Table S4. The results of fit and the data files for the SPFIT program for the S state of the 37Cl1,37Cl2 species of (HCl)2 H2O.

(H2O)(HCl)2 37Cl1+37Cl2 Mon Mar 14 09:58:10 2011

											obs	o-c	error	blends o-c	blends wt	Notes
/ instead of : below denotes (o-c)>3*err																
1:	1	1	1	3	3	0	0	0	3	3	6036.9209	0.0016	0.010			
2:	1	1	1	3	4	0	0	0	3	3	6044.9106	-0.0008	0.010			
3:	1	1	1	3	2	0	0	0	3	3	6053.3162	0.0074	0.010			
!																
4:	2	1	2	3	2	1	0	1	3	2	8788.5079	0.0168	0.010	0.0107	0.40	
5:	2	1	2	2	3	1	0	1	3	2	8788.5079	0.0066	0.010	0.0107	0.60	
6:	2	1	2	0	2	1	0	1	0	1	8791.7670	0.0058	0.010			
7:	2	1	2	3	4	1	0	1	3	4	8792.2218	0.0089	0.010			
8:	2	1	2	1	3	1	0	1	1	2	8798.0921	-0.0045	0.010			
9:	2	1	2	3	5	1	0	1	3	4	8800.0745	0.0038	0.010			
10:	2	1	2	3	3	1	0	1	2	2	8800.5519	-0.0128	0.010			
11:	2	1	2	1	2	1	0	1	1	2	8802.8203	-0.0017	0.010			
12:	2	1	2	2	2	1	0	1	0	1	8803.5238	0.0035	0.010			
13:	2	1	2	2	4	1	0	1	3	3	8804.6512	0.0044	0.010			
!																
14:	4	0	4	2	5	3	1	3	2	4	10971.4316	0.0014	0.010			
15:	4	0	4	1	4	3	1	3	0	3	10971.7655	0.0060	0.010	0.0126	0.78	
16:	4	0	4	3	2	3	1	3	3	1	10971.7655	0.0366	0.010	0.0126	0.22	
17:	4	0	4	3	6	3	1	3	3	5	10972.4071	-0.0032	0.010			
18:	4	0	4	3	7	3	1	3	3	6	10972.8502	-0.0066	0.010	-0.0100	0.65	
19:	4	0	4	0	4	3	1	3	1	3	10972.8502	-0.0162	0.010	-0.0100	0.35	
20:	4	0	4	2	4	3	1	3	2	3	10973.4506	-0.0030	0.010			
21:	4	0	4	3	5	3	1	3	3	4	10974.0557	-0.0069	0.010			
22:	4	0	4	2	3	3	1	3	3	2	10974.1879	0.0100	0.010			
23:	4	0	4	1	5	3	1	3	1	4	10974.3981	-0.0047	0.010			
24:	4	0	4	2	6	3	1	3	2	5	10975.0116	-0.0006	0.010			
!																
25:	3	1	3	1	2	2	0	2	2	1	11291.7144	-0.0208	0.010			
26:	3	1	3	3	2	2	0	2	0	2	11292.0163	-0.0037	0.010			
27:	3	1	3	3	4	2	0	2	1	3	11294.6917	-0.0004	0.010			
28:	3	1	3	1	4	2	0	2	2	3	11294.8408	-0.0013	0.010			
29:	3	1	3	2	4	2	0	2	3	3	11296.0840	-0.0037	0.010			
30:	3	1	3	2	3	2	0	2	2	2	11296.2523	-0.0092	0.010			
31:	3	1	3	3	5	2	0	2	3	4	11298.4230	0.0107	0.010			
32:	3	1	3	3	6	2	0	2	3	5	11298.8394	0.0062	0.010			
33:	3	1	3	0	3	2	0	2	1	2	11301.0660	0.0113	0.010			
!																
34:	5	0	5	2	4	4	1	4	2	3	14295.2060	0.0000	0.010			
35:	5	0	5	2	6	4	1	4	2	5	14295.7160	-0.0024	0.010			
36:	5	0	5	3	5	4	1	4	3	4	14296.4247	-0.0023	0.010	-0.0049	0.27	
37:	5	0	5	0	5	4	1	4	0	4	14296.4247	0.0031	0.010	-0.0049	0.31	
38:	5	0	5	3	7	4	1	4	3	6	14296.4247	-0.0126	0.010	-0.0049	0.42	
39:	5	0	5	3	8	4	1	4	3	7	14296.6756	0.0050	0.010	0.0081	0.65	
40:	5	0	5	2	3	4	1	4	2	3	14296.6756	0.0203	0.010	0.0081	0.04	
41:	5	0	5	1	4	4	1	4	1	3	14296.6756	0.0127	0.010	0.0081	0.31	
42:	5	0	5	1	6	4	1	4	1	5	14297.3805	0.0009	0.010			
43:	5	0	5	2	7	4	1	4	2	6	14297.6041	-0.0011	0.010			
!																
44:	2	2	1	2	4	1	1	0	3	3	15365.4745	0.0074	0.010			
45:	2	2	1	3	2	1	1	0	2	2	15367.6467	-0.0071	0.010			
46:	2	2	1	2	3	1	1	0	1	2	15369.4200	0.0018	0.010			
47:	2	2	1	2	4	1	1	0	2	3	15372.0641	-0.0023	0.010			
48:	2	2	1	3	5	1	1	0	3	4	15377.2676	-0.0018	0.010			
49:	2	2	1	1	2	1	1	0	1	1	15380.0819	-0.0060	0.010			
50:	2	2	1	1	3	1	1	0	2	3	15382.3044	-0.0172	0.010			
51:	2	2	1	3	4	1	1	0	2	3	15383.3083	0.0430	0.010	0.0058	0.69	
52:	2	2	1	2	2	1	1	0	2	2	15383.3083	-0.0761	0.010	0.0058	0.31	
53:	2	2	1	3	3	1	1	0	3	2	15384.5829	-0.0053	0.010			
54:	2	2	1	3	4	1	1	0	3	4	15385.4687	0.0049	0.010			
!																
55:	5	1	5	3	4	4	0	4	2	3	15981.4692	0.0067	0.010			
56:	5	1	5	3	5	4	0	4	3	4	15981.6074	0.0045	0.010			
57:	5	1	5	3	6	4	0	4	3	5	15981.9223	0.0100	0.010			
58:	5	1	5	2	7	4	0	4	2	6	15982.3750	-0.0047	0.010			
59:	5	1	5	2	5	4	0	4	2	4	15982.6685	0.0119	0.010			
60:	5	1	5	2	6	4	0	4	2	5	15984.8973	-0.0267	0.010			
61:	5	1	5	3	7	4	0	4	3	6	15985.1249	0.0064	0.010			
62:	5	1	5	3	8	4	0	4	3	7	15985.5879	-0.0053	0.010			
!																
63:	2	2	0	1	2	1	1	1	1	1	16030.1809	-0.0077	0.010			
64:	2	2	0	2	1	1	1	1	3	2	16031.1913	-0.0038	0.010	-0.0004	0.57	
65:	2	2	0	3	2	1	1	1	3	2	16031.1913	0.0041	0.010	-0.0004	0.43	
66:	2	2	0	2	3	1	1	1	1	2	16036.0963	-0.0046	0.010			
67:	2	2	0	1	3	1	1	1	3	2	16037.1300	-0.0063	0.010			
68:	2	2	0	3	2	1	1	1	2	3	16037.3749	0.0068	0.010			
69:	2	2	0	3	5	1	1	1	3	4	16037.6602	0.0007	0.010			
70:	2	2	0	3	3	1	1	1	1	2	16039.1496	0.0037	0.010			
71:	2	2	0	3	2	1	1	1	0	1	16040.2708	0.0088	0.010			
72:	2	2	0	3	4	1	1	1	2	3	16043.9365	0.0070	0.010			
73:	2	2	0	1	3	1	1	1	1	2	16045.0922	-0.0010	0.010			
74:	2	2	0	2	1	1	1	1	2	1	16048.0070	0.0069	0.010			
75:	2	2	0	3	3	1	1	1	2	2	16049.5506	-0.0066	0.010			
76:	2	2	0	1	3	1	1	1	3	3	16053.5288	0.0029	0.010			
!																
77:	3	2	2	3	5	2	1	1	3	4	18123.6582	-0.0048	0.010			
78:	3	2	2	3	4	2	1	1	1	3	18124.5773	0.0096	0.010			
79:	3	2	2	3	6	2	1	1	3	5	18132.0656	-0.0003	0.010			
80:	3	2	2	2	5	2	1	1	2	4	18134.7043	-0.0016	0.010			

PARAMETERS IN FIT:

10000	A	/MHz	4666.6422(23)	1
20000	B	/MHz	1957.7166(11)	2
30000	C	/MHz	1377.13028(82)	3
200	DJ	/kHz	3.260(19)	4
1100	DJK	/kHz	5.22(27)	5
2000	DK	/kHz	[22.64]	6
40100	dJ	/kHz	[0.992]	7
41000	dK	/kHz	[9.12]	8
110010000	1.5*Xaa	/MHz	-52.065(22)	9
110040000	(Xb-Xc)/4	/MHz	-2.4638(86)	10
110610000	chiab	/MHz	[21.4]	11
220010000	1.5*Xaa	/MHz	20.782(34)	12
220040000	(Xb-Xc)/4	/MHz	-14.3326(62)	13
220610000	chiab	/MHz	[17.7]	14

MICROWAVE AVG = 0.000107 MHz, IR AVG = 0.00000
MICROWAVE RMS = 0.007596 MHz, IR RMS = 0.00000
END OF ITERATION 1 OLD, NEW RMS ERROR= 0.75961 0.75961

distinct frequency lines in fit: 71
distinct parameters of fit: 9

for standard parameter errors previous errors are multiplied by: 0.812875

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

10000	A	/MHz	4666.6422(18)	1
20000	B	/MHz	1957.71668(96)	2
30000	C	/MHz	1377.13028(66)	3
200	DJ	/kHz	3.260(15)	4
1100	DJK	/kHz	5.22(22)	5
2000	DK	/kHz	[22.64]	6
40100	dJ	/kHz	[0.992]	7
41000	dK	/kHz	[9.12]	8
110010000	1.5*Xaa	/MHz	-52.065(18)	9
110040000	(Xb-Xc)/4	/MHz	-2.4638(69)	10
110610000	chiab	/MHz	[21.4]	11
220010000	1.5*Xaa	/MHz	20.782(27)	12
220040000	(Xb-Xc)/4	/MHz	-14.3326(50)	13
220610000	chiab	/MHz	[17.7]	14

CORRELATION COEFFICIENTS, C.ij:

	A	B	C	-DJ	-DJK	1.5*Xaa	(Xb-Xc)/	1.5*Xaa
A	1.0000							
B	-0.6861	1.0000						
C	-0.0449	0.2633	1.0000					
-DJ	0.4814	-0.6588	-0.8272	1.0000				
-DJK	-0.9582	0.7020	-0.0410	-0.4411	1.0000			
1.5*Xaa	-0.0228	0.0517	-0.1889	0.1058	0.0872	1.0000		
(Xb-Xc)/4	0.0473	0.0323	0.0553	-0.0401	-0.0539	-0.1362	0.0000	
1.5*Xaa	-0.0426	-0.0229	-0.2834	0.1833	0.1046	0.3261	-0.4748	0.0000
(Xb-Xc)/4	0.0736	-0.1046	-0.0146	0.0508	-0.1060	-0.0916	-0.2867	0.2469

	(Xb-Xc)/
(Xb-Xc)/4	0.0000

Mean value of |C.ij|, i.ne.j = 0.2316
Mean value of C.ij, i.ne.j = -0.0754

Worst fitting lines (obs-calc/error):

60:	-2.7	25:	-2.1	50:	-1.7	10:	-1.3
15:	1.3	59:	1.2	33:	1.1	4:	1.1
31:	1.1	22:	1.0	57:	1.0	18:	-1.0
78:	1.0	30:	-0.9	7:	0.9	71:	0.9
39:	0.8	63:	-0.8	3:	0.7	44:	0.7
45:	-0.7	72:	0.7	21:	-0.7	74:	0.7
68:	0.7	55:	0.7	75:	-0.7	61:	0.6
67:	-0.6	32:	0.6	49:	-0.6	51:	0.6
6:	0.6	62:	-0.5	53:	-0.5	36:	-0.5
54:	0.5	77:	-0.5	23:	-0.5	58:	-0.5
66:	-0.5	56:	0.4	8:	-0.4	13:	0.4
9:	0.4	29:	-0.4	70:	0.4	26:	-0.4
12:	0.3	17:	-0.3				

/ SPFIT output reformatted with PIFORM