

Table S2. The results of fit and the data files for the SPFIT program for the S state of the 37C11 species of (HCl)2 H2O.

(H2O)(HCl)2 37C11

Mon Mar 14 09:44:19 2011

/ instead of : below denotes (o-c)>3*err										

	obs	o-c	error	bblends	Notes					
				o-c	wt					

1:	1 1 1 2 2	0 0 0 1 1	6099.3777	-0.0003	0.010	-0.0008	0.22			
2:	1 1 1 2 2	0 0 0 2 2	6099.3777	-0.0012	0.010	-0.0008	0.46			
3:	1 1 1 2 2	0 0 0 3 3	6099.3777	-0.0003	0.010	-0.0008	0.32			
4:	1 1 1 3 3	0 0 0 3 3	6101.2454	-0.0061	0.010	-0.0064	0.70			
5:	1 1 1 3 3	0 0 0 2 2	6101.2454	-0.0070	0.010	-0.0064	0.30			
6:	1 1 1 3 4	0 0 0 3 3	6111.7928	-0.0063	0.010					
7:	1 1 1 1 2	0 0 0 1 1	6112.3161	0.0000	0.010	-0.0002	0.84			
8:	1 1 1 1 2	0 0 0 2 2	6112.3161	-0.0008	0.010	-0.0002	0.16			
9:	1 1 1 2 3	0 0 0 2 2	6113.8320	-0.0095	0.010	-0.0092	0.70			
10:	1 1 1 2 3	0 0 0 3 3	6113.8320	-0.0086	0.010	-0.0092	0.30			
11:	1 1 1 1 1	0 0 0 2 2	6121.7268	0.0122	0.010	0.0127	0.47			
12:	1 1 1 1 1	0 0 0 1 1	6121.7268	0.0130	0.010	0.0127	0.53			
13:	1 1 1 3 2	0 0 0 3 3	6122.0243	-0.0042	0.010	-0.0046	0.61			
14:	1 1 1 3 2	0 0 0 2 2	6122.0243	-0.0051	0.010	-0.0046	0.39			
!										
15:	3 0 3 3 6	2 1 2 3 5	7698.7373	0.0000	0.010					
16:	3 0 3 3 4	2 1 2 3 4	7698.9191	-0.0379	0.010	0.0031	0.27			
17:	3 0 3 3 5	2 1 2 3 4	7698.9191	0.0191	0.010	0.0031	0.71			
18:	3 0 3 2 3	2 1 2 3 4	7698.9191	-0.0158	0.010	0.0031	0.02			
19:	3 0 3 3 4	2 1 2 3 3	7700.6630	-0.0097	0.010					
20:	3 0 3 2 5	2 1 2 3 4	7707.8001	0.0039	0.010					
!										
21:	2 2 0 3 1	2 1 1 2 2	8168.8244	-0.0099	0.010					
22:	2 2 0 2 4	2 1 1 3 4	8173.6916	0.0044	0.010					
23:	2 2 0 2 3	2 1 1 1 3	8175.3176	-0.0080	0.010					
24:	2 2 0 3 5	2 1 1 3 4	8175.9505	-0.0139	0.010					
25:	2 2 0 3 3	2 1 1 2 2	8177.7789	0.0118	0.010					
26:	2 2 0 1 1	2 1 1 0 2	8186.2594	0.0000	0.010	0.0057	0.20			
27:	2 2 0 0 2	2 1 1 3 3	8186.2594	0.0045	0.010	0.0057	0.15			
28:	2 2 0 3 3	2 1 1 3 3	8186.2594	0.0047	0.010	0.0057	0.15			
29:	2 2 0 3 3	2 1 1 0 2	8186.2594	0.0089	0.010	0.0057	0.18			
30:	2 2 0 0 2	2 1 1 2 1	8186.2594	0.0085	0.010	0.0057	0.17			
31:	2 2 0 0 2	2 1 1 0 2	8186.2594	0.0087	0.010	0.0057	0.15			
32:	2 2 0 3 5	2 1 1 3 5	8186.9874	0.0016	0.010					
33:	2 2 0 3 3	2 1 1 2 3	8190.3080	0.0040	0.010					
34:	2 2 0 3 3	2 1 1 2 4	8191.1867	0.0145	0.010					
35:	2 2 0 3 4	2 1 1 3 3	8192.7905	-0.0095	0.010	0.0041	0.28			
36:	2 2 0 2 2	2 1 1 3 3	8192.7905	0.0094	0.010	0.0041	0.72			
37:	2 2 0 2 1	2 1 1 2 1	8193.5213	0.0054	0.010	0.0044	0.68			
38:	2 2 0 2 1	2 1 1 2 0	8193.5213	0.0022	0.010	0.0044	0.32			
39:	2 2 0 1 3	2 1 1 2 3	8196.0837	0.0051	0.010					
40:	2 2 0 3 4	2 1 1 2 4	8197.7172	-0.0003	0.010					
!										
41:	2 1 2 3 3	1 0 1 3 2	8902.3452	-0.0069	0.010					
42:	2 1 2 2 2	1 0 1 3 2	8902.8034	0.0011	0.010					
43:	2 1 2 3 3	1 0 1 2 3	8908.0282	0.0035	0.010					
44:	2 1 2 2 1	1 0 1 3 2	8909.4771	-0.0084	0.010	-0.0107	0.13			
45:	2 1 2 3 2	1 0 1 3 2	8909.4771	-0.0037	0.010	-0.0107	0.37			
46:	2 1 2 2 3	1 0 1 3 2	8909.4771	-0.0164	0.010	-0.0107	0.50			
47:	2 1 2 3 4	1 0 1 2 3	8909.7311	-0.0091	0.010					
48:	2 1 2 3 3	1 0 1 1 2	8911.0526	0.0077	0.010					
49:	2 1 2 2 2	1 0 1 0 1	8912.5243	0.0121	0.010					
50:	2 1 2 3 4	1 0 1 3 4	8913.1148	-0.0068	0.010					
51:	2 1 2 2 3	1 0 1 2 3	8915.2060	0.0398	0.010	0.0001	0.28			
52:	2 1 2 2 4	1 0 1 2 3	8915.2060	-0.0150	0.010	0.0001	0.72			
53:	2 1 2 0 2	1 0 1 1 1	8916.7153	0.0019	0.010					
54:	2 1 2 1 1	1 0 1 1 0	8917.3261	-0.0046	0.010					
55:	2 1 2 3 1	1 0 1 3 2	8918.2321	-0.0149	0.010					
56:	2 1 2 3 3	1 0 1 3 3	8918.7226	-0.0085	0.010					
57:	2 1 2 1 3	1 0 1 1 2	8919.9749	-0.0079	0.010					
58:	2 1 2 3 3	1 0 1 2 2	8921.6084	-0.0100	0.010					
59:	2 1 2 3 5	1 0 1 3 4	8922.0803	-0.0065	0.010					

60:	2 1 2 2 4	1 0 1 3 3	8925.9149	-0.0126	0.010					
61:	2 1 2 1 2	1 0 1 0 1	8926.6511	-0.0081	0.010					
62:	2 1 2 3 2	1 0 1 2 1	8926.8718	-0.0015	0.010	-0.0052	0.23			
63:	2 1 2 2 1	1 0 1 2 1	8926.8718	-0.0062	0.010	-0.0052	0.77			
64:	2 1 2 3 2	1 0 1 2 2	8928.7607	0.0134	0.010	0.0053	0.36			
65:	2 1 2 2 3	1 0 1 2 2	8928.7607	0.0007	0.010	0.0053	0.64			
66:	2 1 2 1 2	1 0 1 2 1	8934.3502	0.0084	0.010					
67:	2 1 2 0 2	1 0 1 2 2	8935.1014	-0.0093	0.010					
68:	2 1 2 3 1	1 0 1 2 2	8937.5138	-0.0002	0.010					
69:	3 1 3 1 2	2 1 2 1 1	9278.0025	-0.0123	0.010	0.0015	0.27			
!										
70:	3 1 3 2 5	2 1 2 2 4	9278.0025	0.0067	0.010	0.0015	0.73			
71:	3 1 3 3 5	2 1 2 3 4	9278.6010	0.0193	0.010					
72:	3 1 3 3 6	2 1 2 3 5	9279.0920	0.0090	0.010					
73:	3 1 3 1 3	2 1 2 0 2	9279.2205	0.0026	0.010					
!										
74:	5 1 4 2 7	5 0 5 3 7	9389.4591	0.0078	0.010					
75:	5 1 4 1 4	5 0 5 1 4	9399.2632	-0.0079	0.010					
76:	5 1 4 2 4	5 0 5 3 4	9399.5160	-0.0010	0.010					
77:	5 1 4 3 7	5 0 5 2 7	9400.0692	0.0091	0.010					
78:	5 1 4 3 6	5 0 5 3 6	9403.0724	0.0134	0.010					
!										
79:	2 2 1 1 2	2 1 2 1 2	9894.0136	0.0080	0.010					
80:	2 2 1 2 4	2 1 2 2 3	9896.8252	-0.0490	0.010	-0.0067	0.23			
81:	2 2 1 2 4	2 1 2 2 4	9896.8252	0.0059	0.010	-0.0067	0.77			
82:	2 2 1 3 5	2 1 2 3 5	9897.3358	-0.0047	0.010					
83:	2 2 1 3 5	2 1 2 3 4	9906.3123	0.0064	0.010					
84:	2 2 1 3 3	2 1 2 3 4	9907.4225	-0.0035	0.010					
!										
85:	3 2 2 1 3	3 1 3 1 3	10849.4522	-0.0048	0.010					
86:	3 2 2 2 3	3 1 3 0 3	10850.1909	0.0226	0.010					
87:	3 2 2 3 6	3 1 3 3 6	10852.3912	0.0078	0.010					
88:	3 2 2 1 4	3 1 3 1 4	10855.8333	-0.0122	0.010					
89:	3 2 2 3 4	3 1 3 3 5	10861.8896	-0.0293	0.010	-0.0169	0.23			
90:	3 2 2 3 5	3 1 3 3 5	10861.8896	-0.0131	0.010	-0.0169	0.77			
91:	3 2 2 2 3	3 1 3 2 3	10864.3938	0.0060	0.010					
!										
92:	3 1 2 3 6	2 1 1 3 5	11075.1227	0.0070	0.010					
93:	3 1 2 1 3	2 1 1 1 2	11075.3767	0.0024	0.010					
94:	3 1 2 3 5	2 1 1 3 4	11075.6196	-0.0067	0.010					
!										
95:	4 0 4 3 6	3 1 3 3 6	11256.3934	0.0084	0.010					
96:	4 0 4 3 3	3 1 3 3 2	11259.3951	-0.0064	0.010					
97:	4 0 4 3 6	3 1 3 2 5	11260.9584	0.0017	0.010					
98:	4 0 4 2 5	3 1 3 1 4	11263.1569	0.0045	0.010					
99:	4 0 4 1 4	3 1 3 0 3	11264.1996	0.0013	0.010					
100:	4 0 4 2 5	3 1 3 2 4	11264.4360	0.0001	0.010					
101:	4 0 4 2 2	3 1 3 2 1	11264.9107	0.0073	0.010					
102:	4 0 4 0 4	3 1 3 1 3	11265.6920	-0.0184	0.010	-0.0030	0.35			
103:	4 0 4 3 7	3 1 3 3 6	11265.6920	0.0051	0.010	-0.0030	0.65			
104:	4 0 4 3 6	3 1 3 3 5	11265.8487	-0.0028	0.010					
105:	4 0 4 3 4	3 1 3 3 3	11265.9738	0.0066	0.010					
106:	4 0 4 3 1	3 1 3 3 1	11266.1353	-0.0063	0.010					
107:	4 0 4 1 3	3 1 3 1 2	11266.3585	-0.0188	0.010					
108:	4 0 4 2 4	3 1 3 2 3	11266.9636	0.0155	0.010					
109:	4 0 4 1 5	3 1 3 1 4	11267.4394	-0.0078	0.010					
110:	4 0 4 3 5	3 1 3 3 4	11267.5736	0.0123	0.010					
111:	4 0 4 2 6	3 1 3 2 5	11267.9772	-0.0014	0.010					
112:	4 0 4 3 4	3 1 3 3 4	11270.8767	-0.0130	0.010					
113:	4 0 4 2 3	3 1 3 2 2	11271.3764	0.0027	0.010					
!										
114:	3 1 3 3 5	2 0 2 2 4	11456.0695	-0.0065	0.010					
115:	3 1 3 2 3	2 0 2 0 2	11457.5680	0.0044	0.010					
116:	3 1 3 3 5	2 0 2 3 5	11458.3646	-0.0015	0.010					
117:	3 1 3 2 5	2 0 2 2 4	11460.9684	-0.0025	0.010					
118:	3 1 3 3 3	2 0 2 3 3	11461.2408	-0.0226	0.010	-0.0161	0.43			
119:	3 1 3 3 3	2 0 2 0 2	11461.2408	-0.0111	0.010	-0.0161	0.57			
120:	3 1 3 3 4	2 0 2 1 3	11462.1314	0.0089	0.010					
121:	3 1 3 1 4	2 0 2 2 3	11462.8189	0.0160	0.010					
122:	3 1 3 1 3	2 0 2 3 2	11463.6951	-0.0075	0.010					
123:	3 1 3 2 3	2 0 2 2 2	11464.0972	0.0059	0.010					
124:	3 1 3 2 2	2 0 2 1 1	11464.7157	0.0257	0.010	-0.0029	0.19			

264:	6	0	6	1	5	5	1	5	3	5	17815.8846	-0.0304	0.010	0.0000	0.01
265:	6	0	6	3	8	5	1	5	3	7	17815.8846	0.0141	0.010	0.0000	0.19
266:	6	0	6	3	7	5	1	5	3	6	17815.8846	0.0287	0.010	0.0000	0.17
267:	6	0	6	3	9	5	1	5	3	8	17815.8846	0.0400	0.010	0.0000	0.23
!															
268:	3	2	2	3	4	2	1	1	1	3	18321.7543	-0.0043	0.010	-0.0034	0.87
269:	3	2	2	2	3	2	1	1	1	3	18321.7543	0.0029	0.010	-0.0034	0.13
270:	3	2	2	1	4	2	1	1	3	3	18329.3586	-0.0025	0.010		
271:	3	2	2	1	3	2	1	1	1	2	18331.1732	-0.0096	0.010		
272:	3	2	2	3	6	2	1	1	3	5	18331.8445	0.0027	0.010		
273:	3	2	2	2	4	2	1	1	2	3	18333.4613	0.0110	0.010		
274:	3	2	2	2	5	2	1	1	2	4	18334.3202	-0.0029	0.010		
275:	3	2	2	2	3	2	1	1	3	2	18341.0493	0.0149	0.010	0.0091	0.73
276:	3	2	2	3	2	2	1	1	3	2	18341.0493	-0.0065	0.010	0.0091	0.27
277:	3	2	2	3	1	2	1	1	3	1	18341.2255	-0.0044	0.010	-0.0020	0.45
278:	3	2	2	3	2	2	1	1	3	1	18341.2255	0.0000	0.010	-0.0020	0.55

PARAMETERS IN FIT:

10000	A	/MHz	4705.47947(68)	1
20000	B	/MHz	2006.57149(93)	2
30000	C	/MHz	1404.63530(63)	3
200	DJ	/kHz	3.329(18)	4
1100	DJK	/kHz	6.312(62)	5
2000	DK	/kHz	22.64(11)	6
40100	dJ	/kHz	0.9921(75)	7
41000	dK	/kHz	9.12(29)	8
110010000	1.5*Xaa	/MHz	-50.971(10)	9
110040000	(Xb-Xc)/4	/MHz	-2.6286(40)	10
110610000	chiab	/MHz	21.4(12)	11
220010000	1.5*Xaa	/MHz	27.332(13)	12
220040000	(Xb-Xc)/4	/MHz	-18.3596(30)	13
220610000	chiab	/MHz	20.1(12)	14

MICROWAVE AVG = -0.000065 MHz, IR AVG = 0.00000
 MICROWAVE RMS = 0.008620 MHz, IR RMS = 0.00000
 END OF ITERATION 1 OLD, NEW RMS ERROR= 0.86199 0.86199

distinct frequency lines in fit: 226
 distinct parameters of fit: 14

for standard parameter errors previous errors are multiplied by: 0.889997

PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:

10000	A	/MHz	4705.47947(60)	1
20000	B	/MHz	2006.57149(82)	2
30000	C	/MHz	1404.63530(56)	3
200	DJ	/kHz	3.329(16)	4
1100	DJK	/kHz	6.312(55)	5
2000	DK	/kHz	22.641(98)	6
40100	dJ	/kHz	0.9921(66)	7
41000	dK	/kHz	9.12(26)	8
110010000	1.5*Xaa	/MHz	-50.9719(95)	9
110040000	(Xb-Xc)/4	/MHz	-2.6286(35)	10
110610000	chiab	/MHz	21.4(10)	11
220010000	1.5*Xaa	/MHz	27.332(12)	12
220040000	(Xb-Xc)/4	/MHz	-18.3596(27)	13
220610000	chiab	/MHz	20.1(11)	14

CORRELATION COEFFICIENTS, C.ij:

	A	B	C	-DJ	-DJK	-DK	-dJ	-dK
A	1.0000							
B	-0.0855	1.0000						
C	-0.0159	-0.5203	1.0000					
-DJ	0.1546	-0.9311	0.5344	1.0000				
-DJK	-0.4559	0.3839	-0.2684	-0.4710	1.0000			
-DK	-0.3582	0.2794	-0.1612	-0.2992	-0.3783	1.0000		

-dJ	-0.0257	-0.7679	0.4036	0.6007	-0.3530	0.0635	1.0000		
-dK	0.1181	-0.6497	0.8273	0.7770	-0.3497	-0.3612	0.2213	1.0000	
1.5*Xaa	-0.0812	-0.1344	0.0323	0.0932	0.0073	-0.0220	0.1526	0.0131	
(Xb-Xc)/4	-0.0052	-0.0278	0.0446	0.0313	-0.0116	-0.0333	-0.0425	0.0807	
chiab	-0.1486	-0.0051	-0.0027	-0.0194	0.1138	0.0235	0.0181	-0.0252	
1.5*Xaa	0.0010	0.0149	-0.0565	-0.0174	0.0014	0.0040	0.0032	-0.0543	
(Xb-Xc)/4	0.0315	0.0755	0.0387	-0.0338	-0.0485	0.0648	-0.0089	0.0022	
chiab	0.0437	-0.0988	0.1030	0.1409	0.0038	-0.2173	-0.0414	0.2013	

1.5*Xaa (Xb-Xc)/ chiab 1.5*Xaa (Xb-Xc)/ chiab

1.5*Xaa	1.0000								
(Xb-Xc)/4	-0.3978	1.0000							
chiab	0.0495	-0.0681	1.0000						
1.5*Xaa	0.4307	-0.3839	0.0411	1.0000					
(Xb-Xc)/4	-0.0974	-0.1861	0.0330	-0.0157	1.0000				
chiab	-0.0664	0.1311	-0.7915	-0.0721	-0.0705	1.0000			

Mean value of |C.ij|, i.ne.j = 0.1772
 Mean value of C.ij, i.ne.j = -0.0368

Worst fitting lines (obs-calc/error):

217:	-2.5	171:	-2.5	86:	2.3	204:	2.2
250:	2.2	148:	2.1	168:	1.9	71:	1.9
107:	-1.9	157:	-1.7	89:	-1.7	258:	-1.6
118:	-1.6	153:	1.6	121:	1.6	108:	1.6
214:	1.5	126:	1.5	234:	-1.5	144:	1.5
202:	-1.5	55:	-1.5	151:	-1.4	34:	1.4
182:	1.4	180:	1.4	187:	1.4	24:	-1.4
78:	1.3	112:	-1.3	11:	1.3	60:	-1.3
110:	1.2	88:	-1.2	49:	1.2	176:	1.2
25:	1.2	150:	-1.1	135:	-1.1	139:	-1.1
273:	1.1	44:	-1.1	199:	-1.1	175:	1.0
138:	-1.0	162:	-1.0	172:	1.0	239:	1.0
58:	-1.0	174:	1.0				

SPFIT output reformatted with PIFORM