

Supplementary Information for: “Chirped Pulse Fourier-Transform Microwave Spectroscopy of Alcohol and Water Tetramers”

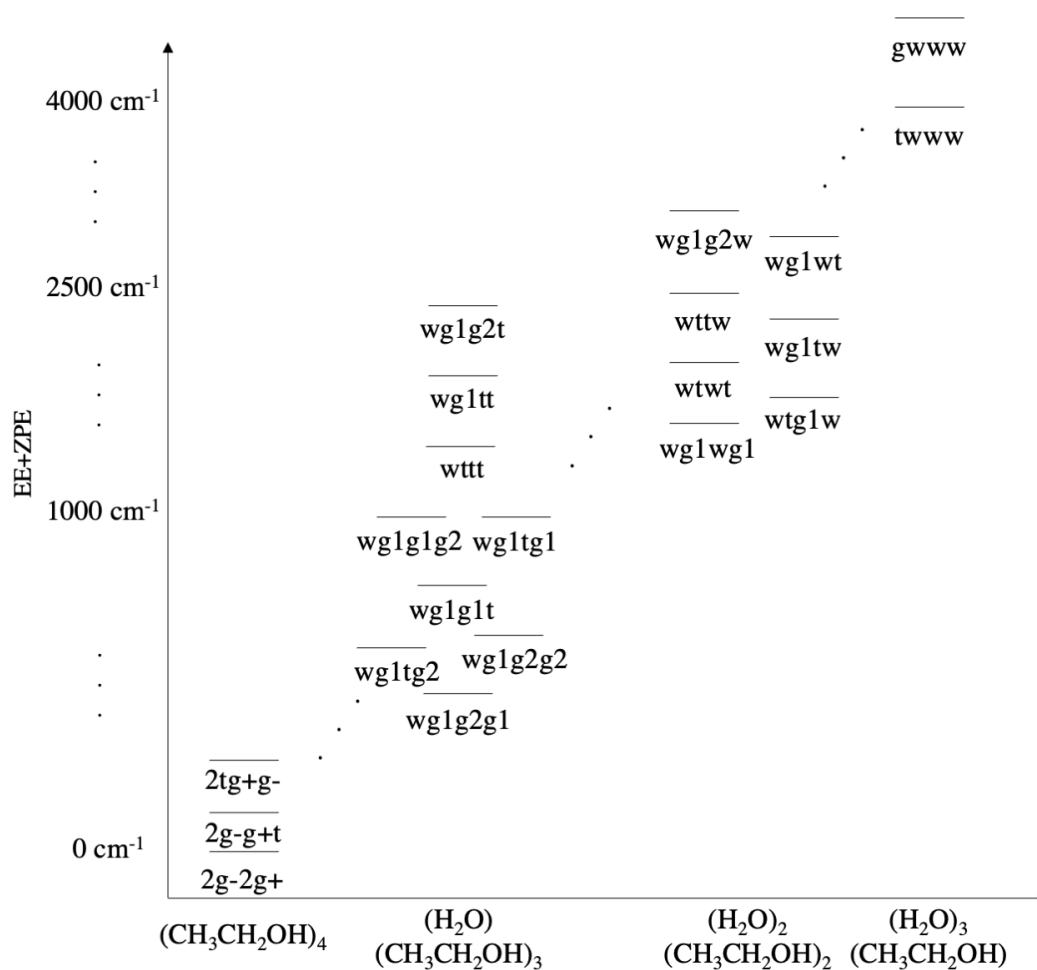
In this supplementary information, the authors include details on computational modeling and spectroscopic fits for ethanol:water tetramers. The sections are listed below, and brief descriptions of each section are included.

Sections:

1. Relative Energy Ordering of all Optimized Tetramer Conformers
2. SPFIT Results
3. Kraitchman Substitution results and calculated O-O distances
4. Images of fitted conformers
5. Sample XIAM results

Section 1: Relative Energy Ordering of all Optimized Tetramer Conformers

Herein is included a figure demonstrating the relative energy of all tetramer conformers optimized via *ab initio* computation. Each conformer geometry was optimized with DFT in Gaussian at the B3LYP level of theory and the 6-311G++(d,p) basis set. Energy of tetramer conformers is increased with addition of water, as shown on the horizontal axis. Energy differences between conformers with a set number of water molecules are small, at less than 400 cm⁻¹. This implies the potential presence of all conformers in experimental expansions, limiting detection of conformers to the dipole moment of each structure.



Relative energy ordering of ethanol:water tetramers investigated herein, expressed as electronic energy (EE) plus zero point correction (ZPE). Gaps between groupings of conformers are on the order of several hundred wavenumbers, while gaps between conformers with the same number of water/ethanol subunits are on the order of 1000s of wavenumbers, as seen in previous studies (Nishi, 1988}. Relative energies between conformers of the same hydration level calculated with Gaussian using B3LYP/6311g++(d,p).

Section 2: SPFIT results for ethanol:water tetramers and their isotopologues

In this section, SPFIT output files are included for all tetramer conformers observed in the experimental data, as well as perdeuterated isotopologues and singly deuterated isotopologues. Files are organized by number of water molecules, with all ethanol tetramer fits first, then one-water tetramers, etc. Each fit is separated by a page break.

SPFIT Details for 2tg+g-

EXP.FREQ. - CALC.FREQ. - DIFF. - EXP.ERR.- EST.ERR.-AVG.
CALC.FREQ. - DIFF. - WT.

1: 10 10 1 9 9 0	10968.73000	10968.72511	0.00489	0.10000	0.00000
2: 11 2 10 10 1 9	10453.03000	10453.07030	-0.04030	0.10000	0.00000
3: 12 12 0 11 11 0	13170.46000	13170.46486	-0.00486	0.10000	0.00000
4: 13 0 13 12 0 12	12158.16000	12158.21198	-0.05198	0.10000	0.00000
5: 13 1 12 12 1 11	12306.68000	12306.64881	0.03119	0.10000	0.00000
6: 13 1 13 12 0 12	12158.16000	12158.21198	-0.05198	0.10000	0.00000
7: 13 2 12 12 1 11	12306.68000	12306.64881	0.03119	0.10000	0.00000
8: 17 17 1 16 16 1	18665.48000	18665.47884	0.00116	0.10000	0.00000
9: 18 0 18 17 0 17	16803.55000	16803.41026	0.13974	0.10000	0.00000
10: 18 5 14 17 4 13	17402.21000	17402.21651	-0.00651	0.10000	0.00000
11: 19 1 19 18 0 18	17732.57000	17732.48319	0.08681	0.10000	0.00000
17732.48319 0.08681 0.5000					
12: 19 1 19 18 1 18	17732.57000	17732.48319	0.08681	0.10000	0.00000
17732.48319 0.08681 0.5000					
13: 20 0 20 19 1 19	18661.40000	18661.55364	-0.15364	0.10000	0.00000
18661.55364 -0.15364 0.5000					
14: 20 0 20 19 0 19	18661.40000	18661.55364	-0.15364	0.10000	0.00000
18661.55364 -0.15364 0.5000					

NORMALIZED DIAGONAL:

1	1.00000E+000	2	8.18444E-001	3	3.66147E-001	4	4.78148E-002	5	9.98447E-001
6	4.05199E-003								
7	1.06679E-001	8	2.95007E-001						

MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00

NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION

1	10000	A	550.825(56)	0.000
2	20000	B	539.159(216)	0.001
3	30000	C	464.6791(134)	-0.0000
4	200	-DeltaJ	-0.012301(228)	-0.000001
5	2000	-DeltaK	-0.027735(216)	-0.000001
6	1100	-DeltaJK	0.03944(48)	0.00000
7	40100	-deltaJ	-9.687(78)E-03	0.000E-03
8	41000	-deltaK	0.02668(156)	-0.00000

MICROWAVE AVG = -0.001189 MHz, IR AVG = 0.00000
MICROWAVE RMS = 0.070553 MHz, IR RMS = 0.00000

SPFIT Details for all ethanol-d6 2tg+g-

	EXP.FREQ.	- CALC.FREQ.	- DIFF.	- EXP.ERR.	- EST.ERR.	-AVG.
CALC.FREQ. - DIFF. - WT.						
1: 18 0 18 17 0 17	14254.99000	14254.98241	0.00759	0.10000	0.09386	
14254.98241 0.00759 0.5000						
2: 18 1 18 17 0 17	14254.99000	14254.98241	0.00759	0.10000	0.09386	
14254.98241 0.00759 0.5000						
3: 19 2 18 18 2 17	15156.32000	15156.35680	-0.03680	0.10000	0.05833	
15156.35680 -0.03680 0.5000						
4: 19 1 18 18 2 17	15156.32000	15156.35680	-0.03680	0.10000	0.05833	
15156.35680 -0.03680 0.5000						
5: 19 2 17 18 2 16	15271.57000	15271.55459	0.01541	0.10000	0.08660	
15271.55460 0.01540 0.5000						
6: 19 3 17 18 2 16	15271.57000	15271.55462	0.01538	0.10000	0.08660	
15271.55460 0.01540 0.5000						
7: 21 1 21 20 1 20	16622.48000	16622.45103	0.02897	0.10000	0.09580	
16622.45103 0.02897 0.5000						
8: 21 0 21 20 1 20	16622.48000	16622.45103	0.02897	0.10000	0.09580	
16622.45103 0.02897 0.5000						
9: 21 2 20 20 2 19	16732.27000	16732.36371	-0.09371	0.10000	0.05195	
16732.36371 -0.09371 0.5000						
10: 21 1 20 20 2 19	16732.27000	16732.36371	-0.09371	0.10000	0.05195	
16732.36371 -0.09371 0.5000						
11: 21 2 19 20 2 18	16846.32000	16846.11733	0.20267	0.10000	0.06113	
16846.11733 0.20267 0.5000						
12: 21 3 19 20 2 18	16846.32000	16846.11733	0.20267	0.10000	0.06113	
16846.11733 0.20267 0.5000						
13: 21 3 18 20 3 17	16962.14000	16962.27891	-0.13891	0.10000	0.07581	
16962.27893 -0.13893 0.5000						
14: 21 4 18 20 3 17	16962.14000	16962.27895	-0.13895	0.10000	0.07581	
16962.27893 -0.13893 0.5000						
15: 21 4 17 20 4 16	17080.19000	17080.15778	0.03222	0.10000	0.09618	
16: 22 2 21 21 2 20	17520.26000	17520.27753	-0.01753	0.10000	0.07617	

NORMALIZED DIAGONAL:

1	1.00000E+000	2	1.13449E-002	3	1.02445E-001	4	6.50228E-004	5	7.22510E-001
6	2.50223E-005	7	2.61584E-002	8	1.82523E-001				

MARQUARDT PARAMETER = 7.18784e-005, TRUST EXPANSION = 1.00

NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION

1	10000	A	492.24(111)	0.00
2	20000	B	430.90(43)	-0.00
3	30000	C	394.1888(157)	-0.0000
4	200	-DeltaJ	0.020343(98)	-0.000000
5	2000	-DeltaK	0.026990(117)	-0.000000
6	1100	-DeltaJK	-0.047647(113)	0.000001

7	40100	-deltaJ	-0.013376(228)	0.000000
8	41000	-deltaK	0.02357(34)	-0.000000
MICROWAVE AVG =			-0.000013 MHz, IR AVG =	0.000000
MICROWAVE RMS =			0.090056 MHz, IR RMS =	0.000000

SPFIT Details for wg1g2t

EXP.FREQ. - CALC.FREQ. - DIFF. - EXP.ERR.- EST.ERR.-AVG.
CALC.FREQ. - DIFF. - WT.

1: 8 3 6 7 2 6	11079.94000	11079.94014	-0.00014	0.10000	0.00000
2: 9 2 8 8 1 8	12443.43000	12443.43003	-0.00003	0.10000	0.00000
3: 11 2 9 10 2 8	10153.98000	10153.97929	0.00071	0.10000	0.00000
4: 11 5 7 10 5 6	10429.67000	10429.66996	0.00004	0.10000	0.00000
5: 13 0 13 12 0 12	10260.36000	10260.30444	0.05556	0.10000	0.00000
6: 13 1 13 12 0 12	10260.39000	10260.44598	-0.05598	0.10000	0.00000
7: 21 3 19 20 2 18	17658.59000	17658.59034	-0.00034	0.10000	0.00000
8: 22 1 22 21 0 21	17132.56000	17132.56524	-0.00524	0.10000	0.00000
9: 22 0 22 21 0 21	17132.57000	17132.56480	0.00520	0.10000	0.00000
10: 23 2 22 22 1 21	18536.55000	18536.54970	0.00030	0.10000	0.00000

NORMALIZED DIAGONAL:

1	1.00000E+000	2	4.80270E-001	3	9.96601E-001	4	5.95483E-003	5	3.27645E-001
6	3.20074E-004	7	6.15607E-001	8	9.51515E-002				

MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00

NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION

1	10000	A	1036.863(157)	0.000
2	20000	B	538.362(48)	-0.000
3	30000	C	381.6686(165)	-0.0000
4	200	-DeltaJ	-2.14(82)E-03	-0.00E-03
5	2000	-DeltaK	-0.1883(33)	-0.0000
6	1100	-DeltaJK	0.1904(41)	0.0000
7	40100	-deltaJ	-0.024522(242)	-0.000000
8	41000	-deltaK	-0.09823(156)	-0.00000

MICROWAVE AVG = 0.000006 MHz, IR AVG = 0.00000

MICROWAVE RMS = 0.025052 MHz, IR RMS = 0.00000

SPFIT Details for wg1g2t with d2o

	EXP.FREQ.	CALC.FREQ.	DIFF.	EXP.ERR.-	EST.ERR.-AVG.
CALC.FREQ. - DIFF. - WT.					
1: 6 6 1 5 5 1	11530.89000	11530.88973	0.00027	0.10000	0.07071
2: 6 6 1 5 5 1	11530.89000	11530.88973	0.00027	0.10000	0.07071
3: 8 8 1 7 7 1	15554.70000	15554.70112	-0.00112	0.10000	0.09999
4: 9 8 2 8 7 2	16478.62000	16478.61912	0.00088	0.10000	0.10000
5: 15 2 13 14 2 12	12937.50000	12937.51295	-0.01295	0.10000	0.09964
6: 17 0 17 16 0 16	13156.03000	13156.03922	-0.00922	0.10000	0.09970
13156.03948 -0.00948 0.5000					
7: 17 1 17 16 0 16	13156.03000	13156.03974	-0.00974	0.10000	0.09970
13156.03948 -0.00948 0.5000					
8: 18 1 17 17 1 16	14546.90000	14546.79699	0.10301	0.10000	0.06915
14546.80464 0.09536 0.5000					
9: 18 2 17 17 1 16	14546.90000	14546.81229	0.08771	0.10000	0.06915
14546.80464 0.09536 0.5000					
10: 19 1 18 18 1 17	15300.50000	15300.58624	-0.08624	0.10000	0.07372
15300.58907 -0.08907 0.5000					
11: 19 2 18 18 1 17	15300.50000	15300.59191	-0.09191	0.10000	0.07372
15300.58907 -0.08907 0.5000					
12: 20 2 18 19 2 17	16695.96000	16695.90700	0.05300	0.10000	0.09973
16695.95118 0.00882 0.5000					
13: 20 3 18 19 2 17	16695.96000	16695.99536	-0.03536	0.10000	0.09973
16695.95118 0.00882 0.5000					
14: 22 0 22 21 0 21	16924.50000	16924.49286	0.00714	0.10000	0.09989
16924.49286 0.00714 0.5000					
15: 22 1 22 21 0 21	16924.50000	16924.49286	0.00714	0.10000	0.09989
16924.49286 0.00714 0.5000					
NORMALIZED DIAGONAL:					
1 1.00000E+000 2 2.72255E-001 3 1.46898E-001 4 1.24383E-002 5 6.45289E-001					
6 2.07548E-003					
7 1.06209E-001 8 9.99424E-001					
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00					
NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION					
1 10000 A 1006.2347(168) 0.0000					
2 20000 B 537.470(122) -0.000					
3 30000 C 377.8764(111) 0.0000					
4 200 -DeltaJ -1.606(212)E-03 0.000E-03					
5 2000 -DeltaK -9.80(63)E-03 -0.00E-03					
6 1100 -DeltaJK 0.01185(80) 0.00000					
7 40100 -deltaJ -1.089(116)E-03 0.000E-03					
8 41000 -deltaK -5.63(45)E-03 -0.00E-03					
MICROWAVE AVG = 0.000013 MHz, IR AVG = 0.00000					
MICROWAVE RMS = 0.041732 MHz, IR RMS = 0.00000					

SPFIT Details for wg1g2t with HDO

EXP.FREQ. - CALC.FREQ. - DIFF. - EXP.ERR.- EST.ERR.-AVG.

CALC.FREQ. - DIFF. - WT.

1: 6 6 0 5 5 1	11783.46000	11783.46730	-0.00730	0.10000	0.00000
11783.46532 -0.00532 0.5000					
2: 6 6 1 5 5 1	11783.46000	11783.46333	-0.00333	0.10000	0.00000
11783.46532 -0.00532 0.5000					
3: 8 7 2 7 6 2	14771.87000	14771.86984	0.00016	0.10000	0.00000
4: 8 8 1 7 7 1	15900.84000	15900.83795	0.00205	0.10000	0.00000
5: 15 2 13 14 2 12	13053.14000	13052.90749	0.23251	0.10000	0.00000
6: 17 0 17 16 0 16	13279.98000	13280.06186	-0.08186	0.10000	0.00000
7: 17 3 15 16 2 14	14567.55000	14567.76733	-0.21733	0.10000	0.00000
8: 21 1 20 20 1 19	16965.84000	16965.73323	0.10677	0.10000	0.00000
16965.73440 0.10560 0.5000					
9: 21 2 20 20 1 19	16965.84000	16965.73557	0.10443	0.10000	0.00000
16965.73440 0.10560 0.5000					
10: 22 0 22 21 0 21	17085.92000	17085.94749	-0.02749	0.10000	0.00000
17085.94749 -0.02749 0.5000					
11: 22 1 22 21 0 21	17085.92000	17085.94750	-0.02750	0.10000	0.00000
17085.94749 -0.02749 0.5000					
12: 24 2 23 24 1 24	14822.16000	14822.16513	-0.00513	0.10000	0.00000

NORMALIZED DIAGONAL:

1 1.00000E+000	2 4.62457E-002	3 2.24027E-001	4 9.95545E-001	5 1.93706E-003
6 1.25979E-002				
7 9.24369E-001	8 2.49410E-002			

MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00

NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION

1	10000	A	1028.7704(225)	-0.0000
2	20000	B	539.141(48)	-0.000
3	30000	C	381.3754(75)	-0.0000
4	200	-DeltaJ	-3.864(171)E-03	-0.000E-03
5	2000	-DeltaK	-7.85(62)E-03	-0.00E-03
6	1100	-DeltaJK	0.01133(75)	0.00000
7	40100	-deltaJ	-3.087(91)E-03	-0.000E-03
8	41000	-deltaK	1.09(38)E-03	-0.00E-03
MICROWAVE AVG =			0.000355 MHz, IR AVG =	0.00000
MICROWAVE RMS =			0.115452 MHz, IR RMS =	0.00000

SPFIT Details for wttt

EXP.FREQ. - CALC.FREQ. - DIFF. - EXP.ERR.- EST.ERR.-AVG.
CALC.FREQ. - DIFF. - WT.

1: 6 6 1 5 5 1	11251.03000	11251.03001	-0.00001	0.10000	0.07071
2: 6 6 1 5 5 1	11251.03000	11251.03001	-0.00001	0.10000	0.07071
3: 7 7 1 6 6 1	13214.40000	13214.39999	0.00001	0.10000	0.10000
4: 14 0 14 13 0 13	10268.40000	10268.43077	-0.03077	0.10000	0.06333
5: 14 1 13 13 1 12	10931.92000	10931.91253	0.00747	0.10000	0.09942
6: 14 1 14 13 0 13	10268.40000	10268.43735	-0.03735	0.10000	0.06329
7: 16 0 16 15 0 15	11685.37000	11685.27693	0.09307	0.10000	0.05236
11685.27735 0.09265 0.5000					
8: 16 1 16 15 0 15	11685.37000	11685.27776	0.09224	0.10000	0.05236
11685.27735 0.09265 0.5000					
9: 18 1 17 17 1 16	13764.26000	13764.26345	-0.00345	0.10000	0.10133
13764.26810 -0.00810 0.5000					
10: 18 2 17 17 1 16	13764.26000	13764.27276	-0.01276	0.10000	0.10133
13764.26810 -0.00810 0.5000					
11: 19 0 19 18 0 18	13808.25000	13808.27805	-0.02805	0.10000	0.09682
13808.27807 -0.02807 0.5000					
12: 19 1 19 18 0 18	13808.25000	13808.27809	-0.02809	0.10000	0.09682
13808.27807 -0.02807 0.5000					
13: 24 2 22 23 2 21	18667.30000	18667.29996	0.00004	0.10000	0.10006
14: 24 1 23 23 1 22	18004.43000	18004.42788	0.00212	0.10000	0.09858

NORMALIZED DIAGONAL:

1	1.00000E+000	2	2.47276E-001	3	5.82286E-001	4	4.95142E-003	5	1.25254E-001
6	2.77648E-004								
7	3.82011E-002	8	9.97532E-001						

MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00

NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION

1	10000	A	982.109(33)	0.000
2	20000	B	528.576(169)	-0.000
3	30000	C	355.1998(100)	0.0000
4	200	-DeltaJ	-5.74(50)E-03	0.00E-03
5	2000	-DeltaK	-0.0237(42)	0.0000
6	1100	-DeltaJK	0.0286(46)	-0.0000
7	40100	-deltaJ	-1.343(172)E-03	0.000E-03
8	41000	-deltaK	-0.01263(301)	0.00000
MICROWAVE AVG =			-0.000183 MHz, IR AVG =	0.00000
MICROWAVE RMS =			0.032809 MHz, IR RMS =	0.00000

SPFIT Details for wttt with d2o

EXP.FREQ. - CALC.FREQ. - DIFF. - EXP.ERR.- EST.ERR.-AVG.	
CALC.FREQ. - DIFF. - WT.	
1: 6 6 1 5 5 1	10951.02000 10951.02026 -0.00026 0.10000 0.00000
2: 6 6 1 5 5 1	10951.02000 10951.02026 -0.00026 0.10000 0.00000
3: 9 8 2 8 7 2	15668.49000 15668.48970 0.00030 0.10000 0.00000
4: 20 1 19 19 1 18	15019.45000 15019.32347 0.12653 0.10000 0.00000
15019.32359 0.12641 0.5000	
5: 20 2 19 19 1 18	15019.45000 15019.32371 0.12629 0.10000 0.00000
15019.32359 0.12641 0.5000	
6: 20 2 18 19 2 17	15681.13000 15681.18762 -0.05762 0.10000 0.00000
7: 20 3 18 19 2 17	15681.14000 15681.20028 -0.06028 0.10000 0.00000
8: 20 3 17 19 3 16	16348.80000 16348.58534 0.21466 0.10000 0.00000
16348.77732 0.02268 0.5000	
9: 20 4 17 19 3 16	16348.80000 16348.96930 -0.16930 0.10000 0.00000
16348.77732 0.02268 0.5000	
10: 21 0 21 20 0 20	15058.94000 15059.01345 -0.07345 0.10000 0.00000
15059.01345 -0.07345 0.5000	
11: 21 1 21 20 0 20	15058.94000 15059.01345 -0.07345 0.10000 0.00000
15059.01345 -0.07345 0.5000	
12: 22 2 20 21 2 19	17079.71000 17079.67081 0.03919 0.10000 0.00000
17079.67155 0.03845 0.5000	
13: 22 3 20 21 2 19	17079.71000 17079.67230 0.03770 0.10000 0.00000
17079.67155 0.03845 0.5000	
14: 22 3 19 21 3 18	17744.01000 17743.96607 0.04393 0.10000 0.00000
17743.99225 0.01775 0.5000	
15: 22 4 19 21 3 18	17744.01000 17744.01844 -0.00844 0.10000 0.00000
17743.99225 0.01775 0.5000	
16: 23 0 23 22 0 22	16458.71000 16458.67983 0.03017 0.10000 0.00000
16458.67983 0.03017 0.5000	
17: 23 1 23 22 0 22	16458.71000 16458.67983 0.03017 0.10000 0.00000
16458.67983 0.03017 0.5000	
18: 23 2 21 22 2 20	17778.57000 17778.61370 -0.04370 0.10000 0.00000
17778.61395 -0.04395 0.5000	
19: 23 3 21 22 2 20	17778.57000 17778.61420 -0.04420 0.10000 0.00000
17778.61395 -0.04395 0.5000	

NORMALIZED DIAGONAL:

1 1.00000E+000 2 1.47065E-001 3 7.76457E-002 4 8.24537E-003 5 6.46130E-001
6 1.85927E-004
7 9.99533E-001 8 6.95583E-002

MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00

NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION

1	10000	A	954.198(82)	0.000
2	20000	B	531.648(213)	0.000

3	30000	C	351.0172(215)	0.0000
4	200	-DeltaJ	3.90(96)E-03	-0.00E-03
5	2000	-DeltaK	0.0234(45)	-0.0000
6	1100	-DeltaJK	-0.0276(54)	0.0000
7	40100	-deltaJ	-3.69(50)E-03	0.00E-03
8	41000	-deltaK	0.0224(42)	-0.0000
MICROWAVE AVG =			-0.000007 MHz, IR AVG =	0.00000
MICROWAVE RMS =			0.052819 MHz, IR RMS =	0.00000

SPFIT Details for wttt with HDO

EXP.FREQ. - CALC.FREQ. - DIFF. - EXP.ERR.- EST.ERR.-AVG.	
CALC.FREQ. - DIFF. - WT.	
1: 6 6 0 5 5 1	11176.20000 11176.19350 0.00650 0.10000 0.09923
11176.18798 0.01202 0.5000	
2: 6 6 1 5 5 1	11176.20000 11176.18247 0.01753 0.10000 0.09923
11176.18798 0.01202 0.5000	
3: 8 5 4 7 4 4	11940.13000 11940.14056 -0.01056 0.10000 0.09116
4: 9 8 2 8 7 2	15978.30000 15978.32409 -0.02409 0.10000 0.08641
5: 9 9 1 8 8 1	17027.29000 17027.27476 0.01524 0.10000 0.09484
6: 14 0 14 13 0 13	10242.49000 10242.51905 -0.02905 0.10000 0.07360
10242.52149 -0.03149 0.5000	
7: 14 1 14 13 0 13	10242.49000 10242.52392 -0.03392 0.10000 0.07360
10242.52149 -0.03149 0.5000	
8: 14 4 11 13 4 10	12216.53000 12216.57718 -0.04718 0.10000 0.09634
9: 17 0 17 16 0 16	12366.11000 12366.24231 -0.13231 0.10000 0.06094
12366.24241 -0.13241 0.5000	
10: 17 1 17 16 0 16	12366.11000 12366.24251 -0.13251 0.10000 0.06094
12366.24241 -0.13241 0.5000	
11: 18 2 16 17 2 15	14401.99000 14401.76069 0.22931 0.10000 0.06064
12: 21 0 21 20 0 20	15197.87000 15197.74646 0.12354 0.10000 0.09012
15197.74646 0.12354 0.5000	
13: 21 1 21 20 0 20	15197.87000 15197.74646 0.12354 0.10000 0.09012
15197.74646 0.12354 0.5000	
14: 21 1 20 20 1 19	15858.02000 15857.99833 0.02167 0.10000 0.06014
15857.99847 0.02153 0.5000	
15: 21 2 20 20 1 19	15858.02000 15857.99861 0.02139 0.10000 0.06014
15857.99847 0.02153 0.5000	
16: 22 1 21 21 1 20	16565.47000 16565.54975 -0.07975 0.10000 0.06676
16565.54980 -0.07980 0.5000	
17: 22 2 21 21 1 20	16565.47000 16565.54985 -0.07985 0.10000 0.06676
16565.54980 -0.07980 0.5000	
18: 22 2 20 21 2 19	17229.02000 17229.10722 -0.08722 0.10000 0.08424
17229.10973 -0.08973 0.5000	
19: 22 3 20 21 2 19	17229.02000 17229.11224 -0.09224 0.10000 0.08424
17229.10973 -0.08973 0.5000	
NORMALIZED DIAGONAL:	
1 1.00000E+000 2 5.88486E-001 3 1.98502E-001 4 1.20337E-002 5 5.08682E-001	
6 4.01691E-003	
7 8.81088E-002 8 9.99012E-001	
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00	
NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION	
1 10000 A 975.1596(178) -0.0000	
2 20000 B 529.494(66) -0.000	
3 30000 C 354.0067(54) 0.0000	

4	200	-DeltaJ	0.625(110)E-03	0.000E-03
5	2000	-DeltaK	0.010510(295)	-0.000000
6	1100	-DeltaJK	-0.01112(33)	0.000000
7	40100	-deltaJ	-0.075(84)E-03	0.000E-03
8	41000	-deltaK	9.306(298)E-03	-0.000E-03
MICROWAVE AVG =			-0.001135 MHz, IR AVG =	0.000000
MICROWAVE RMS =			0.093339 MHz, IR RMS =	0.000000

SPFIT Details for wg1tw

EXP.FREQ. - CALC.FREQ. - DIFF. - EXP.ERR.- EST.ERR.-AVG.
CALC.FREQ. - DIFF. - WT.

1: 4 4 1 3 3 1	10938.25000	10938.25243	-0.00243	0.10000	0.00000
2: 5 4 2 4 3 2	12395.46000	12395.45951	0.00049	0.10000	0.00000
3: 6 6 0 5 5 1	16779.55000	16779.55647	-0.00647	0.10000	0.00000
16779.54792 0.00208 0.5000					
4: 6 6 1 5 5 1	16779.55000	16779.53936	0.01064	0.10000	0.00000
16779.54792 0.00208 0.5000					
5: 7 6 2 6 5 2	18221.87000	18221.87177	-0.00177	0.10000	0.00000
6: 9 2 8 8 1 7	12043.14000	12043.12797	0.01203	0.10000	0.00000
7: 11 0 11 10 0 10	13370.35000	13370.29918	0.05082	0.10000	0.00000
8: 11 1 11 10 0 10	13370.37000	13370.43452	-0.06452	0.10000	0.00000
9: 14 0 14 13 0 13	16883.85000	16883.84384	0.00616	0.10000	0.00000
10: 14 1 13 13 1 12	17818.56000	17818.39988	0.16012	0.10000	0.00000
11: 14 1 14 13 0 13	16883.85000	16883.84865	0.00135	0.10000	0.00000
12: 14 2 13 13 1 12	17818.56000	17818.72408	-0.16408	0.10000	0.00000

NORMALIZED DIAGONAL:

1	1.00000E+000	2	3.21007E-001	3	2.07692E-001	4	1.28770E-002	5	5.34714E-001
6	6.97514E-004								
7	1.17205E-001	8	9.99986E-001						

MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00

NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION

1	10000	A	1458.781(42)	-0.000
2	20000	B	832.488(242)	0.000
3	30000	C	587.0201(174)	-0.0000
4	200	-DeltaJ	-0.03030(211)	-0.00000
5	2000	-DeltaK	-0.0570(49)	-0.0000
6	1100	-DeltaJK	0.0884(70)	0.0000
7	40100	-deltaJ	-6.17(123)E-03	-0.00E-03
8	41000	-deltaK	-9.90(133)E-03	0.00E-03

MICROWAVE AVG = 0.000023 MHz, IR AVG = 0.00000
MICROWAVE RMS = 0.073549 MHz, IR RMS = 0.00000

SPFIT Details for wg1tw with HDO and H2O

	EXP.FREQ.	CALC.FREQ.	DIFF.	EXP.ERR.	EST.ERR.	AVG.
CALC.FREQ. - DIFF. - WT.						
1: 6 3 4 5 2 4	12760.29000	12760.28684	0.00316	0.10000	0.00000	
2: 6 3 4 5 2 4	12760.29000	12760.28684	0.00316	0.10000	0.00000	
3: 7 5 3 6 4 3	16645.30000	16645.31532	-0.01532	0.10000	0.00000	
4: 8 2 6 7 1 6	15618.40000	15618.39005	0.00995	0.10000	0.00000	
5: 10 2 9 9 2 8	13059.02000	13059.10697	-0.08697	0.10000	0.00000	
6: 10 4 7 9 4 6	14434.14000	14434.13628	0.00372	0.10000	0.00000	
7: 11 2 9 10 2 8	15278.29000	15278.20182	0.08818	0.10000	0.00000	
8: 11 3 8 10 3 7	16454.69000	16454.69988	-0.00988	0.10000	0.00000	
9: 13 0 13 12 0 12	15645.39000	15645.36816	0.02184	0.10000	0.00000	
10: 13 1 13 12 0 12	15645.40000	15645.38034	0.01966	0.10000	0.00000	
11: 14 1 13 13 1 12	17737.12000	17737.16110	-0.04110	0.10000	0.00000	

NORMALIZED DIAGONAL:

1	1.00000E+000	2	3.11662E-001	3	2.30822E-001	4	7.12813E-002	5	9.54985E-001
6	5.15537E-003								
7	9.98405E-001	8	5.85250E-001						

MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00

NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION

1	10000	A	1456.4213(310)	-0.0000
2	20000	B	826.5009(111)	0.0000
3	30000	C	583.8551(108)	-0.0000
4	200	-DeltaJ	-0.01406(40)	0.00000
5	2000	-DeltaK	-0.14363(86)	0.00000
6	1100	-DeltaJK	0.15670(125)	-0.00000
7	40100	-deltaJ	-0.934(225)E-03	-0.000E-03
8	41000	-deltaK	-0.12176(67)	0.00000
MICROWAVE AVG =			-0.000326 MHz, IR AVG =	0.00000
MICROWAVE RMS =			0.040851 MHz, IR RMS =	0.00000

SPFIT Details for wttw

EXP.FREQ. - CALC.FREQ. - DIFF. - EXP.ERR.- EST.ERR.-AVG.	
CALC.FREQ. - DIFF. - WT.	
1: 5 5 0 4 4 0	12493.57000 12493.71234 -0.14234 0.10000 0.00000
2: 6 2 4 5 1 4	12156.22000 12156.19065 0.02935 0.10000 0.00000
3: 7 7 0 6 6 1	17719.83000 17719.72152 0.10848 0.10000 0.00000
4: 10 0 10 9 0 9	11568.04000 11567.89253 0.14747 0.10000 0.00000
11567.89499 0.14501 0.5000	
5: 10 1 10 9 0 9	11568.04000 11567.89745 0.14255 0.10000 0.00000
11567.89499 0.14501 0.5000	
6: 12 0 12 11 0 11	13779.45000 13779.44074 0.00926 0.10000 0.00000
13779.44086 0.00914 0.5000	
7: 12 1 12 11 0 11	13779.45000 13779.44098 0.00902 0.10000 0.00000
13779.44086 0.00914 0.5000	
8: 13 2 11 12 2 10	16931.38000 16931.41502 -0.03502 0.10000 0.00000
9: 14 2 12 13 2 11	18035.22000 18035.28052 -0.06052 0.10000 0.00000
18035.31488 -0.09488 0.5000	
10: 14 3 12 13 2 11	18035.22000 18035.34924 -0.12924 0.10000 0.00000
18035.31488 -0.09488 0.5000	
NORMALIZED DIAGONAL:	
1 1.00000E+000 2 9.45806E-001 3 9.90494E-001	
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00	
NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION	
1 10000 A 1305.2633(64) -0.0000	
2 20000 B 897.6755(77) 0.0000	
3 30000 C 552.91483(244) -0.00000	
MICROWAVE AVG = 0.002821 MHz, IR AVG = 0.00000	
MICROWAVE RMS = 0.095790 MHz, IR RMS = 0.00000	

SPFIT Details for wttw with HDO and H2O

EXP.FREQ. - CALC.FREQ. - DIFF. - EXP.ERR.- EST.ERR.-AVG.	
CALC.FREQ. - DIFF. - WT.	
1: 5 4 1 4 3 1	11242.68000 11242.69479 -0.01479 0.10000 0.00000
2: 5 4 1 4 3 1	11242.68000 11242.69479 -0.01479 0.10000 0.00000
3: 6 4 2 5 3 2	12596.10000 12596.06054 0.03946 0.10000 0.00000
4: 7 2 5 6 1 5	14362.91000 14362.91037 -0.00037 0.10000 0.00000
5: 7 7 0 6 6 1	17648.78000 17648.81918 -0.03918 0.10000 0.00000
17648.77792 0.00208 0.5000	
6: 7 7 1 6 6 1	17648.78000 17648.73667 0.04333 0.10000 0.00000
17648.77792 0.00208 0.5000	
7: 8 5 4 7 4 4	17146.63000 17146.63995 -0.00995 0.10000 0.00000
8: 11 0 11 10 0 10	12614.15000 12614.15334 -0.00334 0.10000 0.00000
12614.15390 -0.00390 0.5000	
9: 11 1 11 10 0 10	12614.15000 12614.15446 -0.00446 0.10000 0.00000
12614.15390 -0.00390 0.5000	
10: 12 5 8 11 5 7	17723.40000 17723.40041 -0.00041 0.10000 0.00000
11: 14 1 13 13 1 12	16931.83000 16931.82833 0.00167 0.10000 0.00000
16931.82900 0.00100 0.5000	
12: 14 2 13 13 1 12	16931.83000 16931.82968 0.00032 0.10000 0.00000
16931.82900 0.00100 0.5000	
13: 15 0 15 14 0 14	17022.67000 17022.66915 0.00085 0.10000 0.00000
17022.66915 0.00085 0.5000	
14: 15 1 15 14 0 14	17022.67000 17022.66915 0.00085 0.10000 0.00000
17022.66915 0.00085 0.5000	
NORMALIZED DIAGONAL:	
1 1.00000E+000 2 8.05358E-001 3 2.00194E-001 4 6.54921E-002 5 7.11906E-001	
6 1.12255E-002	
7 3.35756E-001 8 9.98960E-001	
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00	
NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION	
1 10000 A 1300.3416(191) 0.0000	
2 20000 B 892.5002(140) -0.0000	
3 30000 C 550.1164(111) 0.0000	
4 200 -DeltaJ -2.430(116)E-03 -0.000E-03	
5 2000 -DeltaK -5.25(46)E-03 0.00E-03	
6 1100 -DeltaJK 6.57(53)E-03 -0.00E-03	
7 40100 -deltaJ -2.653(84)E-03 0.000E-03	
8 41000 -deltaK 3.42(41)E-03 0.00E-03	
MICROWAVE AVG = -0.000083 MHz, IR AVG = 0.00000	
MICROWAVE RMS = 0.014544 MHz, IR RMS = 0.00000	

SPFIT Details for wttw with d2o

EXP.FREQ. - CALC.FREQ. - DIFF. - EXP.ERR.- EST.ERR.-AVG.	
CALC.FREQ. - DIFF. - WT.	
1: 5 4 1 4 3 1	10636.45000 10636.45612 -0.00612 0.10000 0.06874
2: 5 4 1 4 3 1	10636.45000 10636.45612 -0.00612 0.10000 0.06874
3: 6 4 3 5 3 3	12485.52000 12485.53485 -0.01485 0.10000 0.09208
4: 6 5 1 5 4 2	13253.92000 13253.88702 0.03298 0.10000 0.04823
5: 7 6 2 6 5 2	15624.54000 15624.54799 -0.00799 0.10000 0.09627
6: 7 7 0 6 6 1	16582.38000 16582.48266 -0.10266 0.10000 0.09979
16582.38185 -0.00185 0.5000	
7: 7 7 1 6 6 1	16582.38000 16582.28104 0.09896 0.10000 0.09979
16582.38185 -0.00185 0.5000	
8: 8 5 4 7 4 4	16419.63000 16419.62936 0.00064 0.10000 0.09993
9: 9 1 8 8 1 7	11043.96000 11043.95278 0.00722 0.10000 0.07853
10: 10 1 10 9 0 9	11121.08000 11121.08584 -0.00584 0.10000 0.07249
11: 13 0 13 12 0 12	14306.17000 14306.16820 0.00180 0.10000 0.09630
14306.16820 0.00180 0.5000	
12: 13 1 13 12 0 12	14306.17000 14306.16820 0.00180 0.10000 0.09630
14306.16820 0.00180 0.5000	
13: 14 2 12 13 2 11	17335.28000 17335.27717 0.00283 0.10000 0.09918
17335.28099 -0.00099 0.5000	
14: 14 3 12 13 2 11	17335.28000 17335.28482 -0.00482 0.10000 0.09918
17335.28099 -0.00099 0.5000	
NORMALIZED DIAGONAL:	
1 1.00000E+000 2 2.86015E-001 3 2.60851E-001 4 5.97365E-002 5 9.97031E-001	
6 5.26630E-003	
7 6.88389E-001 8 5.55440E-001	
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00	
NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION	
1 10000 A 1220.9315(273) -0.0000	
2 20000 B 880.320(50) 0.000	
3 30000 C 531.7673(99) -0.0000	
4 200 -DeltaJ -3.59(33)E-03 0.00E-03	
5 2000 -DeltaK -0.03493(124) 0.00000	
6 1100 -DeltaJK 0.03948(154) -0.00000	
7 40100 -deltaJ -0.011605(228) -0.000000	
8 41000 -deltaK -0.03296(128) 0.00000	
MICROWAVE AVG =	-0.000101 MHz, IR AVG = 0.00000
MICROWAVE RMS =	0.011837 MHz, IR RMS = 0.00000

SPFIT Details for twww

	EXP.FREQ.	CALC.FREQ.	DIFF.	EXP.ERR.	EST.ERR.	AVG.
CALC.FREQ. - DIFF. - WT.						
1: 3 2 1 2 1 1	12140.50000	12140.49271	0.00729	0.10000	0.00000	
2: 3 2 1 2 1 1	12140.50000	12140.49271	0.00729	0.10000	0.00000	
3: 4 1 3 3 0 3	11917.81000	11917.82102	-0.01102	0.10000	0.00000	
4: 4 3 1 3 2 1	18554.86000	18554.86683	-0.00683	0.10000	0.00000	
5: 5 0 5 4 0 4	9945.26000	9945.13833	0.12167	0.10000	0.00000	
6: 6 1 6 5 0 5	12172.21000	12172.28677	-0.07677	0.10000	0.00000	
7: 6 2 5 5 2 4	12427.05000	12427.09504	-0.04504	0.10000	0.00000	
8: 7 3 5 7 2 6	11109.76000	11109.75562	0.00438	0.10000	0.00000	
9: 9 2 8 8 2 7	18329.88000	18329.86150	0.01850	0.10000	0.00000	
10: 10 1 10 9 0 9	18929.74000	18929.56889	0.17111	0.10000	0.00000	
11: 10 0 10 9 0 9	18881.28000	18881.45275	-0.17275	0.10000	0.00000	

NORMALIZED DIAGONAL:

1	1.00000E+000	2	6.07113E-001	3	3.61698E-001	4	2.86064E-002	5	7.77550E-001
6	1.87713E-003	7	9.99836E-001	8	2.07839E-001				

MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00

NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION

1	10000	A	3093.503(43)	-0.000
2	20000	B	1190.4341(255)	-0.0000
3	30000	C	903.3326(174)	0.0000
4	200	-DeltaJ	0.04957(253)	0.00000
5	2000	-DeltaK	0.0720(73)	0.0000
6	1100	-DeltaJK	-0.1228(97)	-0.0000
7	40100	-deltaJ	-0.03391(106)	-0.00000
8	41000	-deltaK	0.0574(34)	0.0000
MICROWAVE AVG =			0.001622 MHz, IR AVG =	0.00000
MICROWAVE RMS =			0.086595 MHz, IR RMS =	0.00000

SPFIT Details for twww with d2o

	EXP.FREQ. -	CALC.FREQ. -	DIFF. -	EXP.ERR.-	EST.ERR.-	AVG.
CALC.FREQ. - DIFF. - WT.						
1: 4 2 2 3 1 2	12829.54000	12829.53315	0.00685	0.10000	0.07063	
2: 4 2 2 3 1 2	12829.54000	12829.53315	0.00685	0.10000	0.07063	
3: 4 3 1 3 2 1	16704.29000	16704.29571	-0.00571	0.10000	0.09996	
4: 6 0 6 5 0 5	10960.95000	10961.06459	-0.11459	0.10000	0.08164	
5: 6 2 5 5 2 4	11660.97000	11660.99502	-0.02502	0.10000	0.09920	
6: 7 1 7 6 1 6	12493.10000	12492.94587	0.15413	0.10000	0.06298	
7: 7 1 7 6 0 6	12803.02000	12803.01513	0.00487	0.10000	0.09997	
8: 7 4 4 7 3 5	12386.18000	12386.17896	0.00104	0.10000	0.10000	
9: 9 0 9 8 0 8	15954.70000	15954.74082	-0.04082	0.10000	0.09786	
10: 9 1 8 8 1 7	17648.77000	17648.76305	0.00695	0.10000	0.09988	

NORMALIZED DIAGONAL:

1 1.00000E+000 2 9.99997E-001 3 2.61223E-001 4 8.55465E-002 5 8.98704E-001
6 2.54647E-003
7 4.30675E-001 8 7.58815E-002

MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00

NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION

1	10000	A	2764.333(43)	0.000
2	20000	B	1124.705(40)	-0.000
3	30000	C	843.9835(215)	-0.0000
4	200	-DeltaJ	0.07328(269)	-0.00000
5	2000	-DeltaK	0.2052(82)	-0.0000
6	1100	-DeltaJK	-0.2730(108)	0.0000
7	40100	-deltaJ	-1.12(97)E-03	0.00E-03
8	41000	-deltaK	0.0447(38)	-0.0000
MICROWAVE AVG =			-0.000546 MHz, IR AVG =	0.00000
MICROWAVE RMS =			0.062753 MHz, IR RMS =	0.00000

SPFIT Details for twww with HDO and 2H2O

	EXP.FREQ.	CALC.FREQ.	DIFF.	EXP.ERR.	EST.ERR.	AVG.
CALC.FREQ. - DIFF. - WT.						
1: 3 3 1 2 2 1	16398.86000	16398.85982	0.00018	0.10000	0.07070	
2: 3 3 1 2 2 1	16398.86000	16398.85982	0.00018	0.10000	0.07070	
3: 4 2 2 3 1 2	13961.08000	13961.08639	-0.00639	0.10000	0.08607	
4: 4 2 3 3 1 3	15236.12000	15236.11569	0.00431	0.10000	0.09324	
5: 5 1 5 4 0 4	10509.98000	10509.97480	0.00520	0.10000	0.09304	
6: 6 3 4 5 3 3	12552.62000	12552.62253	-0.00253	0.10000	0.09161	
7: 7 2 6 6 2 5	14285.28000	14285.28410	-0.00410	0.10000	0.09289	
8: 7 3 5 6 3 4	14654.84000	14654.83554	0.00446	0.10000	0.08646	
9: 8 0 8 7 1 7	14905.65000	14905.64569	0.00431	0.10000	0.09307	
10: 8 1 8 7 1 7	15053.93000	15053.93716	-0.00716	0.10000	0.05568	
11: 9 0 9 8 0 8	16927.83000	16927.82812	0.00188	0.10000	0.09477	

NORMALIZED DIAGONAL:

1	1.00000E+000	2	7.40245E-001	3	3.71324E-001	4	2.98228E-002	5	2.87889E-001
6	3.78048E-003	7	1.56966E-001	8	9.99845E-001				

MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00

NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION

1	10000	A	3069.896(63)	-0.000
2	20000	B	1178.521(35)	0.000
3	30000	C	894.5971(212)	0.0000
4	200	-DeltaJ	0.02187(223)	0.00000
5	2000	-DeltaK	-8.6(51)E-03	0.0E-03
6	1100	-DeltaJK	- 0.0154(72)	-0.0000
7	40100	-deltaJ	-0.02172(134)	-0.00000
8	41000	-deltaK	0.01840(278)	0.00000
MICROWAVE AVG =			0.000033 MHz, IR AVG =	0.00000
MICROWAVE RMS =			0.004296 MHz, IR RMS =	0.00000

SPFIT Details for gwww

EXP.FREQ. - CALC.FREQ. - DIFF. - EXP.ERR.- EST.ERR.-AVG.
CALC.FREQ. - DIFF. - WT.

1: 6 0 6 5 1 5	12222.79000	12222.82495	-0.03495	0.10000	0.09067
2: 8 0 8 7 0 7	16581.46000	16581.56142	-0.10142	0.10000	0.07277
3: 8 0 8 7 1 7	16428.24000	16428.27258	-0.03258	0.10000	0.05196
4: 8 1 7 7 1 6	18171.83000	18171.82137	0.00863	0.10000	0.09987
5: 9 0 9 8 1 8	18462.25000	18462.11487	0.13513	0.10000	0.06162

NORMALIZED DIAGONAL:

1 1.00000E+000 2 5.69646E-001 3 9.43440E-001

MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00

NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION

1	10000	A	2780.966(145)	0.000
2	20000	B	1259.2319(256)	0.0000
3	30000	C	990.4445(60)	0.0000

MICROWAVE AVG = -0.005038 MHz, IR AVG = 0.00000

MICROWAVE RMS = 0.078617 MHz, IR RMS = 0.00000

SPFIT Details for gwww with d2o

	EXP.FREQ.	- CALC.FREQ.	- DIFF.	- EXP.ERR.	- EST.ERR.	-AVG.
CALC.FREQ. - DIFF. - WT.						
1: 3 3 0 2 2 0	13592.26000	13592.27343	-0.01343	0.10000	0.06514	
2: 3 3 0 2 2 0	13592.26000	13592.27343	-0.01343	0.10000	0.06514	
3: 4 3 2 3 2 2	15793.37000	15793.34079	0.02921	0.10000	0.08428	
4: 6 0 6 5 0 5	11740.14000	11740.06363	0.07637	0.10000	0.08436	
5: 6 0 6 5 1 5	11410.63000	11410.64540	-0.01540	0.10000	0.09423	
6: 6 1 5 5 1 4	13053.14000	13053.08182	0.05818	0.10000	0.09831	
7: 7 2 6 6 2 5	14451.67000	14451.89947	-0.22947	0.10000	0.06821	
8: 8 2 7 7 2 6	16410.91000	16410.68417	0.22583	0.10000	0.07523	
9: 8 1 7 7 1 6	16886.03000	16886.12373	-0.09373	0.10000	0.08267	
10: 8 3 6 7 3 5	16983.69000	16983.68912	0.00088	0.10000	0.09826	
11: 8 0 8 7 0 7	15364.52000	15364.52479	-0.00479	0.10000	0.06148	
12: 9 1 9 8 1 8	17162.50000	17162.51894	-0.01894	0.10000	0.09038	

NORMALIZED DIAGONAL:

1	1.00000E+000	2	2.70298E-001	3	2.22801E-001	4	3.31616E-002	5	7.95251E-001
6	9.77651E-004								
7	9.99998E-001	8	1.39128E-001						

MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00

NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION

1	10000	A	2513.922(214)	-0.000
2	20000	B	1186.298(57)	-0.000
3	30000	C	917.0280(280)	0.0000
4	200	-DeltaJ	0.1131(86)	0.0000
5	2000	-DeltaK	0.1861(175)	0.0000
6	1100	-DeltaJK	-0.3013(261)	-0.0000
7	40100	-deltaJ	-0.0700(42)	-0.0000
8	41000	-deltaK	0.1217(104)	0.0000
MICROWAVE AVG =			0.000108 MHz, IR AVG =	0.00000
MICROWAVE RMS =			0.101443 MHz, IR RMS =	0.00000

SPFIT Details for gwww with HDO and 2H2O

EXP.FREQ. - CALC.FREQ. - DIFF. - EXP.ERR.- EST.ERR.-AVG.
CALC.FREQ. - DIFF. - WT.

1:	3 3 0 2 2 0	14841.22000	14841.28587	-0.06587	0.10000	0.06868
2:	3 3 0 2 2 0	14841.22000	14841.28587	-0.06587	0.10000	0.06868
3:	4 2 2 3 1 2	13506.13000	13505.90996	0.22004	0.10000	0.08272
4:	4 2 3 3 1 3	14650.38000	14650.52946	-0.14946	0.10000	0.09243
5:	4 3 1 3 2 1	17027.30000	17027.18099	0.11901	0.10000	0.09527
6:	5 2 4 4 2 3	11139.04000	11138.90518	0.13482	0.10000	0.09389
7:	5 1 5 4 0 4	11083.86000	11083.99994	-0.13994	0.10000	0.09340
8:	7 3 5 6 3 4	15841.81000	15841.94014	-0.13014	0.10000	0.09432
9:	8 1 8 7 1 7	16445.31000	16445.30959	0.00041	0.10000	0.10000
10:	8 2 7 7 2 6	17551.87000	17551.79872	0.07128	0.10000	0.09833

NORMALIZED DIAGONAL:

1 1.00000E+000 2 6.78450E-001 3 3.51016E-001 4 3.43171E-002 5 5.68001E-001
6 6.04884E-003
7 1.91890E-001 8 9.99324E-001

MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00

NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION

1	10000	A	2747.692(59)	0.000
2	20000	B	1256.4492(258)	-0.0000
3	30000	C	986.3222(208)	-0.0000
4	200	-DeltaJ	0.04515(208)	-0.00000
5	2000	-DeltaK	0.0453(54)	-0.0000
6	1100	-DeltaJK	-0.0921(72)	0.0000
7	40100	-deltaJ	-0.03020(118)	0.00000
8	41000	-deltaK	0.04162(295)	-0.00000

MICROWAVE AVG = -0.000573 MHz, IR AVG = 0.00000
MICROWAVE RMS = 0.123844 MHz, IR RMS = 0.00000

Section 3: Kraitchman Analysis from singly deuterated isotopologues and O-O distance from calculated structures.

In this section, Kraitchman analysis results from the KRA fitting program are included for every tetramer conformer including at least one water. In each of these conformers, the same water molecule (in regards to relative position around the ring) was substituted with HDO with deuterium in the plane of hydrogen bonding. The results of KRA fitting show the change in position for this deuterium.

In addition, calculated O-O distance is presented in table form for each conformer. These calculated distances show an increase in O-O distance upon inclusion of water into the pure ethanol tetramers, illustrating the strength of the hydrogen bond in pure ethanol tetramers.

Table of Calculated H position vs. Kraitchman fit of H position. ** indicates high error in fit, so value not reported.

Conformer	X	Y	Z	Distance to Center of Mass	Calc. X	Calc. Y	Calc. Z	Calc. Distance to Center of Mass
wg1g2t	0.070527	2.127519	0.455759	2.176930734	**	1.75477	0.85915	1.953805639
wttt	0.95024	1.917036	0.057843	2.140403909	1.18066	2.24931	**	2.540345156
wg1tw	2.457927	0.633641	0.278126	2.553480003	2.09037	0.54486	0.17909	2.167623672
wttw	1.637834	1.281045	0.203628	2.089268022	1.74118	1.29479	0.29507	2.189807124
twww	2.055524	1.168428	0.068512	2.365395696	2.05793	1.12638	0.2348	2.357740195
gwww	0.397353	1.464177	0.361862	1.559694778	0.83698	1.47857	0.63819	1.814935603

Table of Calculated O-O distances, showing trend in increasing O-O distance with inclusion of water

Pure Tetramer	O-O distance	Average
2g-g+t	2.70762	2.71277
	2.71584	
	2.71993	
	2.70769	

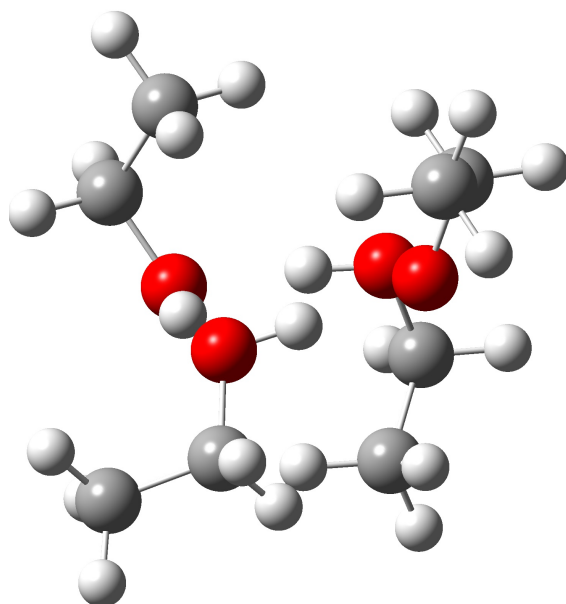
2g-2g+	2.71754	2.717545
	2.71755	
	2.71754	
	2.71755	
2tg+g-	2.69939	2.7092
	2.70873	
	2.72013	
	2.70855	

Mixed Tetramers	O-O distance	Average
wg1g2t	2.73792	2.7522
	2.75396	
	2.75617	
	2.76075	
wttt	2.76929	2.750365
	2.74803	
	2.75897	
	2.72517	
wg1g2w	2.76762	2.749715
	2.75544	
	2.72465	
	2.75115	
wttw	2.75328	2.74954
	2.76111	
	2.75985	
	2.72392	
gwww	2.74019	2.7492125

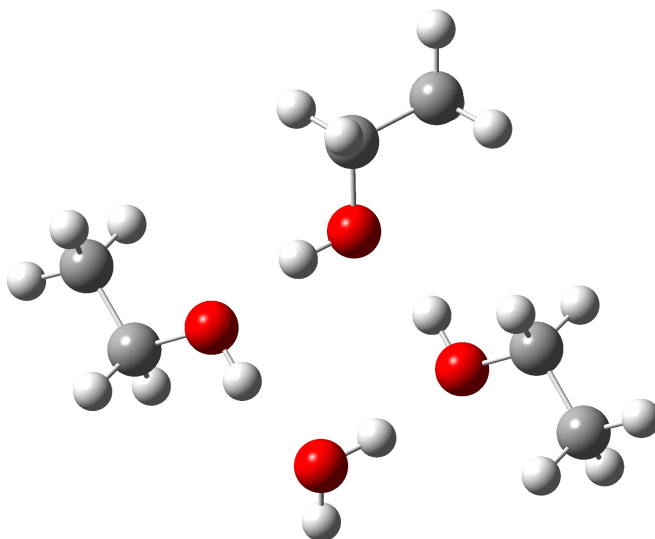
	2.7329	
	2.76598	
	2.75778	
twww	2.72331	2.740305
	2.73695	
	2.74218	
	2.75878	

Section 4: Enlarged Images of Fitted Conformers

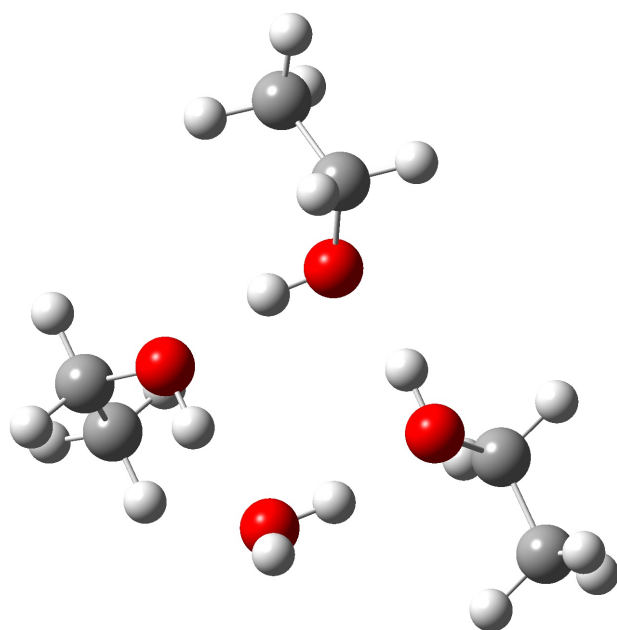
Here, enlarged images of each fitted conformer are included for reference, and to illustrate the relative geometry of ethyl groups distinguishing conformers from each other. *Ab initio* geometries are available upon request.



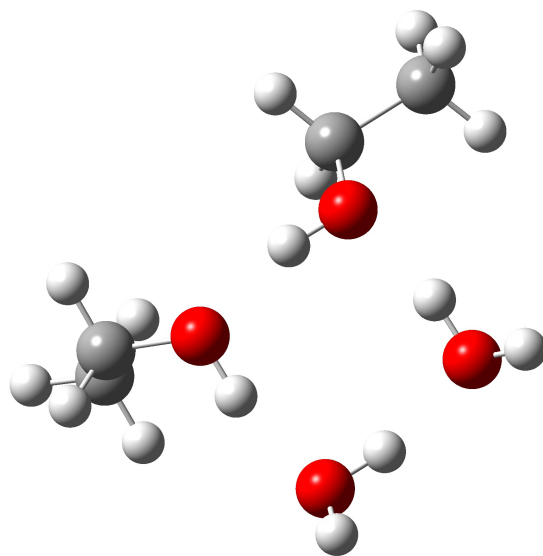
2tg+g-



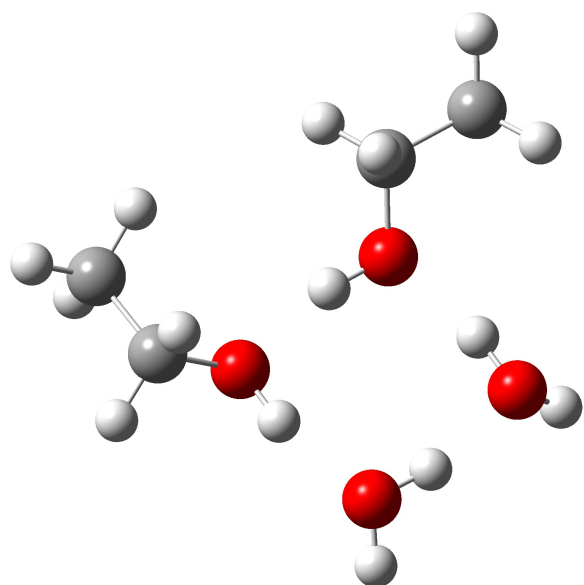
Wttt



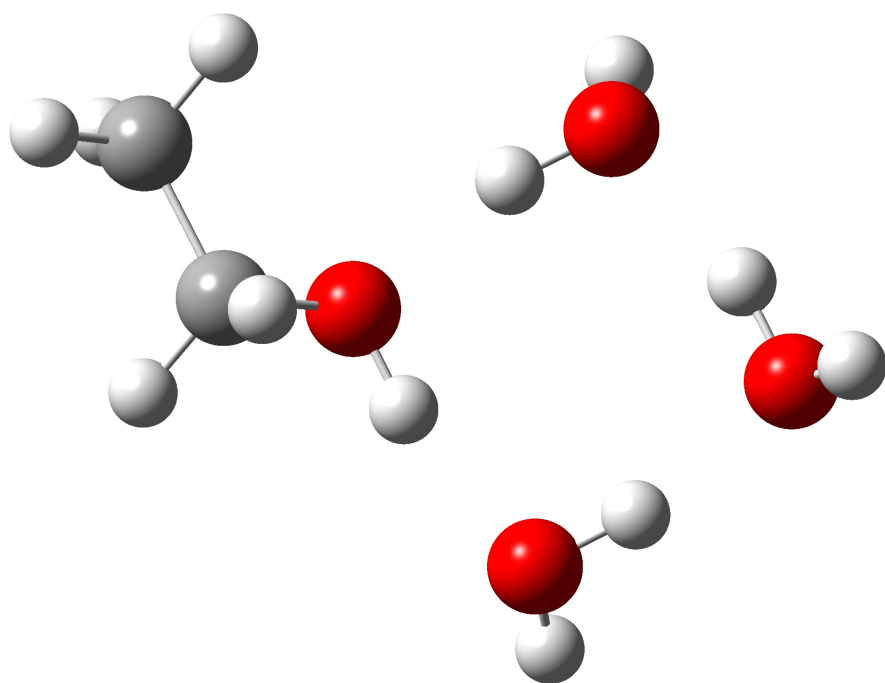
Wg1g2t



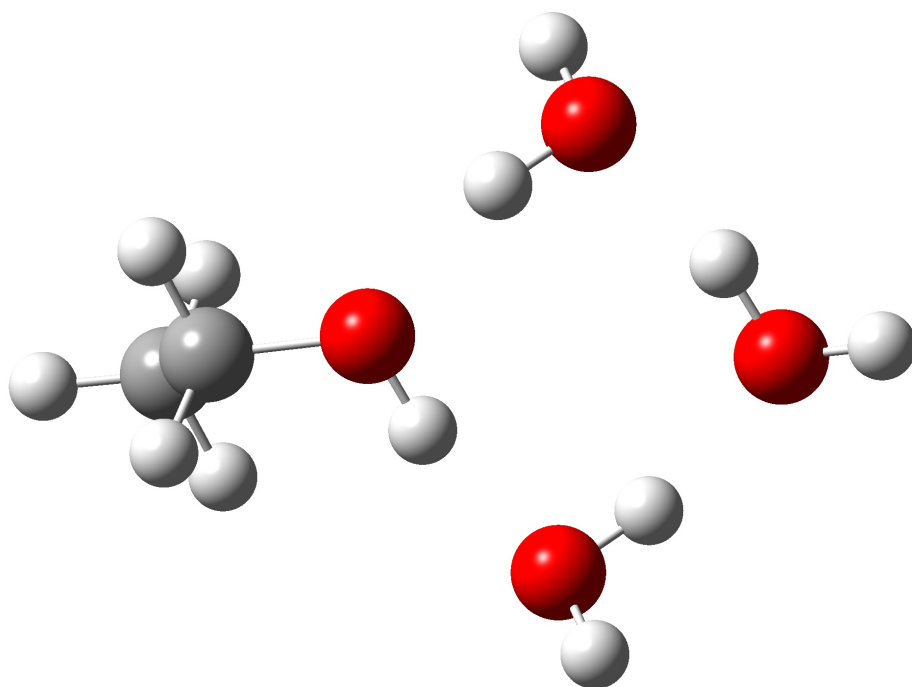
Wg1tw



Wttw



Twwww



Gwww

Section 5: XIAM Results

Finally, samples from the XIAM results are included to demonstrate the calculated magnitude of splitting due to the methyl group rotation. This magnitude of splitting is lower than can be resolved with the current instrumentation, but is large enough, especially for high J states, that it may increase the error in line assignment (and thus SPFIT results) commensurately.

Sample lines fit for the 2tg+g- conformer:

J K- K+ J K- K+ Sym	calc/GHz	diff/MHz	obs/GHz		
1: 10 10 1 9 9 0 S 0	10.9611722	7.5578	10.9687300	Err .1D+01	I .702 rigid-rigid
2: 11 0 11 10 0 10 S 0	10.2946610	-6.1310	10.2885300	Err .1D+01	I 2.002 rigid-rigid
3: 12 0 12 11 0 11 S 0	11.2234430	8.0570	11.2315000	Err .1D+01	I 1.752 rigid-rigid

XIAM predicted splitting for a few sample lines, illustrating a magnitude of splitting too small to resolve with the current instrumentation.

[illegible][illegible][illegible]