Table S5. The results of fit and the data files for the SPFIT program for the S state of the 18O species of (HCl)2 H2O.

(H2 18O)(HCl)2 Mon Mar 14 10:13:01 2011

											obs	o-c	error	blends o-c	Notes wt
/ instead of : below denotes (o-c)>3*err															
!															
1:	3	0	3	1	3	2	1	2	2	2	8156.6952	0.0151	0.010		
2:	3	0	3	2	4	2	1	2	2	3	8157.8183	-0.0028	0.010		
3:	3	0	3	3	5	2	1	2	3	4	8158.6493	0.0027	0.010		
4:	3	0	3	3	6	2	1	2	3	5	8159.9733	0.0212	0.010		
5:	3	0	3	2	5	2	1	2	2	4	8163.1267	-0.0082	0.010		
!															
6:	2	1	2	2	3	1	0	1	3	2	8553.0838	-0.0004	0.010		
7:	2	1	2	3	4	1	0	1	2	3	8554.4134	-0.0100	0.010		
8:	2	1	2	3	4	1	0	1	3	4	8557.7169	-0.0023	0.010		
9:	2	1	2	2	4	1	0	1	2	3	8560.4152	-0.0020	0.010		
10:	2	1	2	1	3	1	0	1	1	2	8565.2161	0.0088	0.010		
11:	2	1	2	3	4	1	0	1	3	3	8567.2456	-0.0046	0.010		
12:	2	1	2	3	5	1	0	1	3	4	8567.6887	-0.0024	0.010		
13:	2	1	2	3	3	1	0	1	2	2	8568.1573	-0.0062	0.010		
14:	2	1	2	2	2	1	0	1	0	1	8572.0633	-0.0020	0.010		
15:	2	1	2	2	3	1	0	1	3	3	8573.2510	-0.0065	0.010		
16:	2	1	2	2	1	1	0	1	2	1	8574.0362	0.0176	0.010		
17:	2	1	2	3	2	1	0	1	2	2	8576.1321	0.0104	0.010		
!															
18:	3	2	2	3	6	3	1	3	3	6	9962.5310	0.0048	0.010		
19:	3	2	2	2	5	3	1	3	2	5	9967.5133	0.0125	0.010		
!															
20:	3	1	3	3	5	2	0	2	3	5	11076.0466	-0.0095	0.010		
21:	3	1	3	2	5	2	0	2	2	4	11080.4379	-0.0079	0.010		
22:	3	1	3	3	4	2	0	2	1	3	11081.9308	0.0083	0.010	0.0083	0.50
23:	3	1	3	3	4	2	0	2	1	3	11081.9308	0.0083	0.010	0.0083	0.50
24:	3	1	3	1	4	2	0	2	2	3	11082.3969	-0.0004	0.010		
25:	3	1	3	1	3	2	0	2	0	2	11082.6219	-0.0083	0.010		
26:	3	1	3	2	3	2	0	2	2	2	11083.8174	-0.0112	0.010	-0.0249	0.50
27:	3	1	3	2	4	2	0	2	3	3	11083.8174	-0.0385	0.010	-0.0249	0.50
28:	3	1	3	3	5	2	0	2	3	4	11086.6460	0.0030	0.010		
29:	3	1	3	3	6	2	0	2	3	5	11087.2507	-0.0032	0.010		
30:	3	1	3	0	3	2	0	2	1	2	11090.0920	0.0038	0.010		
!															
31:	4	2	3	1	4	4	1	4	1	4	11402.7978	0.0103	0.010		
32:	4	2	3	3	7	4	1	4	3	7	11404.9240	-0.0050	0.010		
33:	4	2	3	2	5	4	1	4	1	5	11410.3762	-0.0165	0.010		
34:	4	2	3	1	5	4	1	4	3	5	11418.6991	0.0003	0.010		
!															
35:	4	0	4	2	5	3	1	3	2	4	11643.8545	0.0033	0.010		
36:	4	0	4	1	4	3	1	3	0	3	11644.4018	-0.0076	0.010		
37:	4	0	4	3	4	3	1	3	3	3	11644.5258	0.0089	0.010		
38:	4	0	4	3	6	3	1	3	3	5	11644.9844	-0.0092	0.010		
39:	4	0	4	2	4	3	1	3	2	3	11645.6426	0.0420	0.010	0.0022	0.33
40:	4	0	4	3	7	3	1	3	3	6	11645.6426	-0.0175	0.010	0.0022	0.67
41:	4	0	4	3	5	3	1	3	3	4	11646.0377	-0.0141	0.010		
42:	4	0	4	1	5	3	1	3	1	4	11646.7444	-0.0003	0.010		
43:	4	0	4	2	6	3	1	3	2	5	11647.2304	-0.0043	0.010		
!															
44:	4	1	4	1	3	3	0	3	2	2	13475.0271	0.0392	0.010	0.0207	0.36
45:	4	1	4	3	3	3	0	3	3	2	13475.0271	0.0104	0.010	0.0207	0.64
46:	4	1	4	3	4	3	0	3	3	3	13475.6144	0.0040	0.010		
47:	4	1	4	3	5	3	0	3	3	4	13476.3574	0.0006	0.010		
48:	4	1	4	2	6	3	0	3	2	5	13476.7481	-0.0011	0.010		
49:	4	1	4	0	4	3	0	3	0	3	13480.0119	0.0120	0.010		
50:	4	1	4	2	5	3	0	3	2	4	13480.3358	0.0036	0.010		
51:	4	1	4	3	6	3	0	3	3	5	13480.9729	0.0095	0.010		
52:	4	1	4	3	7	3	0	3	3	6	13481.6871	-0.0027	0.010		
53:	4	1	4	1	4	3	0	3	1	3	13483.3892	-0.0034	0.010		
!															
54:	2	2	1	2	3	1	1	0	1	2	14488.5582	0.0120	0.010		
55:	2	2	1	3	3	1	1	0	3	3	14489.2588	0.0004	0.010		
56:	2	2	1	2	4	1	1	0	2	3	14491.9242	-0.0053	0.010		
57:	2	2	1	2	3	1	1	0	2	3	14493.1513	0.0037	0.010		
58:	2	2	1	2	4	1	1	0	3	4	14494.7142	-0.0023	0.010		
59:	2	2	1	2	2	1	1	0	0	1	14497.3893	-0.0094	0.010		
60:	2	2	1	3	4	1	1	0	3	3	14497.6597	-0.0050	0.010		
61:	2	2	1	3	5	1	1	0	3	4	14498.6167	0.0071	0.010		
62:	2	2	1	1	3	1	1	0	1	2	14500.1594	0.0038	0.010		
63:	2	2	1	1	2	1	1	0	1	1	14502.1235	0.0070	0.010		
64:	2	2	1	1	3	1	1	0	2	2	14504.7383	-0.0221	0.010		
65:	2	2	1	3	4	1	1	0	2	3	14506.0403	-0.0016	0.010		
66:	2	2	1	3	3	1	1	0	3	2	14507.8196	-0.0102	0.010		
67:	2	2	1	3	3	1	1	0	3	2	14507.8203	-0.0095	0.010		
68:	2	2	1	3	4	1	1	0	3	4	14508.8387	0.0097	0.010		
69:	2	2	1	3	4	1	1	0	3	4	14508.8400	0.0110	0.010		
!															
70:	5	0	5	2	4	4	1	4	2	3	14895.4741	-0.0150	0.010		
71:	5	0	5	0	5	4	1	4	0	4	14896.7750	-0.0043	0.010	-0.0082	0.43
72:	5	0	5	3	7	4	1	4	3	6	14896.7750	-0.0111	0.010	-0.0082	0.57
73:	5	0	5	3	8	4	1	4	3	7	14897.1345	0.0007	0.010		
74:	5	0	5	1	6	4	1	4	1	5	14897.3263	0.0171	0.010		
75:	5	0	5	2	7	4	1	4	2	6	14897.4587	-0.0040	0.010		
!															
76:	2	2	0	2	3	1	1	1	3	2	15271.0606	-0.0014	0.010		
77:	2	2	0	1	2	1	1	1	1	1	15273.2851	0.0012	0.010		
78:	2	2	0	0	2	1	1	1	1	2	15273.8231	-0.0064	0.010		
79:	2	2	0	2	4	1	1	1	2	3	15278.4282	0.0128	0.010		
80:	2	2	0	1	3	1	1	1	3	2	15282.1816	-0.0037	0.010		
81:	2	2	0	3	5	1	1	1	3	4	15282.8911	0.0077	0.010		
82:	2	2	0	3	3	1	1	1	1	2	15284.8222	0.0026	0.010		
83:	2	2	0	3	2	1	1	1	0	1	15286.2153	-0.0147	0.010		
84:	2	2	0	2	4	1	1	1	3	3	15291.4098	0.0101	0.010		
85:	2	2	0	1	3	1	1	1	1	2	15292.2718	0.0032	0.010		
86:	2	2	0	3	4	1	1	1	3	4	15293.4796	-0.0126	0.010		
87:	2	2	0	2	3	1	1	1	2	2	15294.4403	0.0113	0.010		
88:	2	2	0	1	3	1	1	1	3	3	15303.1916	0.0087	0.010		
!															
89:	5	1	5	3	6	4	0	4	3	5	15912.2887	-0.0015	0.010		
90:	5	1	5	2	7	4	0	4	2	6	15912.9373	-0.0065	0.010	-0.0017	0.59
91:	5	1	5	2	5	4	0	4	2	4	15912.9373	0.0052	0.010	-0.0017	0.41
92:	5	1	5	2	6	4	0	4	2	5	15915.2532	0.0029	0.010	0.0055	0.67
93:	5	1	5	2	3	4	0	4	2	2	15915.2532	0.0105	0.010	0.0055	0.33
94:	5	1	5	3	7	4	0	4	3	6	15915.4770	0.0031	0.010		
95:	5	1	5	3	8	4	0	4	3	7	15916.0883	0.0057	0.010		
96:	5	1	5	1	5	4	0	4	1	4	15916.8024	-0.0083	0.010		
!															
97:	3	2	2	3	5	2	1	1	3	4	17287.8309	0.0077	0.010		
98:	3	2	2	3	4	2	1	1	1	3	17288.9133	0.0098	0.010		
99:	3	2	2	1	4	2	1	1	3	3	17296.5075	-0.0031	0.010		
100:	3	2	2	0	3	2	1	1	1	2	17297.9613	-0.0237	0.010		
101:	3	2	2	3	6	2	1	1	3	5	17298.7327	0.0038	0.010		
102:	3	2	2	2	4	2	1	1	2	3	17300.8317	-0.0034	0.010		
103:	3	2	2	2	5	2	1	1	2	4	17301.9054	-0.0041	0.010		
104:	3	2	2	2	3	2	1	1	3	2	17308.1914	-0.0031	0.010	0.0002	0.54
105:	3	2	2	1	3	2	1	1	3	2	17308.1914	0.0041	0.010	0.0002	0.46

PARAMETERS IN FIT:

10000	A	/MHz	4366.1667(36)	1
20000	B	/MHz	2064.58178(96)	2
30000	C	/MHz	1399.61390(64)	3
200	DJ	/kHz	3.475(17)	4
1100	DJK	/kHz	5.77(14)	5
2000	DK	/kHz	19.27(63)	6
40100	dJ	/kHz	[1.083]	7
41000	dK	/kHz	[9.488]	8
110010000	1.5*Xaa	/MHz	-64.674(19)	9
110040000	(Xb-Xc)/4	/MHz	-3.3512(84)	10
110610000	chiab	/MHz	[26.76]	11
220010000	1.5*Xaa	/MHz	27.306(26)	12
220040000	(Xb-Xc)/4	/MHz	-18.3564(56)	13
220610000	chiab	/MHz	[21.15]	14

```
 MICROWAVE AVG =        0.000065 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.009105 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        0.91047         0.91047

  distinct frequency lines in fit:    97
       distinct parameters of fit:    10

 for standard parameter errors previous errors are multiplied by:   0.961373

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

        10000            A  /MHz         4366.1667(34)                        1
        20000            B  /MHz         2064.58178(92)                       2
        30000            C  /MHz         1399.61390(61)                       3

          200           DJ  /kHz            3.475(16)                         4
         1100          DJK  /kHz            5.77(13)                          5
         2000           DK  /kHz           19.27(60)                          6
        40100           dJ  /kHz          [ 1.083]                            7
        41000           dK  /kHz          [ 9.488]                            8

    110010000      1.5*Xaa  /MHz          -64.674(18)                         9
    110040000    (Xb-Xc)/4  /MHz           -3.3512(80)                       10
    110610000         chiab /MHz          [26.76]                            11

    220010000      1.5*Xaa  /MHz           27.306(25)                        12
    220040000    (Xb-Xc)/4  /MHz          -18.3564(53)                       13
    220610000         chiab /MHz          [21.15]                            14

 CORRELATION COEFFICIENTS, C.ij:

           A        B        C        -DJ      -DJK     -DK      1.5*Xaa  (Xb-Xc)/

A           1.0000
B           0.4701   1.0000
C          -0.5335   0.1389   1.0000
-DJ         0.4873  -0.2434  -0.9313   1.0000
-DJK       -0.6833  -0.1416   0.4991  -0.5923   1.0000
-DK        -0.9274  -0.5488   0.4498  -0.3535   0.3951   1.0000
1.5*Xaa     0.0480  -0.0107  -0.0082   0.0300  -0.1338   0.0446   1.0000
(Xb-Xc)/4  -0.0529  -0.0753   0.0167  -0.0023   0.0001   0.0343  -0.2678   1.0000
1.5*Xaa     0.0475   0.0553  -0.0368   0.0366  -0.1023   0.0273   0.4562  -0.5261
(Xb-Xc)/4  -0.0823  -0.0530   0.0427  -0.0406   0.0986   0.0614   0.0154  -0.3845

           1.5*Xaa  (Xb-Xc)/

1.5*Xaa     0.0000
(Xb-Xc)/4   0.0952   0.0000

 Mean value of |C.ij|, i.ne.j =   0.2285
 Mean value of  C.ij,  i.ne.j =  -0.0707


 Worst fitting lines (obs-calc/error):

    26:   -2.5        100:   -2.4         64:   -2.2          4:    2.1
    44:    2.1         16:    1.8         74:    1.7         33:   -1.7
     1:    1.5         70:   -1.5         83:   -1.5         41:   -1.4
    79:    1.3         86:   -1.3         19:    1.2         54:    1.2
    49:    1.2         87:    1.1         69:    1.1         17:    1.0
    31:    1.0         66:   -1.0         84:    1.0          7:   -1.0
    98:    1.0         68:    1.0         67:   -0.9         51:    0.9
    20:   -0.9         59:   -0.9         38:   -0.9         37:    0.9
    10:    0.9         88:    0.9         22:    0.8         25:   -0.8
    96:   -0.8         71:   -0.8          5:   -0.8         21:   -0.8
    97:    0.8         81:    0.8         36:   -0.8         61:    0.7
    63:    0.7         15:   -0.6         78:   -0.6         13:   -0.6
    95:    0.6         92:    0.5

                                                  ____________________________________
 ________________________________________________/ SPFIT output reformatted with PIFORM
```