Table S6. The results of fit and the data files for the SPFIT program for the HDO species of (HCl)2 H2O.

(HDO)(HCl)2 Mon Mar 14 10:25:10 2011

											obs	o-c	error	blends o-c	Notes wt
/ instead of : below denotes (o-c)>3*err															
!															
1/	2	1	2	3	4	1	0	1	3	4	8848.5035	0.0312	0.010		
2:	2	1	2	2	4	1	0	1	2	3	8851.3129	-0.0205	0.010		
3:	2	1	2	1	3	1	0	1	1	2	8855.9520	0.0116	0.010		
4:	2	1	2	0	2	1	0	1	2	1	8857.5159	0.0119	0.010		
5:	2	1	2	3	5	1	0	1	3	4	8858.4433	0.0031	0.010		
6:	2	1	2	3	3	1	0	1	2	2	8859.0604	-0.0087	0.010		
7:	2	1	2	2	4	1	0	1	3	3	8864.2886	0.0149	0.010		
8:	2	1	2	2	1	1	0	1	2	1	8864.9684	0.0107	0.010		
9:	2	1	2	2	3	1	0	1	2	2	8867.0109	-0.0289	0.010	-0.0231	0.62
10:	2	1	2	3	2	1	0	1	2	2	8867.0109	-0.0132	0.010	-0.0231	0.38
!															
11:	3	1	3	3	2	2	0	2	3	1	11418.0439	0.0007	0.010		
12:	3	1	3	3	2	2	0	2	0	2	11418.1637	0.0019	0.010		
13:	3	1	3	3	3	2	0	2	3	2	11420.3694	0.0142	0.010	0.0080	0.65
14:	3	1	3	3	3	2	0	2	3	3	11420.3694	-0.0036	0.010	0.0080	0.35
15:	3	1	3	2	5	2	0	2	2	4	11420.8280	0.0006	0.010		
16:	3	1	3	3	4	2	0	2	1	3	11422.4311	-0.0138	0.010		
17:	3	1	3	1	4	2	0	2	2	3	11422.7049	-0.0015	0.010		
18:	3	1	3	3	5	2	0	2	3	4	11426.7962	0.0062	0.010		
19:	3	1	3	3	6	2	0	2	3	5	11427.6922	-0.0071	0.010		
20:	3	1	3	1	3	2	0	2	1	2	11430.3040	-0.0018	0.010		
21:	3	1	3	2	3	2	0	2	1	2	11431.7710	0.0136	0.010		
22:	3	1	3	2	4	2	0	2	1	3	11431.8366	-0.0206	0.010		
!															
23:	4	0	4	2	5	3	1	3	2	4	11648.0289	0.0066	0.010		
24:	4	0	4	1	4	3	1	3	1	3	11648.6822	-0.0034	0.010		
25:	4	0	4	3	6	3	1	3	3	5	11649.5740	-0.0034	0.010		
26:	4	0	4	1	3	3	1	3	1	2	11649.8317	-0.0116	0.010	0.0065	0.28
27:	4	0	4	3	7	3	1	3	3	6	11649.8317	0.0134	0.010	0.0065	0.72
28:	4	0	4	0	4	3	1	3	2	3	11650.1419	0.0182	0.010		
29:	4	0	4	2	4	3	1	3	0	3	11650.2286	0.0056	0.010		
30:	4	0	4	3	5	3	1	3	3	4	11650.6043	-0.0171	0.010		
31:	4	0	4	1	5	3	1	3	1	4	11651.3183	-0.0028	0.010		
32:	4	0	4	2	6	3	1	3	2	5	11651.8088	0.0024	0.010		
!															
33:	4	1	4	3	3	3	0	3	3	2	13850.1200	-0.0182	0.010		
34:	4	1	4	3	4	3	0	3	3	3	13850.8635	-0.0147	0.010		
35:	4	1	4	3	5	3	0	3	3	4	13851.6668	0.0075	0.010		
36:	4	1	4	2	6	3	0	3	2	5	13851.8771	-0.0050	0.010		
37:	4	1	4	1	5	3	0	3	1	4	13852.8777	0.0002	0.010		
38:	4	1	4	0	4	3	0	3	0	3	13855.2793	0.0028	0.010		
39:	4	1	4	1	3	3	0	3	2	3	13855.7215	-0.0087	0.010		
40:	4	1	4	3	6	3	0	3	3	5	13856.4588	0.0011	0.010		
41:	4	1	4	3	7	3	0	3	3	6	13857.0864	0.0033	0.010		
42:	4	1	4	1	4	3	0	3	1	3	13858.8414	0.0001	0.010		
!															
43:	5	0	5	2	4	4	1	4	2	3	15007.7227	-0.0069	0.010		
44:	5	0	5	2	6	4	1	4	2	5	15008.2656	-0.0086	0.010		
45:	5	0	5	3	5	4	1	4	3	4	15008.6244	-0.0011	0.010		
46:	5	0	5	1	5	4	1	4	1	4	15008.8972	0.0043	0.010		
47:	5	0	5	0	5	4	1	4	0	4	15009.1454	-0.0002	0.010		
48:	5	0	5	1	6	4	1	4	1	5	15009.9225	0.0005	0.010		
49:	5	0	5	2	7	4	1	4	2	6	15010.1223	0.0029	0.010		
!															
50:	2	2	1	2	3	1	1	0	1	2	15175.6222	-0.0138	0.010		
51:	2	2	1	3	3	1	1	0	3	3	15176.2877	-0.0102	0.010		
52:	2	2	1	2	4	1	1	0	2	3	15178.7325	0.0059	0.010		
53:	2	2	1	2	2	1	1	0	0	1	15184.2489	-0.0015	0.010		
54:	2	2	1	3	4	1	1	0	3	3	15184.5174	-0.0116	0.010		
55:	2	2	1	3	5	1	1	0	3	4	15185.5934	0.0217	0.010		
56:	2	2	1	1	3	1	1	0	1	2	15187.3403	-0.0116	0.010		
57:	2	2	1	1	2	1	1	0	1	1	15189.4381	0.0187	0.010		
58:	2	2	1	1	3	1	1	0	2	2	15191.9516	-0.0034	0.010		
59:	2	2	1	3	4	1	1	0	2	3	15192.9267	0.0247	0.010		
60:	2	2	1	3	3	1	1	0	3	2	15194.8503	-0.0112	0.010		
61:	2	2	1	3	4	1	1	0	3	4	15195.6969	0.0083	0.010		
62:	2	2	1	2	2	1	1	0	3	2	15203.2654	-0.0002	0.010		
!															
63:	2	2	0	1	2	1	1	1	1	1	15923.3003	-0.0194	0.010		
64:	2	2	0	3	2	1	1	1	3	2	15924.7344	-0.0006	0.010	-0.0062	0.44
65:	2	2	0	2	1	1	1	1	3	2	15924.7344	-0.0105	0.010	-0.0062	0.56
66:	2	2	0	1	3	1	1	1	3	2	15932.3394	0.0090	0.010		
67:	2	2	0	3	3	1	1	1	2	3	15932.5230	-0.0146	0.010		
68:	2	2	0	3	5	1	1	1	3	4	15932.8408	0.0257	0.010		
69:	2	2	0	1	1	1	1	1	1	1	15934.1043	-0.0050	0.010		
70:	2	2	0	3	3	1	1	1	1	2	15934.8039	0.0062	0.010		
71:	2	2	0	3	1	1	1	1	2	2	15936.6263	-0.0181	0.010		
72:	2	2	0	0	2	1	1	1	2	2	15936.7453	-0.0043	0.010		
73:	2	2	0	3	4	1	1	1	2	3	15940.8149	0.0014	0.010		
74:	2	2	0	2	4	1	1	1	3	3	15941.0173	0.0092	0.010		
75:	2	2	0	1	3	1	1	1	1	2	15942.3917	-0.0014	0.010		
76:	2	2	0	3	4	1	1	1	3	4	15943.6377	0.0024	0.010		
77:	2	2	0	2	3	1	1	1	2	2	15944.2319	0.0262	0.010		
78:	2	2	0	3	3	1	1	1	3	3	15945.4398	-0.0050	0.010		
79:	2	2	0	1	3	1	1	1	3	3	15953.0271	-0.0133	0.010		
80:	2	2	0	2	2	1	1	1	2	1	15954.1085	-0.0145	0.010		
!															
81:	5	1	5	3	4	4	0	4	2	3	16299.5014	-0.0029	0.010		
82:	5	1	5	3	5	4	0	4	3	4	16299.6400	0.0076	0.010		
83:	5	1	5	3	6	4	0	4	3	5	16300.1288	0.0003	0.010		
84:	5	1	5	2	7	4	0	4	2	6	16300.7180	0.0054	0.010		
85:	5	1	5	2	5	4	0	4	2	4	16300.8642	-0.0004	0.010		
86:	5	1	5	1	6	4	0	4	1	5	16301.0745	-0.0003	0.010	-0.0066	0.71
87:	5	1	5	3	3	4	0	4	3	2	16301.0745	-0.0221	0.010	-0.0066	0.29
88:	5	1	5	1	4	4	0	4	1	3	16301.4600	-0.0013	0.010		
89:	5	1	5	3	7	4	0	4	3	6	16303.6076	0.0069	0.010		
90:	5	1	5	3	8	4	0	4	3	7	16304.1725	0.0068	0.010		
91:	5	1	5	1	5	4	0	4	1	4	16304.9856	0.0030	0.010		
!															
92:	3	2	2	3	5	2	1	1	3	4	18021.0315	0.0051	0.010		
93:	3	2	2	3	4	2	1	1	1	3	18022.1770	0.0156	0.010		
94:	3	2	2	1	4	2	1	1	3	3	18029.5849	-0.0075	0.010		
95:	3	2	2	3	6	2	1	1	3	5	18031.6904	0.0018	0.010		
96:	3	2	2	2	4	2	1	1	2	3	18033.9565	0.0041	0.010		
97:	3	2	2	2	5	2	1	1	2	4	18035.0836	0.0026	0.010		
98:	3	2	2	2	3	2	1	1	3	2	18041.0893	-0.0155	0.010		

PARAMETERS IN FIT:

10000	A	/MHz	4587.3023(66)	1
20000	B	/MHz	2067.0181(24)	2
30000	C	/MHz	1422.8694(15)	3
200	DJ	/kHz	2.936(73)	4
1100	DJK	/kHz	7.29(27)	5
2000	DK	/kHz	17.9(15)	6
40100	dJ	/kHz	0.938(38)	7
10000	dK	/kHz	[9.488]	8
110010000	1.5*Xaa	/MHz	-66.140(19)	9
110040000	(Xb-Xc)/4	/MHz	-3.1237(74)	10
110610000	chiab	/MHz	27.59(14)	11
220010000	1.5*Xaa	/MHz	26.102(29)	12
220040000	(Xb-Xc)/4	/MHz	-18.1268(50)	13
220610000	chiab	/MHz	21.08(18)	14

MICROWAVE AVG = 0.000088 MHz, IR AVG = 0.00000
MICROWAVE RMS = 0.011045 MHz, IR RMS = 0.00000
END OF ITERATION 1 OLD, NEW RMS ERROR= 1.10450 1.10450

distinct frequency lines in fit: 93
distinct parameters of fit: 13

for standard parameter errors previous errors are multiplied by: 1.190864

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

10000	A	/MHz	4587.3023(78)	1
20000	B	/MHz	2067.0181(28)	2
30000	C	/MHz	1422.8694(17)	3
200	DJ	/kHz	2.936(86)	4
1100	DJK	/kHz	7.29(33)	5
2000	DK	/kHz	17.9(18)	6
40100	dJ	/kHz	0.938(45)	7
10000	dK	/kHz	[9.488]	8
110010000	1.5*Xaa	/MHz	-66.140(23)	9
110040000	(Xb-Xc)/4	/MHz	-3.1237(88)	10
110610000	chiab	/MHz	27.59(17)	11
220010000	1.5*Xaa	/MHz	26.102(34)	12
220040000	(Xb-Xc)/4	/MHz	-18.1268(59)	13
220610000	chiab	/MHz	21.08(21)	14

CORRELATION COEFFICIENTS, C.ij:

	A	B	C	-DJ	-DJK	-DK	-dJ	1.5*Xaa
A	1.0000							
B	-0.0084	1.0000						
C	-0.8376	0.0362	1.0000					
-DJ	0.7478	-0.5305	-0.7985	1.0000				
-DJK	0.0803	0.5946	-0.3298	-0.0035	1.0000			
-DK	-0.9410	-0.1697	0.8758	-0.7029	-0.4020	1.0000		
-dJ	0.6498	-0.5544	-0.6591	0.9630	0.0355	-0.6320	1.0000	
1.5*Xaa	0.1189	-0.0196	-0.0451	0.0597	-0.0605	-0.0703	0.0563	1.0000
(Xb-Xc)/4	-0.0642	-0.0255	0.1269	-0.0851	-0.1229	0.0986	-0.0811	-0.2461
chiab	0.2103	0.0607	-0.2069	0.1530	0.1778	-0.2603	0.1489	0.0351
1.5*Xaa	-0.1009	0.0271	-0.0062	-0.0364	0.0995	0.0566	-0.0356	0.2933
(Xb-Xc)/4	-0.0306	0.0173	-0.0182	0.0051	0.0689	0.0050	0.0180	0.1035
chiab	0.1925	0.0690	-0.1245	0.1008	0.0875	-0.2071	0.1013	0.1534

	(Xb-Xc)/ chiab	1.5*Xaa	(Xb-Xc)/ chiab
(Xb-Xc)/4	1.0000		
chiab	-0.2162	1.0000	
1.5*Xaa	-0.5156	0.1978	1.0000
(Xb-Xc)/4	-0.1994	0.1383	0.2104	1.0000
chiab	0.0146	-0.5848	-0.1092	-0.0710	0.0000

Mean value of |C.ij|, i.ne.j = 0.2218
Mean value of C.ij, i.ne.j = -0.0375

Worst fitting lines (obs-calc/error):

1:	3.1	77:	2.6	68:	2.6	59:	2.5
9:	-2.3	55:	2.2	22:	-2.1	2:	-2.0
63:	-1.9	57:	1.9	28:	1.8	33:	-1.8
71:	-1.8	30:	-1.7	93:	1.6	98:	-1.6
7:	1.5	34:	-1.5	67:	-1.5	80:	-1.4
16:	-1.4	50:	-1.4	21:	1.4	79:	-1.3
4:	1.2	3:	1.2	56:	-1.2	54:	-1.2
60:	-1.1	8:	1.1	51:	-1.0	74:	0.9
66:	0.9	39:	-0.9	6:	-0.9	44:	-0.9
61:	0.8	13:	0.8	82:	0.8	35:	0.8
94:	-0.8	19:	-0.7	89:	0.7	43:	-0.7
90:	0.7	23:	0.7	86:	-0.7	26:	0.6
64:	-0.6	70:	0.6				

SPFIT output reformatted with PIFORM