
70	64	6	69	63	6	637.721670	-0.000248
70	64	7	69	63	7	637.721670	-0.000248
70	64	6	69	63	7	637.721670	-0.000248
70	64	7	69	63	6	637.721670	-0.000248
71	46	26	70	45	26	637.726500	0.000033
71	45	26	70	44	26	637.726500	0.000033
71	45	27	70	44	27	637.733560	0.000326
71	44	27	70	43	27	637.733560	0.000326
71	44	28	70	43	28	637.739750	0.000162
71	43	28	70	42	28	637.739750	0.000162
70	65	5	69	64	5	637.746970	-0.000085
70	65	6	69	64	6	637.746970	-0.000085
70	65	5	69	64	6	637.746970	-0.000085
70	65	6	69	64	5	637.746970	-0.000085
71	42	30	70	41	30	637.751250	-0.000173
71	41	30	70	40	30	637.751250	-0.000173
71	41	31	70	40	31	637.756990	-0.000043
71	40	31	70	39	31	637.756990	-0.000043
71	40	32	70	39	32	637.762490	-0.000006
71	39	32	70	38	32	637.762490	-0.000006
70	66	4	69	65	4	637.772900	0.000732
70	66	5	69	65	5	637.772900	0.000732
70	66	4	69	65	5	637.772900	0.000732
70	66	5	69	65	4	637.772900	0.000732
71	34	37	70	33	37	637.788720	0.000063
71	35	37	70	34	37	637.788720	0.000063
70	67	3	69	66	3	637.797370	0.000047
70	67	4	69	66	4	637.797370	0.000047
70	67	3	69	66	4	637.797370	0.000047
70	67	4	69	66	3	637.797370	0.000047
71	30	41	70	29	41	637.809470	0.000071
71	31	41	70	30	41	637.809470	0.000071
70	68	2	69	67	2	637.822670	0.000104
70	68	3	69	67	3	637.822670	0.000104
70	68	2	69	67	3	637.822670	0.000104
70	68	3	69	67	2	637.822670	0.000104
70	69	1	69	68	1	637.847750	-0.000209
70	69	2	69	68	2	637.847750	-0.000209
70	69	1	69	68	2	637.847750	-0.000209
70	69	2	69	68	1	637.847750	-0.000209
71	62	9	70	61	9	637.851810	-0.000566
71	62	10	70	61	10	637.851810	-0.000566
71	62	9	70	61	10	637.851810	-0.000566

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
71	62	10	70	61	9	637.851810	-0.000565
71	63	8	70	62	8	637.877570	-0.000180
71	63	9	70	62	9	637.877570	-0.000180
71	63	8	70	62	9	637.877570	-0.000180
71	63	9	70	62	8	637.877570	-0.000180
71	64	7	70	63	7	637.902870	0.000041
71	64	8	70	63	8	637.902870	0.000041
71	64	7	70	63	8	637.902870	0.000041
71	64	8	70	63	7	637.902870	0.000041
71	65	6	70	64	6	637.927770	0.000041
71	65	7	70	64	7	637.927770	0.000041
72	47	26	71	46	26	637.927770	0.000462
72	46	26	71	45	26	637.927770	0.000462
71	65	6	70	64	7	637.927770	0.000041
71	65	7	70	64	6	637.927770	0.000041
72	46	27	71	45	27	637.934760	0.000529
72	45	27	71	44	27	637.934760	0.000529
72	45	28	71	44	28	637.940890	0.000156
72	44	28	71	43	28	637.940890	0.000156
71	66	5	70	65	5	637.952750	0.000221
71	66	6	70	65	6	637.952750	0.000221
72	43	30	71	42	30	637.952750	-0.000048
72	42	30	71	41	30	637.952750	-0.000048
71	66	5	70	65	6	637.952750	0.000221
71	66	6	70	65	5	637.952750	0.000221
72	41	32	71	40	32	637.964700	0.000665
72	40	32	71	39	32	637.964700	0.000665
71	67	4	70	66	4	637.977250	-0.000063
71	67	5	70	66	5	637.977250	-0.000063
71	67	4	70	66	5	637.977250	-0.000063
71	67	5	70	66	4	637.977250	-0.000063
72	35	37	71	34	37	637.990340	-0.000113
72	36	37	71	35	37	637.990340	-0.000113
71	68	3	70	67	3	638.001820	-0.000310
71	68	4	70	67	4	638.001820	-0.000310
71	68	3	70	67	4	638.001820	-0.000310
71	68	4	70	67	3	638.001820	-0.000310
72	31	41	71	30	41	638.011540	0.000242
72	32	41	71	31	41	638.011540	0.000242
72	62	10	71	61	10	638.032990	-0.000635
72	62	11	71	61	11	638.032990	-0.000635
72	62	10	71	61	11	638.032990	-0.000635
72	62	11	71	61	10	638.032990	-0.000635
71	70	1	70	69	1	638.051550	-0.000559
71	70	2	70	69	2	638.051550	-0.000559
71	70	1	70	69	2	638.051550	-0.000559

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
71	70	2	70	69	1	638.051550	-0.000559
72	63	9	71	62	9	638.058830	-0.000218
72	63	10	71	62	10	638.058830	-0.000218
72	63	9	71	62	10	638.058830	-0.000219
72	63	10	71	62	9	638.058830	-0.000218
72	64	8	71	63	8	638.083990	-0.000066
72	64	9	71	63	9	638.083990	-0.000066
72	64	8	71	63	9	638.083990	-0.000066
72	64	9	71	63	8	638.083990	-0.000066
72	65	7	71	64	7	638.108380	-0.000414
72	65	8	71	64	8	638.108380	-0.000414
72	65	7	71	64	8	638.108380	-0.000414
72	65	8	71	64	7	638.108380	-0.000414
72	66	6	71	65	6	638.133110	-0.000251
72	66	7	71	65	7	638.133110	-0.000251
72	66	6	71	65	7	638.133110	-0.000251
72	66	7	71	65	6	638.133110	-0.000251
73	47	27	72	46	27	638.135820	0.000781
73	46	27	72	45	27	638.135820	0.000781
72	67	5	71	66	5	638.157710	-0.000127
72	67	6	71	66	6	638.157710	-0.000127
72	67	5	71	66	6	638.157710	-0.000127
72	67	6	71	66	5	638.157710	-0.000127
73	42	32	72	41	32	638.165790	0.000370
73	41	32	72	40	32	638.165790	0.000370
72	68	4	71	67	4	638.181820	-0.000466
72	68	5	71	67	5	638.181820	-0.000466
72	68	4	71	67	5	638.181820	-0.000466
72	68	5	71	67	4	638.181820	-0.000466
73	36	37	72	35	37	638.192620	0.000481
73	37	37	72	36	37	638.192620	0.000481
72	69	3	71	68	3	638.206610	-0.000165
72	69	4	71	68	4	638.206610	-0.000165
72	69	3	71	68	4	638.206610	-0.000165
72	69	4	71	68	3	638.206610	-0.000165
73	32	41	72	31	41	638.213360	0.000263
73	33	41	72	32	41	638.213360	0.000263
73	63	10	72	62	10	638.240020	-0.000428
73	63	11	72	62	11	638.240020	-0.000428
73	63	10	72	62	11	638.240020	-0.000428
73	63	11	72	62	10	638.240020	-0.000428
72	71	1	71	70	1	638.256020	-0.000102
72	71	2	71	70	2	638.256020	-0.000102
72	71	1	71	70	2	638.256020	-0.000102
72	71	2	71	70	1	638.256020	-0.000102
73	64	9	72	63	9	638.265620	0.000108

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
73	64	10	72	63	10	638.265620	0.000108
73	64	9	72	63	10	638.265620	0.000108
73	64	10	72	63	9	638.265620	0.000108
73	65	8	72	64	8	638.289910	-0.000265
73	65	9	72	64	9	638.289910	-0.000265
73	65	8	72	64	9	638.289910	-0.000265
73	65	9	72	64	8	638.289910	-0.000265
73	68	5	72	67	5	638.363020	0.000046
73	68	6	72	67	6	638.363020	0.000046
73	68	5	72	67	6	638.363020	0.000046
73	68	6	72	67	5	638.363020	0.000046
74	43	32	73	42	32	638.367300	0.000669
74	42	32	73	41	32	638.367300	0.000669
73	69	4	72	68	4	638.387070	-0.000030
73	69	5	72	68	5	638.387070	-0.000030
73	69	4	72	68	5	638.387070	-0.000030
73	69	5	72	68	4	638.387070	-0.000030
74	37	37	73	36	37	638.394090	0.000424
74	38	37	73	37	37	638.394090	0.000424
74	33	41	73	32	41	638.414760	-0.000017
74	34	41	73	33	41	638.414760	-0.000017
74	64	10	73	63	10	638.447060	0.000012
74	64	11	73	63	11	638.447060	0.000011
74	64	10	73	63	11	638.447060	0.000011
74	64	11	73	63	10	638.447060	0.000012
73	72	1	72	71	1	638.459750	-0.000224
73	72	2	72	71	2	638.459750	-0.000224
73	72	1	72	71	2	638.459750	-0.000224
73	72	2	72	71	1	638.459750	-0.000224
74	65	9	73	64	9	638.471620	-0.000137
74	65	10	73	64	10	638.471620	-0.000137
74	65	9	73	64	10	638.471620	-0.000137
74	65	10	73	64	9	638.471620	-0.000137
74	66	8	73	65	8	638.496060	-0.000043
74	66	9	73	65	9	638.496060	-0.000043
74	66	8	73	65	9	638.496060	-0.000043
74	66	9	73	65	8	638.496060	-0.000043
74	67	7	73	66	7	638.519690	-0.000488
74	67	8	73	66	8	638.519690	-0.000488
74	67	7	73	66	8	638.519690	-0.000488
74	67	8	73	66	7	638.519690	-0.000488
74	69	5	73	68	5	638.568020	0.000085
74	69	6	73	68	6	638.568020	0.000085
75	44	32	74	43	32	638.568020	0.000392
75	43	32	74	42	32	638.568020	0.000392
74	69	5	73	68	6	638.568020	0.000085

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
74	69	6	73	68	5	638.568020	0.000085
74	70	4	73	69	4	638.592030	0.000278
74	70	5	73	69	5	638.592030	0.000278
74	70	4	73	69	5	638.592030	0.000278
74	70	5	73	69	4	638.592030	0.000278
75	65	10	74	64	10	638.653500	0.000089
75	65	11	74	64	11	638.653500	0.000089
75	65	10	74	64	11	638.653500	0.000089
75	65	11	74	64	10	638.653500	0.000089
74	73	1	73	72	1	638.663270	-0.000413
74	73	2	73	72	2	638.663270	-0.000413
74	73	1	73	72	2	638.663270	-0.000413
74	73	2	73	72	1	638.663270	-0.000413
75	66	9	74	65	9	638.677990	0.000197
75	66	10	74	65	10	638.677990	0.000197
75	66	9	74	65	10	638.677990	0.000197
75	66	10	74	65	9	638.677990	0.000197
75	67	8	74	66	8	638.701870	0.000062
75	67	9	74	66	9	638.701870	0.000062
75	67	8	74	66	9	638.701870	0.000062
75	67	9	74	66	8	638.701870	0.000062
75	68	7	74	67	7	638.725580	-0.000009
75	68	8	74	67	8	638.725580	-0.000009
75	68	7	74	67	8	638.725580	-0.000009
75	68	8	74	67	7	638.725580	-0.000009
76	66	10	75	65	10	638.859810	0.000275
76	66	11	75	65	11	638.859810	0.000275
76	66	10	75	65	11	638.859810	0.000275
76	66	11	75	65	10	638.859810	0.000275
76	67	9	75	66	9	638.883590	-0.000004
76	67	10	75	66	10	638.883590	-0.000004
76	67	9	75	66	10	638.883590	-0.000004
76	67	10	75	66	9	638.883590	-0.000004
76	69	7	75	68	7	638.930680	-0.000110
76	69	8	75	68	8	638.930680	-0.000110
76	69	7	75	68	8	638.930680	-0.000110
76	69	8	75	68	7	638.930680	-0.000110
77	67	10	76	66	10	639.066040	0.000638
77	67	11	76	66	11	639.066040	0.000638
77	67	10	76	66	11	639.066040	0.000638
77	67	11	76	66	10	639.066040	0.000638
77	68	9	76	67	9	639.089610	0.000438
77	68	10	76	67	10	639.089610	0.000438
77	68	9	76	67	10	639.089610	0.000438
77	68	10	76	67	9	639.089610	0.000438
77	70	7	76	69	7	639.136210	0.000427

Continuation, see next page

Continuation of Table 28:$\nu_{22} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
77	70	8	76	69	8	639.136210	0.000427
77	70	7	76	69	8	639.136210	0.000427
77	70	8	76	69	7	639.136210	0.000427
78	69	9	77	68	9	639.295010	0.000519
78	69	10	77	68	10	639.295010	0.000519
78	69	9	77	68	10	639.295010	0.000519
78	69	10	77	68	9	639.295010	0.000519

Table 29: Rovibrational transition wavenumbers $\tilde{\nu}_{obs}$ for the fundamental $\nu_{17} \leftarrow gs$ of dithiine. J'', K_a'' and K_c'' are lower state quantum numbers, J', K_a' and K_c' are upper state quantum numbers, $\tilde{\nu}_{\text{obs.}}$ = observed wavenumber, $\tilde{\nu}_{\text{cal.}}$ = wavenumber calculated with the parameters in Table 10. All wavenumbers are given in cm^{-1}.

Table 29: Rovibrational transitions of $\nu_{17} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
32	9	24	33	8	25	1304.18320	0.00021
32	8	24	33	9	25	1304.18320	0.00021
31	9	22	32	10	23	1304.20211	0.00010
31	10	22	32	9	23	1304.20211	0.00010
30	11	20	31	10	21	1304.22101	0.00008
30	10	20	31	11	21	1304.22101	0.00008
29	11	18	30	12	19	1304.23964	-0.00001
29	12	18	30	11	19	1304.23964	-0.00001
32	7	25	33	8	26	1304.28066	0.00006
32	8	25	33	7	26	1304.28066	0.00006
31	8	23	32	9	24	1304.29990	0.00020
31	9	23	32	8	24	1304.29990	0.00020
30	10	21	31	9	22	1304.31891	0.00016
30	9	21	31	10	22	1304.31891	0.00016
29	10	19	30	11	20	1304.33757	-0.00011
29	11	19	30	10	20	1304.33757	-0.00011
32	7	26	33	6	27	1304.37821	0.00006
32	6	26	33	7	27	1304.37821	0.00006
31	8	24	32	7	25	1304.39732	0.00001
31	7	24	32	8	25	1304.39732	0.00001
30	8	22	31	9	23	1304.41640	-0.00005
30	9	22	31	8	23	1304.41640	-0.00005
29	9	20	30	10	21	1304.43550	-0.00003

Continuation, see next page

Continuation of Table 29: $\nu_{17} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
29	10	20	30	9	21	1304.43550	-0.00003
28	11	18	29	10	19	1304.45457	0.00012
28	10	18	29	11	19	1304.45457	0.00012
31	6	25	32	7	26	1304.49517	0.00031
31	7	25	32	6	26	1304.49517	0.00031
30	7	23	31	8	24	1304.51398	-0.00008
30	8	23	31	7	24	1304.51398	-0.00008
29	8	21	30	9	22	1304.53319	-0.00005
29	9	21	30	8	22	1304.53319	-0.00005
28	10	19	29	9	20	1304.55250	0.00017
28	9	19	29	10	20	1304.55250	0.00017
31	5	26	32	6	27	1304.59222	-0.00014
31	6	26	32	5	27	1304.59222	-0.00014
30	6	24	31	7	25	1304.61145	-0.00016
30	7	24	31	6	25	1304.61145	-0.00016
29	7	22	30	8	23	1304.63090	0.00004
29	8	22	30	7	23	1304.63090	0.00004
28	9	20	29	8	21	1304.65007	0.00000
28	8	20	29	9	21	1304.65007	0.00000
27	9	18	28	10	19	1304.66937	0.00021
27	10	18	28	9	19	1304.66937	0.00021
30	5	25	31	6	26	1304.70931	0.00021
30	6	25	31	5	26	1304.70931	0.00021
29	6	23	30	7	24	1304.72873	0.00033
29	7	23	30	6	24	1304.72873	0.00033
28	7	21	29	8	22	1304.74765	-0.00004
28	8	21	29	7	22	1304.74765	-0.00004
27	8	19	28	9	20	1304.76696	0.00004
27	9	19	28	8	20	1304.76696	0.00004
26	10	17	27	9	18	1304.78623	0.00021
26	9	17	27	10	18	1304.78623	0.00021
30	4	26	31	5	27	1304.80657	0.00001
30	5	26	31	4	27	1304.80657	0.00001
29	5	24	30	6	25	1304.82604	0.00015
29	6	24	30	5	25	1304.82604	0.00015
28	7	22	29	6	23	1304.84535	0.00011
28	6	22	29	7	23	1304.84535	0.00011
27	8	20	28	7	21	1304.86465	0.00009
27	7	20	28	8	21	1304.86465	0.00009
26	9	18	27	8	19	1304.88417	0.00036
26	8	18	27	9	19	1304.88417	0.00036
30	4	27	31	3	28	1304.90416	0.00017
30	3	27	31	4	28	1304.90416	0.00017
29	4	25	30	5	26	1304.92325	-0.00009
29	5	25	30	4	26	1304.92325	-0.00009
28	5	23	29	6	24	1304.94274	0.00002

Continuation, see next page

Continuation of Table 29: $\nu_{17} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
28	6	23	29	5	24	1304.94274	0.00002
27	6	21	28	7	22	1304.96239	0.00028
27	7	21	28	6	22	1304.96239	0.00028
26	7	19	27	8	20	1304.98165	0.00019
26	8	19	27	7	20	1304.98165	0.00019
25	8	17	26	9	18	1305.00072	0.00001
25	9	17	26	8	18	1305.00072	0.00001
30	2	28	31	3	29	1305.00137	-0.00003
30	3	28	31	2	29	1305.00137	-0.00003
24	9	15	25	10	16	1305.01978	0.00003
24	10	15	25	9	16	1305.01978	0.00003
29	4	26	30	3	27	1305.02061	-0.00015
29	3	26	30	4	27	1305.02061	-0.00015
28	4	24	29	5	25	1305.03990	-0.00026
28	5	24	29	4	25	1305.03990	-0.00026
27	5	22	28	6	23	1305.05975	0.00016
27	6	22	28	5	23	1305.05975	0.00016
26	7	20	27	6	21	1305.07901	0.00000
26	6	20	27	7	21	1305.07901	0.00000
25	7	18	26	8	19	1305.09841	0.00003
25	8	18	26	7	19	1305.09841	0.00003
24	9	16	25	8	17	1305.11748	-0.00015
24	8	16	25	9	17	1305.11748	-0.00015
29	2	27	30	3	28	1305.11827	0.00011
29	3	27	30	2	28	1305.11827	0.00011
28	4	25	29	3	26	1305.13745	-0.00012
28	3	25	29	4	26	1305.13745	-0.00012
27	5	23	28	4	24	1305.15703	0.00001
27	4	23	28	5	24	1305.15703	0.00001
26	6	21	27	5	22	1305.17658	0.00009
26	5	21	27	6	22	1305.17658	0.00009
25	6	19	26	7	20	1305.19611	0.00017
25	7	19	26	6	20	1305.19611	0.00017
30	0	30	31	1	31	1305.19639	0.00020
30	1	30	31	0	31	1305.19639	0.00020
18	13	5	19	14	6	1305.21025	-0.00014
24	7	17	25	8	18	1305.21541	0.00008
24	8	17	25	7	18	1305.21541	0.00008
29	2	28	30	1	29	1305.21561	0.00006
29	1	28	30	2	29	1305.21561	0.00006
28	3	26	29	2	27	1305.23483	-0.00013
28	2	26	29	3	27	1305.23483	-0.00013
17	13	4	18	14	5	1305.24130	0.00021
27	4	24	28	3	25	1305.25450	0.00008
27	3	24	28	4	25	1305.25450	0.00008
26	4	22	27	5	23	1305.27407	0.00015

Continuation, see next page

Continuation of Table 29: $\nu_{17} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
26	5	22	27	4	23	1305.27407	0.00015
25	5	20	26	6	21	1305.29331	-0.00011
25	6	20	26	5	21	1305.29331	-0.00011
19	13	7	20	12	8	1305.30158	0.00023
29	0	29	30	1	30	1305.31304	0.00012
29	1	29	30	0	30	1305.31304	0.00012
24	7	18	25	6	19	1305.31304	0.00014
24	6	18	25	7	19	1305.31304	0.00014
28	2	27	29	1	28	1305.33242	0.00009
28	1	27	29	2	28	1305.33242	0.00009
23	8	16	24	7	17	1305.33242	0.00012
23	7	16	24	8	17	1305.33242	0.00012
27	2	25	28	3	26	1305.35194	0.00014
27	3	25	28	2	26	1305.35194	0.00014
26	3	23	27	4	24	1305.37127	-0.00004
26	4	23	27	3	24	1305.37127	-0.00004
25	4	21	26	5	22	1305.39109	0.00025
25	5	21	26	4	22	1305.39109	0.00025
19	11	8	20	12	9	1305.40333	0.00029
19	12	8	20	11	9	1305.40333	-0.00008
24	5	19	25	6	20	1305.41037	-0.00001
24	6	19	25	5	20	1305.41037	-0.00001
28	0	28	29	1	29	1305.42963	-0.00007
28	1	28	29	0	29	1305.42963	-0.00007
23	6	17	24	7	18	1305.42987	-0.00001
23	7	17	24	6	18	1305.42987	-0.00001
27	2	26	28	1	27	1305.44929	0.00013
27	1	26	28	2	27	1305.44929	0.00013
26	2	24	27	3	25	1305.46882	0.00015
26	3	24	27	2	25	1305.46882	0.00015
25	3	22	26	4	23	1305.48825	0.00003
25	4	22	26	3	23	1305.48825	0.00003
24	4	20	25	5	21	1305.50798	0.00018
24	5	20	25	4	21	1305.50798	0.00018
23	5	18	24	6	19	1305.52761	0.00024
23	6	18	24	5	19	1305.52761	0.00024
27	0	27	28	1	28	1305.54664	0.00013
27	1	27	28	0	28	1305.54664	0.00013
22	7	16	23	6	17	1305.54664	-0.00024
22	6	16	23	7	17	1305.54664	-0.00024
26	2	25	27	1	26	1305.56609	0.00007
26	1	25	27	2	26	1305.56609	0.00007
21	8	14	22	7	15	1305.56609	-0.00018
21	7	14	22	8	15	1305.56609	-0.00018
25	3	23	26	2	24	1305.58571	0.00013
25	2	23	26	3	24	1305.58571	0.00013

Continuation, see next page

Continuation of Table 29: $\nu_{17} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
24	3	21	25	4	22	1305.60542	0.00025
24	4	21	25	3	22	1305.60542	0.00025
23	4	19	24	5	20	1305.62469	-0.00009
23	5	19	24	4	20	1305.62469	-0.00009
22	6	17	23	5	18	1305.64458	0.00020
22	5	17	23	6	18	1305.64458	0.00020
26	0	26	27	1	27	1305.66348	0.00012
26	1	26	27	0	27	1305.66348	0.00012
21	7	15	22	6	16	1305.66386	-0.00004
21	6	15	22	7	16	1305.66386	-0.00004
14	12	2	15	13	3	1305.67126	0.00012
25	1	24	26	2	25	1305.68293	0.00001
25	2	24	26	1	25	1305.68293	0.00001
24	3	22	25	2	23	1305.70247	-0.00005
24	2	22	25	3	23	1305.70247	-0.00005
23	3	20	24	4	21	1305.72224	0.00009
23	4	20	24	3	21	1305.72224	0.00009
22	5	18	23	4	19	1305.74178	-0.00001
22	4	18	23	5	19	1305.74178	-0.00001
15	11	4	16	12	5	1305.75379	0.00001
21	5	16	22	6	17	1305.76126	-0.00015
21	6	16	22	5	17	1305.76126	-0.00015
25	0	25	26	1	26	1305.78019	-0.00005
25	1	25	26	0	26	1305.78019	-0.00005
20	7	14	21	6	15	1305.78086	-0.00008
20	6	14	21	7	15	1305.78086	-0.00008
24	1	23	25	2	24	1305.79993	0.00009
24	2	23	25	1	24	1305.79993	0.00009
19	7	12	20	8	13	1305.80016	-0.00009
19	8	12	20	7	13	1305.80016	-0.00009
14	11	3	15	12	4	1305.80400	-0.00003
18	9	10	19	8	11	1305.81900	-0.00003
18	8	10	19	9	11	1305.81900	-0.00003
23	3	21	24	2	22	1305.81952	0.00004
23	2	21	24	3	22	1305.81952	0.00004
22	3	19	23	4	20	1305.83908	-0.00007
22	4	19	23	3	20	1305.83908	-0.00007
21	4	17	22	5	18	1305.85876	-0.00006
21	5	17	22	4	18	1305.85876	-0.00006
20	5	15	21	6	16	1305.87854	0.00008
20	6	15	21	5	16	1305.87854	0.00008
24	1	24	25	0	25	1305.89715	-0.00001
24	0	24	25	1	25	1305.89715	-0.00001
19	6	13	20	7	14	1305.89766	-0.00031
19	7	13	20	6	14	1305.89766	-0.00031
23	1	22	24	2	23	1305.91693	0.00013

Continuation, see next page

Continuation of Table 29: $\nu_{17} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
23	2	22	24	1	23	1305.91693	0.00013
18	7	11	19	8	12	1305.91718	-0.00003
18	8	11	19	7	12	1305.91718	-0.00003
17	9	9	18	8	10	1305.93584	0.00011
17	8	9	18	9	10	1305.93584	0.00011
22	3	20	23	2	21	1305.93647	-0.00001
22	2	20	23	3	21	1305.93647	-0.00001
15	12	4	16	11	5	1305.95110	-0.00003
21	4	18	22	3	19	1305.95624	0.00006
21	3	18	22	4	19	1305.95624	0.00006
20	5	16	21	4	17	1305.97573	-0.00014
20	4	16	21	5	17	1305.97573	-0.00014
19	6	14	20	5	15	1305.99555	0.00003
19	5	14	20	6	15	1305.99555	0.00003
23	1	23	24	0	24	1306.01400	-0.00010
23	0	23	24	1	24	1306.01400	-0.00010
22	2	21	23	1	22	1306.03383	0.00005
22	1	21	23	2	22	1306.03383	0.00005
21	3	19	22	2	20	1306.05361	0.00012
21	2	19	22	3	20	1306.05361	0.00012
13	10	3	14	11	4	1306.05488	0.00006
12	11	1	13	12	2	1306.06170	0.00005
20	3	17	21	4	18	1306.07343	0.00021
20	4	17	21	3	18	1306.07343	0.00021
19	4	15	20	5	16	1306.09296	0.00002
19	5	15	20	4	16	1306.09296	0.00002
18	6	13	19	5	14	1306.11286	0.00027
18	5	13	19	6	14	1306.11286	0.00027
22	0	22	23	1	23	1306.13116	0.00009
22	1	22	23	0	23	1306.13116	0.00009
17	6	11	18	7	12	1306.13233	0.00028
17	7	11	18	6	12	1306.13233	0.00028
12	10	2	13	11	3	1306.14033	0.00013
21	2	20	22	1	21	1306.15077	-0.00002
21	1	20	22	2	21	1306.15077	-0.00002
20	3	18	21	2	19	1306.17058	0.00005
20	2	18	21	3	19	1306.17058	0.00005
19	3	16	20	4	17	1306.19018	-0.00011
19	4	16	20	3	17	1306.19018	-0.00011
18	4	14	19	5	15	1306.20978	-0.00024
18	5	14	19	4	15	1306.20978	-0.00024
17	5	12	18	6	13	1306.22979	0.00012
17	6	12	18	5	13	1306.22979	0.00012
21	1	21	22	0	22	1306.24809	0.00003
21	0	21	22	1	22	1306.24809	0.00003
20	2	19	21	1	20	1306.26791	0.00010

Continuation, see next page

Continuation of Table 29: $\nu_{17} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
20	1	19	21	2	20	1306.26791	0.00010
19	2	17	20	3	18	1306.28758	-0.00001
19	3	17	20	2	18	1306.28758	-0.00001
12	9	3	13	10	4	1306.30488	0.00006
30	3	27	30	4	26	1306.30512	-0.00006
30	4	27	30	5	26	1306.30512	-0.00006
33	7	27	33	8	26	1306.30676	-0.00001
33	6	27	33	7	26	1306.30676	-0.00001
18	3	15	19	4	16	1306.30737	0.00000
18	4	15	19	3	16	1306.30737	0.00000
34	7	27	34	8	26	1306.30737	-0.00003
34	8	27	34	9	26	1306.30737	-0.00003
35	9	27	35	10	26	1306.30818	0.00010
35	8	27	35	9	26	1306.30818	0.00010
17	4	13	18	5	14	1306.32709	-0.00003
17	5	13	18	4	14	1306.32709	-0.00003
13	10	4	14	9	5	1306.33084	0.00005
20	0	20	21	1	21	1306.36491	-0.00017
20	1	20	21	0	21	1306.36491	-0.00017
19	2	18	20	1	19	1306.38491	0.00005
19	1	18	20	2	19	1306.38491	0.00005
26	0	26	26	1	25	1306.40069	-0.00004
26	1	26	26	2	25	1306.40069	-0.00004
29	4	26	29	5	25	1306.40187	-0.00001
29	3	26	29	4	25	1306.40187	-0.00001
31	6	26	31	7	25	1306.40281	-0.00003
31	5	26	31	6	25	1306.40281	-0.00003
13	9	5	14	8	6	1306.40305	-0.00001
33	8	26	33	9	25	1306.40399	0.00000
33	7	26	33	8	25	1306.40399	0.00000
34	8	26	34	9	25	1306.40446	-0.00018
34	9	26	34	10	25	1306.40446	-0.00018
18	3	16	19	2	17	1306.40484	0.00017
18	2	16	19	3	17	1306.40484	0.00017
35	10	26	35	11	25	1306.40540	0.00006
35	9	26	35	10	25	1306.40540	0.00006
17	3	14	18	4	15	1306.42440	-0.00007
17	4	14	18	3	15	1306.42440	-0.00007
16	5	12	17	4	13	1306.44402	-0.00021
16	4	12	17	5	13	1306.44402	-0.00021
19	0	19	20	1	20	1306.48217	0.00005
19	1	19	20	0	20	1306.48217	0.00005
27	3	25	27	4	24	1306.49815	-0.00007
27	2	25	27	3	24	1306.49815	-0.00007
30	5	25	30	6	24	1306.49956	0.00003
30	6	25	30	7	24	1306.49956	0.00003

Continuation, see next page

Continuation of Table 29: $\nu_{17} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
13	7	6	14	8	7	1306.49980	-0.00034
18	1	17	19	2	18	1306.50189	-0.00004
18	2	17	19	1	18	1306.50189	-0.00004
34	9	25	34	10	24	1306.50189	-0.00005
34	10	25	34	11	24	1306.50189	-0.00005
35	11	25	35	12	24	1306.50262	-0.00006
35	10	25	35	11	24	1306.50262	-0.00006
17	3	15	18	2	16	1306.52183	0.00007
17	2	15	18	3	16	1306.52183	0.00007
16	3	13	17	4	14	1306.54146	-0.00012
16	4	13	17	3	14	1306.54146	-0.00012
15	4	11	16	5	12	1306.56161	0.00027
15	5	11	16	4	12	1306.56161	0.00027
18	1	18	19	0	19	1306.59946	0.00029
18	0	18	19	1	19	1306.59946	0.00029
17	1	16	18	2	17	1306.61919	0.00018
17	2	16	18	1	17	1306.61919	0.00018
16	3	14	17	2	15	1306.63865	-0.00021
16	2	14	17	3	15	1306.63865	-0.00021
15	4	12	16	3	13	1306.65905	0.00035
15	3	12	16	4	13	1306.65905	0.00035
17	0	17	18	1	18	1306.71612	-0.00012
17	1	17	18	0	18	1306.71612	-0.00012
15	3	13	16	2	14	1306.75576	-0.00022
15	2	13	16	3	14	1306.75576	-0.00022
14	3	11	15	4	12	1306.77614	0.00031
14	4	11	15	3	12	1306.77614	0.00031
26	4	22	26	5	21	1306.78935	-0.00007
26	5	22	26	6	21	1306.78935	-0.00007
27	6	22	27	7	21	1306.78985	-0.00001
27	5	22	27	6	21	1306.78985	-0.00001
30	8	22	30	9	21	1306.79147	0.00002
30	9	22	30	10	21	1306.79147	0.00002
32	10	22	32	11	21	1306.79288	0.00008
32	11	22	32	12	21	1306.79288	0.00008
34	12	22	34	13	21	1306.79430	-0.00011
34	13	22	34	14	21	1306.79430	-0.00011
37	16	22	37	17	21	1306.79736	-0.00004
37	15	22	37	16	21	1306.79736	-0.00004
12	6	7	13	5	8	1306.81496	0.00010
12	5	7	13	6	8	1306.81496	0.00011
16	1	16	17	0	17	1306.83321	-0.00012
16	0	16	17	1	17	1306.83321	-0.00012
15	1	14	16	2	15	1306.85339	0.00018
15	2	14	16	1	15	1306.85339	0.00018
24	3	21	24	4	20	1306.88587	-0.00003

Continuation, see next page

Continuation of Table 29: $\nu_{17} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
24	4	21	24	5	20	1306.88587	-0.00003
29	9	21	29	10	20	1306.88822	-0.00007
29	8	21	29	9	20	1306.88822	-0.00007
34	13	21	34	14	20	1306.89212	-0.00008
34	14	21	34	15	20	1306.89212	-0.00008
15	0	15	16	1	16	1306.95061	0.00019
15	1	15	16	0	16	1306.95061	0.00019
14	2	13	15	1	14	1306.97050	0.00016
14	1	13	15	2	14	1306.97050	0.00016
13	2	11	14	3	12	1306.99029	0.00004
13	3	11	14	2	12	1306.99029	0.00004
14	0	14	15	1	15	1307.06735	-0.00018
14	1	14	15	0	15	1307.06735	-0.00018
23	5	19	23	6	18	1307.08008	-0.00002
23	4	19	23	5	18	1307.08008	-0.00002
25	7	19	25	8	18	1307.08103	0.00003
25	6	19	25	7	18	1307.08103	0.00003
26	7	19	26	8	18	1307.08149	-0.00005
26	8	19	26	9	18	1307.08149	-0.00005
29	11	19	29	12	18	1307.08361	0.00007
29	10	19	29	11	18	1307.08361	0.00007
30	11	19	30	12	18	1307.08432	-0.00004
30	12	19	30	13	18	1307.08432	-0.00004
13	1	12	14	2	13	1307.08738	-0.00008
13	2	12	14	1	13	1307.08738	-0.00008
11	4	8	12	3	9	1307.12728	0.00005
11	3	8	12	4	9	1307.12728	0.00005
22	4	18	22	5	17	1307.17707	0.00002
22	5	18	22	6	17	1307.17707	0.00002
25	8	18	25	9	17	1307.17835	-0.00017
25	7	18	25	8	17	1307.17835	-0.00017
28	10	18	28	11	17	1307.18060	-0.00001
28	11	18	28	12	17	1307.18060	-0.00001
31	14	18	31	15	17	1307.18319	-0.00028
31	13	18	31	14	17	1307.18319	-0.00028
34	16	18	34	17	17	1307.18750	0.00020
34	17	18	34	18	17	1307.18750	0.00020
38	20	18	38	21	17	1307.19433	0.00001
38	21	18	38	22	17	1307.19433	0.00001
12	1	11	13	2	12	1307.20438	-0.00022
12	2	11	13	1	12	1307.20438	-0.00022
11	2	9	12	3	10	1307.22461	0.00007
11	3	9	12	2	10	1307.22461	0.00007
10	4	7	11	3	8	1307.24432	-0.00003
10	3	7	11	4	8	1307.24432	-0.00003
29	13	17	29	14	16	1307.27991	0.00022

Continuation, see next page

Continuation of Table 29: $\nu_{17} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
29	12	17	29	13	16	1307.27991	0.00022
34	17	17	34	18	16	1307.28654	-0.00011
34	18	17	34	19	16	1307.28654	-0.00011
12	1	12	13	0	13	1307.30184	0.00006
12	0	12	13	1	13	1307.30184	0.00006
11	2	10	12	1	11	1307.32185	0.00010
11	1	10	12	2	11	1307.32185	0.00010
10	3	8	11	2	9	1307.34162	-0.00007
10	2	8	11	3	9	1307.34162	-0.00007
20	4	16	20	5	15	1307.37105	0.00001
20	5	16	20	6	15	1307.37105	0.00001
26	10	16	26	11	15	1307.37505	0.00004
26	11	16	26	12	15	1307.37505	0.00004
29	14	16	29	15	15	1307.37835	0.00001
29	13	16	29	14	15	1307.37835	0.00001
30	14	16	30	15	15	1307.37964	-0.00008
30	15	16	30	16	15	1307.37964	-0.00008
31	16	16	31	17	15	1307.38125	0.00001
31	15	16	31	16	15	1307.38125	0.00001
11	1	11	12	0	12	1307.41869	-0.00023
11	0	11	12	1	12	1307.41869	-0.00023
10	1	9	11	2	10	1307.43861	-0.00029
10	2	9	11	1	10	1307.43861	-0.00029
6	5	1	7	6	2	1307.44096	0.00006
9	2	7	10	3	8	1307.45890	0.00007
9	3	7	10	2	8	1307.45890	0.00007
17	3	15	17	4	14	1307.46733	0.00003
17	2	15	17	3	14	1307.46733	0.00003
18	3	15	18	4	14	1307.46764	-0.00002
18	4	15	18	5	14	1307.46764	-0.00002
19	5	15	19	6	14	1307.46804	-0.00004
19	4	15	19	5	14	1307.46804	-0.00004
22	7	15	22	8	14	1307.46978	-0.00002
22	8	15	22	9	14	1307.46978	-0.00002
26	11	15	26	12	14	1307.47345	-0.00001
26	12	15	26	13	14	1307.47345	-0.00001
28	13	15	28	14	14	1307.47604	-0.00002
28	14	15	28	15	14	1307.47604	-0.00002
8	4	5	9	3	6	1307.47863	0.00012
8	3	5	9	4	6	1307.47863	0.00019
9	2	8	10	1	9	1307.55615	0.00010
9	1	8	10	2	9	1307.55615	0.00010
17	4	14	17	5	13	1307.56455	-0.00015
17	3	14	17	4	13	1307.56455	-0.00015
20	6	14	20	7	13	1307.56626	-0.00003
20	7	14	20	8	13	1307.56626	-0.00003

Continuation, see next page

Continuation of Table 29: $\nu_{17} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
24	10	14	24	11	13	1307.56969	-0.00017
24	11	14	24	12	13	1307.56969	-0.00017
25	12	14	25	13	13	1307.57115	0.00007
25	11	14	25	12	13	1307.57115	0.00007
26	12	14	26	13	13	1307.57265	0.00018
26	13	14	26	14	13	1307.57265	0.00018
28	14	14	28	15	13	1307.57592	0.00013
28	15	14	28	16	13	1307.57592	0.00013
32	18	14	32	19	13	1307.58503	-0.00012
32	19	14	32	20	13	1307.58503	-0.00011
20	7	13	20	8	12	1307.66437	0.00007
20	8	13	20	9	12	1307.66437	0.00007
22	9	13	22	10	12	1307.66625	-0.00004
22	10	13	22	11	12	1307.66625	-0.00004
24	11	13	24	12	12	1307.66899	0.00007
24	12	13	24	13	12	1307.66899	0.00007
17	6	12	17	7	11	1307.75994	-0.00009
17	5	12	17	6	11	1307.75994	-0.00009
21	10	12	21	11	11	1307.76395	-0.00003
21	9	12	21	10	11	1307.76395	-0.00003
23	12	12	23	13	11	1307.76701	-0.00004
23	11	12	23	12	11	1307.76701	-0.00004
8	0	8	9	1	9	1307.77007	-0.00028
8	1	8	9	0	9	1307.77007	-0.00028
7	2	6	8	1	7	1307.79018	-0.00018
7	1	6	8	2	7	1307.79018	-0.00018
11	1	11	11	2	10	1307.85481	0.00001
11	0	11	11	1	10	1307.85481	0.00001
12	1	11	12	2	10	1307.85505	-0.00005
12	2	11	12	3	10	1307.85505	-0.00005
13	3	11	13	4	10	1307.85544	-0.00005
13	2	11	13	3	10	1307.85544	-0.00005
14	3	11	14	4	10	1307.85599	0.00002
14	4	11	14	5	10	1307.85599	0.00002
19	9	11	19	10	10	1307.86046	0.00001
19	8	11	19	9	10	1307.86046	0.00001
22	11	11	22	12	10	1307.86564	0.00006
22	12	11	22	13	10	1307.86564	0.00006
6	2	5	7	1	6	1307.90748	-0.00004
6	1	5	7	2	6	1307.90748	-0.00004
16	6	10	16	7	9	1307.95580	0.00013
16	7	10	16	8	9	1307.95580	0.00013
18	8	10	18	9	9	1307.95829	-0.00011
18	9	10	18	10	9	1307.95829	-0.00011
19	10	10	19	11	9	1307.96004	-0.00012
19	9	10	19	10	9	1307.96004	-0.00013

Continuation, see next page

Continuation of Table 29: $\nu_{17} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
20	10	10	20	11	9	1307.96223	-0.00004
20	11	10	20	12	9	1307.96223	-0.00001
21	12	10	21	13	9	1307.96475	0.00008
21	11	10	21	12	9	1307.96475	0.00000
22	13	10	22	14	9	1307.96737	-0.00013
6	0	6	7	1	7	1308.00481	0.00015
6	1	6	7	0	7	1308.00481	0.00015
5	1	4	6	2	5	1308.02455	-0.00009
5	2	4	6	1	5	1308.02478	0.00010
3	3	0	4	4	1	1308.02929	-0.00005
4	3	2	5	2	3	1308.05115	0.00003
11	3	8	11	4	7	1308.14766	0.00007
11	4	8	11	5	7	1308.14766	0.00007
17	10	8	17	11	7	1308.15825	0.00000
17	9	8	17	10	7	1308.15909	0.00007
19	12	8	19	13	7	1308.16482	-0.00011
24	17	8	24	18	7	1308.17916	-0.00031
5	2	4	4	1	3	1309.60461	-0.00012
22	15	8	22	14	9	1309.65583	0.00003
21	13	8	21	12	9	1309.66110	-0.00019
21	14	8	21	13	9	1309.66299	0.00013
20	13	8	20	12	9	1309.66911	0.00000
19	11	8	19	10	9	1309.67389	-0.00031
13	5	8	13	4	9	1309.69336	0.00016
13	6	8	13	5	9	1309.69336	0.00016
12	4	8	12	3	9	1309.69479	0.00014
12	5	8	12	4	9	1309.69479	0.00014
7	1	7	6	0	6	1309.74191	0.00018
7	0	7	6	1	6	1309.74191	0.00018
6	2	4	5	3	3	1309.81789	-0.00001
6	3	4	5	2	3	1309.81977	0.00000
25	16	10	25	15	11	1309.85394	0.00003
8	0	8	7	1	7	1309.85864	-0.00022
8	1	8	7	0	7	1309.85864	-0.00022
19	10	10	19	9	11	1309.87968	-0.00015
19	9	10	19	8	11	1309.87968	-0.00015
17	8	10	17	7	11	1309.88421	-0.00024
17	7	10	17	6	11	1309.88421	-0.00024
14	5	10	14	4	11	1309.88874	-0.00020
14	4	10	14	3	11	1309.88874	-0.00020
13	4	10	13	3	11	1309.89016	0.00022
13	3	10	13	2	11	1309.89016	0.00022
18	8	11	18	7	12	1309.98197	0.00010
18	7	11	18	6	12	1309.98197	0.00010
17	7	11	17	6	12	1309.98361	0.00010
17	6	11	17	5	12	1309.98361	0.00010

Continuation, see next page

Continuation of Table 29: $\nu_{17} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
13	3	11	13	2	12	1309.98785	0.00008
13	2	11	13	1	12	1309.98785	0.00008
8	2	6	7	3	5	1310.05258	-0.00018
8	3	6	7	2	5	1310.05258	-0.00020
25	13	12	25	12	13	1310.06369	-0.00011
25	14	12	25	13	13	1310.06369	-0.00011
23	12	12	23	11	13	1310.07048	0.00012
23	11	12	23	10	13	1310.07048	0.00012
22	11	12	22	10	13	1310.07307	0.00002
22	10	12	22	9	13	1310.07307	0.00002
16	5	12	16	4	13	1310.08319	0.00007
16	4	12	16	3	13	1310.08319	0.00007
15	4	12	15	3	13	1310.08413	0.00009
15	3	12	15	2	13	1310.08413	0.00009
23	11	13	23	10	14	1310.17076	-0.00006
23	10	13	23	9	14	1310.17076	-0.00006
21	9	13	21	8	14	1310.17488	0.00002
21	8	13	21	7	14	1310.17488	0.00002
15	2	13	15	1	14	1310.18183	0.00000
15	3	13	15	2	14	1310.18183	0.00000
10	1	9	9	2	8	1310.19030	0.00027
10	2	9	9	1	8	1310.19030	0.00027
11	1	11	10	0	10	1310.21008	-0.00019
11	0	11	10	1	10	1310.21008	-0.00019
29	16	14	29	15	15	1310.25437	0.00027
29	15	14	29	14	15	1310.25437	0.00027
27	14	14	27	13	15	1310.26093	0.00010
27	13	14	27	12	15	1310.26093	0.00010
26	12	14	26	11	15	1310.26352	-0.00015
26	13	14	26	12	15	1310.26352	-0.00015
10	2	8	9	3	7	1310.28694	0.00000
10	3	8	9	2	7	1310.28694	0.00000
11	2	10	10	1	9	1310.30687	-0.00029
11	1	10	10	2	9	1310.30687	-0.00029
12	0	12	11	1	11	1310.32724	-0.00017
12	1	12	11	0	11	1310.32724	-0.00017
33	18	15	33	17	16	1310.34120	0.00017
33	19	15	33	18	16	1310.34120	0.00017
32	17	15	32	16	16	1310.34569	0.00032
32	18	15	32	17	16	1310.34569	0.00032
26	11	15	26	10	16	1310.36407	0.00013
26	12	15	26	11	16	1310.36407	0.00013
22	8	15	22	7	16	1310.37084	-0.00015
22	7	15	22	6	16	1310.37084	-0.00015
21	6	15	21	5	16	1310.37227	0.00000
21	7	15	21	6	16	1310.37227	0.00000

Continuation, see next page

Continuation of Table 29: $\nu_{17} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
20	5	15	20	4	16	1310.37345	0.00006
20	6	15	20	5	16	1310.37345	0.00006
19	4	15	19	3	16	1310.37451	0.00015
19	5	15	19	4	16	1310.37451	0.00015
17	3	15	17	2	16	1310.37597	0.00006
17	2	15	17	1	16	1310.37597	0.00006
10	3	7	9	4	6	1310.38404	0.00012
10	4	7	9	3	6	1310.38404	0.00012
11	3	9	10	2	8	1310.40405	0.00001
11	2	9	10	3	8	1310.40405	0.00001
12	1	11	11	2	10	1310.42430	0.00001
12	2	11	11	1	10	1310.42430	0.00001
33	17	16	33	16	17	1310.44424	-0.00031
33	18	16	33	17	17	1310.44424	-0.00031
32	17	16	32	16	17	1310.44808	-0.00005
32	16	16	32	15	17	1310.44808	-0.00005
31	16	16	31	15	17	1310.45137	-0.00001
31	15	16	31	14	17	1310.45137	-0.00001
25	10	16	25	9	17	1310.46526	-0.00002
25	9	16	25	8	17	1310.46526	-0.00002
24	9	16	24	8	17	1310.46667	-0.00016
24	8	16	24	7	17	1310.46667	-0.00016
23	8	16	23	7	17	1310.46828	0.00007
23	7	16	23	6	17	1310.46828	0.00007
22	6	16	22	5	17	1310.46950	0.00007
22	7	16	22	6	17	1310.46950	0.00007
12	2	10	11	3	9	1310.52128	0.00013
12	3	10	11	2	9	1310.52128	0.00013
35	19	17	35	18	18	1310.53989	0.00000
35	18	17	35	17	18	1310.53989	0.00000
33	17	17	33	16	18	1310.54671	-0.00002
33	16	17	33	15	18	1310.54671	-0.00002
32	15	17	32	14	18	1310.54977	0.00006
32	16	17	32	15	18	1310.54977	0.00006
30	13	17	30	12	18	1310.55495	0.00004
30	14	17	30	13	18	1310.55495	0.00004
29	13	17	29	12	18	1310.55703	-0.00012
29	12	17	29	11	18	1310.55703	-0.00012
14	0	14	13	1	13	1310.56186	0.00015
14	1	14	13	0	13	1310.56186	0.00015
21	4	17	21	3	18	1310.56861	0.00007
21	5	17	21	4	18	1310.56861	0.00007
19	2	17	19	1	18	1310.56978	-0.00026
19	3	17	19	2	18	1310.56978	-0.00026
11	5	7	10	4	6	1310.59799	-0.00006
11	4	7	10	5	6	1310.59799	-0.00004

Continuation, see next page

Continuation of Table 29: $\nu_{17} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
13	3	11	12	2	10	1310.63829	0.00002
13	2	11	12	3	10	1310.63829	0.00002
25	7	18	25	6	19	1310.66276	0.00011
25	8	18	25	7	19	1310.66276	0.00011
23	5	18	23	4	19	1310.66489	0.00012
23	6	18	23	5	19	1310.66489	0.00012
22	5	18	22	4	19	1310.66558	-0.00007
22	4	18	22	3	19	1310.66558	-0.00007
21	4	18	21	3	19	1310.66630	-0.00014
21	3	18	21	2	19	1310.66630	-0.00014
15	1	15	14	0	14	1310.67911	0.00025
15	0	15	14	1	14	1310.67911	0.00025
14	2	12	13	3	11	1310.75528	-0.00011
14	3	12	13	2	11	1310.75528	-0.00011
29	11	19	29	10	20	1310.75577	-0.00012
29	10	19	29	9	20	1310.75577	-0.00012
28	9	19	28	8	20	1310.75764	0.00028
28	10	19	28	9	20	1310.75764	0.00028
27	8	19	27	7	20	1310.75882	0.00013
27	9	19	27	8	20	1310.75882	0.00013
25	6	19	25	5	20	1310.76093	-0.00003
25	7	19	25	6	20	1310.76093	-0.00003
23	4	19	23	3	20	1310.76284	0.00006
15	2	14	14	1	13	1310.77544	-0.00026
15	1	14	14	2	13	1310.77544	-0.00026
16	0	16	15	1	15	1310.79629	0.00026
16	1	16	15	0	15	1310.79629	0.00026
13	5	9	12	4	8	1310.83208	0.00004
13	4	9	12	5	8	1310.83208	0.00004
35	16	20	35	15	21	1310.84410	0.00001
35	15	20	35	14	21	1310.84410	0.00001
33	14	20	33	13	21	1310.84848	0.00021
33	13	20	33	12	21	1310.84848	0.00021
31	12	20	31	11	21	1310.85204	0.00025
31	11	20	31	10	21	1310.85204	0.00025
14	3	11	13	4	10	1310.85227	0.00004
14	4	11	13	3	10	1310.85227	0.00004
30	11	20	30	10	21	1310.85321	-0.00011
30	10	20	30	9	21	1310.85321	-0.00011
24	5	20	24	4	21	1310.85981	-0.00012
24	4	20	24	3	21	1310.85981	-0.00012
23	4	20	23	3	21	1310.86075	0.00008
23	3	20	23	2	21	1310.86075	0.00008
22	2	20	22	1	21	1310.86140	0.00006
22	3	20	22	2	21	1310.86140	0.00006
21	2	20	21	1	21	1310.86192	0.00000

Continuation, see next page

Continuation of Table 29: $\nu_{17} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
21	1	20	21	0	21	1310.86192	0.00000
15	3	13	14	2	12	1310.87241	-0.00012
15	2	13	14	3	12	1310.87241	-0.00012
16	1	15	15	2	14	1310.89278	-0.00007
16	2	15	15	1	14	1310.89278	-0.00007
17	1	17	16	0	16	1310.91300	-0.00020
17	0	17	16	1	16	1310.91300	-0.00020
35	14	21	35	13	22	1310.94405	-0.00008
35	15	21	35	14	22	1310.94405	-0.00008
14	4	10	13	5	9	1310.94892	-0.00018
14	5	10	13	4	9	1310.94892	-0.00018
32	12	21	32	11	22	1310.94926	-0.00006
32	11	21	32	10	22	1310.94926	-0.00006
31	11	21	31	10	22	1310.95067	-0.00010
31	10	21	31	9	22	1310.95067	-0.00010
30	9	21	30	8	22	1310.95209	0.00000
30	10	21	30	9	22	1310.95209	0.00000
29	8	21	29	7	22	1310.95326	-0.00004
29	9	21	29	8	22	1310.95326	-0.00004
26	5	21	26	4	22	1310.95632	0.00003
26	6	21	26	5	22	1310.95632	0.00003
25	4	21	25	3	22	1310.95703	-0.00007
25	5	21	25	4	22	1310.95703	-0.00007
15	4	12	14	3	11	1310.96957	0.00022
15	3	12	14	4	11	1310.96957	0.00022
16	2	14	15	3	13	1310.98952	-0.00014
16	3	14	15	2	13	1310.98952	-0.00014
18	0	18	17	1	17	1311.03035	-0.00003
18	1	18	17	0	17	1311.03035	-0.00003
38	17	22	38	16	23	1311.03804	0.00001
38	16	22	38	15	23	1311.03804	0.00001
37	16	22	37	15	23	1311.03990	-0.00019
37	15	22	37	14	23	1311.03990	-0.00019
35	14	22	35	13	23	1311.04390	0.00016
35	13	22	35	12	23	1311.04390	0.00016
34	12	22	34	11	23	1311.04523	-0.00014
34	13	22	34	12	23	1311.04523	-0.00014
29	8	22	29	7	23	1311.05166	-0.00002
29	7	22	29	6	23	1311.05166	-0.00002
28	6	22	28	5	23	1311.05261	-0.00003
28	7	22	28	6	23	1311.05261	-0.00003
24	3	22	24	2	23	1311.05552	-0.00011
24	2	22	24	1	23	1311.05552	-0.00011
15	5	11	14	4	10	1311.06626	0.00008
15	4	11	14	5	10	1311.06626	0.00008
16	3	13	15	4	12	1311.08650	0.00003

Continuation, see next page

Continuation of Table 29: $\nu_{17} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
16	4	13	15	3	12	1311.08650	0.00003
17	3	15	16	2	14	1311.10677	-0.00004
17	2	15	16	3	14	1311.10677	-0.00004
13	7	6	12	8	5	1311.12323	-0.00019
18	1	17	17	2	16	1311.12746	0.00028
18	2	17	17	1	16	1311.12746	0.00028
13	8	6	12	7	5	1311.12746	0.00002
19	1	19	18	0	18	1311.14755	-0.00002
19	0	19	18	1	18	1311.14755	-0.00002
16	4	12	15	5	11	1311.18342	0.00014
16	5	12	15	4	11	1311.18342	0.00014
17	4	14	16	3	13	1311.20357	-0.00003
17	3	14	16	4	13	1311.20357	-0.00003
19	2	18	18	1	17	1311.24447	0.00011
19	1	18	18	2	17	1311.24447	0.00011
20	0	20	19	1	19	1311.26494	0.00016
20	1	20	19	0	19	1311.26494	0.00016
17	5	13	16	4	12	1311.30049	0.00010
17	4	13	16	5	12	1311.30049	0.00010
18	3	15	17	4	14	1311.32074	0.00000
18	4	15	17	3	14	1311.32074	0.00000
35	10	25	35	9	26	1311.34075	-0.00002
35	11	25	35	10	26	1311.34075	-0.00002
19	3	17	18	2	16	1311.34124	0.00010
19	2	17	18	3	16	1311.34124	0.00010
33	9	25	33	8	26	1311.34287	0.00005
33	8	25	33	7	26	1311.34287	0.00005
32	8	25	32	7	26	1311.34382	0.00009
32	7	25	32	6	26	1311.34382	0.00009
28	3	25	28	2	26	1311.34663	-0.00005
28	4	25	28	3	26	1311.34663	-0.00005
27	3	25	27	2	26	1311.34729	0.00002
27	2	25	27	1	26	1311.34729	0.00002
20	1	19	19	2	18	1311.36149	-0.00007
20	2	19	19	1	18	1311.36149	-0.00007
21	1	21	20	0	20	1311.38194	-0.00006
21	0	21	20	1	20	1311.38194	-0.00006
17	6	12	16	5	11	1311.39740	0.00021
17	5	12	16	6	11	1311.39740	0.00021
14	9	5	13	10	4	1311.40689	0.00020
18	4	14	17	5	13	1311.41756	0.00005
18	5	14	17	4	13	1311.41756	0.00005
13	10	4	12	9	3	1311.42950	0.00004
19	4	16	18	3	15	1311.43797	0.00007
19	3	16	18	4	15	1311.43797	0.00007
33	8	26	33	7	27	1311.44103	-0.00012

Continuation, see next page

Continuation of Table 29: $\nu_{17} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
33	7	26	33	6	27	1311.44103	-0.00012
29	4	26	29	3	27	1311.44397	0.00000
29	3	26	29	2	27	1311.44397	0.00000
28	2	26	28	1	27	1311.44456	0.00002
28	3	26	28	2	27	1311.44456	0.00002
27	1	26	27	0	27	1311.44503	-0.00003
27	2	26	27	1	27	1311.44503	-0.00003
20	2	18	19	3	17	1311.45845	0.00013
20	3	18	19	2	17	1311.45845	0.00013
21	2	20	20	1	19	1311.47860	-0.00017
21	1	20	20	2	19	1311.47860	-0.00017
17	7	11	16	6	10	1311.49400	-0.00005
17	6	11	16	7	10	1311.49400	-0.00005
22	0	22	21	1	21	1311.49913	-0.00011
22	1	22	21	0	21	1311.49913	-0.00011
18	5	13	17	6	12	1311.51424	-0.00005
18	6	13	17	5	12	1311.51424	-0.00005
19	5	15	18	4	14	1311.53449	-0.00016
19	4	15	18	5	14	1311.53449	-0.00016
38	11	27	38	10	28	1311.53503	0.00006
38	12	27	38	11	28	1311.53503	0.00006
34	7	27	34	6	28	1311.53873	0.00012
34	8	27	34	7	28	1311.53873	0.00012
32	5	27	32	4	28	1311.54016	0.00010
32	6	27	32	5	28	1311.54016	0.00010
31	4	27	31	3	28	1311.54061	-0.00009
31	5	27	31	4	28	1311.54061	-0.00009
29	2	27	29	1	28	1311.54179	-0.00006
29	3	27	29	2	28	1311.54179	-0.00006
20	3	17	19	4	16	1311.55541	0.00034
20	4	17	19	3	16	1311.55541	0.00034
21	3	19	20	2	18	1311.57545	-0.00007
21	2	19	20	3	18	1311.57545	-0.00007
22	1	21	21	2	20	1311.59616	0.00017
22	2	21	21	1	20	1311.59616	0.00017
13	11	3	12	10	2	1311.60488	-0.00013
18	6	12	17	7	11	1311.61131	0.00022
18	7	12	17	6	11	1311.61131	0.00022
23	1	23	22	0	22	1311.61640	-0.00009
23	0	23	22	1	22	1311.61640	-0.00009
19	6	14	18	5	13	1311.63162	0.00022
19	5	14	18	6	13	1311.63162	0.00022
20	4	16	19	5	15	1311.65195	0.00015
20	5	16	19	4	15	1311.65195	0.00015
21	4	18	20	3	17	1311.67242	0.00017
21	3	18	20	4	17	1311.67242	0.00017

Continuation, see next page

Continuation of Table 29: $\nu_{17} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
22	2	20	21	3	19	1311.69268	-0.00005
22	3	20	21	2	19	1311.69268	-0.00005
18	7	11	17	8	10	1311.70798	-0.00001
18	8	11	17	7	10	1311.70798	-0.00001
23	2	22	22	1	21	1311.71316	-0.00008
23	1	22	22	2	21	1311.71316	-0.00008
19	7	13	18	6	12	1311.72799	-0.00018
19	6	13	18	7	12	1311.72799	-0.00018
24	0	24	23	1	23	1311.73364	-0.00013
24	1	24	23	0	23	1311.73364	-0.00013
20	5	15	19	6	14	1311.74858	0.00005
20	6	15	19	5	14	1311.74858	0.00005
21	5	17	20	4	16	1311.76871	-0.00026
21	4	17	20	5	16	1311.76871	-0.00026
22	3	19	21	4	18	1311.78940	-0.00005
22	4	19	21	3	18	1311.78940	-0.00005
18	8	10	17	9	9	1311.80497	-0.00013
18	9	10	17	8	9	1311.80497	-0.00013
23	3	21	22	2	20	1311.81015	0.00019
23	2	21	22	3	20	1311.81015	0.00019
19	8	12	18	7	11	1311.82450	-0.00049
19	7	12	18	8	11	1311.82450	-0.00049
24	1	23	23	2	22	1311.83054	0.00004
24	2	23	23	1	22	1311.83054	0.00004
20	6	14	19	7	13	1311.84523	-0.00004
20	7	14	19	6	13	1311.84523	-0.00004
25	1	25	24	0	24	1311.85098	-0.00009
25	0	25	24	1	24	1311.85098	-0.00009
21	6	16	20	5	15	1311.86571	0.00003
21	5	16	20	6	15	1311.86571	0.00003
22	4	18	21	5	17	1311.88588	-0.00027
22	5	18	21	4	17	1311.88588	-0.00027
23	4	20	22	3	19	1311.90647	-0.00020
23	3	20	22	4	19	1311.90647	-0.00020
24	2	22	23	3	21	1311.92720	-0.00001
24	3	22	23	2	21	1311.92720	-0.00001
25	2	24	24	1	23	1311.94757	-0.00021
25	1	24	24	2	23	1311.94757	-0.00021
21	7	15	20	6	14	1311.96211	-0.00028
21	6	15	20	7	14	1311.96211	-0.00028
26	0	26	25	1	25	1311.96835	-0.00004
26	1	26	25	0	25	1311.96835	-0.00004
22	5	17	21	6	16	1311.98286	0.00001
22	6	17	21	5	16	1311.98286	0.00001
23	5	19	22	4	18	1312.00343	0.00007
23	4	19	22	5	18	1312.00343	0.00007

Continuation, see next page

Continuation of Table 29: $\nu_{17} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
24	3	21	23	4	20	1312.02383	-0.00007
24	4	21	23	3	20	1312.02383	-0.00007
25	3	23	24	2	22	1312.04453	0.00005
25	2	23	24	3	22	1312.04453	0.00005
21	8	14	20	7	13	1312.05909	-0.00003
21	7	14	20	8	13	1312.05909	-0.00003
26	1	25	25	2	24	1312.06500	-0.00009
26	2	25	25	1	24	1312.06500	-0.00009
22	6	16	21	7	15	1312.07964	0.00011
22	7	16	21	6	15	1312.07964	0.00011
27	1	27	26	0	26	1312.08582	0.00008
27	0	27	26	1	26	1312.08582	0.00008
23	6	18	22	5	17	1312.09996	-0.00007
23	5	18	22	6	17	1312.09996	-0.00007
24	4	20	23	5	19	1312.12063	0.00005
24	5	20	23	4	19	1312.12063	0.00005
25	4	22	24	3	21	1312.14104	-0.00012
25	3	22	24	4	21	1312.14104	-0.00012
26	2	24	25	3	23	1312.16164	-0.00014
26	3	24	25	2	23	1312.16164	-0.00014
22	7	15	21	8	14	1312.17623	0.00000
22	8	15	21	7	14	1312.17623	0.00000
27	2	26	26	1	25	1312.18233	-0.00010
27	1	26	26	2	25	1312.18233	-0.00010
23	7	17	22	6	16	1312.19669	-0.00001
23	6	17	22	7	16	1312.19669	-0.00001
28	0	28	27	1	27	1312.20305	-0.00007
28	1	28	27	0	27	1312.20305	-0.00007
24	5	19	23	6	18	1312.21717	-0.00007
24	6	19	23	5	18	1312.21717	-0.00007
25	5	21	24	4	20	1312.23765	-0.00018
25	4	21	24	5	20	1312.23765	-0.00018
21	10	12	20	9	11	1312.25294	0.00013
21	9	12	20	10	11	1312.25294	0.00013
26	3	23	25	4	22	1312.25836	-0.00009
26	4	23	25	3	22	1312.25836	-0.00009
22	8	14	21	9	13	1312.27273	-0.00023
22	9	14	21	8	13	1312.27273	-0.00023
27	3	25	26	2	24	1312.27909	-0.00001
27	2	25	26	3	24	1312.27909	-0.00001
23	8	16	22	7	15	1312.29352	0.00015
23	7	16	22	8	15	1312.29352	0.00015
28	1	27	27	2	26	1312.29980	0.00000
28	2	27	27	1	26	1312.29980	0.00000
24	6	18	23	7	17	1312.31404	0.00015
24	7	18	23	6	17	1312.31404	0.00015

Continuation, see next page

Continuation of Table 29: $\nu_{17} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
29	1	29	28	0	28	1312.32033	-0.00020
29	0	29	28	1	28	1312.32033	-0.00020
25	6	20	24	5	19	1312.33441	-0.00006
25	5	20	24	6	19	1312.33441	-0.00006
26	4	22	25	5	21	1312.35486	-0.00024
26	5	22	25	4	21	1312.35486	-0.00024
27	4	24	26	3	23	1312.37546	-0.00030
27	3	24	26	4	23	1312.37546	-0.00030
28	2	26	27	3	25	1312.39632	-0.00014
28	3	26	27	2	25	1312.39632	-0.00014
24	7	17	23	8	16	1312.41044	-0.00009
24	8	17	23	7	16	1312.41044	-0.00009
29	2	28	28	1	27	1312.41730	0.00011
29	1	28	28	2	27	1312.41730	0.00011
25	7	19	24	6	18	1312.43114	0.00004
25	6	19	24	7	18	1312.43114	0.00004
30	0	30	29	1	29	1312.43799	0.00002
30	1	30	29	0	29	1312.43799	0.00002
26	5	21	25	6	20	1312.45173	0.00000
26	6	21	25	5	20	1312.45173	0.00000
27	5	23	26	4	22	1312.47204	-0.00035
27	4	23	26	5	22	1312.47204	-0.00035
18	14	5	17	13	4	1312.48037	-0.00011
28	3	25	27	4	24	1312.49292	-0.00018
28	4	25	27	3	24	1312.49292	-0.00018
24	8	16	23	9	15	1312.50696	-0.00023
24	9	16	23	8	15	1312.50696	-0.00023
29	3	27	28	2	26	1312.51394	0.00010
29	2	27	28	3	26	1312.51394	0.00010
25	8	18	24	7	17	1312.52779	0.00006
25	7	18	24	8	17	1312.52779	0.00006
30	1	29	29	2	28	1312.53484	0.00022
30	2	29	29	1	28	1312.53484	0.00022
26	6	20	25	7	19	1312.54832	-0.00002
26	7	20	25	6	19	1312.54832	-0.00002
27	6	22	26	5	21	1312.56882	-0.00019
27	5	22	26	6	21	1312.56882	-0.00019
28	4	24	27	5	23	1312.58937	-0.00035
28	5	24	27	4	23	1312.58937	-0.00035
29	4	26	28	3	25	1312.61050	0.00003
29	3	26	28	4	25	1312.61050	0.00003
25	9	17	24	8	16	1312.62435	0.00000
25	8	17	24	9	16	1312.62435	0.00000
30	2	28	29	3	27	1312.63126	0.00000
30	3	28	29	2	27	1312.63126	0.00000
26	7	19	25	8	18	1312.64486	-0.00008

Continuation, see next page

Continuation of Table 29: $\nu_{17} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
26	8	19	25	7	18	1312.64486	-0.00008
27	7	21	26	6	20	1312.66571	0.00010
27	6	21	26	7	20	1312.66571	0.00010
28	5	23	27	6	22	1312.68614	-0.00018
28	6	23	27	5	22	1312.68614	-0.00018
29	5	25	28	4	24	1312.70706	-0.00002
29	4	25	28	5	24	1312.70706	-0.00002
30	3	27	29	4	26	1312.72777	-0.00010
30	4	27	29	3	26	1312.72777	-0.00010
26	8	18	25	9	17	1312.74112	-0.00042
26	9	18	25	8	17	1312.74112	-0.00042
27	8	20	26	7	19	1312.76196	-0.00023
27	7	20	26	8	19	1312.76196	-0.00023
28	6	22	27	7	21	1312.78286	-0.00004
28	7	22	27	6	21	1312.78286	-0.00004
29	6	24	28	5	23	1312.80354	-0.00012
29	5	24	28	6	23	1312.80354	-0.00012
27	9	19	26	8	18	1312.85863	-0.00014
27	8	19	26	9	18	1312.85863	-0.00014
28	7	21	27	8	20	1312.87941	-0.00006
28	8	21	27	7	20	1312.87941	-0.00006
29	7	23	28	6	22	1312.90009	-0.00014
29	6	23	28	7	22	1312.90009	-0.00014
30	5	25	29	6	24	1312.92105	0.00001
30	6	25	29	5	24	1312.92105	0.00001
27	10	18	26	9	17	1312.95518	-0.00016
27	9	18	26	10	17	1312.95518	-0.00016
28	8	20	27	9	19	1312.97608	0.00006
28	9	20	27	8	19	1312.97608	0.00006
29	8	22	28	7	21	1312.99677	-0.00001
29	7	22	28	8	21	1312.99677	-0.00001
30	6	24	29	7	23	1313.01756	-0.00003
30	7	24	29	6	23	1313.01756	-0.00003
28	9	19	27	10	18	1313.07265	0.00008
28	10	19	27	9	18	1313.07265	0.00008
29	9	21	28	8	20	1313.09343	0.00012
29	8	21	28	9	20	1313.09343	0.00012
30	7	23	29	8	22	1313.11408	-0.00004
30	8	23	29	7	22	1313.11408	-0.00004
31	7	25	30	6	24	1313.13502	0.00003
31	6	25	30	7	24	1313.13502	0.00003
28	10	18	27	11	17	1313.16917	0.00005
28	11	18	27	10	17	1313.16917	0.00005
29	10	20	28	9	19	1313.18998	0.00015
29	9	20	28	10	19	1313.18998	0.00015
30	8	22	29	9	21	1313.21048	-0.00016

Continuation, see next page

Continuation of Table 29: $\nu_{17} \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
30	9	22	29	8	21	1313.21048	-0.00016
31	8	24	30	7	23	1313.23155	0.00004
31	7	24	30	8	23	1313.23155	0.00004
32	6	26	31	7	25	1313.25250	0.00008
32	7	26	31	6	25	1313.25250	0.00008
30	9	21	29	10	20	1313.30705	-0.00009
30	10	21	29	9	20	1313.30705	-0.00009
31	9	23	30	8	22	1313.32783	-0.00017
31	8	23	30	9	22	1313.32783	-0.00017
29	12	18	28	11	17	1313.38292	0.00003
29	11	18	28	12	17	1313.38292	0.00003
30	10	20	29	11	19	1313.40367	0.00004
30	11	20	29	10	19	1313.40367	0.00004
31	10	22	30	9	21	1313.42428	-0.00020
31	9	22	30	10	21	1313.42428	-0.00020
32	8	24	31	9	23	1313.44507	-0.00033
32	9	24	31	8	23	1313.44507	-0.00033

Table 30: Rovibrational transition wavenumbers $\tilde{\nu}_{obs}$ for the fundamental $\nu_3 \leftarrow gs$ of dithiine. J'', K_a'' and K_c'' are lower state quantum numbers, J', K_a' and K_c' are upper state quantum numbers, $\tilde{\nu}_{\text{obs.}}$ = observed wavenumber, $\tilde{\nu}_{\text{cal.}}$ = wavenumber calculated with the parameters in Table 10. All wavenumbers are given in cm^{-1}.

Table 30: Rovibrational transitions of $\nu_3 \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
38	2	36	39	2	37	1539.97354	0.00060
38	3	36	39	3	37	1539.97354	0.00060
37	3	34	38	3	35	1539.99497	0.00000
37	4	34	38	4	35	1539.99497	0.00000
36	4	32	37	4	33	1540.01757	0.00042
36	5	32	37	5	33	1540.01757	0.00042
35	5	30	36	5	31	1540.03961	0.00015
35	6	30	36	6	31	1540.03961	0.00015
39	1	39	40	1	40	1540.05259	0.00047
39	0	39	40	0	40	1540.05259	0.00047
34	7	28	35	7	29	1540.06159	-0.00030
34	6	28	35	6	29	1540.06159	-0.00030
37	3	35	38	3	36	1540.09592	0.00028

Continuation, see next page

Continuation of Table 30: $\nu_3 \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
37	2	35	38	2	36	1540.09592	0.00028
32	9	24	33	9	25	1540.10734	0.00030
32	8	24	33	8	25	1540.10734	0.00030
36	3	33	37	3	34	1540.11809	0.00046
36	4	33	37	4	34	1540.11809	0.00046
31	10	22	32	10	23	1540.12978	0.00010
31	9	22	32	9	23	1540.12978	0.00010
35	4	31	36	4	32	1540.14014	0.00037
35	5	31	36	5	32	1540.14014	0.00037
30	11	20	31	11	21	1540.15194	-0.00034
30	10	20	31	10	21	1540.15194	-0.00034
34	6	29	35	6	30	1540.16200	-0.00005
34	5	29	35	5	30	1540.16200	-0.00005
38	1	38	39	1	39	1540.17489	0.00014
38	0	38	39	0	39	1540.17489	0.00014
29	11	18	30	11	19	1540.17489	0.00014
29	12	18	30	12	19	1540.17489	0.00014
33	6	27	34	6	28	1540.18433	-0.00012
33	7	27	34	7	28	1540.18433	-0.00012
37	1	36	38	1	37	1540.19706	0.00066
37	2	36	38	2	37	1540.19706	0.00066
28	12	16	29	12	17	1540.19706	0.00017
28	13	16	29	13	17	1540.19706	0.00017
32	7	25	33	7	26	1540.20710	0.00016
32	8	25	33	8	26	1540.20710	0.00016
35	4	32	36	4	33	1540.24026	0.00009
35	3	32	36	3	33	1540.24026	0.00009
30	10	21	31	10	22	1540.25139	-0.00069
30	9	21	31	9	22	1540.25139	-0.00069
34	4	30	35	4	31	1540.26190	-0.00038
34	5	30	35	5	31	1540.26190	-0.00038
29	10	19	30	10	20	1540.27461	0.00001
29	11	19	30	11	20	1540.27461	0.00001
33	5	28	34	5	29	1540.28475	0.00023
33	6	28	34	6	29	1540.28475	0.00023
36	2	35	37	2	36	1540.31898	0.00011
36	1	35	37	1	36	1540.31898	0.00011
27	12	15	28	12	16	1540.31898	0.00011
27	13	15	28	13	16	1540.31898	0.00011
31	8	24	32	8	25	1540.32893	-0.00039
31	7	24	32	7	25	1540.32893	-0.00039
30	8	22	31	8	23	1540.35172	-0.00011
30	9	22	31	9	23	1540.35172	-0.00011
34	4	31	35	4	32	1540.36307	0.00049
34	3	31	35	3	32	1540.36307	0.00049
29	9	20	30	9	21	1540.37409	-0.00025

Continuation, see next page

Continuation of Table 30: $\nu_3 \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
29	10	20	30	10	21	1540.37409	-0.00025
33	5	29	34	5	30	1540.38464	-0.00001
33	4	29	34	4	30	1540.38464	-0.00001
28	11	18	29	11	19	1540.39680	0.00002
28	10	18	29	10	19	1540.39680	0.00002
32	5	27	33	5	28	1540.40682	-0.00004
32	6	27	33	6	28	1540.40682	-0.00004
27	11	16	28	11	17	1540.41894	-0.00003
27	12	16	28	12	17	1540.41894	-0.00003
36	0	36	37	0	37	1540.41966	0.00001
36	1	36	37	1	37	1540.41966	0.00001
31	6	25	32	6	26	1540.42930	0.00013
31	7	25	32	7	26	1540.42930	0.00013
26	13	14	27	13	15	1540.44060	-0.00003
26	12	14	27	12	15	1540.44060	-0.00003
34	2	32	35	2	33	1540.46334	0.00037
34	3	32	35	3	33	1540.46334	0.00037
33	4	30	34	4	31	1540.48495	0.00009
33	3	30	34	3	31	1540.48495	0.00009
28	10	19	29	10	20	1540.49663	0.00015
28	9	19	29	9	20	1540.49663	0.00015
32	4	28	33	4	29	1540.50704	0.00014
32	5	28	33	5	29	1540.50704	0.00014
27	10	17	28	10	18	1540.51913	0.00033
27	11	17	28	11	18	1540.51913	0.00033
31	5	26	32	5	27	1540.52890	-0.00017
31	6	26	32	6	27	1540.52890	-0.00017
35	1	35	36	1	36	1540.54170	-0.00020
35	0	35	36	0	36	1540.54170	-0.00020
30	6	24	31	6	25	1540.55124	-0.00010
30	7	24	31	7	25	1540.55124	-0.00010
34	1	33	35	1	34	1540.56395	0.00050
34	2	33	35	2	34	1540.56395	0.00050
29	7	22	30	7	23	1540.57384	0.00014
29	8	22	30	8	23	1540.57384	0.00014
33	3	31	34	3	32	1540.58536	0.00020
33	2	31	34	2	32	1540.58536	0.00020
28	9	20	29	9	21	1540.59644	0.00034
28	8	20	29	8	21	1540.59644	0.00034
32	4	29	33	4	30	1540.60694	-0.00008
32	3	29	33	3	30	1540.60694	-0.00008
27	9	18	28	9	19	1540.61842	-0.00005
27	10	18	28	10	19	1540.61842	-0.00005
31	4	27	32	4	28	1540.62923	0.00021
31	5	27	32	5	28	1540.62923	0.00021
26	11	16	27	11	17	1540.64069	0.00001

Continuation, see next page

Continuation of Table 30: $\nu_3 \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
26	10	16	27	10	17	1540.64069	0.00001
30	5	25	31	5	26	1540.65152	0.00037
30	6	25	31	6	26	1540.65152	0.00037
25	11	14	26	11	15	1540.66259	0.00010
25	12	14	26	12	15	1540.66259	0.00010
34	1	34	35	1	35	1540.66345	-0.00058
34	0	34	35	0	35	1540.66345	-0.00058
29	6	23	30	6	24	1540.67381	0.00042
29	7	23	30	7	24	1540.67381	0.00042
33	1	32	34	1	33	1540.68566	0.00011
33	2	32	34	2	33	1540.68566	0.00011
28	7	21	29	7	22	1540.69554	-0.00016
28	8	21	29	8	22	1540.69554	-0.00016
32	3	30	33	3	31	1540.70755	0.00033
32	2	30	33	2	31	1540.70755	0.00033
27	8	19	28	8	20	1540.71806	0.00002
27	9	19	28	9	20	1540.71806	0.00002
31	4	28	32	4	29	1540.72891	-0.00014
31	3	28	32	3	29	1540.72891	-0.00014
26	10	17	27	10	18	1540.74023	-0.00008
26	9	17	27	9	18	1540.74023	-0.00008
30	4	26	31	4	27	1540.75119	0.00017
30	5	26	31	5	27	1540.75119	0.00017
29	6	24	30	6	25	1540.77320	0.00009
29	5	24	30	5	25	1540.77320	0.00009
33	1	33	34	1	34	1540.78588	-0.00015
33	0	33	34	0	34	1540.78588	-0.00015
28	7	22	29	7	23	1540.79505	-0.00025
28	6	22	29	6	23	1540.79505	-0.00025
32	1	31	33	1	32	1540.80760	0.00009
32	2	31	33	2	32	1540.80760	0.00009
27	8	20	28	8	21	1540.81722	-0.00034
27	7	20	28	7	21	1540.81722	-0.00034
31	3	29	32	3	30	1540.82936	0.00020
31	2	29	32	2	30	1540.82936	0.00020
26	9	18	27	9	19	1540.83975	-0.00008
26	8	18	27	8	19	1540.83975	-0.00008
30	4	27	31	4	28	1540.85086	-0.00009
30	3	27	31	3	28	1540.85086	-0.00009
25	9	16	26	9	17	1540.86265	0.00064
25	10	16	26	10	17	1540.86265	0.00064
29	4	25	30	4	26	1540.87288	0.00000
29	5	25	30	5	26	1540.87288	0.00000
28	5	23	29	5	24	1540.89510	0.00017
28	6	23	29	6	24	1540.89510	0.00017
32	0	32	33	0	33	1540.90767	-0.00023

Continuation, see next page

Continuation of Table 30: $\nu_3 \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
32	1	32	33	1	33	1540.90767	-0.00023
31	1	30	32	1	31	1540.92926	-0.00009
31	2	30	32	2	31	1540.92926	-0.00009
26	7	19	27	7	20	1540.93919	-0.00010
26	8	19	27	8	20	1540.93919	-0.00010
30	2	28	31	2	29	1540.95093	-0.00003
30	3	28	31	3	29	1540.95093	-0.00003
25	8	17	26	8	18	1540.96184	0.00035
25	9	17	26	9	18	1540.96184	0.00035
29	4	26	30	4	27	1540.97264	-0.00008
29	3	26	30	3	27	1540.97264	-0.00008
28	4	24	29	4	25	1540.99490	0.00029
28	5	24	29	5	25	1540.99490	0.00029
27	5	22	28	5	23	1541.01657	-0.00005
27	6	22	28	6	23	1541.01657	-0.00005
31	0	31	32	0	32	1541.03006	0.00042
31	1	31	32	1	32	1541.03006	0.00042
26	7	20	27	7	21	1541.03853	-0.00020
26	6	20	27	6	21	1541.03853	-0.00020
30	2	29	31	2	30	1541.05130	0.00024
30	1	29	31	1	30	1541.05130	0.00024
25	7	18	26	7	19	1541.06090	0.00002
25	8	18	26	8	19	1541.06090	0.00002
29	2	27	30	2	28	1541.07267	0.00004
29	3	27	30	3	28	1541.07267	0.00004
24	9	16	25	9	17	1541.08332	0.00032
24	8	16	25	8	17	1541.08332	0.00032
28	4	25	29	4	26	1541.09430	-0.00005
28	3	25	29	3	26	1541.09430	-0.00005
27	5	23	28	5	24	1541.11645	0.00024
27	4	23	28	4	24	1541.11645	0.00024
26	6	21	27	6	22	1541.13795	-0.00023
26	5	21	27	5	22	1541.13795	-0.00023
30	0	30	31	0	31	1541.15107	-0.00018
30	1	30	31	1	31	1541.15107	-0.00018
25	6	19	26	6	20	1541.16044	0.00020
25	7	19	26	7	20	1541.16044	0.00020
29	2	28	30	2	29	1541.17247	-0.00016
29	1	28	30	1	29	1541.17247	-0.00016
24	7	17	25	7	18	1541.18231	-0.00002
24	8	17	25	8	18	1541.18231	-0.00002
28	3	26	29	3	27	1541.19417	0.00000
28	2	26	29	2	27	1541.19417	0.00000
23	9	15	24	9	16	1541.20442	0.00006
23	8	15	24	8	16	1541.20442	0.00006
27	4	24	28	4	25	1541.21600	0.00014

Continuation, see next page

Continuation of Table 30: $\nu_3 \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
27	3	24	28	3	25	1541.21600	0.00014
26	4	22	27	4	23	1541.23795	0.00027
26	5	22	27	5	23	1541.23795	0.00027
25	5	20	26	5	21	1541.25995	0.00034
25	6	20	26	6	21	1541.25995	0.00034
29	0	29	30	0	30	1541.27324	0.00051
29	1	29	30	1	30	1541.27324	0.00051
24	7	18	25	7	19	1541.28133	-0.00029
24	6	18	25	6	19	1541.28133	-0.00029
28	2	27	29	2	28	1541.29393	-0.00014
28	1	27	29	1	28	1541.29393	-0.00014
23	8	16	24	8	17	1541.30363	-0.00001
23	7	16	24	7	17	1541.30363	-0.00001
27	2	25	28	2	26	1541.31561	0.00003
27	3	25	28	3	26	1541.31561	0.00003
22	9	14	23	9	15	1541.32526	-0.00030
22	8	14	23	8	15	1541.32526	-0.00030
26	3	23	27	3	24	1541.33762	0.00039
26	4	23	27	4	24	1541.33762	0.00039
25	4	21	26	4	22	1541.35890	-0.00011
25	5	21	26	5	22	1541.35890	-0.00011
24	5	19	25	5	20	1541.38056	-0.00034
24	6	19	25	6	20	1541.38056	-0.00034
28	0	28	29	0	29	1541.39397	-0.00010
28	1	28	29	1	29	1541.39397	-0.00010
23	6	17	24	6	18	1541.40307	0.00021
23	7	17	24	7	18	1541.40307	0.00021
22	8	15	23	8	16	1541.42516	0.00036
22	7	15	23	7	16	1541.42516	0.00036
26	2	24	27	2	25	1541.43699	0.00014
26	3	24	27	3	25	1541.43699	0.00014
21	8	13	22	8	14	1541.44673	0.00013
21	9	13	22	9	14	1541.44673	0.00013
25	3	22	26	3	23	1541.45854	0.00007
25	4	22	26	4	23	1541.45854	0.00007
24	4	20	25	4	21	1541.48046	0.00025
24	5	20	25	5	21	1541.48046	0.00025
23	5	18	24	5	19	1541.50195	-0.00011
23	6	18	24	6	19	1541.50195	-0.00011
27	0	27	28	0	28	1541.51518	-0.00010
27	1	27	28	1	28	1541.51518	-0.00010
22	7	16	23	7	17	1541.52416	0.00021
22	6	16	23	6	17	1541.52416	0.00021
26	2	25	27	2	26	1541.53651	-0.00005
26	1	25	27	1	26	1541.53651	-0.00005
21	8	14	22	8	15	1541.54630	0.00048

Continuation, see next page

Continuation of Table 30: $\nu_3 \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
21	7	14	22	7	15	1541.54630	0.00048
25	3	23	26	3	24	1541.55842	0.00043
25	2	23	26	2	24	1541.55842	0.00043
24	3	21	25	3	22	1541.57925	-0.00032
24	4	21	25	4	22	1541.57925	-0.00032
23	4	19	24	4	20	1541.60083	-0.00044
23	5	19	24	5	20	1541.60083	-0.00044
22	6	17	23	6	18	1541.62282	-0.00025
22	5	17	23	5	18	1541.62282	-0.00025
26	0	26	27	0	27	1541.63636	0.00001
26	1	26	27	1	27	1541.63636	0.00001
21	7	15	22	7	16	1541.64509	0.00018
21	6	15	22	6	16	1541.64509	0.00018
25	1	24	26	1	25	1541.65759	0.00000
25	2	24	26	2	25	1541.65759	0.00000
20	7	13	21	7	14	1541.66696	0.00028
20	8	13	21	8	14	1541.66696	0.00028
24	3	22	25	3	23	1541.67885	-0.00014
24	2	22	25	2	23	1541.67885	-0.00014
19	8	11	20	8	12	1541.68779	-0.00034
19	9	11	20	9	12	1541.68779	-0.00034
23	3	20	24	3	21	1541.70076	0.00022
23	4	20	24	4	21	1541.70076	0.00022
22	4	18	23	4	19	1541.72208	-0.00012
22	5	18	23	5	19	1541.72208	-0.00012
21	5	16	22	5	17	1541.74358	-0.00037
21	6	16	22	6	17	1541.74358	-0.00037
25	0	25	26	0	26	1541.75705	-0.00024
25	1	25	26	1	26	1541.75705	-0.00024
20	7	14	21	7	15	1541.76562	-0.00010
20	6	14	21	6	15	1541.76562	-0.00010
24	1	23	25	1	24	1541.77878	0.00028
24	2	23	25	2	24	1541.77878	0.00028
23	3	21	24	3	22	1541.79986	0.00000
23	2	21	24	2	22	1541.79986	0.00000
22	3	19	23	3	20	1541.82125	-0.00012
22	4	19	23	4	20	1541.82125	-0.00012
21	4	17	22	4	18	1541.84288	-0.00011
21	5	17	22	5	18	1541.84288	-0.00011
20	5	15	21	5	16	1541.86487	0.00018
20	6	15	21	6	16	1541.86487	0.00018
24	1	24	25	1	25	1541.87825	0.00016
24	0	24	25	0	25	1541.87825	0.00016
19	6	13	20	6	14	1541.88665	0.00027
19	7	13	20	7	14	1541.88665	0.00027
23	1	22	24	1	23	1541.89927	0.00001

Continuation, see next page

Continuation of Table 30: $\nu_3 \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
23	2	22	24	2	23	1541.89927	0.00001
18	7	11	19	7	12	1541.90790	0.00001
18	8	11	19	8	12	1541.90790	0.00001
22	3	20	23	3	21	1541.92050	-0.00009
22	2	20	23	2	21	1541.92050	-0.00009
21	4	18	22	4	19	1541.94225	0.00019
21	3	18	22	3	19	1541.94225	0.00019
20	5	16	21	5	17	1541.96373	0.00009
20	4	16	21	4	17	1541.96373	0.00009
19	6	14	20	6	15	1541.98499	-0.00029
19	5	14	20	5	15	1541.98499	-0.00029
23	1	23	24	1	24	1541.99863	-0.00012
23	0	23	24	0	24	1541.99863	-0.00012
18	7	12	19	7	13	1542.00701	0.00012
18	6	12	19	6	13	1542.00701	0.00012
22	2	21	23	2	22	1542.01990	0.00001
22	1	21	23	1	22	1542.01990	0.00001
21	3	19	22	3	20	1542.04071	-0.00047
21	2	19	22	2	20	1542.04071	-0.00047
20	3	17	21	3	18	1542.06273	0.00012
20	4	17	21	4	18	1542.06273	0.00012
19	4	15	20	4	16	1542.08410	-0.00005
19	5	15	20	5	16	1542.08410	-0.00005
18	6	13	19	6	14	1542.10594	0.00021
18	5	13	19	5	14	1542.10594	0.00021
22	0	22	23	0	23	1542.11913	-0.00014
22	1	22	23	1	23	1542.11913	-0.00014
17	6	11	18	6	12	1542.12744	0.00021
17	7	11	18	7	12	1542.12744	0.00021
21	2	20	22	2	21	1542.14071	0.00033
21	1	20	22	1	21	1542.14071	0.00033
19	3	16	20	3	17	1542.18281	-0.00022
19	4	16	20	4	17	1542.18281	-0.00022
18	4	14	19	4	15	1542.20464	0.00012
18	5	14	19	5	15	1542.20464	0.00012
17	5	12	18	5	13	1542.22582	-0.00021
17	6	12	18	6	13	1542.22582	-0.00021
21	0	21	22	0	22	1542.24024	0.00058
21	1	21	22	1	22	1542.24024	0.00058
16	7	10	17	7	11	1542.24764	0.00024
16	6	10	17	6	11	1542.24764	0.00024
20	1	19	21	1	20	1542.26104	0.00031
20	2	19	21	2	20	1542.26104	0.00031
15	7	8	16	7	9	1542.26771	-0.00045
15	8	8	16	8	9	1542.26771	-0.00046
19	3	17	20	3	18	1542.28205	0.00010

Continuation, see next page

Continuation of Table 30: $\nu_3 \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
19	2	17	20	2	18	1542.28205	0.00010
18	3	15	19	3	16	1542.30355	0.00025
18	4	15	19	4	16	1542.30355	0.00025
17	4	13	18	4	14	1542.32443	-0.00031
17	5	13	18	5	14	1542.32443	-0.00031
16	6	11	17	6	12	1542.34639	0.00021
16	5	11	17	5	12	1542.34639	0.00021
20	0	20	21	0	21	1542.36039	0.00049
20	1	20	21	1	21	1542.36039	0.00049
15	7	9	16	7	10	1542.36789	0.00051
15	6	9	16	6	10	1542.36789	0.00051
19	2	18	20	2	19	1542.38101	0.00007
19	1	18	20	1	19	1542.38101	0.00007
18	3	16	19	3	17	1542.40251	0.00038
18	2	16	19	2	17	1542.40251	0.00038
17	3	14	18	3	15	1542.42385	0.00041
17	4	14	18	4	15	1542.42385	0.00041
16	5	12	17	5	13	1542.44461	-0.00021
16	4	12	17	4	13	1542.44461	-0.00021
15	5	10	16	5	11	1542.46654	0.00038
15	6	10	16	6	11	1542.46654	0.00038
19	0	19	20	0	20	1542.47994	-0.00007
19	1	19	20	1	20	1542.47994	-0.00007
18	1	17	19	1	18	1542.50084	-0.00017
18	2	17	19	2	18	1542.50084	-0.00017
13	8	6	14	8	7	1542.50641	-0.00041
13	7	6	14	7	7	1542.50641	0.00014
17	3	15	18	3	16	1542.52232	0.00016
17	2	15	18	2	16	1542.52232	0.00016
16	3	13	17	3	14	1542.54329	-0.00014
16	4	13	17	4	14	1542.54329	-0.00014
15	4	11	16	4	12	1542.56469	-0.00006
15	5	11	16	5	12	1542.56469	-0.00006
14	6	9	15	6	10	1542.58564	-0.00034
14	5	9	15	5	10	1542.58564	-0.00034
18	1	18	19	1	19	1542.59976	-0.00021
18	0	18	19	0	19	1542.59976	-0.00021
13	6	7	14	6	8	1542.60607	-0.00055
13	7	7	14	7	8	1542.60607	-0.00057
17	1	16	18	1	17	1542.62099	0.00005
17	2	16	18	2	17	1542.62099	0.00005
16	3	14	17	3	15	1542.64214	0.00009
16	2	14	17	2	15	1542.64214	0.00009
15	4	12	16	4	13	1542.66356	0.00029
15	3	12	16	3	13	1542.66356	0.00029
14	5	10	15	5	11	1542.68466	0.00013

Continuation, see next page

Continuation of Table 30: $\nu_3 \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
14	4	10	15	4	11	1542.68466	0.00013
13	5	8	14	5	9	1542.70549	-0.00012
13	6	8	14	6	9	1542.70549	-0.00012
17	0	17	18	0	18	1542.71982	0.00002
17	1	17	18	1	18	1542.71982	0.00002
12	7	6	13	7	7	1542.72524	-0.00059
12	6	6	13	6	7	1542.72524	-0.00038
16	2	15	17	2	16	1542.74090	0.00017
16	1	15	17	1	16	1542.74090	0.00017
15	3	13	16	3	14	1542.76160	-0.00020
15	2	13	16	2	14	1542.76160	-0.00020
14	3	11	15	3	12	1542.78298	0.00001
14	4	11	15	4	12	1542.78298	0.00001
13	4	9	14	4	10	1542.80413	-0.00002
13	5	9	14	5	10	1542.80413	-0.00002
16	0	16	17	0	17	1542.83950	0.00002
16	1	16	17	1	17	1542.83950	0.00002
15	2	14	16	2	15	1542.86024	-0.00013
15	1	14	16	1	15	1542.86024	-0.00013
14	2	12	15	2	13	1542.88090	-0.00051
14	3	12	15	3	13	1542.88090	-0.00051
13	3	10	14	3	11	1542.90289	0.00036
13	4	10	14	4	11	1542.90289	0.00036
12	5	8	13	5	9	1542.92389	0.00028
12	4	8	13	4	9	1542.92389	0.00028
11	6	6	12	6	7	1542.94445	0.00027
11	5	6	12	5	7	1542.94445	0.00034
10	6	4	11	6	5	1542.95598	-0.00017
10	7	4	11	7	5	1542.96630	0.00016
13	2	11	14	2	12	1543.00102	0.00015
13	3	11	14	3	12	1543.00102	0.00015
12	3	9	13	3	10	1543.02167	-0.00026
12	4	9	13	4	10	1543.02167	-0.00026
14	0	14	15	0	15	1543.07830	-0.00011
14	1	14	15	1	15	1543.07830	-0.00011
13	1	12	14	1	13	1543.09908	-0.00016
13	2	12	14	2	13	1543.09908	-0.00016
12	3	10	13	3	11	1543.12048	0.00029
12	2	10	13	2	11	1543.12048	0.00029
11	4	8	12	4	9	1543.14102	-0.00016
11	3	8	12	3	9	1543.14102	-0.00016
10	5	6	11	5	7	1543.16153	-0.00042
10	4	6	11	4	7	1543.16153	-0.00040
13	0	13	14	0	14	1543.19747	-0.00020
13	1	13	14	1	14	1543.19747	-0.00020
12	1	11	13	1	12	1543.21849	0.00004

Continuation, see next page

Continuation of Table 30: $\nu_3 \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
12	2	11	13	2	12	1543.21849	0.00004
10	4	7	11	4	8	1543.26043	0.00016
10	3	7	11	3	8	1543.26043	0.00016
9	4	5	10	4	6	1543.28035	-0.00025
8	5	3	9	5	4	1543.28575	0.00001
8	6	3	9	6	4	1543.30882	0.00025
8	5	4	7	5	3	1546.26292	0.00016
9	3	6	8	3	5	1546.28462	-0.00007
9	4	6	8	4	5	1546.28462	-0.00002
10	2	8	9	2	7	1546.30337	-0.00026
10	3	8	9	3	7	1546.30337	-0.00026
11	2	10	10	2	9	1546.32257	-0.00036
11	1	10	10	1	9	1546.32257	-0.00036
12	0	12	11	0	11	1546.34253	0.00012
12	1	12	11	1	11	1546.34253	0.00012
9	5	5	8	5	4	1546.38090	-0.00008
9	4	5	8	4	4	1546.38231	-0.00017
8	5	3	7	5	2	1546.38679	-0.00009
10	3	7	9	3	6	1546.39991	0.00006
10	4	7	9	4	6	1546.39991	0.00007
11	3	9	10	3	8	1546.41904	0.00018
11	2	9	10	2	8	1546.41904	0.00018
12	1	11	11	1	10	1546.43837	0.00024
12	2	11	11	2	10	1546.43837	0.00024
13	1	13	12	1	12	1546.45769	0.00012
13	0	13	12	0	12	1546.45769	0.00012
10	4	6	9	4	5	1546.49625	-0.00025
10	5	6	9	5	5	1546.49625	-0.00008
11	4	8	10	4	7	1546.51461	-0.00032
11	3	8	10	3	7	1546.51461	-0.00032
12	2	10	11	2	9	1546.53374	-0.00021
12	3	10	11	3	9	1546.53374	-0.00021
13	2	12	12	2	11	1546.55351	0.00032
13	1	12	12	1	11	1546.55351	0.00032
14	0	14	13	0	13	1546.57263	0.00004
14	1	14	13	1	13	1546.57263	0.00004
10	6	5	9	6	4	1546.59235	0.00004
11	5	7	10	5	6	1546.61173	0.00052
11	4	7	10	4	6	1546.61173	0.00051
12	3	9	11	3	8	1546.63014	0.00026
12	4	9	11	4	8	1546.63014	0.00026
15	1	15	14	1	14	1546.68749	0.00003
15	0	15	14	0	14	1546.68749	0.00003
11	6	6	10	6	5	1546.70788	0.00005
11	5	6	10	5	5	1546.70812	-0.00020
10	6	4	9	6	3	1546.71071	-0.00006

Continuation, see next page

Continuation of Table 30: $\nu_3 \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
12	4	8	11	4	7	1546.72601	0.00003
12	5	8	11	5	7	1546.72601	0.00003
13	4	10	12	4	9	1546.74489	0.00019
13	3	10	12	3	9	1546.74489	0.00019
14	2	12	13	2	11	1546.76408	0.00039
14	3	12	13	3	11	1546.76408	0.00039
15	2	14	14	2	13	1546.78274	-0.00012
15	1	14	14	1	13	1546.78274	-0.00012
16	0	16	15	0	15	1546.80187	-0.00031
16	1	16	15	1	15	1546.80187	-0.00031
13	5	9	12	5	8	1546.84065	0.00001
13	4	9	12	4	8	1546.84065	0.00001
14	3	11	13	3	10	1546.85949	0.00011
14	4	11	13	4	10	1546.85949	0.00011
15	3	13	14	3	12	1546.87805	-0.00029
15	2	13	14	2	12	1546.87805	-0.00029
16	1	15	15	1	14	1546.89753	0.00006
16	2	15	15	2	14	1546.89753	0.00006
17	1	17	16	1	16	1546.91690	0.00014
17	0	17	16	0	16	1546.91690	0.00014
13	6	8	12	6	7	1546.93647	-0.00034
13	5	8	12	5	7	1546.93647	-0.00034
14	4	10	13	4	9	1546.95494	-0.00024
14	5	10	13	5	9	1546.95494	-0.00024
15	4	12	14	4	11	1546.97431	0.00039
15	3	12	14	3	11	1546.97431	0.00039
16	2	14	15	2	13	1546.99316	0.00031
16	3	14	15	3	13	1546.99316	0.00031
17	2	16	16	2	15	1547.01231	0.00037
17	1	16	16	1	15	1547.01231	0.00037
18	0	18	17	0	17	1547.03118	0.00000
18	1	18	17	1	17	1547.03118	0.00000
13	6	7	12	6	6	1547.03298	-0.00057
13	7	7	12	7	6	1547.03298	-0.00042
14	5	9	13	5	8	1547.05111	-0.00005
14	6	9	13	6	8	1547.05111	-0.00005
15	5	11	14	5	10	1547.06956	-0.00004
15	4	11	14	4	10	1547.06956	-0.00004
16	3	13	15	3	12	1547.08841	0.00010
16	4	13	15	4	12	1547.08841	0.00010
17	3	15	16	3	14	1547.10754	0.00033
17	2	15	16	2	14	1547.10754	0.00033
18	1	17	17	1	16	1547.12595	-0.00031
18	2	17	17	2	16	1547.12595	-0.00031
19	1	19	18	1	18	1547.14546	-0.00001
19	0	19	18	0	18	1547.14546	-0.00001

Continuation, see next page

Continuation of Table 30: $\nu_3 \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
15	6	10	14	6	9	1547.16528	-0.00013
15	5	10	14	5	9	1547.16528	-0.00013
16	4	12	15	4	11	1547.18385	-0.00002
16	5	12	15	5	11	1547.18385	-0.00002
17	4	14	16	4	13	1547.20259	0.00003
17	3	14	16	3	13	1547.20259	0.00003
18	2	16	17	2	15	1547.22155	0.00012
18	3	16	17	3	15	1547.22155	0.00012
19	2	18	18	2	17	1547.24056	0.00012
19	1	18	18	1	17	1547.24056	0.00012
20	0	20	19	0	19	1547.25992	0.00032
20	1	20	19	1	19	1547.25992	0.00032
15	7	9	14	7	8	1547.26086	-0.00059
15	6	9	14	6	8	1547.26086	-0.00059
16	5	11	15	5	10	1547.27946	-0.00008
16	6	11	15	6	10	1547.27946	-0.00008
18	3	15	17	3	14	1547.31640	-0.00027
18	4	15	17	4	14	1547.31640	-0.00027
19	3	17	18	3	16	1547.33562	0.00012
19	2	17	18	2	16	1547.33562	0.00012
20	1	19	19	1	18	1547.35464	0.00017
20	2	19	19	2	18	1547.35464	0.00017
21	1	21	20	1	20	1547.37390	0.00031
21	0	21	20	0	20	1547.37390	0.00031
16	6	10	15	6	9	1547.37507	-0.00032
16	7	10	15	7	9	1547.37507	-0.00032
17	6	12	16	6	11	1547.39363	0.00008
17	5	12	16	5	11	1547.39363	0.00008
18	4	14	17	4	13	1547.41217	0.00017
18	5	14	17	5	13	1547.41217	0.00017
19	4	16	18	4	15	1547.43085	0.00021
19	3	16	18	3	15	1547.43085	0.00021
20	2	18	19	2	17	1547.44948	0.00006
20	3	18	19	3	17	1547.44948	0.00006
21	2	20	20	2	19	1547.46821	-0.00015
21	1	20	20	1	19	1547.46821	-0.00015
16	7	9	15	7	8	1547.47116	-0.00037
16	8	9	15	8	8	1547.47116	-0.00036
22	0	22	21	0	21	1547.48773	0.00029
22	1	22	21	1	21	1547.48773	0.00029
17	7	11	16	7	10	1547.48874	-0.00049
17	6	11	16	6	10	1547.48874	-0.00049
18	5	13	17	5	12	1547.50760	0.00017
18	6	13	17	6	12	1547.50760	0.00017
19	5	15	18	5	14	1547.52617	0.00031
19	4	15	18	4	14	1547.52617	0.00031

Continuation, see next page

Continuation of Table 30: $\nu_3 \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
20	3	17	19	3	16	1547.54443	-0.00002
20	4	17	19	4	16	1547.54443	-0.00002
21	3	19	20	3	18	1547.56341	0.00021
21	2	19	20	2	18	1547.56341	0.00021
22	1	21	21	1	20	1547.58249	0.00039
22	2	21	21	2	20	1547.58249	0.00039
17	8	10	16	8	9	1547.58502	-0.00011
17	7	10	16	7	9	1547.58502	-0.00011
23	1	23	22	1	22	1547.60120	0.00006
23	0	23	22	0	22	1547.60120	0.00006
18	6	12	17	6	11	1547.60291	-0.00006
18	7	12	17	7	11	1547.60291	-0.00006
19	6	14	18	6	13	1547.62104	-0.00012
19	5	14	18	5	13	1547.62104	-0.00012
20	4	16	19	4	15	1547.63920	-0.00037
20	5	16	19	5	15	1547.63920	-0.00037
21	4	18	20	4	17	1547.65796	-0.00017
21	3	18	20	3	17	1547.65796	-0.00017
22	2	20	21	2	19	1547.67692	0.00008
22	3	20	21	3	19	1547.67692	0.00008
23	2	22	22	2	21	1547.69555	-0.00015
23	1	22	22	1	21	1547.69555	-0.00015
18	7	11	17	7	10	1547.69899	0.00032
18	8	11	17	8	10	1547.69899	0.00032
24	0	24	23	0	23	1547.71483	0.00013
24	1	24	23	1	23	1547.71483	0.00013
19	7	13	18	7	12	1547.71614	-0.00043
19	6	13	18	6	12	1547.71614	-0.00043
20	5	15	19	5	14	1547.73444	-0.00032
20	6	15	19	6	14	1547.73444	-0.00032
21	5	17	20	5	16	1547.75286	-0.00028
21	4	17	20	4	16	1547.75286	-0.00028
22	3	19	21	3	18	1547.77176	0.00010
22	4	19	21	4	18	1547.77176	0.00010
23	3	21	22	3	20	1547.79014	-0.00020
23	2	21	22	2	20	1547.79014	-0.00020
24	1	23	23	1	22	1547.80926	0.00011
24	2	23	23	2	22	1547.80926	0.00011
25	1	25	24	1	24	1547.82767	-0.00044
25	0	25	24	0	24	1547.82767	-0.00044
20	6	14	19	6	13	1547.83044	0.00039
20	7	14	19	7	13	1547.83044	0.00039
21	6	16	20	6	15	1547.84828	0.00006
21	5	16	20	5	15	1547.84828	0.00006
22	4	18	21	4	17	1547.86607	-0.00049
22	5	18	21	5	17	1547.86607	-0.00049

Continuation, see next page

Continuation of Table 30: $\nu_3 \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
23	4	20	22	4	19	1547.88468	-0.00037
23	3	20	22	3	19	1547.88468	-0.00037
24	2	22	23	2	21	1547.90376	0.00007
24	3	22	23	3	21	1547.90376	0.00007
25	2	24	24	2	23	1547.92250	0.00004
25	1	24	24	1	23	1547.92250	0.00004
20	7	13	19	7	12	1547.92588	0.00042
20	8	13	19	8	12	1547.92588	0.00042
26	0	26	25	0	25	1547.94096	-0.00042
26	1	26	25	1	25	1547.94096	-0.00042
21	7	15	20	7	14	1547.94307	-0.00033
21	6	15	20	6	14	1547.94307	-0.00033
22	5	17	21	5	16	1547.96148	-0.00006
22	6	17	21	6	16	1547.96148	-0.00006
23	5	19	22	5	18	1547.97978	-0.00007
23	4	19	22	4	18	1547.97978	-0.00007
24	3	21	23	3	20	1547.99802	-0.00028
24	4	21	23	4	20	1547.99802	-0.00028
25	3	23	24	3	22	1548.01725	0.00036
25	2	23	24	2	22	1548.01725	0.00036
20	8	12	19	8	11	1548.02076	-0.00026
20	9	12	19	9	11	1548.02076	-0.00026
26	1	25	25	1	24	1548.03547	-0.00016
26	2	25	25	2	24	1548.03547	-0.00016
21	8	14	20	8	13	1548.03865	-0.00002
21	7	14	20	7	13	1548.03865	-0.00002
27	1	27	26	1	26	1548.05474	0.00023
27	0	27	26	0	26	1548.05474	0.00023
22	6	16	21	6	15	1548.05607	-0.00053
22	7	16	21	7	15	1548.05607	-0.00053
23	6	18	22	6	17	1548.07470	-0.00002
23	5	18	22	5	17	1548.07470	-0.00002
24	4	20	23	4	19	1548.09295	-0.00004
24	5	20	23	5	19	1548.09295	-0.00004
25	4	22	24	4	21	1548.11146	0.00005
25	3	22	24	3	21	1548.11146	0.00005
26	2	24	25	2	23	1548.13011	0.00015
26	3	24	25	3	23	1548.13011	0.00015
27	2	26	26	2	25	1548.14863	-0.00002
27	1	26	26	1	25	1548.14863	-0.00002
22	7	15	21	7	14	1548.15198	0.00022
22	8	15	21	8	14	1548.15198	0.00022
28	0	28	27	0	27	1548.16769	0.00020
28	1	28	27	1	27	1548.16769	0.00020
23	7	17	22	7	16	1548.16973	0.00006
23	6	17	22	6	16	1548.16973	0.00006

Continuation, see next page

Continuation of Table 30: $\nu_3 \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
24	5	19	23	5	18	1548.18794	0.00018
24	6	19	23	6	18	1548.18794	0.00018
25	5	21	24	5	20	1548.20603	0.00003
25	4	21	24	4	20	1548.20603	0.00003
26	3	23	25	3	22	1548.22439	0.00002
26	4	23	25	4	22	1548.22439	0.00002
21	10	12	20	10	11	1548.22980	0.00013
21	9	12	20	9	11	1548.22980	0.00013
27	3	25	26	3	24	1548.24278	-0.00010
27	2	25	26	2	24	1548.24278	-0.00010
28	1	27	27	1	26	1548.26126	-0.00028
28	2	27	27	2	26	1548.26126	-0.00028
29	1	29	28	1	28	1548.28004	-0.00029
29	0	29	28	0	28	1548.28004	-0.00029
24	6	18	23	6	17	1548.28223	-0.00038
24	7	18	23	7	17	1548.28223	-0.00038
25	6	20	24	6	19	1548.30090	0.00024
25	5	20	24	5	19	1548.30090	0.00024
26	4	22	25	4	21	1548.31904	0.00018
26	5	22	25	5	21	1548.31904	0.00018
27	4	24	26	4	23	1548.33702	-0.00018
27	3	24	26	3	23	1548.33702	-0.00018
22	9	13	21	9	12	1548.34273	0.00029
22	10	13	21	10	12	1548.34273	0.00029
28	2	26	27	2	25	1548.35582	0.00015
28	3	26	27	3	25	1548.35582	0.00015
23	9	15	22	9	14	1548.35963	-0.00022
23	8	15	22	8	14	1548.35963	-0.00022
29	2	28	28	2	27	1548.37433	0.00005
29	1	28	28	1	27	1548.37433	0.00005
24	7	17	23	7	16	1548.37757	0.00004
24	8	17	23	8	16	1548.37757	0.00004
30	0	30	29	0	29	1548.39292	-0.00011
30	1	30	29	1	29	1548.39292	-0.00011
25	7	19	24	7	18	1548.39514	-0.00026
25	6	19	24	6	18	1548.39514	-0.00026
26	5	21	25	5	20	1548.41342	0.00000
26	6	21	25	6	20	1548.41342	0.00000
27	5	23	26	5	22	1548.43186	0.00028
27	4	23	26	4	22	1548.43186	0.00028
28	3	25	27	3	24	1548.44988	0.00000
28	4	25	27	4	24	1548.44988	0.00000
23	10	14	22	10	13	1548.45509	-0.00002
23	9	14	22	9	13	1548.45509	-0.00002
29	3	27	28	3	26	1548.46823	-0.00008
29	2	27	28	2	26	1548.46823	-0.00008

Continuation, see next page

Continuation of Table 30: $\nu_3 \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
24	8	16	23	8	15	1548.47302	0.00047
24	9	16	23	9	15	1548.47302	0.00047
30	1	29	29	1	28	1548.48686	-0.00002
30	2	29	29	2	28	1548.48686	-0.00002
25	8	18	24	8	17	1548.49021	-0.00001
25	7	18	24	7	17	1548.49021	-0.00001
31	1	31	30	1	30	1548.50579	0.00020
31	0	31	30	0	30	1548.50579	0.00020
26	6	20	25	6	19	1548.50782	-0.00024
26	7	20	25	7	19	1548.50782	-0.00024
27	6	22	26	6	21	1548.52583	-0.00022
27	5	22	26	5	21	1548.52583	-0.00022
28	4	24	27	4	23	1548.54428	0.00011
28	5	24	27	5	23	1548.54428	0.00011
29	4	26	28	4	25	1548.56260	0.00018
29	3	26	28	3	25	1548.56260	0.00018
24	9	15	23	9	14	1548.56768	0.00001
24	10	15	23	10	14	1548.56768	0.00001
30	2	28	29	2	27	1548.58071	-0.00010
30	3	28	29	3	27	1548.58071	-0.00010
25	9	17	24	9	16	1548.58488	-0.00024
25	8	17	24	8	16	1548.58488	-0.00024
31	2	30	30	2	29	1548.59924	-0.00010
31	1	30	30	1	29	1548.59924	-0.00010
26	7	19	25	7	18	1548.60293	0.00015
26	8	19	25	8	18	1548.60293	0.00015
32	0	32	31	0	31	1548.61765	-0.00036
32	1	32	31	1	31	1548.61765	-0.00036
27	7	21	26	7	20	1548.62035	-0.00023
27	6	21	26	6	20	1548.62035	-0.00023
28	5	23	27	5	22	1548.63855	0.00002
28	6	23	27	6	22	1548.63855	0.00002
29	5	25	28	5	24	1548.65683	0.00022
29	4	25	28	4	24	1548.65683	0.00022
30	3	27	29	3	26	1548.67461	-0.00022
30	4	27	29	4	26	1548.67461	-0.00022
25	10	16	24	10	15	1548.68016	0.00004
25	9	16	24	9	15	1548.68016	0.00004
31	3	29	30	3	28	1548.69332	0.00014
31	2	29	30	2	28	1548.69332	0.00014
26	8	18	25	8	17	1548.69766	0.00009
26	9	18	25	9	17	1548.69766	0.00009
32	1	31	31	1	30	1548.71105	-0.00062
32	2	31	31	2	30	1548.71105	-0.00062
27	8	20	26	8	19	1548.71545	0.00026
27	7	20	26	7	19	1548.71545	0.00026

Continuation, see next page

Continuation of Table 30: $\nu_3 \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
33	1	33	32	1	32	1548.73005	-0.00024
33	0	33	32	0	32	1548.73005	-0.00024
28	6	22	27	6	21	1548.73312	0.00015
28	7	22	27	7	21	1548.73312	0.00015
29	6	24	28	6	23	1548.75073	-0.00015
29	5	24	28	5	23	1548.75073	-0.00015
30	4	26	29	4	25	1548.76861	-0.00031
30	5	26	29	5	25	1548.76861	-0.00031
25	11	15	24	11	14	1548.77527	0.00004
25	10	15	24	10	14	1548.77527	0.00004
31	4	28	30	4	27	1548.78739	0.00029
31	3	28	30	3	27	1548.78739	0.00029
26	9	17	25	9	16	1548.79267	0.00023
26	10	17	25	10	16	1548.79267	0.00023
32	2	30	31	2	29	1548.80540	0.00000
32	3	30	31	3	29	1548.80540	0.00000
27	9	19	26	9	18	1548.80958	-0.00030
27	8	19	26	8	18	1548.80958	-0.00030
28	7	21	27	7	20	1548.82751	0.00003
28	8	21	27	8	20	1548.82751	0.00003
34	0	34	33	0	33	1548.84185	-0.00058
34	1	34	33	1	33	1548.84185	-0.00058
29	7	23	28	7	22	1548.84532	0.00010
29	6	23	28	6	22	1548.84532	0.00010
30	5	25	29	5	24	1548.86260	-0.00049
30	6	25	29	6	24	1548.86260	-0.00049
31	5	27	30	5	26	1548.88122	0.00013
31	4	27	30	4	26	1548.88122	0.00013
26	10	16	25	10	15	1548.88779	0.00037
26	11	16	25	11	15	1548.88779	0.00037
32	3	29	31	3	28	1548.89903	-0.00020
32	4	29	31	4	28	1548.89903	-0.00020
27	10	18	26	10	17	1548.90471	0.00007
27	9	18	26	9	17	1548.90471	0.00007
33	3	31	32	3	30	1548.91741	-0.00008
33	2	31	32	2	30	1548.91741	-0.00008
28	8	20	27	8	19	1548.92178	-0.00028
28	9	20	27	9	19	1548.92178	-0.00028
34	1	33	33	1	32	1548.93556	-0.00034
34	2	33	33	2	32	1548.93556	-0.00034
29	8	22	28	8	21	1548.93945	-0.00017
29	7	22	28	7	21	1548.93945	-0.00017
35	1	35	34	1	34	1548.95396	-0.00048
35	0	35	34	0	34	1548.95396	-0.00048
30	6	24	29	6	23	1548.95677	-0.00056
30	7	24	29	7	23	1548.95677	-0.00056

Continuation, see next page

Continuation of Table 30: $\nu_3 \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
31	6	26	30	6	25	1548.97502	-0.00014
31	5	26	30	5	25	1548.97502	-0.00014
26	11	15	25	11	14	1548.98240	-0.00013
26	12	15	25	12	14	1548.98240	-0.00013
32	4	28	31	4	27	1548.99291	-0.00022
32	5	28	31	5	27	1548.99291	-0.00022
27	11	17	26	11	16	1548.99946	-0.00003
27	10	17	26	10	16	1548.99946	-0.00003
33	4	30	32	4	29	1549.01116	-0.00006
33	3	30	32	3	29	1549.01116	-0.00006
28	9	19	27	9	18	1549.01664	-0.00007
28	10	19	27	10	18	1549.01664	-0.00007
34	2	32	33	2	31	1549.02940	-0.00004
34	3	32	33	3	31	1549.02940	-0.00004
29	9	21	28	9	20	1549.03396	-0.00014
29	8	21	28	8	20	1549.03396	-0.00014
30	7	23	29	7	22	1549.05185	0.00021
30	8	23	29	8	22	1549.05185	0.00021
36	0	36	35	0	35	1549.06568	-0.00062
36	1	36	35	1	35	1549.06568	-0.00062
31	7	25	30	7	24	1549.06927	-0.00004
31	6	25	30	6	24	1549.06927	-0.00004
32	5	27	31	5	26	1549.08698	-0.00012
32	6	27	31	6	26	1549.08698	-0.00012
27	12	16	26	12	15	1549.09498	0.00052
27	11	16	26	11	15	1549.09498	0.00052
33	5	29	32	5	28	1549.10486	-0.00016
33	4	29	32	4	28	1549.10486	-0.00016
28	10	18	27	10	17	1549.11166	0.00021
28	11	18	27	11	17	1549.11166	0.00021
34	3	31	33	3	30	1549.12312	0.00005
34	4	31	33	4	30	1549.12312	0.00005
29	10	20	28	10	19	1549.12906	0.00041
29	9	20	28	9	19	1549.12906	0.00041
30	8	22	29	8	21	1549.14549	-0.00053
30	9	22	29	9	21	1549.14549	-0.00053
25	14	11	24	14	10	1549.15872	0.00002
25	15	11	24	15	10	1549.15872	0.00006
31	8	24	30	8	23	1549.16302	-0.00050
31	7	24	30	7	23	1549.16302	-0.00050
32	6	26	31	6	25	1549.18107	-0.00008
32	7	26	31	7	25	1549.18107	-0.00008
33	6	28	32	6	27	1549.19881	-0.00009
33	5	28	32	5	27	1549.19881	-0.00009
28	11	17	27	11	16	1549.20646	0.00018
28	12	17	27	12	16	1549.20646	0.00018

Continuation, see next page

Continuation of Table 30: $\nu_3 \leftarrow gs$ of dithiine.

$J^{'}$	$K_a^{'}$	$K_c^{'}$	$J^{''}$	$K_a^{''}$	$K_c^{''}$	$\tilde{\nu}_{obs}$ /cm^{-1}	$(\tilde{\nu}_{obs} - \tilde{\nu}_{cal})$ /cm^{-1}
34	4	30	33	4	29	1549.21668	-0.00011
34	5	30	33	5	29	1549.21668	-0.00011
29	11	19	28	11	18	1549.22289	-0.00039
29	10	19	28	10	18	1549.22289	-0.00039
35	4	32	34	4	31	1549.23453	-0.00027
35	3	32	34	3	31	1549.23453	-0.00027
36	2	34	35	2	33	1549.25265	-0.00029
36	3	34	35	3	33	1549.25265	-0.00029
37	2	36	36	2	35	1549.27102	-0.00019
37	1	36	36	1	35	1549.27102	-0.00019
32	7	25	31	7	24	1549.27561	0.00034
32	8	25	31	8	24	1549.27561	0.00034
33	7	27	32	7	26	1549.29245	-0.00041
33	6	27	32	6	26	1549.29245	-0.00041
34	5	29	33	5	28	1549.31066	0.00009
34	6	29	33	6	28	1549.31066	0.00009
29	12	18	28	12	17	1549.31821	0.00022
29	11	18	28	11	17	1549.31821	0.00022
35	5	31	34	5	30	1549.32850	0.00009
35	4	31	34	4	30	1549.32850	0.00009
30	10	20	29	10	19	1549.33472	-0.00026
30	11	20	29	11	19	1549.33472	-0.00026
31	10	22	30	10	21	1549.35223	0.00008
31	9	22	30	9	21	1549.35223	0.00008
32	8	24	31	8	23	1549.36944	-0.00001
32	9	24	31	9	23	1549.36944	-0.00001
33	8	26	32	8	25	1549.38660	-0.00028
33	7	26	32	7	25	1549.38660	-0.00028
34	6	28	33	6	27	1549.40420	-0.00023
34	7	28	33	7	27	1549.40420	-0.00023
35	6	30	34	6	29	1549.42182	-0.00029
35	5	30	34	5	29	1549.42182	-0.00029
36	4	32	35	4	31	1549.43980	-0.00011
36	5	32	35	5	31	1549.43980	-0.00011