

Table S7. The results of fit and the data files for the SPFIT program for the W state of the parent isotopic species of (HC1)2 H2O.

(H2O)(HC1)2, W state

Mon Mar 14 10:33:20 2011

		obs	o-c	error	blends	Notes
					o-c wt	
-----						
/ instead of : below denotes (o-c)>3*err						
-----						
!						
1:	1 1 1 2 1	0 0 0 2 2	6147.1417	0.0059	0.010	
2:	1 1 1 3 3	0 0 0 3 3	6147.6420	0.0039	0.010	
3:	1 1 1 0 1	0 0 0 0 0	6156.9884	-0.0069	0.010	
4:	1 1 1 3 4	0 0 0 3 3	6157.8499	-0.0009	0.010	
5:	1 1 1 1 2	0 0 0 1 1	6158.4226	0.0085	0.010	
6:	1 1 1 2 3	0 0 0 2 2	6160.6161	0.0036	0.010	
7:	1 1 1 3 2	0 0 0 3 3	6168.5044	-0.0092	0.010	
!						
8:	3 2 1 3 5	3 1 2 3 5	7561.4395	0.0050	0.010	
9:	3 2 1 1 4	3 1 2 2 4	7572.4842	-0.0030	0.010	
10:	3 2 1 2 5	3 1 2 2 5	7574.5042	-0.0004	0.010	
!						
11:	3 0 3 3 5	2 1 2 2 4	7990.6502	0.0236	0.010	0.0121 0.75
12:	3 0 3 1 2	2 1 2 2 1	7990.6502	-0.0228	0.010	0.0121 0.25
13:	3 0 3 2 4	2 1 2 1 3	7993.8824	-0.0105	0.010	
14:	3 0 3 2 3	2 1 2 0 2	7997.9639	-0.0241	0.010	-0.0087 0.25
15:	3 0 3 3 6	2 1 2 3 5	7997.9639	-0.0035	0.010	-0.0087 0.75
16:	3 0 3 2 5	2 1 2 2 4	8001.7687	0.0118	0.010	-0.0036 0.69
17:	3 0 3 1 4	2 1 2 2 3	8001.7687	-0.0383	0.010	-0.0036 0.31
18:	3 0 3 3 3	2 1 2 3 3	8003.7501	0.0020	0.010	
19:	3 0 3 2 5	2 1 2 3 4	8007.7426	-0.0044	0.010	
!						
20:	2 2 0 2 3	2 1 1 1 3	8051.9735	0.0172	0.010	
21:	2 2 0 1 2	2 1 1 0 2	8061.4762	0.0106	0.010	
22:	2 2 0 3 5	2 1 1 3 5	8062.9986	-0.0010	0.010	
23:	2 2 0 3 4	2 1 1 1 3	8064.0289	0.0198	0.010	
!						
24:	2 1 2 3 3	1 0 1 3 2	9006.3126	0.0043	0.010	
25:	2 1 2 0 2	1 0 1 3 2	9006.7962	-0.0184	0.010	
26:	2 1 2 3 4	1 0 1 2 3	9015.7734	0.0208	0.010	
27:	2 1 2 3 4	1 0 1 3 4	9018.9636	0.0006	0.010	
28:	2 1 2 1 2	1 0 1 1 1	9022.9579	-0.0035	0.010	
29:	2 1 2 1 1	1 0 1 1 0	9025.7476	0.0053	0.010	
30:	2 1 2 1 3	1 0 1 1 2	9026.4341	0.0001	0.010	
31:	2 1 2 3 4	1 0 1 3 3	9028.6695	0.0062	0.010	
32:	2 1 2 3 5	1 0 1 3 4	9028.9298	0.0003	0.010	
33:	2 1 2 2 2	1 0 1 0 1	9033.3063	-0.0029	0.010	
34:	2 1 2 1 3	1 0 1 3 3	9036.6534	0.0007	0.010	
35:	2 1 2 2 2	1 0 1 2 2	9044.9409	0.0033	0.010	
36:	2 1 2 3 1	1 0 1 2 2	9047.2344	0.0055	0.010	
!						
37:	5 1 4 3 8	5 0 5 3 8	9734.9268	0.0057	0.010	
38:	5 1 4 1 6	5 0 5 1 6	9745.8634	-0.0105	0.010	
!						
39:	3 0 3 2 5	2 0 2 2 4	10119.9117	-0.0034	0.010	
40:	3 0 3 1 3	2 0 2 1 2	10122.8301	0.0004	0.010	
!						
41:	3 2 2 2 4	3 1 3 2 4	10864.9026	0.0007	0.010	
42:	3 2 2 3 4	3 1 3 3 4	10874.2970	-0.0083	0.010	
!						
43:	3 1 3 3 5	2 0 2 2 4	11611.4127	0.0122	0.010	
44:	3 1 3 3 5	2 0 2 3 5	11613.4883	-0.0023	0.010	
45:	3 1 3 2 5	2 0 2 2 4	11617.7760	-0.0057	0.010	
46:	3 1 3 2 4	2 0 2 3 3	11621.3325	-0.0062	0.010	
47:	3 1 3 2 3	2 0 2 2 2	11621.4667	0.0145	0.010	
48:	3 1 3 2 1	2 0 2 2 1	11621.6886	0.0052	0.010	
!						
49:	4 2 3 0 4	4 1 4 0 4	12215.7687	-0.0154	0.010	
50:	4 2 3 3 7	4 1 4 3 7	12217.4397	-0.0058	0.010	
51:	4 2 3 3 5	4 1 4 2 5	12222.4273	0.0067	0.010	
!						
52:	4 2 3 3 6	4 1 4 3 6	12225.1100	0.0135	0.010	
53:	4 2 3 1 5	4 1 4 3 5	12231.0402	0.0024	0.010	
54:	4 2 3 3 5	4 1 4 3 5	12232.0398	-0.0020	0.010	
!						
55:	4 3 1 2 5	4 2 2 2 5	13873.5726	-0.0155	0.010	
56:	4 3 1 3 6	4 2 2 2 6	13875.8995	-0.0134	0.010	
!						
57:	4 1 4 3 3	3 0 3 3 2	14066.1314	-0.0033	0.010	
58:	4 1 4 3 4	3 0 3 3 3	14066.8819	-0.0037	0.010	
59:	4 1 4 1 5	3 0 3 1 4	14068.9049	-0.0005	0.010	
60:	4 1 4 2 4	3 0 3 2 3	14069.0948	0.0008	0.010	
61:	4 1 4 3 2	3 0 3 3 1	14069.6734	-0.0032	0.010	
62:	4 1 4 2 5	3 0 3 2 4	14071.8410	0.0012	0.010	
63:	4 1 4 1 4	3 0 3 1 3	14075.0861	0.0012	0.010	
64:	4 1 4 1 4	3 0 3 1 3	14075.0893	0.0043	0.010	
!						
65:	3 3 0 2 4	3 2 1 2 4	14427.8726	0.0023	0.010	
66:	3 3 0 3 6	3 2 1 3 6	14433.4432	-0.0064	0.010	
67:	3 3 0 3 5	3 2 1 2 5	14446.4700	0.0065	0.010	
!						
68:	3 3 1 2 5	3 2 2 3 5	14901.3838	-0.0021	0.010	
69:	3 3 1 3 6	3 2 2 3 6	14906.0054	-0.0130	0.010	
70:	3 3 1 3 5	3 2 2 2 5	14919.2775	-0.0173	0.010	
!						
71:	2 2 1 3 2	1 1 0 2 2	15587.4442	-0.0071	0.010	
72:	2 2 1 1 1	1 1 0 1 0	15587.5696	0.0086	0.010	
73:	2 2 1 1 2	1 1 0 0 1	15588.8489	0.0085	0.010	
74:	2 2 1 3 3	1 1 0 3 3	15590.3294	-0.0008	0.010	
75:	2 2 1 2 4	1 1 0 2 3	15592.9767	0.0049	0.010	
76:	2 2 1 2 3	1 1 0 2 3	15594.2487	0.0051	0.010	
77:	2 2 1 2 2	1 1 0 0 1	15598.5091	0.0143	0.010	
78:	2 2 1 3 4	1 1 0 3 3	15598.7763	-0.0032	0.010	
79:	2 2 1 1 2	1 1 0 1 1	15603.2436	-0.0044	0.010	
80:	2 2 1 1 2	1 1 0 2 1	15606.5101	0.0099	0.010	
81:	2 2 1 3 4	1 1 0 2 3	15607.1633	0.0122	0.010	
82:	2 2 1 3 3	1 1 0 3 2	15608.8972	0.0058	0.010	
!						
83:	2 2 0 3 1	1 1 1 3 2	16306.9231	-0.0016	0.010	
84:	2 2 0 2 3	1 1 1 3 2	16314.3980	-0.0021	0.010	
85:	2 2 0 1 2	1 1 1 1 1	16316.8764	-0.0013	0.010	
86:	2 2 0 2 1	1 1 1 3 2	16318.2058	-0.0047	0.010	-0.0004 0.57
87:	2 2 0 3 2	1 1 1 3 2	16318.2058	0.0053	0.010	-0.0004 0.43
88:	2 2 0 0 2	1 1 1 0 1	16318.5735	0.0048	0.010	
89:	2 2 0 2 4	1 1 1 3 4	16324.3339	0.0087	0.010	
90:	2 2 0 2 3	1 1 1 1 2	16324.5031	0.0034	0.010	
91:	2 2 0 1 3	1 1 1 3 2	16325.7150	0.0007	0.010	
92:	2 2 0 3 2	1 1 1 2 3	16326.0924	-0.0102	0.010	
93:	2 2 0 2 2	1 1 1 3 2	16326.3960	0.0609	0.010	0.0053 0.17
94:	2 2 0 3 5	1 1 1 3 4	16326.3960	-0.0062	0.010	0.0053 0.83
95:	2 2 0 1 1	1 1 1 3 2	16327.0657	0.0044	0.010	
96:	2 2 0 3 1	1 1 1 2 2	16330.2679	-0.0026	0.010	
97:	2 2 0 3 4	1 1 1 2 3	16334.3457	-0.0092	0.010	
98:	2 2 0 2 4	1 1 1 3 3	16334.5383	0.0003	0.010	
99:	2 2 0 1 3	1 1 1 1 2	16335.8139	0.0000	0.010	
100:	2 2 0 3 4	1 1 1 3 4	16337.1201	0.0043	0.010	
101:	2 2 0 1 2	1 1 1 2 1	16337.7467	0.0213	0.010	
102:	2 2 0 3 3	1 1 1 3 3	16339.0839	0.0074	0.010	0.0075 0.65
103:	2 2 0 3 2	1 1 1 3 3	16339.0839	0.0076	0.010	0.0075 0.35
104:	2 2 0 2 1	1 1 1 2 1	16339.5723	-0.0170	0.010	-0.0139 0.60
105:	2 2 0 2 0	1 1 1 2 1	16339.5723	-0.0092	0.010	-0.0139 0.40
106:	2 2 0 3 3	1 1 1 2 2	16341.5426	-0.0040	0.010	-0.0039 0.47
107:	2 2 0 3 2	1 1 1 2 2	16341.5426	-0.0037	0.010	-0.0039 0.53
!						
108:	5 1 5 3 5	4 0 4 3 4	16521.5378	-0.0076	0.010	
109:	5 1 5 1 4	4 0 4 1 3	16523.5363	-0.0086	0.010	
110:	5 1 5 1 5	4 0 4 1 4	16527.1723	-0.0088	0.010	
!						
111:	3 2 2 1 2	2 1 1 1 1	18468.1785	-0.0024	0.010	0.0002 0.21
112:	3 2 2 3 3	2 1 1 0 2	18468.1785	-0.0032	0.010	0.0002 0.29
113:	3 2 2 1 4	2 1 1 3 3	18468.1785	0.0033	0.010	0.0002 0.50
114:	3 2 2 3 6	2 1 1 3 5	18470.3265	-0.0078	0.010	
115:	3 2 2 2 4	2 1 1 2 3	18472.5422	-0.0016	0.010	
116:	3 2 2 2 3	2 1 1 3 2	18479.7929	-0.0145	0.010	
117:	3 2 2 3 1	2 1 1 3 1	18480.1030	0.0023	0.010	0.0051 0.47

118: 3 2 2 3 2 2 1 1 3 1 18480.1030 0.0074 0.010 0.0051 0.53

50: -0.6 82: 0.6 37: 0.6 45: -0.6  
36: 0.5 29: 0.5

PARAMETERS IN FIT:

10000	A	/MHz	4721.40834(38)	1
20000	B	/MHz	2066.82336(42)	2
30000	C	/MHz	1434.96669(24)	3
200	DJ	/kHz	[ 3.52898182]	4
1100	DJK	/kHz	[ 6.026340396]	5
2000	DK	/kHz	[23.531208]	6
40100	dJ	/kHz	[ 1.08301351]	7
41000	dK	/kHz	[ 9.487819961]	8
110010000	1.5*Xaa	/MHz	[-65.599810085]	9
110040000	(Xb-Xc)/4	/MHz	[-3.182375443]	10
110610000	chiab	/MHz	[26.767689394]	11
220010000	1.5*Xaa	/MHz	[26.69161547]	12
220040000	(Xb-Xc)/4	/MHz	[-18.253092415]	13
220610000	chiab	/MHz	[21.147879983]	14

MICROWAVE AVG = 0.000263 MHz, IR AVG = 0.00000  
MICROWAVE RMS = 0.008120 MHz, IR RMS = 0.00000  
END OF ITERATION 1 OLD, NEW RMS ERROR= 0.81201 0.81201

distinct frequency lines in fit: 107  
distinct parameters of fit: 3

for standard parameter errors previous errors are multiplied by: 0.823638

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

10000	A	/MHz	4721.40834(31)	1
20000	B	/MHz	2066.82336(34)	2
30000	C	/MHz	1434.96669(20)	3
200	DJ	/kHz	[ 3.52898182]	4
1100	DJK	/kHz	[ 6.026340396]	5
2000	DK	/kHz	[23.531208]	6
40100	dJ	/kHz	[ 1.08301351]	7
41000	dK	/kHz	[ 9.487819961]	8
110010000	1.5*Xaa	/MHz	[-65.599810085]	9
110040000	(Xb-Xc)/4	/MHz	[-3.182375443]	10
110610000	chiab	/MHz	[26.767689394]	11
220010000	1.5*Xaa	/MHz	[26.69161547]	12
220040000	(Xb-Xc)/4	/MHz	[-18.253092415]	13
220610000	chiab	/MHz	[21.147879983]	14

CORRELATION COEFFICIENTS, C.ij:

	A	B	C
A	1.0000		
B	0.0943	1.0000	
C	0.0580	0.3923	1.0000

Mean value of |C.ij|, i.ne.j = 0.1815  
Mean value of C.ij, i.ne.j = 0.1815

Worst fitting lines (obs-calc/error):

101:	2.1	26:	2.1	23:	2.0	25:	-1.8
70:	-1.7	20:	1.7	55:	-1.6	49:	-1.5
116:	-1.4	47:	1.4	77:	1.4	104:	-1.4
52:	1.3	56:	-1.3	69:	-1.3	81:	1.2
43:	1.2	11:	1.2	21:	1.1	13:	-1.1
38:	-1.1	92:	-1.0	80:	1.0	97:	-0.9
7:	-0.9	110:	-0.9	14:	-0.9	89:	0.9
72:	0.9	109:	-0.9	73:	0.9	5:	0.9
42:	-0.8	114:	-0.8	108:	-0.8	102:	0.8
71:	-0.7	3:	-0.7	51:	0.7	67:	0.6
66:	-0.6	31:	0.6	46:	-0.6	1:	0.6

SPFIT output reformatted with PIFORM