Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplemental Information for: "Supersonic Jet Chirped Pulse Microwave Spectroscopy of Ring-Like Methanol:Water Pentamers"

Additional tables of fits and fitting information is included in this document. Images of every conformer and calculated O-O distances for each conformer are also included for reference.

Sections:

Section 1: Tables of D2O, D4, and HDO ab initio and fitted constants

Reported here are tables with rotational constants, distortion constants, dipole moment, and relative energy ordering calculated with B3LYP/6-311++G(d,p) followed by the experimentally fit rotational constants with number of lines used and rms error for each fit. The fits were performed with spfit and the values in parentheses are the errors reported by the fitting program.

D4	Ab initio	Experimental
A /MHz	568.085	568.07 (13)
B /MHz	558.812	558.80 (8)
C /MHz	342.082	342.06 (8)
Δ_J /kHz	1.49E-01	-
Δ_K /kHz	-2.23E-01	-
Δ_{JK} /kHz	1.77E-01	-
δ_J /kHz	1.44E-03	-
δ_K /kHz	7.73E+00	-
μ_A /D	-0.29	y
μ_B /D	0.10	y
μ_C /D	0.63	y
N	-	19
Error /kHz	-	36

SI Table 1. Calculated and fitted constants for the $(CD_3OD)_5$ isotopologue conformers.

Ab initio	wdudu	wuduu	wuudu	wduud	wudud
A /MHz	882.995	892.738	885.074	870.248	889.992
B /MHz	683.627	686.911	697.47	725.958	679.818
C /MHz	464.58	452.929	449.691	438.869	460.168
Δ_J /kHz	2.43E-01	3.59E-01	1.28E+00	1.43E+00	2.49E-01
Δ_K /kHz	5.03E-02	2.64E-01	4.26E+00	5.61E+00	1.05E-01
Δ_{JK} /kHz	-4.67E-02	-4.32E-01	-5.28E+00	-6.92E+00	-8.45E-02
δ_J /kHz	2.44E-02	1.97E-02	1.79E-02	8.98E-03	3.03E-02
δ_K /kHz	4.32E-01	1.74E-01	-4.73E+00	-1.00E+01	3.64E-01
μ_A /D	0.17	-0.27	0.31	-0.12	-0.18
μ_B /D	-0.015	0.0082	-0.016	0.53	0.025
μ_C /D	-0.84	0.47	0.49	0.63	-0.87
Rel. E. /cm^{-1}	0.0	20.0	33.4	37.6	55.1
Experimental	wdudu	wuduu	wuudu	wduud	wudud
A /MHz	882.46 (10)	893.10 (21)	884.95 (4)	870.17 (10)	890.27 (15)
B /MHz	684.23 (7)	685.62 (6)	697.46 (6)	725.48 (13)	678.50 (8)
C /MHz	464.56 (8)	453.13 (9)	449.72 (4)	438.74 (7)	460.16 (7)
μ_A /D	y	y	y	y	y
μ_B /D	n	n	y	y	n
μ_C /D	y	y	y	y	y
N	15	16	24	19	15
Error /kHz	22	29	66	87	84

SI Table 2. Calculated and fitted constants for the $(D_2O)(CH_3OH)_4$ isotopologue conformers.

Ab initio	wduud	wudud	wuudu	wuduu	wdudu
A /MHz	770.634	790.928	787.373	795.453	784.956
B /MHz	623.875	575.115	593.838	582.456	577.767
C /MHz	382.28	405.3	393.949	397.554	409.831
Δ_J /kHz	1.12E+00	1.85E-01	8.76E-01	3.01E-01	1.85E-01
Δ_K /kHz	4.39E+00	5.88E-02	2.60E+00	2.58E-01	5.88E-02
Δ_{JK} /kHz	-5.41E+00	9.57E-03	-3.26E+00	-3.95E-01	3.57E-01
δ_J /kHz	1.70E-02	2.54E-02	2.37E-02	1.35E-02	2.54E-02
δ_K /kHz	-6.68E+00	3.07E-01	-2.12E+00	9.99E-02	3.12E-01
μ_A /D	-0.14	0.21	0.28	-0.30	0.20
μ_B /D	0.54	-0.011	-0.020	-0.0066	0.0023
μ_C /D	0.62	-0.89	0.51	0.45	-0.84
Rel. E. /cm^{-1}	0.0	4.8	24.6	67.6	84.8
Experimental	wduud	wudud	wuudu	wuduu	wdudu
A /MHz	771.05 (9)	790.73 (11)	787.10 (10)	794.77 (12)	785.23 (3)
B /MHz	623.79 (14)	575.11 (10)	592.98 (9)	585.09 (12)	577.81 (12)
C /MHz	382.28 (4)	405.50 (7)	394.21 (11)	397.51 (15)	410.00 (11)
μ_A /D	y	y	y	y	y
μ_B /D	y	n	n	n	n
μ_C /D	y	y	y	y	y
N	20	13	14	15	14
Error /kHz	7.6	18	31	37	61

SI Table 3. Calculated and fitted constants for the $(H_2O)(CD_3OD)_4$ isotopologue conformers.

Ab initio	wduud	wudud	wuudu	wuduu	wdudu
A /MHz	886.658	907.611	902.367	910.315	900.677
B /MHz	729.693	680.71	699.631	688.583	684.19
C /MHz	441.669	464.425	453.202	456.688	469.169
Δ_J /kHz	1.48E+00	2.54E-01	1.31E+00	3.79E-01	2.48E-01
Δ_K /kHz	5.82E+00	9.91E-02	4.30E+00	2.90E-01	3.78E-02
Δ_{JK} /kHz	-7.17E+00	-6.44E-02	-5.34E+00	-4.72E-01	4.42E-01
δ_J /kHz	1.07E-02	3.17E-02	1.88E-02	2.10E-02	2.71E-02
δ_K /kHz	-9.71E+00	3.87E-01	-4.42E+00	1.62E-01	4.41E-01
μ_A /D	-0.14	-0.21	0.29	-0.29	0.21
μ_B /D	0.53	-0.012	-0.0076	0.0066	0.0007
μ_C /D	0.64	-0.89	0.53	0.47	-0.84
Rel. E. /cm^{-1}	0.0	8.6	19.3	66.5	88.1
Experimental	wduud	wudud	wuudu	wuduu	wdudu
A /MHz	886.79 (13)	908.06 (4)	902.59 (3)	910.57 (10)	900.68 (9)
B /MHz	729.41 (16)	680.41 (26)	699.44 (12)	688.58 (28)	684.12 (3)
C /MHz	441.76 (5)	464.27 (6)	453.00 (27)	456.66 (21)	469.02 (6)
μ_A /D	y	y	y	y	y
μ_B /D	y	y	y	y	y
μ_C /D	y	n	y	y	y
N	6	5	12	15	5
Error /kHz	46	364	1345	99	211

SI Table 4. Calculated and fitted constants for the $(HDO)(CH_3OH)_4$ isotopologue conformers.

Ab initio	wwduu	wuwuu	wwuud	wwdud	wuwud	wwudu	wuwdu
A /MHz	1092.66	1136.68	1082.5	1021.56	1160.711	1040.101	1151.373
B /MHz	814.721	771.467	831.888	838.828	744.375	826.279	754.495
C /MHz	516.441	506.493	510.202	552.976	505.89	540.928	510.27
ΔJ /kHz	6.43E-01	5.90E-01	7.54E-01	6.21E-01	4.13E-01	7.34E-01	4.92E-01
ΔK /kHz	1.20E+00	-1.24E+00	1.29E+00	1.28E+00	-8.18E-02	1.79E+00	1.86E-01
ΔJK /kHz	-1.58E+00	8.21E-01	-1.89E+00	-1.57E+00	-1.70E-01	-2.10E+00	-4.90E-01
δJ /kHz	7.16E-02	8.22E-02	2.31E-02	5.49E-02	6.45E-02	1.13E-01	5.08E-02
δK /kHz	-6.27E-01	1.96E+00	-8.55E-01	-1.15E+00	3.72E-01	-1.56E+00	1.76E-01
μ_A /D	0.44	-0.32	-0.35	-0.060	-0.28	0.19	0.13
μ_B /D	-0.30	-0.083	-0.36	-0.10	0.22	-0.029	0.11
μ_C /D	0.47	0.41	0.56	-1.03	-0.70	0.78	-0.74
Rel. E. /cm-1	0.0	0.4	19.5	34.9	45.5	53.1	84.6
Experimental	wwduu	wuwuu	wwuud	wwdud	wuwud	wwudu	wuwdu
A /MHz	1092.72 (14)	1139.53 (11)	1083.03 (6)	1021.48 (7)	1160.51 (4)	1040.12 (9)	1153.38 (4)
B /MHz	814.59 (20)	770.44 (3)	831.53 (4)	838.80 (8)	744.32 (12)	826.19 (4)	753.83 (13)
C /MHz	516.27 (4)	506.48 (6)	510.17 (28)	552.91 (5)	505.76 (5)	540.76 (6)	510.32 (24)
μ_A /D	y	y	y	n	y	n	y
μ_B /D	y	y	y	y	n	y	y
μ_C /D	y	y	y	y	y	y	y
N	4	9	11	4	4	5	10
Error /kHz	35	38	41	123	220	211	22

SI Table 5. Calculated and fitted constants for the $(D_2O)_2(CH_3OH)_3$ isotopologue conformers.

Ab initio	wuwuu	wwduu	wwuud	wwdud	wuwud	wwudu	wuwdu
A /MHz	1075.106	1049.482	1044.785	965.155	1092.464	985.474	1082.715
B /MHz	671.894	713.533	727.624	739.637	646.672	725.291	657.236
C /MHz	457.207	472.832	466.337	513.368	452.655	500.473	457.208
ΔJ /kHz	5.65E-01	6.01E-01	6.93E-01	5.90E-01	3.45E-01	7.40E-01	4.24E-01
ΔK /kHz	-1.60E+00	1.22E+00	1.24E+00	1.35E+00	-2.90E-01	2.04E+00	2.44E-02
ΔJK /kHz	1.20E+00	-1.57E+00	-1.79E+00	-1.62E+00	7.97E-02	-2.33E+00	-2.87E-01
δJ /kHz	9.64E-02	9.60E-02	4.29E-02	7.59E-02	5.65E-02	1.52E-01	4.34E-02
δK /kHz	1.96E+00	-5.43E-01	-6.37E-01	-1.01E+00	4.45E-01	-1.51E+00	2.20E-01
μ_A /D	-0.28	0.40	-0.38	-0.027	-0.24	0.16	0.17
μ_B /D	-0.061	-0.31	-0.34	-0.087	0.22	-0.014	0.14
μ_C /D	0.39	0.47	0.57	-1.04	-0.67	0.76	-0.72
Rel. E. /cm-1	0.0	5.5	22.2	24.4	39.8	49.9	78.6
Experimental	wuwuu	wwduu	wwuud	wwdud	wuwud	wwudu	wuwdu
A /MHz	1068.31 (18)	1049.54 (7)	1045.20 (5)	964.96 (13)	1092.62 (22)	985.44 (10)	1083.57 (6)
B /MHz	673.87 (6)	713.47 (23)	727.43 (18)	739.71 (29)	646.52 (5)	725.20 (7)	656.88 (16)
C /MHz	457.36 (4)	472.77 (15)	466.29 (4)	513.24 (4)	452.42 (3)	500.20 (28)	456.99 (5)
μ_A /D	y	y	y	y	y	y	n
μ_B /D	y	y	y	y	y	y	y
μ_C /D	y	y	y	y	y	y	y
N	11	10	10	10	5	4	4
Error /kHz	101	7.9	85	22	512	13	365

SI Table 6. Calculated and fitted constants for the $(H_2O)_2(CD_3OD)_3$ isotopologue conformers.

Ab initio	wuwuu	wwduu	wwuud	wwdud	wuwud	wwudu	wuwdu
A /MHz	1194.66	1144.26	1136.665	1065.697	1217.936	1085.752	1208.863
B /MHz	778.983	829.35	845.323	856.08	751.859	841.11	761.839
C /MHz	517.125	530.176	523.437	569.988	514.848	557.139	519.806
ΔJ /kHz	6.64E-01	7.19E-01	8.34E-01	7.00E-01	4.49E-01	8.28E-01	5.31E-01
ΔK /kHz	-1.52E+00	1.39E+00	1.46E+00	1.45E+00	-1.65E-01	2.10E+00	1.26E-01
ΔJK /kHz	1.04E+00	-1.83E+00	-2.12E+00	-1.79E+00	-1.19E-01	-2.44E+00	-4.59E-01
δJ /kHz	1.03E-01	9.25E-02	3.63E-02	7.12E-02	7.46E-02	1.41E-01	6.11E-02
δK /kHz	2.16E+00	-7.15E-01	-8.94E-01	-1.20E+00	4.38E-01	-1.72E+00	2.28E-01
μ_A /D	-0.28	0.41	-0.38	-0.036	0.24	0.16	0.17
μ_B /D	-0.062	-0.31	-0.34	-0.089	0.22	-0.014	0.14
μ_C /D	0.39	0.47	0.57	-1.04	0.67	0.76	-0.72
Rel. E. /cm-1	0.0	0.7	19.8	28.8	43.5	51.2	80.8
Experimental	wuwuu	wwduu	wwuud	wwdud	wuwud	wwudu	wuwdu
A /MHz	1194.24 (13)	1144.25 (7)	-	1065.75 (17)	1217.61 (26)	1085.72 (20)	1209.17 (25)
B /MHz	778.92 (16)	829.27 (8)	-	855.96 (16)	751.84 (7)	841.06 (14)	761.61 (12)
C /MHz	516.64 (4)	529.87 (4)	-	569.86 (13)	514.67 (4)	557.02 (9)	519.53 (5)
μ_A /D	y	y	-	n	y	y	y
μ_B /D	y	y	-	y	n	y	y
μ_C /D	y	y	-	y	y	n	y
N	4	6	-	4	4	4	4
Error /kHz	1486	182	-	11	71	223	348

SI Table 7. Calculated and fitted constants for the $(HDO)(H_2O)(CH_3OH)_3$ isotopologue conformers.

Ab initio	wwwdd	wwdwu	wwuwu	wwwdu	wwuwd	wwwud	wwdwd
A /MHz	1212.914	1556.513	1502.66	1183.054	1560.575	1173.188	1476.019
B /MHz	1076.859	844.342	859.945	1081.603	850.31	1082.469	874.642
C /MHz	603.85	583.942	592.01	622.391	587.443	634.822	603.259
ΔJ /kHz	6.77E-01	2.96E-01	1.42E+00	6.17E-01	3.03E-01	5.60E-01	1.42E+00
ΔK /kHz	-1.66E+00	1.57E+00	2.89E+00	-8.53E-01	8.56E-01	-1.59E-01	2.94E+00
ΔJK /kHz	1.15E+00	-1.90E-01	-4.04E+00	-3.34E-01	1.28E-01	-9.82E-02	-4.03E+00
δJ /kHz	5.47E-02	6.80E-02	3.87E-01	3.41E-02	6.81E-02	9.48E-03	3.16E-01
δK /kHz	8.69E+00	-1.30E-01	-1.87E+00	3.43E+00	-1.70E-01	4.22E+00	-1.94E+00
μ_A /D	0.54	-0.45	-0.15	0.35	-0.28	-0.044	-0.18
μ_B /D	-0.0029	-0.13	-0.25	-0.32	-0.23	-0.16	-0.15
μ_C /D	0.44	-0.77	0.63	-0.81	0.83	-0.94	0.64
Rel. E. /cm-1	0.0	6.4	57.5	63.7	72.0	74.0	101.0
Experimental	wwwdd	wwdwu	wwuwu	wwwdu	wwuwd	wwwud	wwdwd
A /MHz	1212.93 (9)	-	1502.66 (13)	1183.09 (25)	1560.55 (12)	1173.54 (11)	-
B /MHz	1076.72 (4)	-	859.96 (17)	1081.65 (15)	850.27 (21)	1082.29 (9)	-
C /MHz	603.74 (10)	-	591.76 (20)	622.56 (3)	587.36 (5)	634.44 (4)	-
μ_A /D	y	-	y	y	y	y	-
μ_B /D	y	-	n	y	y	y	-
μ_C /D	n	-	y	n	y	y	-
N	4	-	4	12	6	10	-
Error /kHz	64	-	244	3.8	32	20	-

SI Table 8. Calculated and fitted constants for the $(D_2O)_3(CH_3OH)_2$ isotopologue conformers.

Ab initio	wwdwu	wwwdd	wwuwu	wwwdu	wwuwd	wwwud	wwdwd
A /MHz	1653.203	1169.31	1579.279	1131.072	1664.598	1116.305	1541.017
B /MHz	746.173	1050.833	763.41	1056.898	750.156	1065.689	780.632
C /MHz	547.438	586.644	557.885	605.682	550.809	617.93	570.952
ΔJ /kHz	2.64E-01	7.72E-01	4.80E-01	6.92E-01	2.59E-01	5.34E-01	5.85E-01
ΔK /kHz	2.42E+00	-1.73E+00	4.43E+00	5.23E-01	1.03E+00	-3.02E-01	4.14E+00
ΔJK /kHz	-3.20E-01	1.13E+00	-1.75E+00	-7.79E-01	1.93E-01	6.47E-02	-1.95E+00
δJ /kHz	5.33E-02	6.43E-02	8.04E-02	4.60E-02	4.89E-02	2.16E-04	1.01E-01
δK /kHz	-6.29E-02	1.03E+01	-6.26E-02	2.58E+00	-8.74E-02	8.22E+00	-6.97E-02
μ_A /D	-0.41	0.51	-0.19	0.31	-0.33	-0.016	-0.14
μ_B /D	-0.085	0.011	-0.20	-0.31	-0.19	-0.14	-0.11
μ_C /D	-0.77	0.44	0.63	-0.80	0.84	-0.92	0.64
Rel. E. /cm-1	0.0	8.8	51.4	60.8	64.4	65.5	94.9
Experimental	wwdwu	wwwdd	wwuwu	wwwdu	wwuwd	wwwud	wwdwd
A /MHz	1653.23 (25)	1169.36 (7)	1579.45 (26)	-	1664.24 (16)	1112.59 (8)	1540.47 (5)
B /MHz	746.09 (5)	1050.69 (4)	763.24 (13)	-	750.043 (4)	1068.93 (7)	780.65 (11)
C /MHz	547.32 (4)	586.42 (9)	557.78 (5)	-	550.80 (9)	617.96 (25)	570.83 (4)
μ_A /D	y	n	y	-	y	n	n
μ_B /D	y	y	y	-	y	y	y
μ_C /D	y	y	y	-	y	y	y
N	4	5	4	-	9	12	4
Error /kHz	124	75	400	-	35	36	39

SI Table 9. Calculated and fitted constants for the $(H_2O)_3(CD_3OD)_2$ isotopologue conformers.

Ab initio	wwdwu	wwwdd	wwuwu	wwwdu	wwuwd	wwwud	wwdwd
A /MHz	1702.438	1278.16	1638.89	1245.657	1710.932	1235.64	1605.489
B /MHz	861.881	1142.421	878.418	1146.279	866.477	1150.44	895.375
C /MHz	606.1	635.283	615.162	655.476	609.808	668.11	627.836
ΔJ /kHz	3.28E-01	7.61E-01	5.25E-01	6.76E-01	3.25E-01	6.55E-01	6.42E-01
ΔK /kHz	2.26E+00	-2.20E+00	3.85E+00	-1.76E-02	1.09E+00	-2.18E-01	3.77E+00
ΔJK /kHz	-2.98E-01	1.62E+00	-1.50E+00	-1.80E-01	2.04E-01	-1.07E-01	-1.79E+00
δJ /kHz	7.68E-02	6.61E-02	1.04E-01	3.59E-02	7.15E-02	1.36E-02	1.29E-01
δK /kHz	-1.16E-01	1.18E+01	-1.22E-01	5.06E+00	-1.55E-01	5.65E+00	-1.35E-01
μ_A /D	-0.41	0.51	-0.19	-0.32	0.33	-0.017	-0.14
μ_B /D	-0.085	0.0098	-0.20	-0.32	-0.19	-0.14	-0.11
μ_C /D	-0.77	0.44	0.64	0.80	-0.84	-0.92	0.64
Rel. E. /cm-1	0.0	0.9	51.6	60.4	65.7	66.3	96.4
Experimental	wwdwu	wwwdd	wwuwu	wwwdu	wwuwd	wwwud	wwdwd
A /MHz	-	-	-	-	-	1235.39 (10)	1605.51 (3)
B /MHz	-	-	-	-	-	1150.78 (15)	895.28 (8)
C /MHz	-	-	-	-	-	667.98 (19)	627.65 (4)
μ_A /D	-	-	-	-	-	y	n
μ_B /D	-	-	-	-	-	y	y
μ_C /D	-	-	-	-	-	n	y
N	-	-	-	-	-	5	4
Error /kHz	-	-	-	-	-	80	18

SI Table 10. Calculated and fitted constants for the $(HDO)(H_2O)_2(CH_3OH)_2$ isotopologue conformers.

Ab initio	wwwwu	wwwwd'	wwwwd
A /MHz	1748.802	1684.05	1723.683
B /MHz	1139.581	1173.7	1157.954
C /MHz	715.919	744.609	728.64
ΔJ /kHz	1.59E+00	1.58E-03	1.86E+00
ΔK /kHz	2.65E+00	2.58E-03	3.55E+00
ΔJK /kHz	-4.03E+00	-3.86E-03	-5.08E+00
δJ /kHz	3.35E-01	2.39E-04	3.32E-01
δK /kHz	-1.84E+00	-1.85E-03	-2.71E+00
μ_A /D	-0.45	-0.077	-0.40
μ_B /D	0.057	-0.086	0.088
μ_C /D	0.73	0.84	0.73
Rel. E. /cm-1	0.0	14.5	36.0
Experimental	wwwwu	wwwwd'	wwwwd
A /MHz	1748.68 (11)	1683.21 (5)	1723.00 (28)
B /MHz	1139.58 (5)	1173.55 (13)	1158.26 (13)
C /MHz	715.90 (18)	744.33 (4)	728.87 (11)
μ_A /D	y	y	y
μ_B /D	y	y	y
μ_C /D	y	n	y
N	10	8	10
Error /kHz	28	139	29

SI Table 11. Calculated and fitted constants for the $(D_2O)_4(CH_3OH)$ isotopologue conformers.

Ab initio	wwwwu	wwwwd'	wwwwd
A /MHz	1945.668	1864.589	1911.504
B /MHz	1113.595	1154.347	1134.358
C /MHz	732.854	766.768	748.392
ΔJ /kHz	1.99E+00	1.96E-03	2.42E+00
ΔK /kHz	3.72E+00	3.59E-03	5.14E+00
ΔJK /kHz	-5.44E+00	-5.19E-03	-7.12E+00
δJ /kHz	5.14E-01	3.86E-04	5.59E-01
δK /kHz	-2.41E+00	-2.40E-03	-3.55E+00
μ_A /D	-0.43	-0.058	-0.37
μ_B /D	0.017	-0.052	0.13
μ_C /D	0.72	0.82	0.74
Rel. E. /cm-1	0.0	6.4	34.9
Experimental	wwwwu	wwwwd'	wwwwd
A /MHz	1945.61 (14)	1864.60 (18)	1911.57 (20)
B /MHz	1113.52 (10)	1154.07 (6)	1134.55 (6)
C /MHz	732.66 (8)	766.68 (7)	747.94 (6)
μ_A /D	y	n	y
μ_B /D	y	y	y
μ_C /D	y	y	y
N	4	4	4
Error /kHz	169	150	89

SI Table 12. Calculated and fitted constants for the $(H_2O)_4(CD_3OD)$ isotopologue conformers.

Ab initio	wwwwd	wwwwd'	wwwwu
A /MHz	1919.109	1844.654	1948.036
B /MHz	1234.117	1250.24	1214.465
C /MHz	785.318	798.815	770.69
ΔJ /kHz	2.61E+00	1.94E+00	2.02E+00
ΔK /kHz	5.79E+00	3.30E+00	3.49E+00
ΔJK /kHz	-7.98E+00	-4.89E+00	-5.25E+00
δJ /kHz	4.81E-01	3.18E-01	4.68E-01
δK /kHz	-4.44E+00	-2.35E+00	-2.35E+00
μ_A /D	-0.36	-0.058	-0.43
μ_B /D	0.12	-0.051	0.016
μ_C /D	0.74	0.82	0.72
Rel. E. /cm-1	0.0	30.7	36.7
Experimental	wwwwd	wwwwd'	wwwwu
A /MHz	1919.04 (14)	1844.41 (11)	-
B /MHz	1233.98 (5)	1250.22 (14)	-
C /MHz	784.90 (4)	798.88 (4)	-
μ_A /D	n	y	-
μ_B /D	y	y	-
μ_C /D	n	y	-
N	4	11	-
Error /kHz	971	87	-

SI Table 13. Calculated and fitted constants for the $(HDO)(H_2O)_3(CH_3OH)$ isotopologue conformers.

Ab initio	wwwwu	wwwwd'	wwwwd
A /MHz	1974.882	1875.205	1945.393
B /MHz	1199.241	1229.914	1218.721
C /MHz	768.668	794.843	783.37
ΔJ /kHz	2.05E+00	1.96E+00	2.42E+00
ΔK /kHz	3.57E+00	3.25E+00	4.79E+00
ΔJK /kHz	-5.36E+00	-4.86E+00	-6.79E+00
δJ /kHz	4.95E-01	3.39E-01	5.14E-01
δK /kHz	-2.35E+00	-2.19E+00	-3.40E+00
μ_A /D	-0.43	-0.057	-0.37
μ_B /D	0.013	-0.047	0.13
μ_C /D	0.72	0.82	0.74
Rel. E. /cm-1	0.0	32.3	35.6
Experimental	wwwwu	wwwwd'	wwwwd
A /MHz	1975.78 (9)	1875.16 (6)	1945.36 (29)
B /MHz	1199.11 (22)	1229.78 (8)	1218.32 (28)
C /MHz	768.27 (3)	794.79 (8)	783.16 (9)
μ_A /D	y	n	y
μ_B /D	y	y	y
μ_C /D	n	y	n
N	5	5	4
Error /kHz	42	245	617

SI Table 14. Calculated and fitted constants for the $(H_2O)(HDO)(H_2O)_2(CH_3OH)$ isotopologue conformers.

Section 2: Kraitchman Substitution Results and Calculated O-O Distances

The KRA fitting program was used to empirically find the position of a single hydrogen for comparison to calculation. The hydrogen used for comparison is the hydrogen participating in hydrogen bonding attached to the first water in the ring based on the naming scheme. The agreement between the fit and the calculated coordinates suggests the calculated O-O positions, and therefore separation, would be in good agreement with experiment. Kraitchman analysis was only performed on conformers in which both the normal isotopologues and HDO isotopologues had error within experimental expectation.

SI Table 15. Calculated H position vs Kraitchman fit of H position. * indicates high error due to close proximity of atom to the principal axis, so the value is not reported.

Conformer	Kra. X	Kra. Y	Kra. Z	D to CoM	Calc. X	Calc. Y	Calc. Z	D to CoM	Difference (Å)	% error
wduud	0.8619	1.8690	0.8774	2.2374	0.8528	-1.9659	0.6852	2.2498	0.0124	0.6
wuduu	0.7146	2.1355	*	2.2519	0.5662	-2.1407	-0.2979	2.2342	0.0177	0.8
wuwud	1.4375	1.5857	0.1335	2.1445	1.3729	-1.5371	0.3121	2.0844	0.0600	2.8
wwdud	*	2.2889	0.8818	2.4529	-0.4493	2.4320	-0.5018	2.5236	0.0707	2.9
wwdwd	0.5933	2.2074	*	2.2857	-0.3931	2.1793	-0.0821	2.2160	0.0698	3.1
wwwwu	2.4234	0.4876	*	2.4719	2.3741	-0.5065	0.1277	2.4309	0.0411	1.7

SI Tables 16-21. Calculated O-O distances for each pentamer and one table showing the average O-O distance trending upward with the addition of water. Distances are in units of Angstroms.

0W:5M	**uduud**
Average	**2.713**
	2.707
	2.710
	2.728
	2.710
	2.708

1W:4M	**wduud**	**wuduu**	**wdudu**	**wudud**	**wuudu**
Average	**2.715**	**2.714**	**2.714**	**2.715**	**2.715**
	2.697	2.698	2.699	2.716	2.701
	2.709	2.706	2.707	2.709	2.726
	2.725	2.711	2.708	2.709	2.710
	2.715	2.726	2.712	2.709	2.711
	2.728	2.731	2.742	2.730	2.729

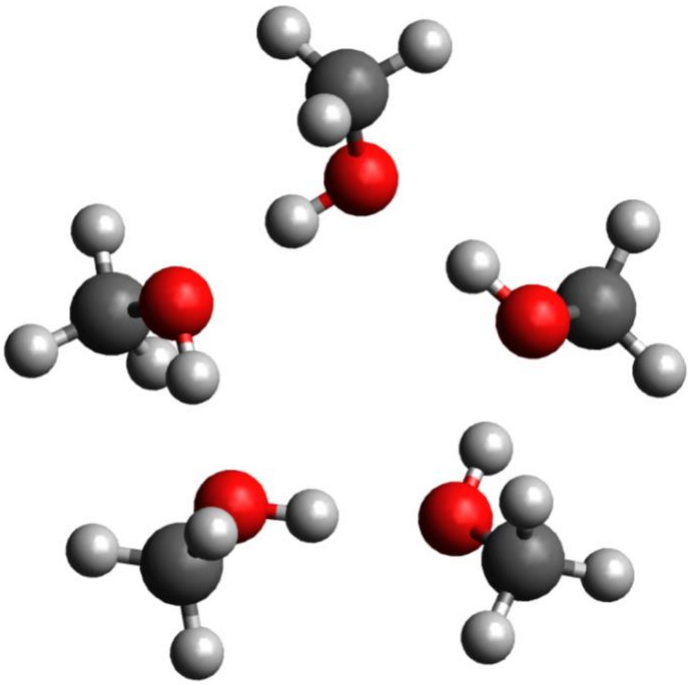
2W:3M	**wwdud**	**wuwud**	**wwduu**	**wwudu**	**wuwdu**	**wuwuu**	**wwuud**
Average	**2.717**	**2.717**	**2.717**	**2.716**	**2.716**	**2.717**	**2.718**
	2.736	2.717	2.719	2.720	2.702	2.701	2.719
	2.698	2.729	2.696	2.697	2.741	2.727	2.699
	2.707	2.699	2.710	2.707	2.699	2.701	2.728
	2.710	2.708	2.727	2.713	2.709	2.726	2.713
	2.732	2.731	2.735	2.745	2.729	2.732	2.731

3W:2M	wwdwd	wwwud	wwwdu	wwuwd	wwwdd	wwuwu	wwdwu
Average	**2.719**	**2.720**	**2.719**	**2.719**	**2.720**	**2.720**	**2.720**
	2.721	2.723	2.724	2.720	2.722	2.722	2.720
	2.699	2.734	2.717	2.701	2.717	2.716	2.698
	2.728	2.699	2.696	2.742	2.699	2.730	2.730
	2.703	2.710	2.712	2.702	2.726	2.701	2.717
	2.744	2.732	2.746	2.730	2.736	2.729	2.733

4W:1M	wwwwu	wwwwd
Average	**2.723**	**2.722**
	2.723	2.725
	2.720	2.721
	2.720	2.718
	2.717	2.702
	2.734	2.745

Water per Cluster	Average O-O distance
0	2.713
1	2.715
2	2.717
3	2.719
4	2.723

Section 3: Images of Geometry Optimized Conformers



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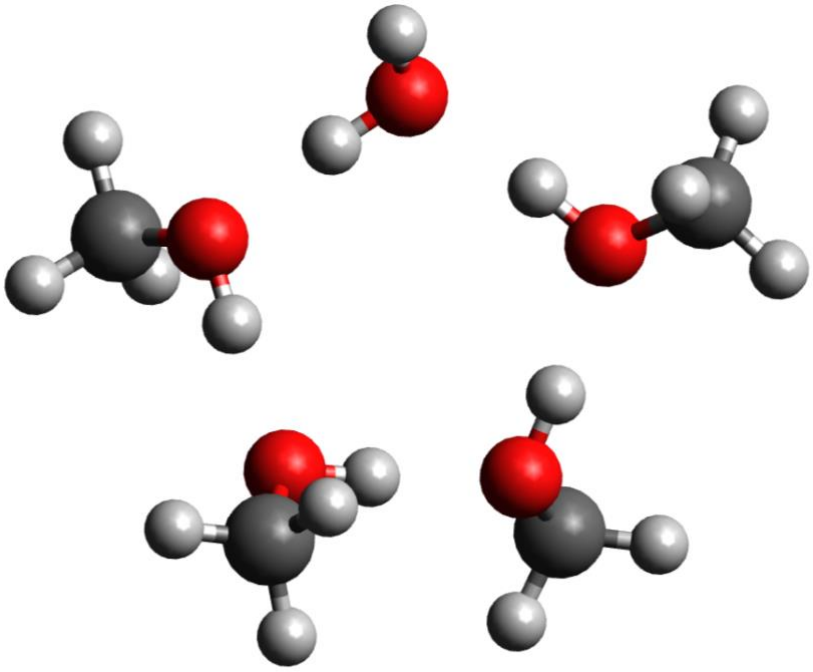
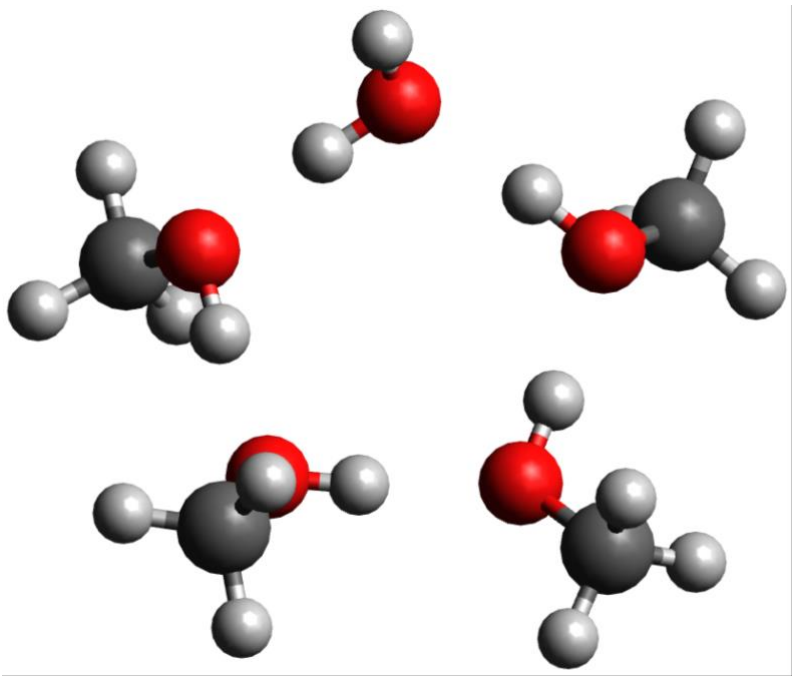
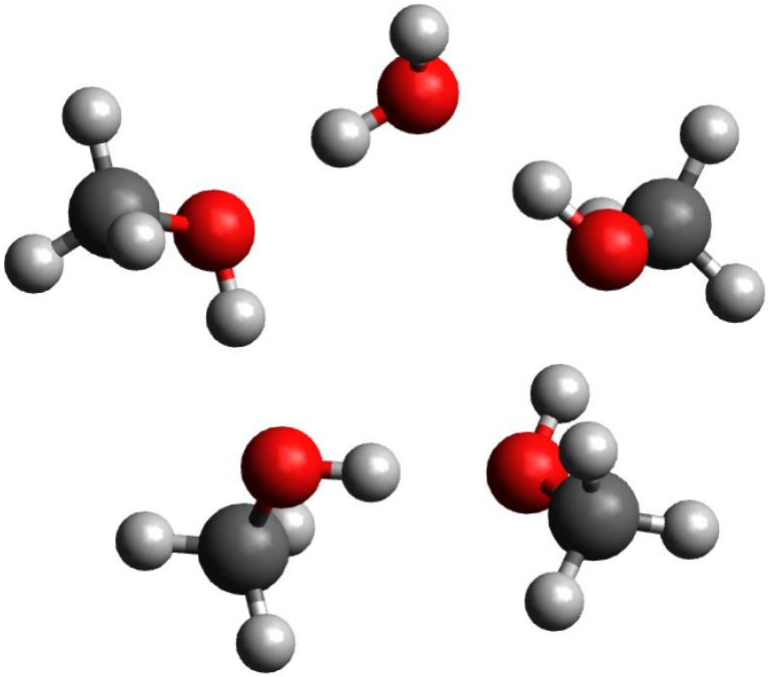


wdudu



wduud



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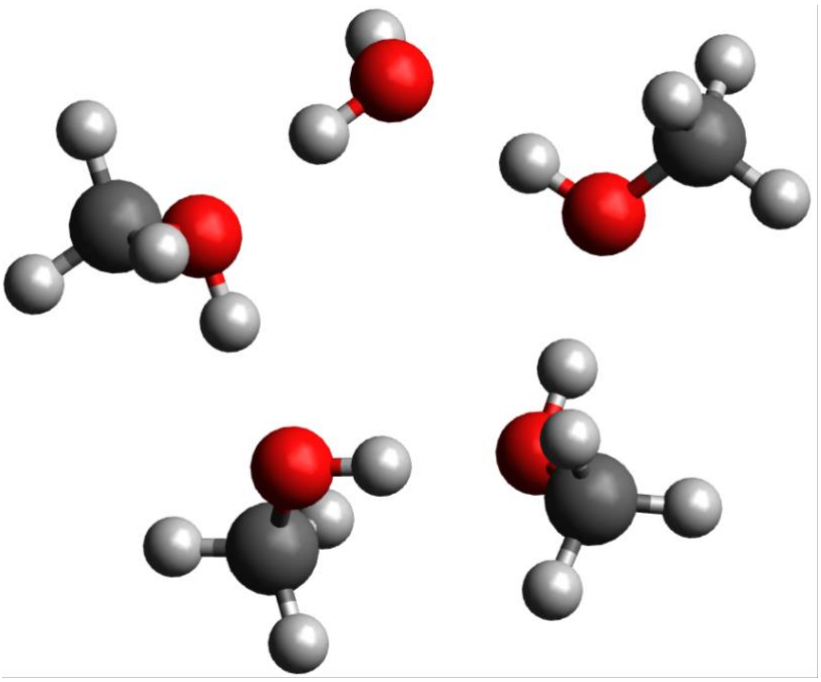

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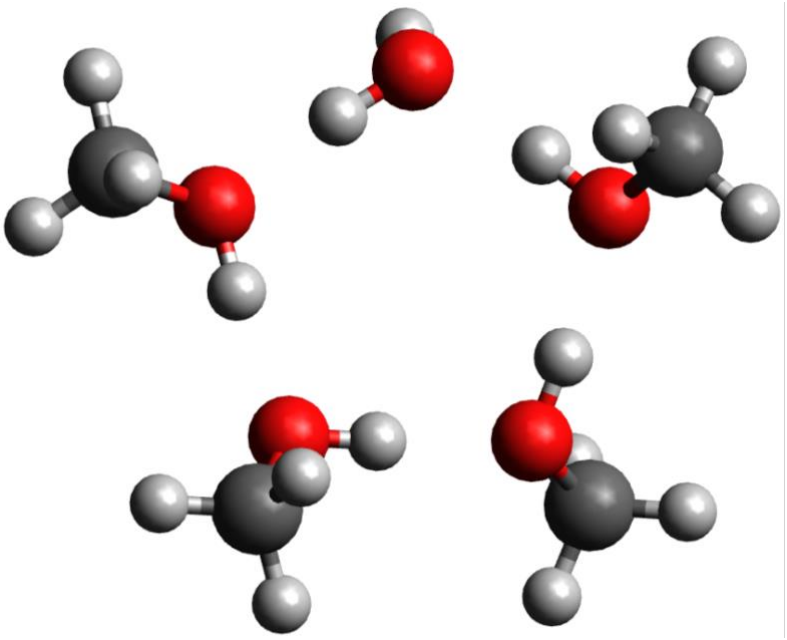

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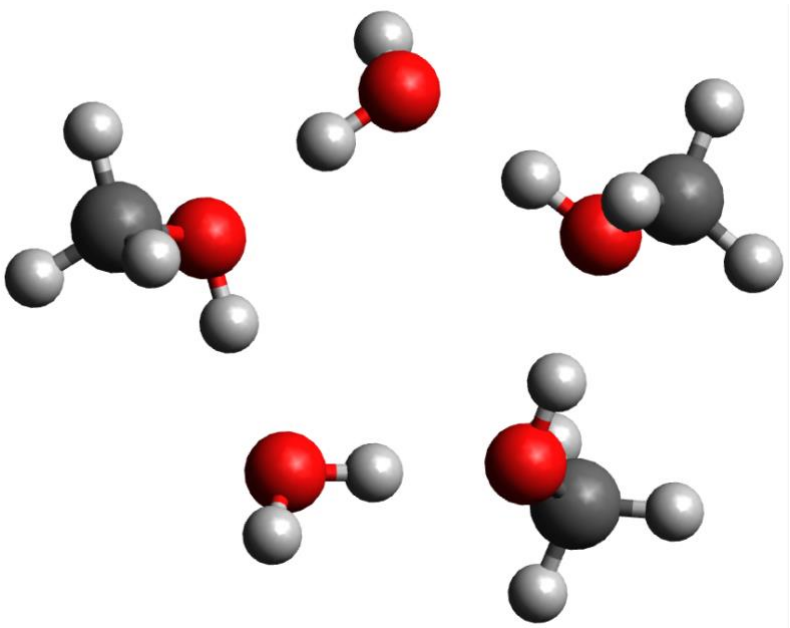

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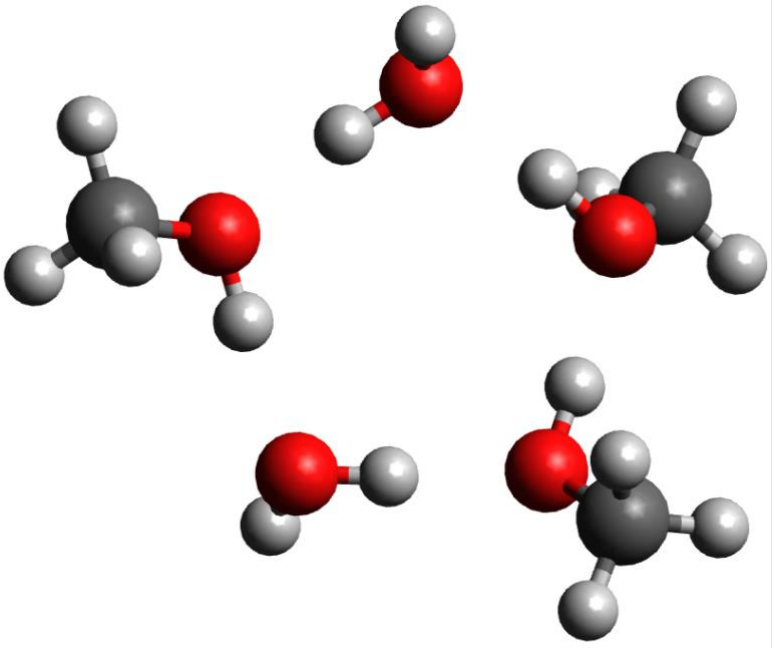

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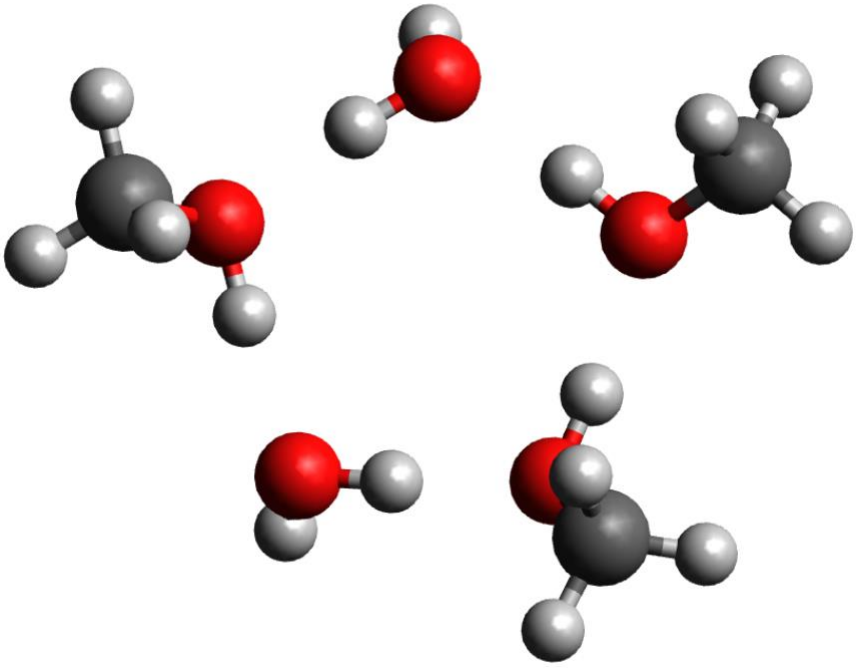

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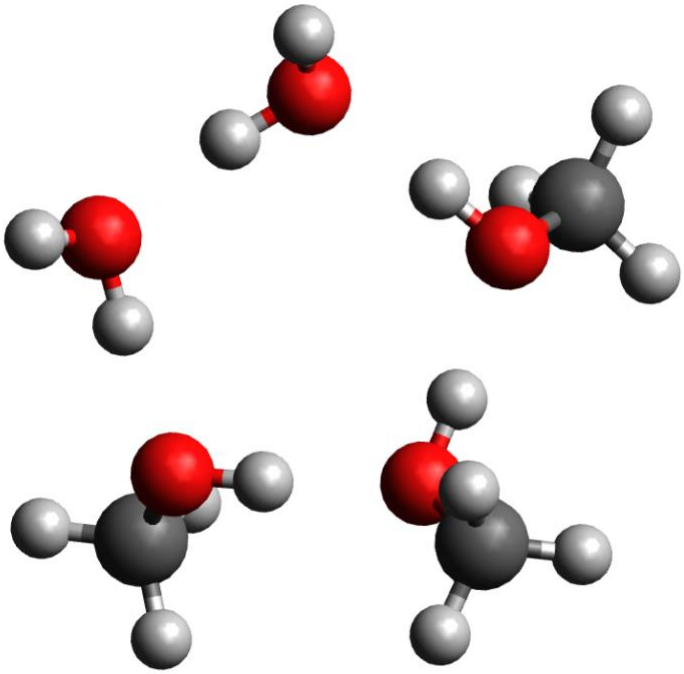
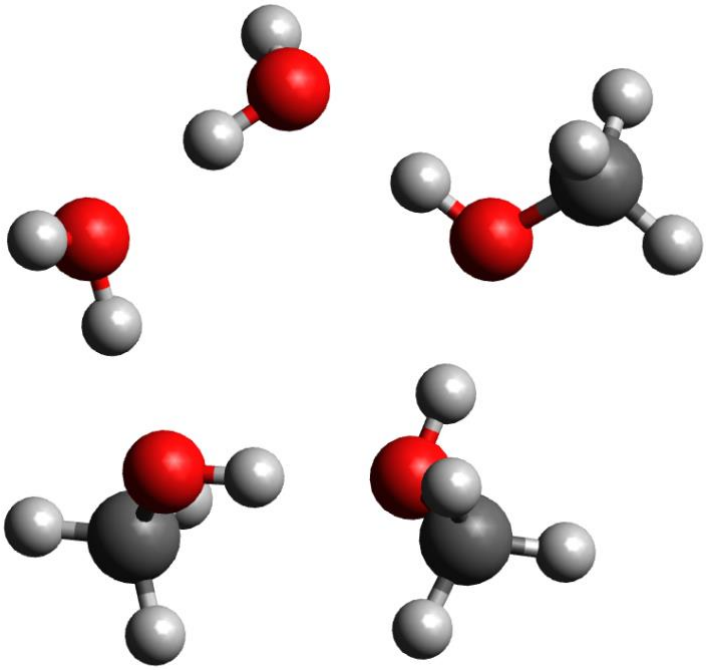


wwdud



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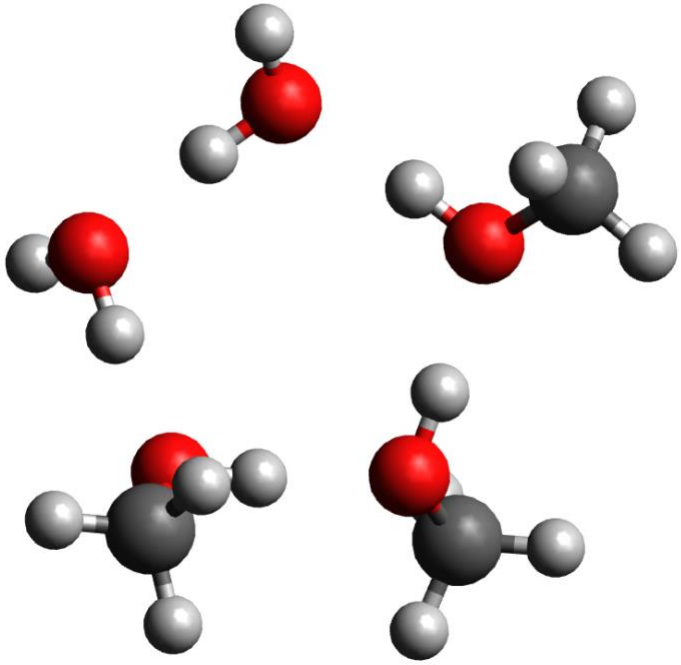

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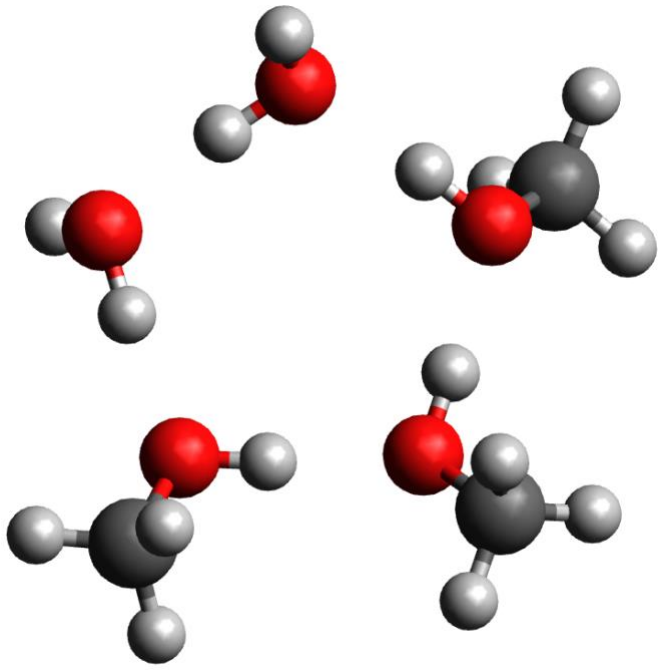

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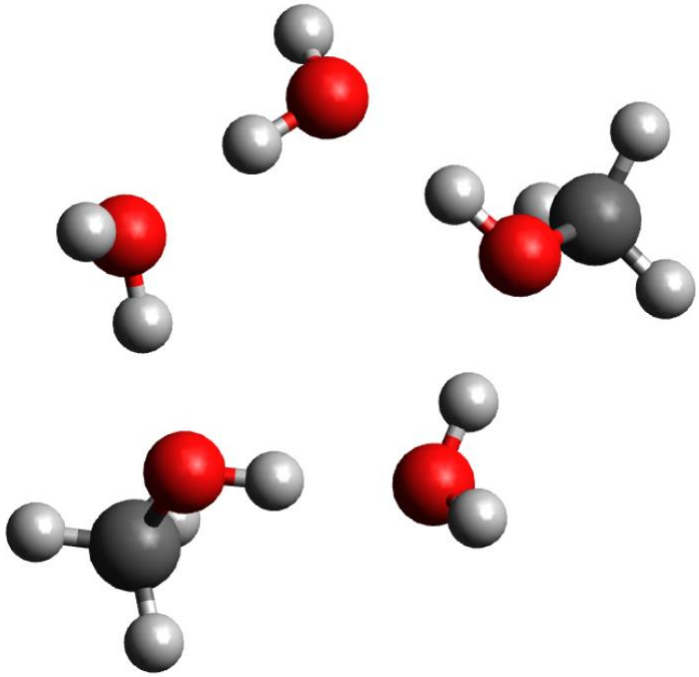

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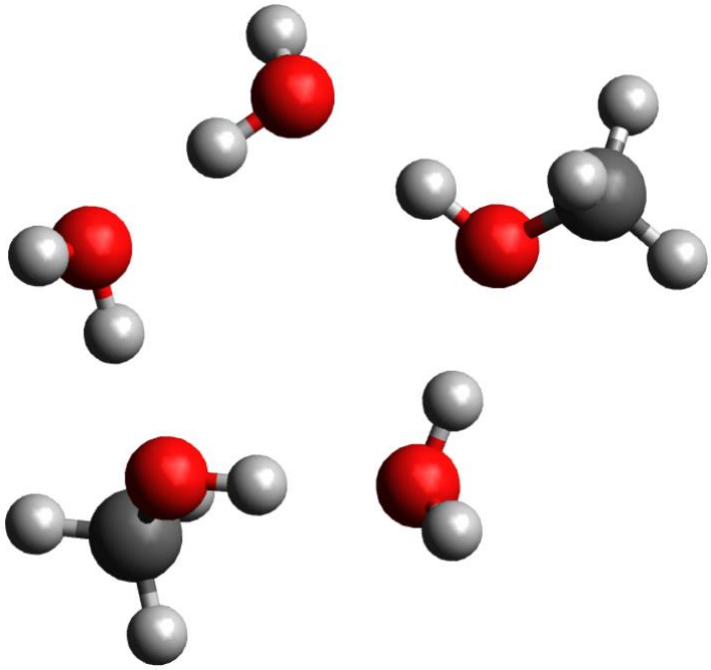

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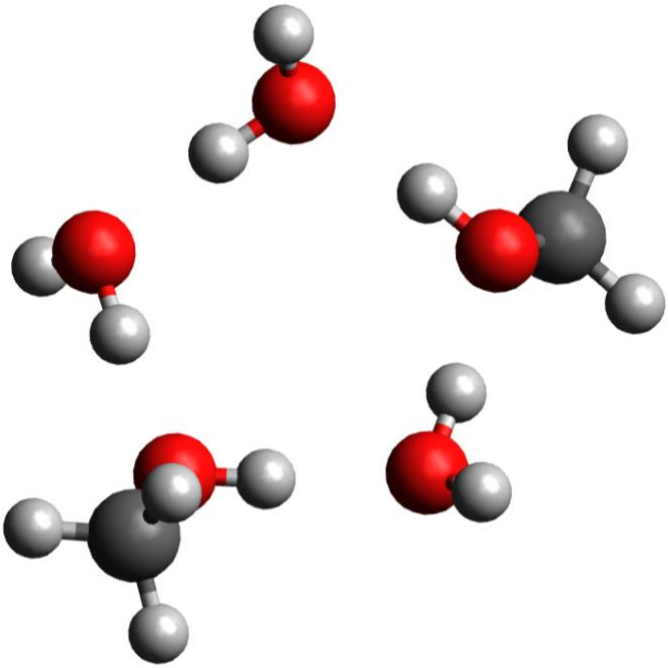

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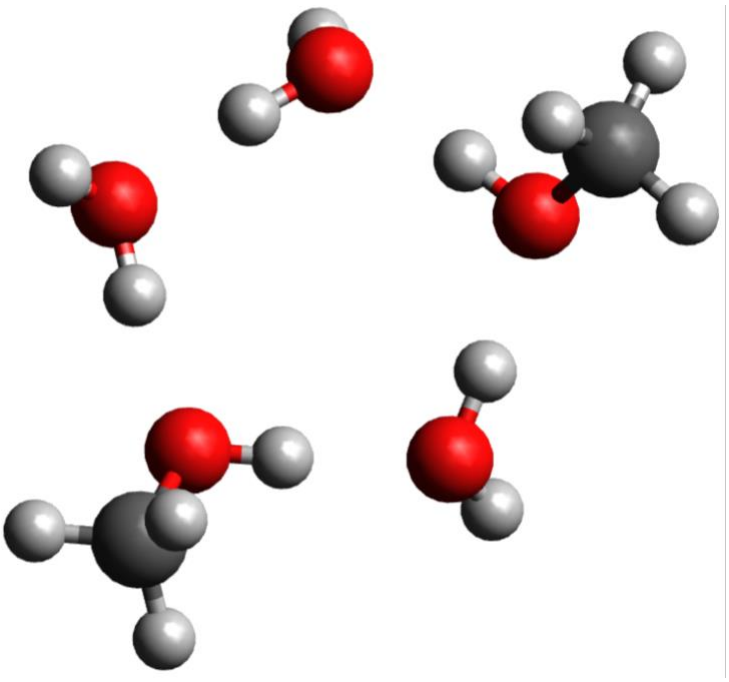

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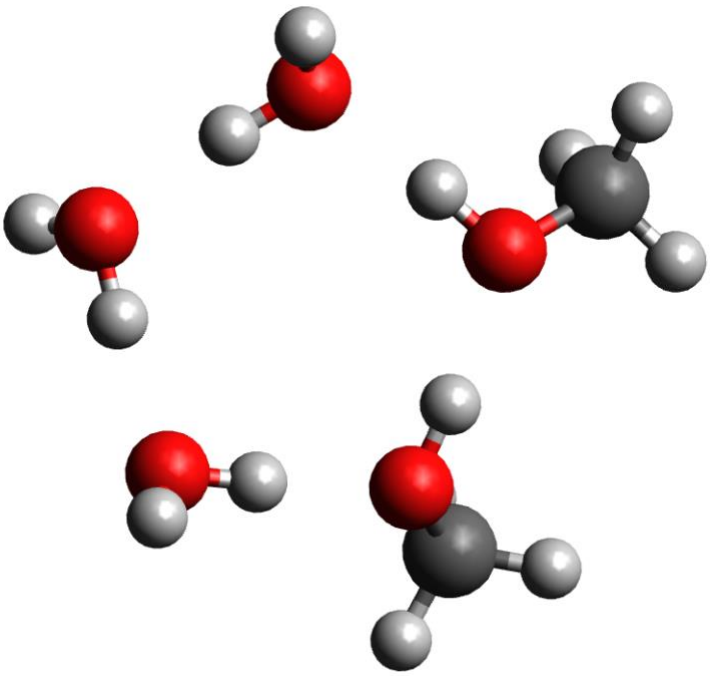

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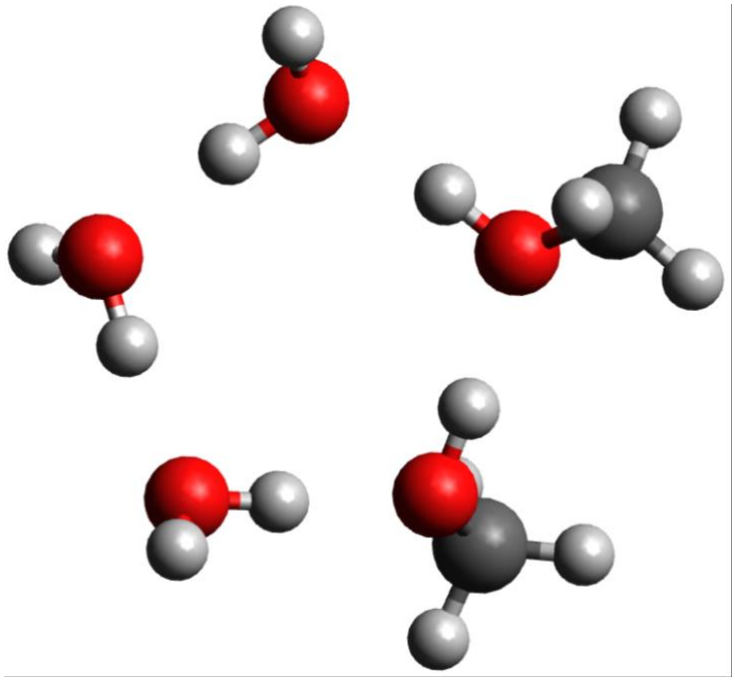

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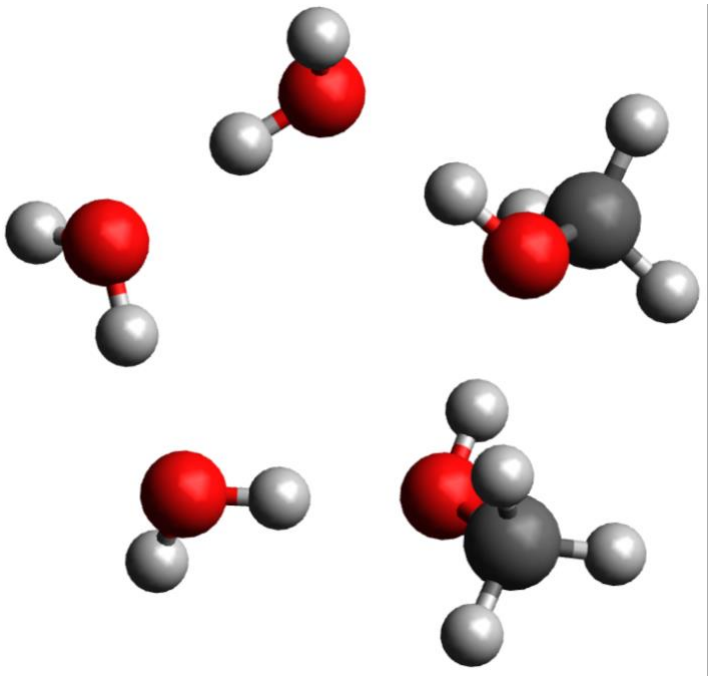

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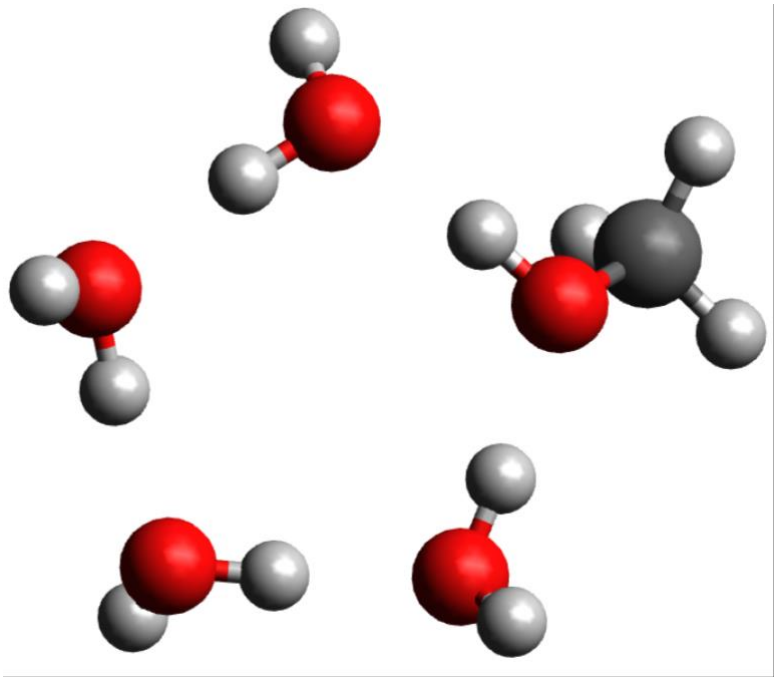

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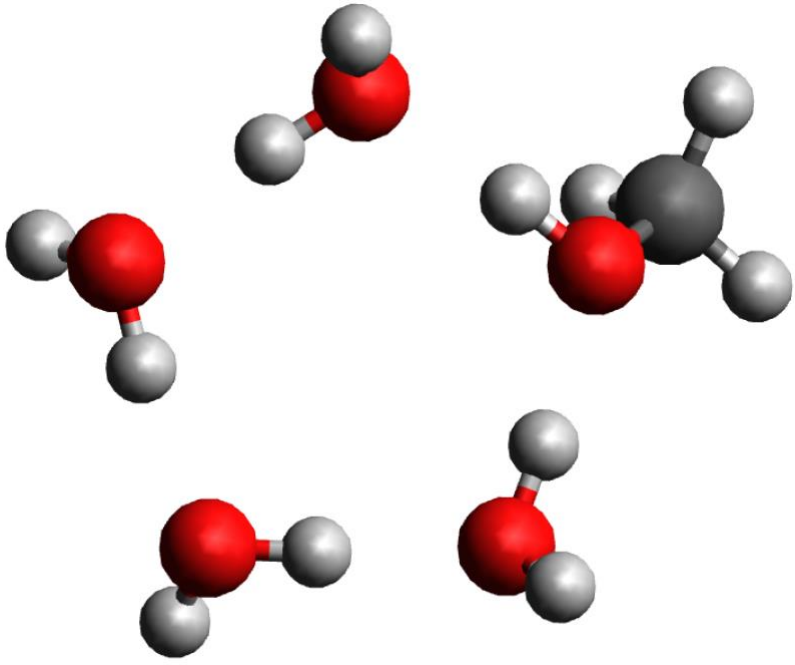

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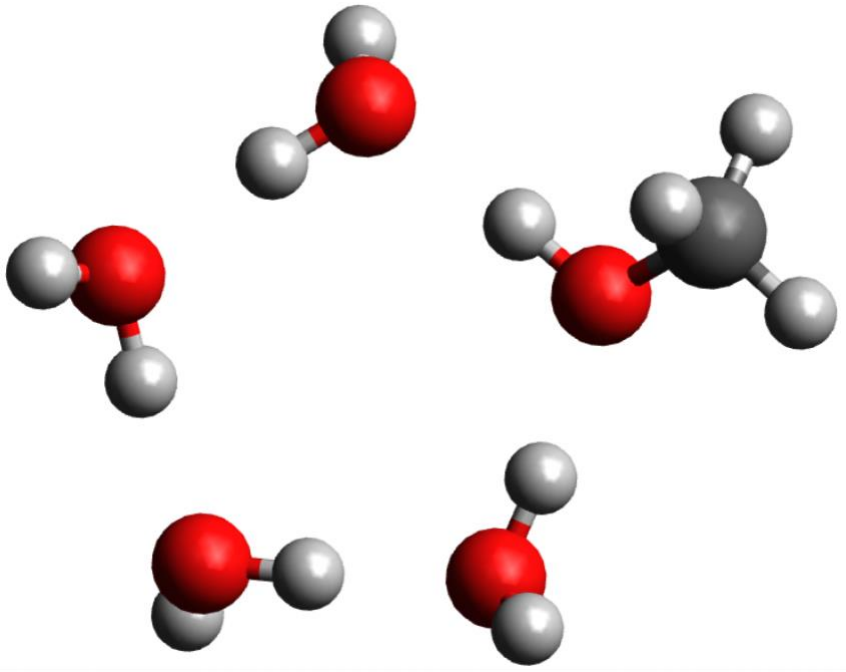


wwwwu

Section 4: Final SPFIT Results

SPFIT output is included for every fitted pentamer conformer. The first 23 fits are normal isotopologues, the next 22 fits are for perdeuterated methanol and normal water clusters, the following 20 fits are perdeuterated water and normal methanol clusters, and the final 18 fits are normal methanol and normal water with a single HDO substitution. HDO1 implies the first water in the naming scheme is replaced with HDO. Likewise, HDO2 conveys the second water in each conformer is replaced with HDO.

uduud SPFIT Output

```
                    EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  10  6  4  9  5  4          13403.18000   13403.05728    0.12272    0.10000   0.09405   13403.12372    0.05628 0.5000
  2:  10  7  4  9  6  4          13403.18000   13403.19016   -0.01016    0.10000   0.09405   13403.12372    0.05628 0.5000
  3:  12  5  7 11  5  6          12580.57000   12580.55470    0.01530    0.10000   0.08154   12580.55466    0.01534 0.5000
  4:  12  6  7 11  6  6          12580.57000   12580.55462    0.01538    0.10000   0.08154   12580.55466    0.01534 0.5000
  5:  12  9  3 11  9  2          14836.27000   14836.35317   -0.08317    0.10000   0.08451
  6:  12 12  1 11 11  1          16164.42000   16164.40859    0.01141    0.10000   0.05571
  7:  13  9  4 12  8  4          17419.53000   17419.65378   -0.12378    0.10000   0.07552
  8:  13 13  1 12 12  1          17513.34000   17513.25312    0.08688    0.10000   0.07255
  9:  14  3 11 13  3 10          13104.22000   13104.23727   -0.01727    0.10000   0.07190   13104.23727   -0.01727 0.5000
 10:  14  4 11 13  4 10          13104.22000   13104.23727   -0.01727    0.10000   0.07190   13104.23727   -0.01727 0.5000
 11:  14 10  5 13 10  4          16344.68000   16344.62286    0.05714    0.10000   0.09066
 12:  19  0 19 18  0 18          15492.08000   15492.07813    0.00187    0.10000   0.09952   15492.07813    0.00187 0.4000
 13:  19  0 19 18  1 18          15492.08000   15492.07813    0.00187    0.10000   0.09952   15492.07813    0.00187 0.2000
 14:  19  1 19 18  0 18          15492.08000   15492.07813    0.00187    0.10000   0.09952   15492.07813    0.00187 0.2000
 15:  19  1 19 18  1 18          15492.08000   15492.07813    0.00187    0.10000   0.09952   15492.07813    0.00187 0.2000
NORMALIZED DIAGONAL:
  1  1.00000E+000    2  8.86697E-001    3  4.07596E-001    4  9.74177E-002    5  9.99359E-001    6  1.31981E-002
  7  1.00000E+000    8  1.00000E+000
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                    NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1       10000         A        675.5123(108)          0.0000
  2       20000         B        665.2199(106)         -0.0000
  3       30000         C         400.325( 40)          -0.000
  4         200    -DeltaJ          -0.282( 34)E-03       -0.000E-03
  5        2000    -DeltaK          -1.538(209)E-03       -0.000E-03
  6        1100   -DeltaJK           2.141(274)E-03        0.000E-03
  7       40100    -deltaJ     0.022800000(  0)E-03 -0.000000000E-03
  8       41000    -deltaK    -0.487000000(  0)E-03  0.000000000E-03
 MICROWAVE AVG =        0.000524 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.064020 MHz, IR RMS =        0.00000
```

wduud SPFIT Output

```
                    EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  7  7  0  6  6  1          12238.79000   12238.79217   -0.00217    0.10000   0.09896
  2:  8  4  5  7  3  5          12749.02000   12748.95153    0.06847    0.10000   0.07467
  3:  9  3  6  8  4  5          10480.21000   10480.32679   -0.11679    0.10000   0.06424
  4: 10  6  5  9  7  2          13712.52000   13712.51300    0.00700    0.10000   0.09874
  5: 12  0 12 11  1 11          11000.91000   11000.85716    0.05284    0.10000   0.06420   11000.85716    0.05284 0.5000
  6: 12  1 12 11  0 11          11000.91000   11000.85716    0.05284    0.10000   0.06420   11000.85716    0.05284 0.5000
  7: 16  2 14 15  2 13          15988.04000   15988.05159   -0.01159    0.10000   0.09768   15988.05159   -0.01159 0.2500
  8: 16  2 14 15  3 13          15988.04000   15988.05158   -0.01158    0.10000   0.09768   15988.05159   -0.01159 0.2500
  9: 16  3 14 15  2 13          15988.04000   15988.05159   -0.01159    0.10000   0.09768   15988.05159   -0.01159 0.2500
 10: 16  3 14 15  3 13          15988.04000   15988.05158   -0.01158    0.10000   0.09768   15988.05159   -0.01159 0.2500
 11: 22  5 17 22  4 18          12445.56000   12445.62889   -0.06889    0.10000   0.06525
 12: 22  6 16 22  5 17          11675.03000   11675.05955   -0.02955    0.10000   0.05488   11675.05962   -0.02962 0.5000
 13: 22  7 16 22  6 17          11675.03000   11675.05969   -0.02969    0.10000   0.05488   11675.05962   -0.02962 0.5000
 14: 23  8 15 23  7 16          10825.16000   10825.01515    0.14485    0.10000   0.06218   10825.02411    0.13589 0.5000
 15: 23  9 15 23  8 16          10825.16000   10825.03307    0.12693    0.10000   0.06218   10825.02411    0.13589 0.5000
 16: 26  8 18 26  7 19          13017.39000   13017.47695   -0.08695    0.10000   0.08022   13017.47701   -0.08701 0.5000
 17: 26  9 18 26  8 19          13017.39000   13017.47708   -0.08708    0.10000   0.08022   13017.47701   -0.08701 0.5000
 18: 28  5 23 28  4 24          16778.15000   16778.10535    0.04465    0.10000   0.09758   16778.10535    0.04465 0.5000
 19: 28  6 23 28  5 24          16778.15000   16778.10535    0.04465    0.10000   0.09758   16778.10535    0.04465 0.5000
NORMALIZED DIAGONAL:
  1 1.00000E+000   2 6.12524E-001   3 1.66391E-001   4 9.53605E-001   5 2.58456E-001   6 6.86698E-003
  7 9.60321E-001   8 9.84001E-001
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                    NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1       10000        A       893.4325( 75)        -0.0000
  2       20000        B       731.0180( 93)         0.0000
  3       30000        C       443.4066( 64)        -0.0000
  4         200   -DeltaJ        -0.749( 43)E-03      -0.000E-03
  5        2000   -DeltaK        -1.735(207)E-03      -0.000E-03
  6        1100   -DeltaJK        2.345(247)E-03       0.000E-03
  7       40100    -deltaJ       -0.01199(100)E-03    -0.00000E-03
  8       41000    -deltaK        -1.14( 38)E-03       -0.00E-03
 MICROWAVE AVG =      -0.000657 MHz, IR AVG =       0.00000
 MICROWAVE RMS =       0.070687 MHz, IR RMS =       0.00000
```

wuduu SPFIT Output

```
                        EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  7  7  1  6  6  1              12525.84000   12525.86925   -0.02925    0.10000   0.06636
  2:  8  3  5  7  2  5              12113.02000   12113.12046   -0.10046    0.10000   0.06016
  3:  9  7  3  8  6  3              14900.03000   14900.01850    0.01150    0.10000   0.05521
  4: 10  6  5  9  7  3              16730.21000   16730.15298    0.05702    0.10000   0.07380
  5: 10 10  0  9  8  1              12462.51000   12462.42598    0.08402    0.10000   0.08250
  6: 12 12  0 11 10  1              15365.97000   15365.98099   -0.01099    0.10000   0.08715
  7: 15  3 12 14  3 11              16044.26000   16044.43046   -0.17046    0.10000   0.09551   16044.29489   -0.03489 0.5000
  8: 15  4 12 14  4 11              16044.26000   16044.15932    0.10068    0.10000   0.09551   16044.29489   -0.03489 0.5000
  9: 18  0 18 17  0 17              16834.46000   16834.45159    0.00841    0.10000   0.09975   16834.45159    0.00841 0.5000
 10: 18  1 18 17  1 17              16834.46000   16834.45159    0.00841    0.10000   0.09975   16834.45159    0.00841 0.5000
NORMALIZED DIAGONAL:
  1 1.00000E+000   2 9.99152E-001   3 3.09776E-001   4 5.22737E-002   5 9.96906E-001   6 1.00000E+000
  7 1.00000E+000   8 1.00000E+000
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                        NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1       10000        A       917.9111( 94)        -0.0000
  2       20000        B       688.9699(135)        -0.0000
  3       30000        C        458.761( 32)        -0.000
  4         200   -DeltaJ         -0.439( 67)E-03       0.000E-03
  5        2000   -DeltaK         -0.3058(252)E-03     -0.0000E-03
  6        1100   -DeltaJK     0.483000000(  0)E-03 -0.000000000E-03
  7       40100    -deltaJ    -0.022000000(  0)E-03  0.000000000E-03
  8       41000    -deltaK    -0.156000000(  0)E-03  0.000000000E-03
 MICROWAVE AVG =      -0.001831 MHz, IR AVG =       0.00000
 MICROWAVE RMS =       0.053385 MHz, IR RMS =       0.00000
```

wdudu SPFIT Output

```
                        EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  6  6  1  5  5  1              10585.02000   10585.02975   -0.00975    0.10000   0.09978
  2:  7  2  6  6  1  6              10818.09000   10818.01240    0.07760    0.10000   0.07868
  3:  8  5  4  7  4  4              12499.04000   12499.12926   -0.08926    0.10000   0.06626
  4:  8  7  1  7  6  1              12131.26000   12131.20121    0.05879    0.10000   0.07664
  5: 11  3  8 10  2  8               16862.49000   16862.51409   -0.02409    0.10000   0.08967
  6: 12 12  0 11 10  1               15330.50000   15330.50041   -0.00041    0.10000   0.06565
  7: 13  0 13 12  0 12               12556.47000   12556.45375    0.01625    0.10000   0.09916   12556.45373    0.01627 0.5000
  8: 13  1 13 12  1 12               12556.47000   12556.45371    0.01629    0.10000   0.09916   12556.45373    0.01627 0.5000
  9: 13  3 10 12  3  9               14407.77000   14407.84538   -0.07538    0.10000   0.07954
 10: 13 13  0 12 11  1               16460.40000   16460.39270    0.00730    0.10000   0.08348
 11: 14  5  9 13  5  8               16746.88000   16746.82983    0.05017    0.10000   0.09006
NORMALIZED DIAGONAL:
  1 1.00000E+000   2 9.93726E-001   3 1.84773E-001   4 1.15477E-001   5 9.85304E-001   6 4.55094E-002
  7 1.00000E+000   8 7.28180E-001
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                    NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1       10000        A       908.1121( 99)         0.0000
  2       20000        B       684.6154(120)        -0.0000
  3       30000        C       471.3651(223)        -0.0000
  4         200   -DeltaJ        -0.352( 49)E-03       0.000E-03
  5        2000   -DeltaK        -1.855(181)E-03       0.000E-03
  6        1100  -DeltaJK         1.642(196)E-03      -0.000E-03
  7       40100   -deltaJ    -0.027900000(  0)E-03 -0.000000000E-03
  8       41000   -deltaK        -1.109(275)E-03       0.000E-03
 MICROWAVE AVG =       0.001125 MHz, IR AVG =       0.00000
 MICROWAVE RMS =       0.051611 MHz, IR RMS =       0.00000
```

wudud SPFIT Output

```
                        EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  7  2  6  6  1  6            10818.09000   10818.20423   -0.11423    0.10000   0.07401
  2:  8  3  6  7  2  6            12301.67000   12301.54523    0.12477    0.10000   0.06786
  3:  9  7  2  8  8  0            16142.68000   16142.67572    0.00428    0.10000   0.07070
  4:  9  8  1  8  6  2            11359.56000   11359.55860    0.00140    0.10000   0.09999
  5:  9  9  1  8  8  1            16142.68000   16142.68765   -0.00765    0.10000   0.07070
  6: 11 11  0 10 10  0               16132.68000   16132.69504   -0.01504    0.10000   0.09961
  7: 13  0 13 12  0 12               12438.22000   12438.21933    0.00067    0.10000   0.10000   12438.21931    0.00069 0.5000
  8: 13  1 13 12  1 12               12438.22000   12438.21928    0.00072    0.10000   0.10000   12438.21931    0.00069 0.5000
  9: 14  3 11 13  3 10               15247.08000   15247.08173   -0.00173    0.10000   0.09999
NORMALIZED DIAGONAL:
  1 1.00000E+000   2 9.64929E-001   3 1.74687E-001   4 2.85167E-001   5 9.98101E-001   6 9.22865E-002
  7 1.00000E+000   8 1.00000E+000
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                     NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1       10000        A       914.8522( 67)        -0.0000
  2       20000        B       681.3245( 74)         0.0000
  3       30000        C       466.6182(203)         0.0000
  4         200    -DeltaJ        -0.428( 38)E-03      -0.000E-03
  5        2000    -DeltaK        -0.905( 68)E-03      -0.000E-03
  6        1100   -DeltaJK         0.820(100)E-03       0.000E-03
  7       40100    -deltaJ    -0.032300000(  0)E-03 -0.000000000E-03
  8       41000    -deltaK    -0.390000000(  0)E-03 -0.000000000E-03
 MICROWAVE AVG =      -0.000940 MHz, IR AVG =       0.00000
 MICROWAVE RMS =       0.060129 MHz, IR RMS =       0.00000
```

wuudu SPFIT Output

```
                        EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  7  7  0  6  6  0              12421.73000   12421.76426   -0.03426    0.10000   0.07019
  2:  8  1  7  7  0  7              12580.57000   12580.41534    0.15466    0.10000   0.08455
  3:  8  4  5  7  3  5              12486.20000   12486.36409   -0.16409    0.10000   0.05799
  4: 10  4  6  9  4  5              12379.56000   12379.57745   -0.01745    0.10000   0.07593
  5: 10  5  5  9  8  1              15896.65000   15896.70653   -0.05653    0.10000   0.07077
  6: 11  1 10 10  1  9              11015.57000   11015.43059    0.13941    0.10000   0.08704   11015.41755    0.15245 0.5000
  7: 11  2 10 10  2  9              11015.57000   11015.40452    0.16548    0.10000   0.08704   11015.41755    0.15245 0.5000
  8: 11  3  9 10  3  8              11686.92000   11687.07232   -0.15232    0.10000   0.05125
  9: 11  4  7 10  4  6              13188.17000   13187.99004    0.17996    0.10000   0.06502
 10: 11 10  1 10  9  1              16428.60000   16428.47814    0.12186    0.10000   0.07427
 11: 11 10  1 10 10  0              14258.78000   14258.83936   -0.05936    0.10000   0.08309
 12: 12  4  9 11  4  8              13272.75000   13272.88444   -0.13444    0.10000   0.08327
NORMALIZED DIAGONAL:
  1 1.00000E+000   2 9.30469E-001   3 2.84088E-001   4 1.42493E-001   5 9.74021E-001   6 1.12697E-001
  7 1.00000E+000   8 1.00000E+000
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                        NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1       10000        A       909.3415( 75)        -0.0000
  2       20000        B       700.4932(110)         0.0000
  3       30000        C       455.0353(215)         0.0000
  4         200    -DeltaJ        -0.202( 46)E-03      -0.000E-03
  5        2000    -DeltaK        -0.464(110)E-03       0.000E-03
  6        1100   -DeltaJK         1.040(118)E-03      -0.000E-03
  7       40100    -deltaJ    -0.019800000(  0)E-03 -0.000000000E-03
  8       41000    -deltaK     0.019500000(  0)E-03 -0.000000000E-03
 MICROWAVE AVG =      -0.000867 MHz, IR AVG =       0.00000
 MICROWAVE RMS =       0.124608 MHz, IR RMS =       0.00000
```

wuwdu SPFIT Output

```
                        EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  5  4  2  4  3  2            10502.95000   10503.13545   -0.18545    0.10000   0.05350
  2:  6  3  4  5  2  4            11228.24000   11228.17066    0.06934    0.10000   0.04818
  3:  6  4  2  5  3  2            11629.69000   11629.59694    0.09306    0.10000   0.07912
  4:  9  1  8  8  0  8            16621.88000   16621.88215   -0.00215    0.10000   0.09310
  5: 12  8  4 12  7  6             10480.21000   10480.07709    0.13291    0.10000   0.06777
  6: 13  7  6 13  8  6             11603.10000   11603.22191   -0.12191    0.10000   0.06804
  7: 15  9  7 15  6  9             11456.09000   11456.05519    0.03481    0.10000   0.05511
  8: 17  8 10 17  7 10              12499.04000   12499.07264   -0.03264    0.10000   0.08776
  9: 18  7 11 17  4 13              16634.19000   16634.18956    0.00044    0.10000   0.10000
 10: 19  6 14 18 13  6              17003.09000   17003.09188   -0.00188    0.10000   0.09997
 11: 19 12  7 19 11  9              17155.33000   17155.31962    0.01038    0.10000   0.09966   17155.31961    0.01039 0.5000
 12: 19 12  8 19  9 10              17155.33000   17155.31960    0.01040    0.10000   0.09966   17155.31961    0.01039 0.5000
NORMALIZED DIAGONAL:
  1 1.00000E+000   2 6.90079E-001   3 2.74417E-001   4 9.98190E-001   5 1.00000E+000   6 7.62985E-002
  7 2.37008E-001   8 1.90028E-001
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                     NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1       10000        A       1214.9160( 69)         0.0000
  2       20000        B        764.9376( 53)        -0.0000
  3       30000        C        521.8436(163)         0.0000
  4         200    -DeltaJ        -0.4775(178)E-03      0.0000E-03
  5        2000    -DeltaK     -0.139000000(  0)E-03 -0.000000000E-03
  6        1100   -DeltaJK          0.817( 47)E-03      -0.000E-03
  7       40100    -deltaJ         -0.0769( 64)E-03      0.0000E-03
  8       41000    -deltaK          -0.438( 37)E-03       0.000E-03
 MICROWAVE AVG =       -0.000280 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.086749 MHz, IR RMS =        0.00000
```

wuwuu SPFIT Output

		EXP.FREQ.	- CALC.FREQ.	- DIFF.	- EXP.ERR.	- EST.ERR.	-AVG. CALC.FREQ.	- DIFF.	- WT.
1:	6 3 3 5 4 1	12794.97000	12794.92116	0.04884	0.10000	0.07813			
2:	6 3 4 5 2 4	11300.96000	11301.02084	-0.06084	0.10000	0.08437			
3:	7 1 6 6 0 6	13021.47000	13021.44829	0.02171	0.10000	0.09906			
4:	7 7 1 6 6 1	16288.97000	16288.98790	-0.01790	0.10000	0.09645			
5:	8 4 5 7 4 4	10749.06000	10748.97527	0.08473	0.10000	0.08839			
6:	8 8 0 7 6 1	11368.94000	11368.90208	0.03792	0.10000	0.09685			
7:	9 7 3 8 5 4	12212.46000	12212.64305	-0.18305	0.10000	0.05635			
8:	10 8 3 9 6 4	13586.82000	13586.75060	0.06940	0.10000	0.09423			
9:	12 2 10 11 2 9	14599.05000	14598.96601	0.08399	0.10000	0.07095			
10:	12 3 10 11 3 9	14588.44000	14588.52253	-0.08253	0.10000	0.07083			

NORMALIZED DIAGONAL:

1 1.00000E+000 2 9.11291E-001 3 3.82572E-001 4 8.93125E-002 5 1.11084E-001 6 2.90607E-002
7 1.78251E-001 8 9.97313E-001

MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00

			NEW PARAMETER (EST. ERROR)	-- CHANGE THIS ITERATION
1	10000	A	1201.8005(199)	0.0000
2	20000	B	781.4729(215)	-0.0000
3	30000	C	519.6128(227)	0.0000
4	200	-DeltaJ	-0.454(130)E-03	0.000E-03
5	2000	-DeltaK	3.86(46)E-03	0.00E-03
6	1100	-DeltaJK	-2.93(51)E-03	-0.00E-03
7	40100	-deltaJ	-0.079(91)E-03	0.000E-03
8	41000	-deltaK	-0.66(51)E-03	0.00E-03

MICROWAVE AVG = 0.000228 MHz, IR AVG = 0.00000
MICROWAVE RMS = 0.082271 MHz, IR RMS = 0.00000

wwdud SPFIT Output

```
                        EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  6  2  4  5  1  4              11205.43000   11205.54643   -0.11643    0.10000   0.05936
  2:  6  4  3  5  3  3              11520.72000   11520.60723    0.11277    0.10000   0.05814
  3:  7  2  6  6  1  6              13286.13000   13286.11138    0.01862    0.10000   0.09802
  4:  7  3  4  6  2  4              12883.95000   12883.91421    0.03579    0.10000   0.08476
  5:  7  5  2  6  4  2              13272.75000   13272.80765   -0.05765    0.10000   0.08900
  6:  8  6  2  7  5  2              10554.43000   10554.42103    0.00897    0.10000   0.09953
  7: 10  9  1  9  8  1               13403.18000   13403.18274   -0.00274    0.10000   0.09856
  8: 15  0 15 14  0 14                 17597.44000   17597.43999    0.00001    0.10000   0.10000
  9: 19 12  7 19 13  7                 10058.26000   10058.25902    0.00098    0.10000   0.09619
 10: 20 13  7 20 12  9                  10737.50000   10737.51601   -0.01601    0.10000   0.09751   10737.50056   -0.00056 0.5000
 11: 20 13  8 20 12  8                  10737.50000   10737.48512    0.01488    0.10000   0.09751   10737.50056   -0.00056 0.5000
NORMALIZED DIAGONAL:
  1 1.00000E+000   2 5.19641E-001   3 9.94831E-002   4 9.99211E-001   5 1.96533E-002   6 9.89339E-002
  7 1.46993E-001   8 7.87303E-001
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                     NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1       10000        A       1079.4438(212)        -0.0000
  2       20000        B        856.7747(116)         0.0000
  3       30000        C        573.1190(316)        -0.0000
  4         200    -DeltaJ         -0.359(112)E-03       0.000E-03
  5        2000    -DeltaK          -3.31( 41)E-03       -0.00E-03
  6        1100   -DeltaJK           5.56( 37)E-03        0.00E-03
  7       40100    -deltaJ        -0.3157(261)E-03     -0.0000E-03
  8       41000    -deltaK          -3.37( 38)E-03       -0.00E-03
 MICROWAVE AVG =      -0.000023 MHz, IR AVG =       0.00000
 MICROWAVE RMS =       0.055957 MHz, IR RMS =       0.00000
```

wwuud SPFIT Output

```
                    EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  6  2  4  5  1  4          11294.94000   11295.04441   -0.10441    0.10000   0.05330
  2:  6  2  5  5  1  5          11603.10000   11603.25373   -0.15373    0.10000   0.05033
  3:  6  5  1  5  4  1          12457.00000   12456.97596    0.02404    0.10000   0.03984
  4:  6  5  2  5  4  1          12421.73000   12421.71387    0.01613    0.10000   0.04199
  5:  6  6  1  5  5  1          13385.09000   13385.04800    0.04200    0.10000   0.04906
  6:  8  2  7  7  1  7          15492.08000   15491.90152    0.17848    0.10000   0.07021
  7:  8  4  4  7  5  3          16328.56000   16328.72300   -0.16300    0.10000   0.04917
  8:  8  6  3  7  5  3          16267.51000   16267.41029    0.09971    0.10000   0.04932
  9:  8  6  3  7  6  2          11586.38000   11586.33501    0.04499    0.10000   0.05411
 10:  9  1  8  8  1  7          10821.86000   10821.86147   -0.00147    0.10000   0.08133
 11:  9  4  5  8  6  2          13812.51000   13812.54715   -0.03715    0.10000   0.05297
 12: 10 10  0  9  8  1          15111.26000   15111.21874    0.04126    0.10000   0.09096
 13: 12  0 12 11  0 11          13087.50000   13087.47363    0.02637    0.10000   0.09844   13087.47355    0.02645 0.2500
 14: 12  0 12 11  1 11          13087.50000   13087.47343    0.02657    0.10000   0.09844   13087.47355    0.02645 0.2500
 15: 12  1 12 11  0 11          13087.50000   13087.47367    0.02633    0.10000   0.09844   13087.47355    0.02645 0.2500
 16: 12  1 12 11  1 11          13087.50000   13087.47347    0.02653    0.10000   0.09844   13087.47355    0.02645 0.2500
 17: 12  9  3 11  9  2          17192.21000   17192.21326   -0.00326    0.10000   0.09825   17192.20970    0.00030 0.5000
 18: 12 11  2 11 11  1          17192.21000   17192.20613    0.00387    0.10000   0.09825   17192.20970    0.00030 0.5000
 19: 13  4 10 12  4  9          16834.46000   16834.50725   -0.04725    0.10000   0.09552
NORMALIZED DIAGONAL:
  1 1.00000E+000   2 7.19586E-001   3 2.58850E-001   4 9.70619E-001   5 4.35612E-001   6 7.34782E-002
  7 1.00000E+000   8 9.99916E-001
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                    NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1       10000        A       1151.9068( 46)         0.0000
  2       20000        B        844.5618( 66)         0.0000
  3       30000        C        526.6232(110)         0.0000
  4         200   -DeltaJ         -0.091( 54)E-03      -0.000E-03
  5        2000   -DeltaK         -0.817(114)E-03      -0.000E-03
  6        1100   -DeltaJK         1.234(153)E-03       0.000E-03
  7       40100    -deltaJ    -0.043700000(  0)E-03 -0.000000000E-03
  8       41000    -deltaK          0.520( 74)E-03       0.000E-03
 MICROWAVE AVG =      -0.002242 MHz, IR AVG =       0.00000
 MICROWAVE RMS =       0.087002 MHz, IR RMS =       0.00000
```

wuwud SPFIT Output

```
                    EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  7  2  5  6  1  5          12170.29000   12170.28634    0.00366    0.10000   0.09241
  2:  9  2  8  8  2  7          10532.44000   10532.40388    0.03612    0.10000   0.07213
  3: 11 10  2 10  8  3          14537.53000   14537.54139   -0.01139    0.10000   0.06475
  4: 12  0 12 11  0 11          12818.62000   12818.66602   -0.04602    0.10000   0.07321   12818.65523   -0.03523 0.2500
  5: 12  0 12 11  1 11          12818.62000   12818.63496   -0.01496    0.10000   0.07321   12818.65523   -0.03523 0.2500
  6: 12  1 12 11  0 11          12818.62000   12818.67549   -0.05549    0.10000   0.07321   12818.65523   -0.03523 0.2500
  7: 12  1 12 11  1 11          12818.62000   12818.64444   -0.02444    0.10000   0.07321   12818.65523   -0.03523 0.2500
  8: 13  3 10 12  4  9          16201.69000   16201.68817    0.00183    0.10000   0.08774
  9: 13  6  7 13  7  7          10784.31000   10784.31126   -0.00126    0.10000   0.09970
 10: 16  0 16 15  0 15          16953.67000   16953.65924    0.01076    0.10000   0.09745   16953.65915    0.01085 0.2500
 11: 16  0 16 15  1 15          16953.67000   16953.65899    0.01101    0.10000   0.09745   16953.65915    0.01085 0.2500
 12: 16  1 16 15  0 15          16953.67000   16953.65932    0.01068    0.10000   0.09745   16953.65915    0.01085 0.2500
 13: 16  1 16 15  1 15          16953.67000   16953.65906    0.01094    0.10000   0.09745   16953.65915    0.01085 0.2500
 14: 16 13  3 16 12  5          16682.13000   16682.13261   -0.00261    0.10000   0.09919
 15: 17  8 10 17  7 10          12962.50000   12962.49724    0.00276    0.10000   0.09864
NORMALIZED DIAGONAL:
  1  1.00000E+000    2  6.41492E-001    3  3.80460E-001    4  1.58626E-001    5  9.46790E-001    6  1.00000E+000
  7  1.77849E-001    8  1.00000E+000
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                    NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1       10000         A       1225.0097(141)         -0.0000
  2       20000         B        754.1996( 73)         -0.0000
  3       30000         C        517.0787( 76)         -0.0000
  4         200    -DeltaJ        -0.4888(303)E-03       0.0000E-03
  5        2000    -DeltaK         0.2868(269)E-03      -0.0000E-03
  6        1100   -DeltaJK     0.091200000(  0)E-03 -0.000000000E-03
  7       40100    -deltaJ        -0.0824(149)E-03       0.0000E-03
  8       41000    -deltaK        -0.3835(261)E-03       0.0000E-03
 MICROWAVE AVG =       0.000526 MHz, IR AVG =       0.00000
 MICROWAVE RMS =       0.017718 MHz, IR RMS =       0.00000
```

wwduu SPFIT Output

```
                        EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  6  1  5  5  0  5            11456.09000   11456.17016  -0.08016    0.10000   0.05927
  2:  6  2  4  5  1  4            11113.73000   11113.80763  -0.07763    0.10000   0.05929
  3:  6  3  4  5  2  4            11504.55000   11504.39904   0.15096    0.10000   0.05055
  4:  8  3  6  7  2  6            15247.08000   15247.03708   0.04292    0.10000   0.06713
  5:  8  5  3  7  4  3            17192.21000   17192.24174  -0.03174    0.10000   0.09839
  6:  9  4  5  8  4  4            13050.90000   13050.85195   0.04805    0.10000   0.07781
  7:  9  6  4  8  6  3            12931.25000   12931.30351  -0.05351    0.10000   0.06279
  8: 10  0 10  9  0  9             11100.96000   11100.96408  -0.00408    0.10000   0.08901   11100.95901    0.00099 0.2500
  9: 10  0 10  9  1  9             11100.96000   11100.95111   0.00889    0.10000   0.08901   11100.95901    0.00099 0.2500
 10: 10  1 10  9  0  9             11100.96000   11100.96690  -0.00690    0.10000   0.08901   11100.95901    0.00099 0.2500
 11: 10  1 10  9  1  9             11100.96000   11100.95393   0.00607    0.10000   0.08901   11100.95901    0.00099 0.2500
 12: 10  3  8  9  3  7            12831.09000   12831.09015  -0.00015    0.10000   0.09321
 13: 12  0 12 11  0 11              13234.95000   13234.95088  -0.00088    0.10000   0.09810   13234.95064   -0.00064 0.2500
 14: 12  0 12 11  1 11              13234.95000   13234.95028  -0.00028    0.10000   0.09810   13234.95064   -0.00064 0.2500
 15: 12  1 12 11  0 11              13234.95000   13234.95101  -0.00101    0.10000   0.09810   13234.95064   -0.00064 0.2500
 16: 12  1 12 11  1 11              13234.95000   13234.95041  -0.00041    0.10000   0.09810   13234.95064   -0.00064 0.2500
NORMALIZED DIAGONAL:
  1 1.00000E+000   2 9.50611E-001   3 9.99009E-001   4 1.30775E-001   5 3.18722E-001   6 5.92889E-002
  7 1.00000E+000   8 1.00000E+000
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                        NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1       10000         A       1160.2860(101)          0.0000
  2       20000         B        829.6372( 98)          0.0000
  3       30000         C        533.4808(175)         -0.0000
  4         200    -DeltaJ         -0.330( 79)E-03      -0.000E-03
  5        2000    -DeltaK         -0.690(179)E-03      -0.000E-03
  6        1100   -DeltaJK          1.037(213)E-03       0.000E-03
  7       40100    -deltaJ    -0.099700000(  0)E-03 -0.000000000E-03
  8       41000    -deltaK     0.705000000(  0)E-03 -0.000000000E-03
 MICROWAVE AVG =       -0.000092 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.065774 MHz, IR RMS =        0.00000
```

wwudu SPFIT Output

```
                        EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  6  3  3  5  2  3              10818.09000   10817.86565    0.22435    0.10000   0.08198
  2:  6  4  2  5  3  2              11165.62000   11165.70568   -0.08568    0.10000   0.09366
  3:  6  4  3  5  3  3              11553.57000   11553.78950   -0.21950    0.10000   0.05643
  4:  6  5  2  5  4  2              12106.44000   12106.37389    0.06611    0.10000   0.08541
  5:  9  4  6  8  3  6              16887.46000   16887.60821   -0.14821    0.10000   0.08583
  6:  9  6  4  8  5  4              17289.13000   17288.96497    0.16503    0.10000   0.08164
  7: 12  4  9 11  4  8               16196.74000   16196.74526   -0.00526    0.10000   0.09998
NORMALIZED DIAGONAL:
  1 1.00000E+000   2 6.45338E-001   3 6.29570E-002   4 1.75425E-001   5 9.82020E-001   6 1.00000E+000
  7 1.00000E+000   8 1.00000E+000
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                    NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1       10000        A       1099.9200(213)         -0.0000
  2       20000        B        841.9109(137)          0.0000
  3       30000        C         561.918( 94)          0.000
  4         200    -DeltaJ         -0.782( 76)E-03       0.000E-03
  5        2000    -DeltaK        -0.01217( 79)        -0.00000
  6        1100   -DeltaJK     2.540000000(  0)E-03 -0.000000000E-03
  7       40100    -deltaJ    -0.152000000(  0)E-03 -0.000000000E-03
  8       41000    -deltaK     1.750000000(  0)E-03 -0.000000000E-03
 MICROWAVE AVG =      -0.000451 MHz, IR AVG =        0.00000
 MICROWAVE RMS =       0.150927 MHz, IR RMS =        0.00000
```

wwuwu SPFIT Output

```
                        EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  5  2  4  4  1  4              11493.78000   11493.77968    0.00032    0.10000   0.07403
  2:  7  4  4  6  3  4              17082.38000   17082.34895    0.03105    0.10000   0.07494
  3:  9  2  8  8  2  7              12665.57000   12665.52778    0.04222    0.10000   0.06691
  4: 10  1 10  9  0  9               12890.39000   12890.36405    0.02595    0.10000   0.06384
  5: 10  9  1  9  8  1               11579.51000   11579.49323    0.01677    0.10000   0.09314
  6: 11  5  7 10  5  6               16834.46000   16834.38640    0.07360    0.10000   0.06641
  7: 11 10  2 10  8  3               16792.26000   16792.43347   -0.17347    0.10000   0.04711
  8: 12  1 12 11  1 11               15356.67000   15356.68925   -0.01925    0.10000   0.09365
  9: 12  4  8 12  5  8               13333.34000   13333.32328    0.01672    0.10000   0.09341
 10: 15  6 10 14  7  8               12434.88000   12434.87407    0.00593    0.10000   0.09916
 11: 16  4 12 16  5 12               12866.27000   12866.27898   -0.00898    0.10000   0.08989
 12: 17  4 14 16  5 12               15137.97000   15137.95739    0.01261    0.10000   0.09817
NORMALIZED DIAGONAL:
  1 1.00000E+000   2 8.13693E-001   3 2.02882E-001   4 2.06796E-001   5 9.40170E-001   6 2.27801E-002
  7 1.50284E-001   8 4.58860E-001
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                     NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1       10000        A       1663.8654(136)        -0.0000
  2       20000        B        879.0923( 74)         0.0000
  3       30000        C        618.6094(107)        -0.0000
  4         200    -DeltaJ         -1.774( 70)E-03      -0.000E-03
  5        2000    -DeltaK         -6.190(180)E-03      -0.000E-03
  6        1100   -DeltaJK          5.766(248)E-03       0.000E-03
  7       40100    -deltaJ          0.449( 38)E-03      -0.000E-03
  8       41000    -deltaK         -1.058(115)E-03       0.000E-03
 MICROWAVE AVG =       0.001956 MHz, IR AVG =       0.00000
 MICROWAVE RMS =       0.057831 MHz, IR RMS =       0.00000
```

wwdwd SPFIT Output

```
                    EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  7  2  5  6  5  1          16537.48000   16537.59496   -0.11496    0.10000   0.07095
  2:  8  5  3  8  6  3          11062.45000   11062.33661    0.11339    0.10000   0.05281
  3:  8  6  2  8  7  2          12815.64000   12815.66617   -0.02617    0.10000   0.07869   12815.65812   -0.01812 0.5000
  4:  8  8  1  8  5  3          12815.64000   12815.65006   -0.01006    0.10000   0.07869   12815.65812   -0.01812 0.5000
  5:  9  5  5  9  4  5          11000.91000   11000.91351   -0.00351    0.10000   0.05042
  6: 10  1 10  9  1  9           13139.50000   13139.42921    0.07079    0.10000   0.08094
  7: 10  2  9  9  2  8           14161.38000   14161.34682    0.03318    0.10000   0.06936
  8: 11  5  6 10  5  5           17192.21000   17192.13739    0.07261    0.10000   0.08646
  9: 12  1 11 11  1 10           16700.90000   16700.96638   -0.06638    0.10000   0.08191
 10: 12  4  8 12  5  8           12573.30000   12573.34172   -0.04172    0.10000   0.06302
 11: 14  3 12 13 12  2           10480.21000   10480.22694   -0.01694    0.10000   0.09605
 12: 16 12  4 16 11  6           13196.84000   13196.85535   -0.01535    0.10000   0.09917
 13: 17  4 13 17  5 13           12113.02000   12112.96460    0.05540    0.10000   0.07682
 14: 21 18  3 21 17  5           15058.29000   15058.31579   -0.02579    0.10000   0.09468
NORMALIZED DIAGONAL:
  1 1.00000E+000   2 9.14076E-001   3 1.29434E-001   4 9.99747E-001   5 6.25221E-002   6 1.78570E-002
  7 2.48723E-001   8 5.86764E-001
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                    NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1       10000        A       1630.1266(144)         0.0000
  2       20000        B        895.6917(175)         0.0000
  3       30000        C        631.7337(192)        -0.0000
  4         200    -DeltaJ        -1.416( 90)E-03      -0.000E-03
  5        2000    -DeltaK        -3.219(168)E-03      -0.000E-03
  6        1100   -DeltaJK         2.062(263)E-03       0.000E-03
  7       40100    -deltaJ         0.257( 34)E-03       0.000E-03
  8       41000    -deltaK        -0.671(115)E-03      -0.000E-03
 MICROWAVE AVG =       0.003276 MHz, IR AVG =       0.00000
 MICROWAVE RMS =       0.060891 MHz, IR RMS =       0.00000
```

wwuwd SPFIT Output

```
                    EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  8  5  3  8  4  5          12804.99000   12805.06233   -0.07233    0.10000   0.06851
  2:  8  6  2  8  7  2          14816.40000   14816.43668   -0.03668    0.10000   0.06608   14816.43250   -0.03250 0.2000
  3:  8  8  1  8  5  3          14816.40000   14816.43146   -0.03146    0.10000   0.06608   14816.43250   -0.03250 0.8000
  4:  9  1  8  8  1  7          12737.52000   12737.51465    0.00535    0.10000   0.06142
  5:  9  1  9  8  0  8          11579.51000   11579.50925    0.00075    0.10000   0.04744
  6: 10  1 10  9  0  9           12799.09000   12798.96912    0.12088    0.10000   0.06951
  7: 10  3  7  9  3  6           15274.78000   15274.76750    0.01250    0.10000   0.06455
  8: 11  2 10 10  2  9           15082.33000   15082.34437   -0.01437    0.10000   0.04561
  9: 11  7  4 11  6  6           16731.27000   16731.24684    0.02316    0.10000   0.06733   16731.23381    0.03619 0.5000
 10: 11  7  5 11  4  7           16731.27000   16731.22078    0.04922    0.10000   0.06733   16731.23381    0.03619 0.5000
 11: 13  5  8 13  6  8           16621.88000   16621.84974    0.03026    0.10000   0.07510
 12: 13 13  0 12 12  0           10625.00000   10625.15190   -0.15190    0.10000   0.07381
 13: 15  3 12 15  4 12           12301.67000   12301.71641   -0.04641    0.10000   0.05727
 14: 15 11  4 15 10  6           14488.45000   14488.37342    0.07658    0.10000   0.09288
 15: 17  3 14 16  4 12           12368.74000   12368.69624    0.04376    0.10000   0.09767
 16: 17  3 14 17  4 14           12684.51000   12684.58206   -0.07206    0.10000   0.08256
 17: 25 20  6 25 21  4           15137.97000   15137.96015    0.00985    0.10000   0.09976
NORMALIZED DIAGONAL:
  1  1.00000E+000   2  1.75705E-001   3  9.87771E-001   4  8.84008E-001   5  8.05712E-002   6  1.87466E-002
  7  4.37870E-001   8  5.90973E-001
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                    NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1       10000        A       1737.4850(148)        -0.0000
  2       20000        B        866.9146( 56)        -0.0000
  3       30000        C        613.2547( 73)        -0.0000
  4         200    -DeltaJ        -0.813( 57)E-03       0.000E-03
  5        2000    -DeltaK        -1.710(146)E-03       0.000E-03
  6        1100   -DeltaJK         0.997(166)E-03      -0.000E-03
  7       40100    -deltaJ         0.2717(251)E-03     -0.0000E-03
  8       41000    -deltaK        -0.485( 60)E-03       0.000E-03
 MICROWAVE AVG =      -0.003563 MHz, IR AVG =       0.00000
 MICROWAVE RMS =       0.064195 MHz, IR RMS =       0.00000
```

wwwdd SPFIT Output

```
                    EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  7  4  4  6  4  3          12931.25000   12931.24752    0.00248    0.10000   0.09999
  2:  8  7  1  7  7  0          16164.42000   16164.42307   -0.00307    0.10000   0.09999
  3: 10  1  9  9  1  8          14523.34000   14523.33973    0.00027    0.10000   0.07071
  4: 10  1  9 10  1 10          10909.20000   10909.32869   -0.12869    0.10000   0.07861
  5: 10  2  9  9  2  8          14523.34000   14523.33955    0.00045    0.10000   0.07071
  6: 13  3 10 13  3 11          12026.68000   12026.52980    0.15020    0.10000   0.06927   12026.52983    0.15017 0.6667
  7: 13  4 10 13  2 11          12026.68000   12026.52991    0.15009    0.10000   0.06927   12026.52983    0.15017 0.3333
  8: 17  3 14 17  3 15          16628.15000   16628.15868   -0.00868    0.10000   0.09992   16628.15868   -0.00868 0.5000
  9: 17  4 14 17  2 15          16628.15000   16628.15868   -0.00868    0.10000   0.09992   16628.15868   -0.00868 0.5000
 10: 20  7 13 20  7 14          15376.74000   15376.73865    0.00135    0.10000   0.09993   15376.73870    0.00130 0.5000
 11: 20  8 13 20  6 14          15376.74000   15376.73875    0.00125    0.10000   0.09993   15376.73870    0.00130 0.5000
 12: 22 11 11 22 11 12          12844.58000   12844.63341   -0.05341    0.10000   0.09669
 13: 22 13 10 22 11 11          11566.97000   11566.93409    0.03591    0.10000   0.09850
NORMALIZED DIAGONAL:
  1 1.00000E+000   2 5.93398E-001   3 9.89076E-002   4 9.99938E-001   5 2.62638E-001   6 4.22835E-003
  7 2.21624E-001   8 9.53733E-001
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                    NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1       10000        A       1289.219( 44)         -0.000
  2       20000        B       1148.9067(149)         0.0000
  3       30000        C        640.0460(175)        -0.0000
  4         200    -DeltaJ        -3.111(289)E-03       0.000E-03
  5        2000    -DeltaK         -7.02( 80)E-03       0.00E-03
  6        1100   -DeltaJK          9.51(104)E-03      -0.00E-03
  7       40100    -deltaJ         0.980(137)E-03      -0.000E-03
  8       41000    -deltaK        -0.01680(244)         0.00000
 MICROWAVE AVG =      -0.000327 MHz, IR AVG =       0.00000
 MICROWAVE RMS =       0.065838 MHz, IR RMS =       0.00000
```

wwdwu SPFIT Output

```
                    EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  4  4  0  3  3  0          12844.58000   12844.69507   -0.11507    0.10000   0.08937
  2:  8  1  7  7  1  6          11488.77000   11488.65123    0.11877    0.10000   0.09775   11488.70851    0.06149 0.5000
  3:  9  1  9  8  1  8          11488.77000   11488.76579    0.00421    0.10000   0.09775   11488.70851    0.06149 0.5000
  4:  9  7  2  9  8  2          16731.27000   16731.27536   -0.00536    0.10000   0.07088   16731.27513   -0.00513 0.5000
  5:  9  9  1  9  6  3          16731.27000   16731.27490   -0.00490    0.10000   0.07088   16731.27513   -0.00513 0.5000
  6: 10  4  7  9  4  6          15022.28000   15022.34293   -0.06293    0.10000   0.05071
  7: 10  7  3 10  6  5          16704.24000   16704.19779    0.04221    0.10000   0.06608
  8: 11  4  7 10  6  4          16441.28000   16441.29719   -0.01719    0.10000   0.05371
  9: 11  5  7 10  5  6          16495.48000   16495.35230    0.12770    0.10000   0.04964
 10: 11  6  6 10  6  5          16441.28000   16441.27551    0.00449    0.10000   0.05371
 11: 12  0 12 11  0 11          15137.97000   15137.86874    0.10126    0.10000   0.08214
 12: 12  4  8 12  5  8          14565.79000   14565.89261   -0.10261    0.10000   0.05088
 13: 12 12  0 12 11  2          10532.44000   10532.28112    0.15888    0.10000   0.06153
 14: 14  3 11 14  4 11          12286.91000   12287.01219   -0.10219    0.10000   0.07335
 15: 16 10  7 15  9  7          12434.88000   12434.98259   -0.10259    0.10000   0.08782
 16: 17  3 14 16  4 12          12271.85000   12271.97336   -0.12336    0.10000   0.08727
 17: 20 15  6 19 14  6          16804.03000   16803.93894    0.09106    0.10000   0.09179
NORMALIZED DIAGONAL:
  1  1.00000E+000   2  7.03643E-001   3  9.26018E-001   4  1.32055E-001   5  2.12669E-001   6  2.75650E-002
  7  8.28099E-002   8  6.41196E-001
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                    NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1       10000        A       1729.2085(151)        -0.0000
  2       20000        B        862.1585(121)         0.0000
  3       30000        C        609.0836(138)        -0.0000
  4         200   -DeltaJ         -0.571( 63)E-03      -0.000E-03
  5        2000   -DeltaK         -2.537( 95)E-03       0.000E-03
  6        1100   -DeltaJK         0.827(164)E-03       0.000E-03
  7       40100    -deltaJ         0.1757(250)E-03     -0.0000E-03
  8       41000    -deltaK         -0.403( 54)E-03      -0.000E-03
 MICROWAVE AVG =      -0.002933 MHz, IR AVG =       0.00000
 MICROWAVE RMS =       0.093063 MHz, IR RMS =       0.00000
```

wwwdu SPFIT Output

```
                    EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  5  5  1  4  4  1          12349.90000   12349.88393    0.01607    0.10000   0.09991
  2:  6  3  4  5  3  3          10625.00000   10624.76064    0.23936    0.10000   0.07735
  3:  8  2  6  7  2  5          13275.00000   13275.26652   -0.26652    0.10000   0.06610   13275.28341   -0.28341 0.5000
  4:  8  3  6  7  2  5          13275.00000   13275.30030   -0.30030    0.10000   0.06610   13275.28341   -0.28341 0.5000
  5:  8  6  2  7  6  1          17192.21000   17192.21120   -0.00120    0.10000   0.10000
  6: 11  0 11 10  0 10             15065.50000   15065.43087    0.06913    0.10000   0.09831   15065.43087    0.06913 0.2500
  7: 11  0 11 10  1 10             15065.50000   15065.43087    0.06913    0.10000   0.09831   15065.43087    0.06913 0.2500
  8: 11  1 11 10  0 10             15065.50000   15065.43087    0.06913    0.10000   0.09831   15065.43087    0.06913 0.2500
  9: 11  1 11 10  1 10             15065.50000   15065.43087    0.06913    0.10000   0.09831   15065.43087    0.06913 0.2500
NORMALIZED DIAGONAL:
  1 1.00000E+000   2 8.01660E-001   3 2.29972E-001   4 9.99839E-001   5 1.00000E+000   6 1.00000E+000
  7 1.00000E+000   8 1.00000E+000
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                    NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1       10000        A       1255.4737(107)         -0.0000
  2       20000        B       1153.5225( 79)          0.0000
  3       30000        C        660.3352(176)          0.0000
  4         200    -DeltaJ         -1.183( 76)E-03      -0.000E-03
  5        2000    -DeltaK     -1.160000000(  0)E-03 -0.000000000E-03
  6        1100   -DeltaJK      1.600000000(  0)E-03 -0.000000000E-03
  7       40100    -deltaJ      0.044200000(  0)E-03 -0.000000000E-03
  8       41000    -deltaK     -0.094900000(  0)E-03  0.000000000E-03
 MICROWAVE AVG =       0.007988 MHz, IR AVG =       0.00000
 MICROWAVE RMS =       0.168910 MHz, IR RMS =       0.00000
```

wwwud SPFIT Output

```
                        EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  6  5  2  5  4  2              14458.78000   14458.89935   -0.11935    0.10000   0.08898
  2:  7  4  3  6  3  3              16692.42000   16692.52508   -0.10508    0.10000   0.09157
  3:  7  4  4  6  3  4              16770.32000   16770.11231    0.20769    0.10000   0.06079
  4: 11  1 10 10  2  9                16385.84000   16385.84019   -0.00019    0.10000   0.10000   16385.84019   -0.00019 0.5000
  5: 11  2 10 10  1  9                16385.84000   16385.84020   -0.00020    0.10000   0.10000   16385.84019   -0.00019 0.5000
NORMALIZED DIAGONAL:
  1 1.00000E+000   2 4.82895E-001   3 9.91164E-001   4 1.00000E+000   5 1.00000E+000   6 1.00000E+000
  7 1.00000E+000   8 1.00000E+000
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                        NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1       10000        A       1243.0912(207)         -0.0000
  2       20000        B       1159.5080(146)          0.0000
  3       30000        C        673.0738( 53)          0.0000
  4         200    -DeltaJ     -0.897000000(  0)E-03 -0.000000000E-03
  5        2000    -DeltaK     -0.943000000(  0)E-03  0.000000000E-03
  6        1100   -DeltaJK      1.500000000(  0)E-03  0.000000000E-03
  7       40100    -deltaJ      8.600000000(  0)E-06 -0.000000000E-06
  8       41000    -deltaK     -0.122000000(  0)E-03  0.000000000E-03
 MICROWAVE AVG =       -0.004235 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.130786 MHz, IR RMS =        0.00000
```

wwwwd' SPFIT Output

```
                        EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  3  3  0  2  2  0            10516.03000   10515.97987    0.05013    0.10000   0.09031
  2:  4  2  2  3  1  2            11263.93000   11264.02222   -0.09222    0.10000   0.06220
  3:  5  3  2  4  3  1            11191.69000   11191.64018    0.04982    0.10000   0.07425
  4:  6  4  3  5  4  2            12862.47000   12862.45926    0.01074    0.10000   0.06243
  5:  8  1  7  7  1  6            15058.30000   15058.31911   -0.01911    0.10000   0.09296
  6: 10  0 10  9  0  9              16854.97000   16855.00107   -0.03107    0.10000   0.09963   16854.96421    0.00579 0.2500
  7: 10  0 10  9  1  9              16854.97000   16854.90163    0.06837    0.10000   0.09963   16854.96421    0.00579 0.2500
  8: 10  1 10  9  0  9              16854.97000   16855.02680   -0.05680    0.10000   0.09963   16854.96421    0.00579 0.2500
  9: 10  1 10  9  1  9              16854.97000   16854.92735    0.04265    0.10000   0.09963   16854.96421    0.00579 0.2500
 10: 12  4  9 12  3 10              12580.58000   12580.57951    0.00049    0.10000   0.09999
NORMALIZED DIAGONAL:
  1 1.00000E+000   2 8.48551E-001   3 3.69263E-001   4 9.93270E-001   5 1.83724E-001   6 1.00000E+000
  7 1.00000E+000   8 1.00000E+000
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                        NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1       10000        A       1903.7763(184)         -0.0000
  2       20000        B       1255.0177(104)          0.0000
  3       30000        C        807.8090(133)         -0.0000
  4         200    -DeltaJ         -1.687( 66)E-03      -0.000E-03
  5        2000    -DeltaK          -4.304(111)E-03       0.000E-03
  6        1100   -DeltaJK     5.180000000(  0)E-03  0.000000000E-03
  7       40100    -deltaJ    -0.359000000(  0)E-03 -0.000000000E-03
  8       41000    -deltaK     2.390000000(  0)E-03  0.000000000E-03
 MICROWAVE AVG =       0.000804 MHz, IR AVG =       0.00000
 MICROWAVE RMS =       0.044745 MHz, IR RMS =       0.00000
```

wwwwu SPFIT Output

```
                          EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  5  4  1  4  3  1              16804.03000   16804.07097   -0.04097    0.10000   0.09860
  2:  6  5  1  5  2  3              16746.88000   16746.84524    0.03476    0.10000   0.09898
  3:  7  1  7  6  1  6              11584.02000   11584.03449   -0.01449    0.10000   0.09983
  4:  7  7  1  7  4  3              12360.68000   12360.67869    0.00131    0.10000   0.10000
  5:  8  0  8  7  0  7              13139.50000   13139.44462    0.05538    0.10000   0.09747
  6:  8  4  4  7  4  3              16499.97000   16499.98619   -0.01619    0.10000   0.09979
  7:  9  9  0  8  8  0              14862.51000   14862.53399   -0.02399    0.10000   0.09951
  8: 13  2 11 13  2 12                 16196.74000   16196.57099    0.16901    0.10000   0.07315
  9: 13  3 11 13  1 12                 16201.69000   16201.84952   -0.15952    0.10000   0.07602
NORMALIZED DIAGONAL:
  1 1.00000E+000   2 3.01866E-002   3 1.78586E-001   4 9.99192E-001   5 1.02958E-001   6 2.45571E-003
  7 9.27772E-001   8 3.97164E-001
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                        NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1       10000        A       1976.920( 32)          0.000
  2       20000        B        1216.80( 39)          -0.00
  3       30000        C        775.399( 70)          0.000
  4         200    -DeltaJ          -8.37(188)E-03        0.00E-03
  5        2000    -DeltaK         -0.0152( 35)          0.0000
  6        1100   -DeltaJK          0.0240( 55)         -0.0000
  7       40100    -deltaJ          -5.08(159)E-03        0.00E-03
  8       41000    -deltaK          0.0123( 34)         -0.0000
 MICROWAVE AVG =       0.000591 MHz, IR AVG =       0.00000
 MICROWAVE RMS =       0.082335 MHz, IR RMS =       0.00000
```

wwwwd SPFIT Output

```
                        EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  5  3  2  4  2  2          14606.25000   14606.25200   -0.00200    0.10000   0.09957
  2:  5  4  1  4  4  0          10516.02000   10516.00768    0.01232    0.10000   0.08189
  3:  6  3  4  5  3  3          12379.56000   12379.57628   -0.01628    0.10000   0.06511
  4:  7  2  5  6  2  4          15022.28000   15022.27439    0.00561    0.10000   0.09653
  5:  9  0  9  8  0  8          14945.49000   14945.71377   -0.22377    0.10000   0.10000   14945.48988    0.00012 0.5000
  6:  9  1  9  8  1  8          14945.49000   14945.26600    0.22400    0.10000   0.10000   14945.48988    0.00012 0.5000
  7:  9  5  4  9  6  4          11474.61000   11474.60906    0.00094    0.10000   0.09990
  8:  9  9  0  8  8  0          15303.33000   15303.32788    0.00212    0.10000   0.09952
  9: 10  7  4  9  6  4           11586.38000   11586.38133   -0.00133    0.10000   0.09981
 10: 12  6  6 12  5  8            12945.01000   12945.01097   -0.00097    0.10000   0.09990
NORMALIZED DIAGONAL:
  1 1.00000E+000   2 3.14768E-001   3 1.97473E-001   4 6.34188E-001   5 9.61090E-001   6 1.02783E-002
  7 5.72427E-002   8 3.64298E-001
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                    NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1       10000        A       1946.976( 36)          0.000
  2       20000        B       1235.962( 45)          0.000
  3       30000        C        789.894( 66)         -0.000
  4         200   -DeltaJ         -6.51( 57)E-03       -0.00E-03
  5        2000   -DeltaK       -0.01753(192)        -0.00000
  6        1100  -DeltaJK        0.02606(276)         0.00000
  7       40100   -deltaJ         -1.329(143)E-03      -0.000E-03
  8       41000   -deltaK           3.96( 66)E-03       -0.00E-03
 MICROWAVE AVG =       0.000058 MHz, IR AVG =       0.00000
 MICROWAVE RMS =       0.007152 MHz, IR RMS =       0.00000
```

D4_uduud SPFIT Output

```
                    EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1: 11  7  4 10  6  4          12390.74000   12390.77150   -0.03150    0.10000   0.04583
  2: 12  7  5 11  7  4          11532.27000   11532.20620    0.06380    0.10000   0.05283
  3: 13  9  4 12  8  4          14641.35000   14641.35110   -0.00110    0.10000   0.04129
  4: 13 10  4 12  9  4          14642.32000   14642.41037   -0.09037    0.10000   0.04369
  5: 13 13  0 12 12  1          14758.17000   14758.16240    0.00760    0.10000   0.09927
  6: 14  4 10 13  3 10          15774.66000   15774.61313    0.04687    0.10000   0.07031
  7: 14  8  7 13  7  6          12898.91000   12898.88257    0.02743    0.10000   0.04946
  8: 14 11  3 13 10  4          17250.80000   17250.78883    0.01117    0.10000   0.09945
  9: 16  6 11 15  5 10          13381.14000   13381.18346   -0.04346    0.10000   0.06116
 10: 17  9  8 16  9  7          15837.43000   15837.39254    0.03746    0.10000   0.05448   15837.39255    0.03745 0.5000
 11: 17 10  8 16  9  7          15837.43000   15837.39255    0.03745    0.10000   0.05448   15837.39255    0.03745 0.5000
 12: 18  7 11 17  7 10          15635.19000   15635.21512   -0.02512    0.10000   0.04639   15635.21512   -0.02512 0.5000
 13: 18  8 11 17  7 10          15635.19000   15635.21512   -0.02512    0.10000   0.04639   15635.21512   -0.02512 0.5000
 14: 19  8 11 18  8 10          16762.32000   16762.32033   -0.00033    0.10000   0.07128
 15: 20  5 16 19  4 15          15675.25000   15675.27265   -0.02265    0.10000   0.05525
 16: 21  0 21 20  0 20          14588.93000   14588.92178    0.00822    0.10000   0.09959   14588.92178    0.00822 0.5000
 17: 21  1 21 20  0 20          14588.93000   14588.92178    0.00822    0.10000   0.09959   14588.92178    0.00822 0.5000
 18: 22  4 18 21  4 17          17043.73000   17043.71736    0.01264    0.10000   0.08625
 19: 29 23  7 30 14 16          11857.85000   11857.84980    0.00020    0.10000   0.09999
NORMALIZED DIAGONAL:
  1 1.00000E+000   2 1.87293E-001   3 6.81362E-002   4 9.20200E-001   5 2.60338E-001   6 1.36467E-002
  7 4.23302E-001   8 5.22129E-002
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                    NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1       10000        A       568.0733(130)         0.0000
  2       20000        B       558.7972( 79)         0.0000
  3       30000        C       342.0587( 81)         0.0000
  4         200   -DeltaJ          0.5(107)E-06       -0.0E-06
  5        2000   -DeltaK        -0.2005(275)E-03      0.0000E-03
  6        1100   -DeltaJK        0.232( 36)E-03      -0.000E-03
  7       40100    -deltaJ        0.0398(191)E-03     -0.0000E-03
  8       41000    -deltaK         -3.73( 59)E-03       0.00E-03
 MICROWAVE AVG =       0.000053 MHz, IR AVG =       0.00000
 MICROWAVE RMS =       0.036249 MHz, IR RMS =       0.00000
```

D4_wudud SPFIT Output

```
                    EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  8  6  3  7  5  3          11215.08000   11215.07709    0.00291    0.10000   0.00000
  2:  8  6  3  7  5  3          11215.08000   11215.07709    0.00291    0.10000   0.00000
  3:  9  3  6  8  2  6          11501.14000   11501.14541   -0.00541    0.10000   0.00000
  4:  9  9  1  8  8  1          13945.15000   13945.15363   -0.00363    0.10000   0.00000
  5: 12  5  7 11  4  7           14982.40000   14982.39474    0.00526    0.10000   0.00000
  6: 12 11  2 11 10  2           18112.50000   18112.49799    0.00201    0.10000   0.00000
  7: 13  1 12 12  1 11           11308.88000   11308.84339    0.03661    0.10000   0.00000   11308.84592    0.03408 0.5000
  8: 13  2 12 12  1 11           11308.88000   11308.84845    0.03155    0.10000   0.00000   11308.84592    0.03408 0.5000
  9: 15  3 12 14  3 11           13962.24000   13962.03362    0.20638    0.10000   0.00000   13962.27953   -0.03953 0.5000
 10: 15  4 12 14  3 11           13962.24000   13962.52543   -0.28543    0.10000   0.00000   13962.27953   -0.03953 0.5000
 11: 19  0 19 18  0 18           15661.28000   15661.29429   -0.01429    0.10000   0.00000   15661.29429   -0.01429 0.5000
 12: 19  1 19 18  0 18           15661.28000   15661.29429   -0.01429    0.10000   0.00000   15661.29429   -0.01429 0.5000
 13: 20  2 18 19  2 17           17492.22000   17492.20154    0.01846    0.10000   0.00000   17492.20155    0.01845 0.5000
 14: 20  3 18 19  2 17           17492.22000   17492.20156    0.01844    0.10000   0.00000   17492.20155    0.01845 0.5000
NORMALIZED DIAGONAL:
  1 1.00000E+000   2 9.75160E-001   3 2.54893E-001   4 8.97902E-002   5 9.98066E-001   6 1.17145E-002
  7 2.66032E-001   8 6.44877E-001
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                    NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1       10000        A       790.7318(108)        -0.0000
  2       20000        B       575.1071(104)         0.0000
  3       30000        C       405.4978( 67)        -0.0000
  4         200   -DeltaJ         0.115( 36)E-03      -0.000E-03
  5        2000   -DeltaK         1.361(195)E-03      -0.000E-03
  6        1100  -DeltaJK        -1.557(222)E-03       0.000E-03
  7       40100   -deltaJ        -0.0288(213)E-03     -0.0000E-03
  8       41000   -deltaK         0.282(231)E-03      -0.000E-03
 MICROWAVE AVG =       0.000276 MHz, IR AVG =       0.00000
 MICROWAVE RMS =       0.018328 MHz, IR RMS =       0.00000
```

D4_wuudu SPFIT Output

```
                    EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  7  7  1  6  6  1          10744.88000   10744.88292   -0.00292    0.10000   0.00000
  2:  7  7  1  6  6  1          10744.88000   10744.88292   -0.00292    0.10000   0.00000
  3:  9  8  2  8  7  2          13342.25000   13342.23748    0.01252    0.10000   0.00000
  4: 10  7  4  9  6  4          13829.39000   13829.39713   -0.00713    0.10000   0.00000
  5: 11 11  1 10 10  1          17046.32000   17046.32173   -0.00173    0.10000   0.00000
  6: 15  1 14 14  1 13          12662.51000   12662.52180   -0.01180    0.10000   0.00000   12662.52181   -0.01181 0.5000
  7: 15  2 14 14  1 13          12662.51000   12662.52182   -0.01182    0.10000   0.00000   12662.52181   -0.01181 0.5000
  8: 16  0 16 15  0 15          12891.15000   12891.18438   -0.03438    0.10000   0.00000   12891.18438   -0.03438 0.5000
  9: 16  1 16 15  0 15          12891.15000   12891.18438   -0.03438    0.10000   0.00000   12891.18438   -0.03438 0.5000
 10: 18  1 17 17  1 16          15025.59000   15025.50894    0.08106    0.10000   0.00000   15025.50894    0.08106 0.5000
 11: 18  2 17 17  1 16          15025.59000   15025.50894    0.08106    0.10000   0.00000   15025.50894    0.08106 0.5000
 12: 19  5 14 18  5 13          18081.09000   18081.00531    0.08469    0.10000   0.00000   18081.08400    0.00600 0.5000
 13: 19  6 14 18  5 13          18081.09000   18081.16268   -0.07268    0.10000   0.00000   18081.08400    0.00600 0.5000
 14: 20  2 18 19  2 17          17160.90000   17160.94137   -0.04137    0.10000   0.00000   17160.94137   -0.04137 0.5000
 15: 20  3 18 19  2 17          17160.90000   17160.94137   -0.04137    0.10000   0.00000   17160.94137   -0.04137 0.5000
NORMALIZED DIAGONAL:
  1  1.00000E+000   2  5.39988E-001   3  1.66235E-001   4  3.31494E-002   5  5.80645E-001   6  3.04726E-003
  7  2.57526E-001   8  9.99697E-001
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                    NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1       10000         A        787.0991(103)          0.0000
  2       20000         B         592.981( 94)          0.000
  3       30000         C        394.2108(112)         -0.0000
  4         200    -DeltaJ          2.089(112)E-03       0.000E-03
  5        2000    -DeltaK           1.62( 71)E-03       0.00E-03
  6        1100   -DeltaJK          -3.87( 79)E-03       -0.00E-03
  7       40100    -deltaJ          0.527( 53)E-03       0.000E-03
  8       41000    -deltaK          -2.79( 79)E-03       0.00E-03
 MICROWAVE AVG =       -0.000268 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.031412 MHz, IR RMS =        0.00000
```

D4_wuduu SPFIT Output

```
                    EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  7  7  1  6  6  1          10842.82000   10842.82015   -0.00015    0.10000   0.00000
  2:  7  7  1  6  6  1          10842.82000   10842.82015   -0.00015    0.10000   0.00000
  3: 10  9  2  9  8  2           15037.50000   15037.49996    0.00004    0.10000   0.00000
  4: 11 11  1 10 10  1            17217.60000   17217.59990    0.00010    0.10000   0.00000
  5: 15  1 14 14  1 13            12741.43000   12741.37297    0.05703    0.10000   0.00000   12741.37301    0.05699 0.5000
  6: 15  2 14 14  1 13            12741.43000   12741.37305    0.05695    0.10000   0.00000   12741.37301    0.05699 0.5000
  7: 16  3 13 15  3 12            14633.90000   14633.91827   -0.01827    0.10000   0.00000   14633.93984   -0.03984 0.5000
  8: 16  4 13 15  3 12            14633.90000   14633.96142   -0.06142    0.10000   0.00000   14633.93984   -0.03984 0.5000
  9: 17  0 17 16  0 16            13787.49000   13787.53856   -0.04856    0.10000   0.00000   13787.53856   -0.04856 0.5000
 10: 17  1 17 16  0 16             13787.49000   13787.53856   -0.04856    0.10000   0.00000   13787.53856   -0.04856 0.5000
 11: 19  4 15 18  4 14             17566.11000   17566.05408    0.05592    0.10000   0.00000   17566.06393    0.04607 0.5000
 12: 19  5 15 18  4 14             17566.11000   17566.07378    0.03622    0.10000   0.00000   17566.06393    0.04607 0.5000
 13: 20  1 19 19  1 18             16713.22000   16713.17914    0.04086    0.10000   0.00000   16713.17914    0.04086 0.5000
 14: 20  2 19 19  1 18             16713.22000   16713.17914    0.04086    0.10000   0.00000   16713.17914    0.04086 0.5000
 15: 20  3 17 19  3 16             17804.33000   17804.38413   -0.05413    0.10000   0.00000   17804.38420   -0.05420 0.5000
 16: 20  4 17 19  3 16             17804.33000   17804.38427   -0.05427    0.10000   0.00000   17804.38420   -0.05420 0.5000
NORMALIZED DIAGONAL:
  1 1.00000E+000   2 2.25785E-001   3 1.34924E-001   4 2.44986E-002   5 5.96865E-001   6 4.20162E-003
  7 2.58077E-001   8 9.96925E-001
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                    NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1      10000        A       794.7696(117)         0.0000
  2      20000        B        585.089(118)         -0.000
  3      30000        C       397.5055(149)         0.0000
  4        200   -DeltaJ         4.403(108)E-03      -0.000E-03
  5       2000   -DeltaK        0.01432( 44)        -0.00000
  6       1100  -DeltaJK       -0.01861( 50)         0.00000
  7      40100    -deltaJ        -0.293( 59)E-03       0.000E-03
  8      41000    -deltaK        0.01020( 43)        -0.00000
 MICROWAVE AVG =       0.000117 MHz, IR AVG =       0.00000
 MICROWAVE RMS =       0.037313 MHz, IR RMS =       0.00000
```

D4_wdudu SPFIT Output

```
                    EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  9  9  1  8  8  1          13851.28000   13851.29920   -0.01920    0.10000   0.00000
  2:  9  9  1  8  8  1          13851.28000   13851.29920   -0.01920    0.10000   0.00000
  3: 10 10  1  9  9  1          15421.06000   15420.99639    0.06361    0.10000   0.00000
  4: 11 11  1 10 10  1          16990.62000   16990.64648   -0.02648    0.10000   0.00000
  5: 12  2 10 11  2  9          11098.74000   11098.79815   -0.05815    0.10000   0.00000
  6: 13  0 13 12  0 12          10906.82000   10906.83386   -0.01386    0.10000   0.00000   10906.83387   -0.01387 0.5000
  7: 13  1 13 12  0 12          10906.82000   10906.83389   -0.01389    0.10000   0.00000   10906.83387   -0.01387 0.5000
  8: 14  2 12 13  2 11          12734.10000   12734.01918    0.08082    0.10000   0.00000
  9: 19  0 19 18  0 18          15817.40000   15817.44027   -0.04027    0.10000   0.00000   15817.44027   -0.04027 0.5000
 10: 19  1 19 18  0 18          15817.40000   15817.44027   -0.04027    0.10000   0.00000   15817.44027   -0.04027 0.5000
 11: 19  1 18 18  1 17          16318.88000   16318.79207    0.08793    0.10000   0.00000   16318.79207    0.08793 0.5000
 12: 19  2 18 18  1 17          16318.88000   16318.79207    0.08793    0.10000   0.00000   16318.79207    0.08793 0.5000
 13: 19  3 16 18  3 15          17328.21000   17328.32253   -0.11253    0.10000   0.00000   17328.32308   -0.11308 0.5000
 14: 19  4 16 18  3 15          17328.21000   17328.32363   -0.11363    0.10000   0.00000   17328.32308   -0.11308 0.5000
 15: 19  4 15 18  4 14          17839.44000   17839.38787    0.05213    0.10000   0.00000
NORMALIZED DIAGONAL:
  1 1.00000E+000   2 2.63529E-001   3 1.44163E-001   4 2.00148E-002   5 7.04968E-001   6 1.12313E-003
  7 1.47727E-001   8 9.97840E-001
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                    NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1       10000         A         785.234( 32)          -0.000
  2       20000         B         577.807(119)           0.000
  3       30000         C        410.0023(105)           0.0000
  4         200    -DeltaJ          1.837(114)E-03       -0.000E-03
  5        2000    -DeltaK         0.01847(186)         -0.00000
  6        1100   -DeltaJK        -0.02075(192)          0.00000
  7       40100    -deltaJ          0.749( 58)E-03       -0.000E-03
  8       41000    -deltaK         0.02174(298)         -0.00000
 MICROWAVE AVG =       -0.000524 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.060639 MHz, IR RMS =        0.00000
```

D4_wduud SPFIT Output

```
                    EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  7  7  1  6  6  1          10553.27000   10553.31651   -0.04651    0.10000   0.00000
  2:  7  7  1  6  6  1          10553.27000   10553.31651   -0.04651    0.10000   0.00000
  3:  8  4  4  7  3  4          10624.71000   10624.72442   -0.01442    0.10000   0.00000
  4: 10  8  3  9  7  3          14225.14000   14225.03952    0.10048    0.10000   0.00000
  5: 11  6  5 10  5  5          14507.79000   14507.79613   -0.00613    0.10000   0.00000
  6: 11 11  1 10 10  1          16713.22000   16713.13200    0.08800    0.10000   0.00000
  7: 12 11  2 11 10  2          17774.87000   17774.97277   -0.10277    0.10000   0.00000
  8: 14  3 12 13  2 11          12233.38000   12233.32256    0.05744    0.10000   0.00000
  9: 15  0 15 14  0 14          11771.15000   11771.10288    0.04712    0.10000   0.00000   11771.10288    0.04712 0.5000
 10: 15  1 15 14  0 14          11771.15000   11771.10288    0.04712    0.10000   0.00000   11771.10288    0.04712 0.5000
 11: 17  0 17 16  0 16          13298.38000   13298.54150   -0.16150    0.10000   0.00000   13298.54150   -0.16150 0.5000
 12: 17  1 17 16  0 16          13298.38000   13298.54150   -0.16150    0.10000   0.00000   13298.54150   -0.16150 0.5000
 13: 19  0 19 18  0 18          14825.58000   14825.54593    0.03407    0.10000   0.00000   14825.54593    0.03407 0.5000
 14: 19  0 19 18  1 18          14825.58000   14825.54593    0.03407    0.10000   0.00000   14825.54593    0.03407 0.5000
 15: 17  3 14 16  3 13          15137.52000   15137.50815    0.01185    0.10000   0.00000   15137.50817    0.01183 0.5000
 16: 17  4 14 16  3 13          15137.52000   15137.50819    0.01181    0.10000   0.00000   15137.50817    0.01183 0.5000
 17: 18  3 16 17  2 15          15286.92000   15286.82873    0.09127    0.10000   0.00000
 18: 20  2 18 19  2 17          16812.92000   16813.02660   -0.10660    0.10000   0.00000   16813.02660   -0.10660 0.5000
 19: 20  3 18 19  2 17          16812.92000   16813.02660   -0.10660    0.10000   0.00000   16813.02660   -0.10660 0.5000
 20: 23  1 23 22  1 22          17878.09000   17878.04784    0.04216    0.10000   0.00000   17878.04784    0.04216 0.5000
 21: 23  0 23 22  1 22          17878.09000   17878.04784    0.04216    0.10000   0.00000   17878.04784    0.04216 0.5000
NORMALIZED DIAGONAL:
  1 1.00000E+000   2 9.61765E-001   3 2.53278E-001   4 5.76259E-002   5 9.98015E-001   6 8.00406E-003
  7 2.97597E-001   8 7.45278E-001
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                    NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1       10000        A       771.0529( 87)         0.0000
  2       20000        B       623.7929(136)        -0.0000
  3       30000        C       382.2803( 44)         0.0000
  4         200   -DeltaJ        -1.375( 45)E-03       0.000E-03
  5        2000   -DeltaK        -1.734(144)E-03       0.000E-03
  6        1100   -DeltaJK        2.848(182)E-03      -0.000E-03
  7       40100    -deltaJ        0.4463(242)E-03      0.0000E-03
  8       41000    -deltaK        -2.627(230)E-03       0.000E-03
 MICROWAVE AVG =      -0.000805 MHz, IR AVG =       0.00000
 MICROWAVE RMS =       0.076310 MHz, IR RMS =       0.00000
```

D4_wwduu SPFIT Output

```
                          EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  8  3  5  7  2  5              12698.86000   12698.85367    0.00633    0.10000   0.09634
  2:  8  4  5  7  3  5              13383.40000   13383.39430    0.00570    0.10000   0.09703
  3:  8  6  3  7  5  3              14592.76000   14592.75944    0.00056    0.10000   0.09997
  4:  9  2  8  8  1  8              15122.06000   15122.05137    0.00863    0.10000   0.09307
  5:  9  3  7  8  2  7              15003.19000   15003.20991   -0.01991    0.10000   0.05363
  6: 10  3  8  9  3  7              11318.19000   11318.19297   -0.00297    0.10000   0.09921
  7: 12  4  8 11  4  7              15023.42000   15023.41897    0.00103    0.10000   0.09992
  8: 13  4 10 12  3  9              14955.66000   14955.65833    0.00167    0.10000   0.09974
  9: 14  0 14 13  0 13              13605.03000   13605.03023   -0.00023    0.10000   0.09999   13605.03025   -0.00025 0.5000
 10: 14  1 14 13  0 13              13605.03000   13605.03027   -0.00027    0.10000   0.09999   13605.03025   -0.00025 0.5000
NORMALIZED DIAGONAL:
  1 1.00000E+000   2 3.73296E-001   3 1.73101E-001   4 3.16977E-002   5 9.91559E-001   6 5.83192E-003
  7 8.54996E-001   8 5.50536E-001
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                      NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1       10000        A       1049.542( 65)          0.000
  2       20000        B       713.4666(229)         -0.0000
  3       30000        C       472.7719(150)         -0.0000
  4         200    -DeltaJ         -2.08( 36)E-03        0.00E-03
  5        2000    -DeltaK         -6.15(110)E-03        0.00E-03
  6        1100   -DeltaJK          7.70(139)E-03       -0.00E-03
  7       40100    -deltaJ         1.064(229)E-03        0.000E-03
  8       41000    -deltaK         -5.90(112)E-03        0.00E-03
 MICROWAVE AVG =       0.000087 MHz, IR AVG =       0.00000
 MICROWAVE RMS =       0.007865 MHz, IR RMS =       0.00000
```

D4_wwudu SPFIT Output

```
                        EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  7  6  2  6  5  2              12731.46000   12731.46005   -0.00005    0.10000   0.10000
  2: 13  2 11 12  2 10                14663.08000   14663.06127    0.01873    0.10000   0.07066
  3: 13  2 11 12  3 10                14662.49000   14662.50870   -0.01870    0.10000   0.07076
  4: 25  3 23 25  2 24                15415.21000   15415.20998    0.00002    0.10000   0.10000
NORMALIZED DIAGONAL:
  1  1.00000E+000    2  4.12490E-001    3  7.79589E-001
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                    NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1       10000        A       985.4447(102)        -0.0000
  2       20000        B       725.1953( 67)        -0.0000
  3       30000        C       500.20201(278)       -0.00000
 MICROWAVE AVG =      -0.000002 MHz, IR AVG =       0.00000
 MICROWAVE RMS =       0.013233 MHz, IR RMS =       0.00000
```

D4_wwdud SPFIT Output

```
                    EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  6  6  0  5  5  0          11260.56000   11260.77672  -0.21672   0.10000   0.07107   11260.51443   0.04557 0.5000
  2:  6  6  1  5  5  0          11260.56000   11260.25215   0.30785   0.10000   0.07107   11260.51443   0.04557 0.5000
  3:  6  6  1  5  5  1          11262.51000   11262.55602  -0.04602   0.10000   0.07037
  4:  8  7  2  7  6  2          14482.99000   14482.98976   0.00024   0.10000   0.10000
  5:  9  5  5  8  5  4          11755.02000   11755.02025  -0.00025   0.10000   0.10000
  6: 10  2  8  9  3  7           11866.66000   11866.65912   0.00088   0.10000   0.09986
  7: 10  3  7  9  2  7           16413.86000   16413.85962   0.00038   0.10000   0.10000
  8: 10  3  8  9  2  7           11880.92000   11880.92024  -0.00024   0.10000   0.10013
  9: 11  3  8 10  3  7            13576.86000   13576.86057  -0.00057   0.10000   0.09999
 10: 11  4  7 10  3  7            17888.10000   17888.10008  -0.00008   0.10000   0.09999
NORMALIZED DIAGONAL:
  1 1.00000E+000   2 8.37657E-001   3 3.14849E-001   4 1.00222E-001   5 1.20894E-001   6 4.08107E-003
  7 1.62530E-001   8 9.99330E-001
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                    NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1      10000        A       964.962(133)          0.000
  2      20000        B       739.7062(288)         0.0000
  3      30000        C       513.243( 43)          0.000
  4        200   -DeltaJ          1.23(125)E-03      -0.00E-03
  5       2000   -DeltaK          7.0( 40)E-03       -0.0E-03
  6       1100  -DeltaJK          -7.4( 51)E-03       0.0E-03
  7      40100    -deltaJ         -0.98( 70)E-03       0.00E-03
  8      41000    -deltaK          7.3( 57)E-03       -0.0E-03
 MICROWAVE AVG =      -0.000011 MHz, IR AVG =       0.00000
 MICROWAVE RMS =       0.021592 MHz, IR RMS =       0.00000
```

D4_wwuud SPFIT Output

```
                    EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  7  1  6  6  0  6          11872.92000   11872.93144   -0.01144    0.10000   0.09984
  2:  7  2  6  6  1  6          11888.27000   11888.25873    0.01127    0.10000   0.09996
  3:  8  6  3  7  5  3          14584.00000   14583.99985    0.00015    0.10000   0.10000
  4:  9  3  6  8  2  6          14833.87000   14833.86902    0.00098    0.10000   0.09999
  5: 10  1  9  9  1  8          10494.12000   10493.93987    0.18013    0.10000   0.07110
  6: 10  2  8  9  3  7          11262.51000   11262.51681   -0.00681    0.10000   0.09986
  7: 10  2  9  9  1  8          10494.12000   10494.30139   -0.18139    0.10000   0.07067
  8: 12  1 11 11  2 10          12355.83000   12355.81100    0.01900    0.10000   0.10036   12355.82285    0.00715 0.5000
  9: 12  2 11 11  2 10          12355.83000   12355.83471   -0.00471    0.10000   0.10036   12355.82285    0.00715 0.5000
 10: 19  0 19 18  1 18          18092.02000   18092.02072   -0.00072    0.10000   0.09992   18092.02072   -0.00072 0.5000
 11: 19  1 19 18  1 18          18092.02000   18092.02072   -0.00072    0.10000   0.09992   18092.02072   -0.00072 0.5000
NORMALIZED DIAGONAL:
  1 1.00000E+000   2 1.05371E-001   3 2.73420E-001   4 2.76957E-003   5 9.98288E-001   6 2.05202E-004
  7 9.46740E-001   8 5.76492E-001
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                    NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1       10000        A        1045.20( 47)          -0.00
  2       20000        B        727.431(175)           0.000
  3       30000        C        466.294( 43)          -0.000
  4         200    -DeltaJ          -7.0( 37)E-03       -0.0E-03
  5        2000    -DeltaK        -0.0221(143)          -0.0000
  6        1100   -DeltaJK         0.0285(178)          0.0000
  7       40100    -deltaJ          4.12(236)E-03        0.00E-03
  8       41000    -deltaK        -0.0245(155)          -0.0000
 MICROWAVE AVG =      -0.000076 MHz, IR AVG =       0.00000
 MICROWAVE RMS =       0.085443 MHz, IR RMS =       0.00000
```

D4_wuwuu SPFIT Output

```
                    EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  7  2  6  6  1  6          11376.50000   11376.49687    0.00313    0.10000   0.10000
  2:  9  6  4  8  5  4          15855.49000   15855.49275   -0.00275    0.10000   0.10000
  3:  12  3 10 11  3  9           12795.59000   12795.47051    0.11949    0.10000   0.08761
  4:  13  4 10 12  4  9           14433.87000   14433.94520   -0.07520    0.10000   0.09553
  5:  14  3 12 13  2 11           14625.11000   14625.25173   -0.14173    0.10000   0.08420
  6:  16  3 13 15  4 12           17180.91000   17180.79227    0.11773    0.10000   0.09279
  7:  16  4 13 15  3 12           17196.79000   17196.71326    0.07674    0.10000   0.09269
  8:  17  3 14 16  3 13           18097.03000   18096.94928    0.08072    0.10000   0.06703
  9:  17  4 14 16  4 13           18094.00000   18094.18842   -0.18842    0.10000   0.06656
 10:  18  1 17 17  1 16           17527.66000   17527.64577    0.01423    0.10000   0.10033   17527.64597    0.01403 0.5000
 11:  18  2 17 17  1 16           17527.66000   17527.64617    0.01383    0.10000   0.10033   17527.64597    0.01403 0.5000
NORMALIZED DIAGONAL:
  1 1.00000E+000   2 6.14682E-001   3 1.76946E-001   4 2.68423E-003   5 9.38945E-001   6 9.54786E-005
  7 4.23325E-001   8 5.74557E-002
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                    NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1       10000        A        1068.31(184)         -0.01
  2       20000        B         673.87( 55)          0.00
  3       30000        C         457.357( 41)         0.000
  4         200    -DeltaJ         0.0344(113)         0.0000
  5        2000    -DeltaK         0.0505(206)         0.0001
  6        1100   -DeltaJK         -0.086( 32)         -0.000
  7       40100    -deltaJ         -0.0232( 72)        -0.0000
  8       41000    -deltaK          0.0386(168)         0.0001
 MICROWAVE AVG =       0.000374 MHz, IR AVG =       0.00000
 MICROWAVE RMS =       0.100996 MHz, IR RMS =       0.00000
```

D4_wuwdu SPFIT Output

```
                        EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  11  4  8 10  3  8              17354.08000   17354.06345    0.01655    0.10000   0.09997
  2:  13  2 12 12  1 11               12947.63000   12947.03373    0.59627    0.10000   0.05774
  3:  14  1 14 13  0 13               13149.78000   13149.92107   -0.14107    0.10000   0.09813
  4:  15  2 13 14  3 12               15486.79000   15487.18724   -0.39724    0.10000   0.08385
NORMALIZED DIAGONAL:
  1  1.00000E+000    2  3.00086E-002    3  9.82319E-001
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                     NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1       10000        A       1083.57( 61)          0.00
  2       20000        B       656.876(160)         -0.000
  3       30000        C       456.9931( 46)        -0.0000
 MICROWAVE AVG =       0.018629 MHz, IR AVG =       0.00000
 MICROWAVE RMS =       0.365210 MHz, IR RMS =       0.00000
```

D4_wuwud SPFIT Output

```
                        EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  9  2  7  8  1  7              13902.63000   13902.25653    0.37347    0.10000   0.08355
  2:  10  4  7  9  3  7             15719.56000   15719.97422   -0.41422    0.10000   0.08123
  3:  13  3 11 12  2 10              13566.34000   13565.71795    0.62205    0.10000   0.05899
  4:  13  4 10 12  3  9             14576.25000   14575.97043    0.27957    0.10000   0.08521
  5:  15  2 13 14  2 12              15347.45000   15348.17941   -0.72941    0.10000   0.07545
NORMALIZED DIAGONAL:
  1  1.00000E+000    2  6.61543E-001    3  8.66810E-001
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                    NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1       10000        A       1092.6220(217)        -0.0000
  2       20000        B        646.5223( 54)         0.0000
  3       30000        C        452.4241( 34)        -0.0000
 MICROWAVE AVG =       0.026292 MHz, IR AVG =       0.00000
 MICROWAVE RMS =       0.511508 MHz, IR RMS =       0.00000
```

D4_wwuwd SPFIT Output

```
                        EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  5  4  2  4  3  2              13622.12000   13622.12006   -0.00006    0.10000   0.10000
  2:  7  3  5  6  2  5              14741.29000   14741.29754   -0.00754    0.10000   0.09975
  3:  9  2  8  8  2  7              11235.09000   11235.07411    0.01589    0.10000   0.09888
  4:  9  3  7  8  2  7              18073.97000   18073.96185    0.00815    0.10000   0.09971
  5: 10  1 10  9  0  9               11498.95000   11498.94818    0.00182    0.10000   0.09999
  6: 11  2  9 10  3  8               13131.24000   13131.28710   -0.04710    0.10000   0.08965
  7: 12  3 10 11  2  9               16548.29000   16548.33788   -0.04788    0.10000   0.08928
  8: 12  3 10 11  3  9               15434.38000   15434.30002    0.07998    0.10000   0.06587
  9: 14  2 13 13  2 12               16835.51000   16835.51348   -0.00348    0.10000   0.09995
NORMALIZED DIAGONAL:
  1 1.00000E+000   2 1.50716E-001   3 8.76886E-001   4 3.83819E-002   5 3.35732E-001   6 1.09222E-003
  7 9.96737E-001   8 2.57714E-001
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                    NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1       10000        A       1664.241(155)         -0.000
  2       20000        B        750.043( 40)          0.000
  3       30000        C        550.7996( 90)         0.0000
  4         200    -DeltaJ          4.09(276)E-03       0.00E-03
  5        2000    -DeltaK           5.0( 51)E-03        0.0E-03
  6        1100   -DeltaJK          -9.2( 78)E-03       -0.0E-03
  7       40100    -deltaJ         -1.60(150)E-03       -0.00E-03
  8       41000    -deltaK           1.1( 32)E-03        0.0E-03
 MICROWAVE AVG =      -0.000023 MHz, IR AVG =       0.00000
 MICROWAVE RMS =       0.035434 MHz, IR RMS =       0.00000
```

D4_wwwud SPFIT Output

```
                    EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  5  1  4  4  0  4          10900.36000   10900.39500   -0.03500    0.10000   0.09448
  2:  6  4  3  5  3  3          13074.53000   13074.44476    0.08524    0.10000   0.06023
  3:  7  3  4  6  4  3          11953.61000   11953.64074   -0.03074    0.10000   0.09580
  4:  8  3  5  7  2  5          17433.97000   17434.01090   -0.04090    0.10000   0.09234
  5:  8  3  5  7  4  4          13193.78000   13193.72226    0.05774    0.10000   0.09930   13193.76824    0.01176 0.5000
  6:  8  4  5  7  4  4          13193.78000   13193.81421   -0.03421    0.10000   0.09930   13193.76824    0.01176 0.5000
  7:  8  8  0  7  7  0          17682.83000   17682.83084   -0.00084    0.10000   0.09999
  8: 10  3  7  9  3  6          15663.20000   15663.18790    0.01210    0.10000   0.09928   15663.18814    0.01186 0.5000
  9: 10  4  7  9  3  6          15663.20000   15663.18838    0.01162    0.10000   0.09928   15663.18814    0.01186 0.5000
 10: 15  5 11 15  3 12          10856.23000   10856.22655    0.00345    0.10000   0.10002   10856.22655    0.00345 0.5000
 11: 15  5 11 15  4 12          10856.23000   10856.22655    0.00345    0.10000   0.10002   10856.22655    0.00345 0.5000
 12: 18  8 11 18  7 12          10842.81000   10842.81152   -0.00152    0.10000   0.10057
NORMALIZED DIAGONAL:
  1 1.00000E+000   2 1.12460E-002   3 1.56334E-001   4 8.13395E-001   5 2.84001E-001   6 4.86962E-003
  7 9.97725E-001   8 4.70601E-001
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                    NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1       10000        A        1112.59( 78)          0.00
  2       20000        B        1068.93( 68)         -0.00
  3       30000        C       617.9649(246)          0.0000
  4         200   -DeltaJ         -1.059(308)E-03       0.000E-03
  5        2000   -DeltaK          -9.66(170)E-03        0.00E-03
  6        1100  -DeltaJK        0.01032(207)        -0.00000
  7       40100   -deltaJ         -0.0165( 35)          0.0000
  8       41000   -deltaK          -0.0659( 93)          0.0000
 MICROWAVE AVG =       0.000368 MHz, IR AVG =       0.00000
 MICROWAVE RMS =       0.035594 MHz, IR RMS =       0.00000
```

D4_wwdwd SPFIT Output

```
                        EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  9  2  8  8  1  8              18080.84000   18080.84041   -0.00041    0.10000   0.10000
  2:  10  0 10  9  1  9              11865.03000   11864.97617    0.05383    0.10000   0.07198
  3:  10  1 10  9  0  9              11872.92000   11872.97579   -0.05579    0.10000   0.06946
  4:  13  3 11 12  2 10              17374.42000   17374.41821    0.00179    0.10000   0.09997
NORMALIZED DIAGONAL:
  1  1.00000E+000    2  4.38800E-001    3  9.54873E-001
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                    NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1       10000        A       1540.465( 52)         -0.000
  2       20000        B       780.6484(114)          0.0000
  3       30000        C       570.8311( 38)         -0.0000
 MICROWAVE AVG =      -0.000144 MHz, IR AVG =       0.00000
 MICROWAVE RMS =       0.038774 MHz, IR RMS =       0.00000
```

D4_wwwdd SPFIT Output

```
                        EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  7  6  1  6  5  1            15490.73000   15490.61214    0.11786    0.10000   0.06934
  2:  8  3  6  7  2  6            17683.89000   17684.00244   -0.11244    0.10000   0.07385
  3: 10  5  5  9  6  4            17393.62000   17393.61102    0.00898    0.10000   0.05832
  4: 10  5  6  9  4  5            16437.25000   16437.27515   -0.02515    0.10000   0.08270
  5: 10  6  4  9  7  3            17774.87000   17774.84638    0.02362    0.10000   0.09746
NORMALIZED DIAGONAL:
  1  1.00000E+000    2  7.57617E-001    3  9.91303E-001
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                    NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1       10000        A       1169.3579( 67)         0.0000
  2       20000        B       1050.6906( 44)        -0.0000
  3       30000        C        586.4166( 88)         0.0000
 MICROWAVE AVG =       0.002574 MHz, IR AVG =       0.00000
 MICROWAVE RMS =       0.074572 MHz, IR RMS =       0.00000
```

D4_wwdwu SPFIT Output

```
                        EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  6  1  5  5  0  5              11162.50000   11162.37368    0.12632    0.10000   0.08601
  2:  7  3  5  6  2  5              14651.32000   14651.36764   -0.04764    0.10000   0.09813
  3: 12  1 12 11  1 11                 13605.03000   13604.88834    0.14166    0.10000   0.08202
  4: 14  2 12 13  3 11                 17393.62000   17393.77174   -0.15174    0.10000   0.07902
NORMALIZED DIAGONAL:
  1  1.00000E+000    2  8.39711E-001    3  9.98053E-001
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                    NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1       10000        A       1653.2342(247)        -0.0000
  2       20000        B        746.0877( 51)         0.0000
  3       30000        C        547.3222( 36)        -0.0000
 MICROWAVE AVG =       0.017151 MHz, IR AVG =       0.00000
 MICROWAVE RMS =       0.123813 MHz, IR RMS =       0.00000
```

D4_wwuwu SPFIT Output

```
                        EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  6  3  4  5  2  4              12891.14000   12891.15058   -0.01058    0.10000   0.09999
  2: 10  2  9  9  1  8              12718.20000   12718.02126    0.17874    0.10000   0.09755
  3: 10  3  8  9  3  7              13189.64000   13189.11694    0.52306    0.10000   0.07580
  4: 12  3 10 11  3  9              15590.68000   15591.25943   -0.57943    0.10000   0.06904
NORMALIZED DIAGONAL:
  1  1.00000E+000    2  6.24299E-001    3  9.42117E-001
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                    NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1       10000        A       1579.4473(261)        -0.0000
  2       20000        B        763.2353(126)         0.0000
  3       30000        C        557.7811( 49)        -0.0000
 MICROWAVE AVG =       0.027947 MHz, IR AVG =       0.00000
 MICROWAVE RMS =       0.400436 MHz, IR RMS =       0.00000
```

D4_wwwwd SPFIT Output

```
                        EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  3  3  1  2  2  1              10561.49000   10561.45656    0.03344    0.10000   0.09821
  2:  6  1  5  5  2  4              10442.81000   10442.68505    0.12495    0.10000   0.07100
  3:  7  3  5  6  3  4              13309.46000   13309.58143   -0.12143    0.10000   0.07291
  4: 16  4 13 16  2 14                 17176.64000   17176.64243   -0.00243    0.10000   0.09999
NORMALIZED DIAGONAL:
  1  1.00000E+000    2  7.00067E-001    3  5.35856E-001
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                    NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1       10000        A       1911.5654(200)         0.0000
  2       20000        B       1134.5525( 63)        -0.0000
  3       30000        C        747.9365( 55)         0.0000
 MICROWAVE AVG =       0.008631 MHz, IR AVG =       0.00000
 MICROWAVE RMS =       0.088713 MHz, IR RMS =       0.00000
```

D4_wwwwd' SPFIT Output

```
                        EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  4  3  2  3  2  2              12455.04000   12454.99132    0.04868    0.10000   0.09867
  2:  7  2  5  6  3  4              12355.84000   12355.86782   -0.02782    0.10000   0.09957
  3: 12  2 10 12  1 11                 13164.88000   13165.09418   -0.21418    0.10000   0.06979
  4: 13  3 10 13  2 11                 12718.21000   12718.00894    0.20106    0.10000   0.07403
NORMALIZED DIAGONAL:
  1  1.00000E+000    2  8.83191E-001    3  3.72474E-001
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                    NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1       10000        A       1864.6016(183)         0.0000
  2       20000        B       1154.0660( 62)         0.0000
  3       30000        C        766.6754( 74)         0.0000
 MICROWAVE AVG =       0.001936 MHz, IR AVG =       0.00000
 MICROWAVE RMS =       0.149537 MHz, IR RMS =       0.00000
```

D4_wwwwu SPFIT Output

		EXP.FREQ.	- CALC.FREQ.	- DIFF.	- EXP.ERR.	- EST.ERR.	-AVG. CALC.FREQ.	- DIFF.	- WT.
1:	4 1 3 3 0 3		10442.81000	10442.91486	-0.10486	0.10000			0.09505
2:	4 4 0 3 3 0		14550.84000	14550.77842	0.06158	0.10000			0.09832
3:	7 1 6 6 1 5		12449.21000	12449.41991	-0.20991	0.10000			0.07831
4:	7 1 6 6 2 5		11985.73000	11985.49526	0.23474	0.10000			0.07187

NORMALIZED DIAGONAL:

1 1.00000E+000 2 9.20356E-001 3 9.93595E-001

MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00

			NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
1	10000	A	1945.6061(142) 0.0000
2	20000	B	1113.5160(102) -0.0000
3	30000	C	732.6576(77) 0.0000

MICROWAVE AVG = -0.004613 MHz, IR AVG = 0.00000

MICROWAVE RMS = 0.168786 MHz, IR RMS = 0.00000

D2O_wdudu SPFIT Output

```
                    EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  7  4  4  6  3  4          10701.77000   10701.76973    0.00027    0.10000   0.00000
  2:  7  4  4  6  3  4          10701.77000   10701.76973    0.00027    0.10000   0.00000
  3:  8  6  3  7  5  3          12705.98000   12705.99022   -0.01022    0.10000   0.00000
  4:  9  6  4  8  5  4          13952.61000   13952.58894    0.02106    0.10000   0.00000
  5:  9  8  2  8  7  2          15025.84000   15025.84027   -0.00027    0.10000   0.00000
  6: 10  6  5  9  5  5          15262.50000   15262.51275   -0.01275    0.10000   0.00000
  7: 11  1 10 10  1  9          11128.03000   11127.98108    0.04892    0.10000   0.00000   11127.98555    0.04445 0.5000
  8: 11  2 10 10  1  9          11128.03000   11127.99001    0.03999    0.10000   0.00000   11127.98555    0.04445 0.5000
  9: 14  0 14 13  0 13          13306.15000   13306.15252   -0.00252    0.10000   0.00000   13306.15252   -0.00252 0.5000
 10: 14  1 14 13  0 13          13306.15000   13306.15252   -0.00252    0.10000   0.00000   13306.15252   -0.00252 0.5000
 11: 14  1 13 13  1 12          13912.51000   13912.56045   -0.05045    0.10000   0.00000   13912.56048   -0.05048 0.5000
 12: 14  2 13 13  1 12          13912.51000   13912.56052   -0.05052    0.10000   0.00000   13912.56048   -0.05048 0.5000
 13: 17  3 14 16  3 13          17912.49000   17912.48163    0.00837    0.10000   0.00000   17912.48259    0.00741 0.5000
 14: 17  4 14 16  3 13          17912.49000   17912.48354    0.00646    0.10000   0.00000   17912.48259    0.00741 0.5000
 15: 19  0 19 18  0 18          17945.32000   17945.31235    0.00765    0.10000   0.00000   17945.31235    0.00765 0.5000
 16: 19  1 19 18  0 18          17945.32000   17945.31235    0.00765    0.10000   0.00000   17945.31235    0.00765 0.5000
NORMALIZED DIAGONAL:
  1 1.00000E+000   2 2.23809E-001   3 2.81865E-001   4 3.34117E-002   5 9.97202E-001   6 1.44996E-003
  7 8.83935E-001   8 5.65206E-001
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                    NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1      10000        A       882.460(100)          0.000
  2      20000        B       684.232( 68)         -0.000
  3      30000        C       464.5505( 75)         0.0000
  4        200   -DeltaJ         1.462(309)E-03       0.000E-03
  5       2000   -DeltaK          4.84(179)E-03       0.00E-03
  6       1100   -DeltaJK        -6.68(209)E-03       -0.00E-03
  7      40100    -deltaJ        -1.813(309)E-03       0.000E-03
  8      41000    -deltaK         6.64(197)E-03       0.00E-03
 MICROWAVE AVG =       0.000443 MHz, IR AVG =       0.00000
 MICROWAVE RMS =       0.022065 MHz, IR RMS =       0.00000
```

D2O_wuduu SPFIT Output

```
                    EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  7  6  2  6  5  2          11601.34000  11601.35505  -0.01505   0.10000  0.06431
  2:  7  6  2  6  5  2          11601.34000  11601.35505  -0.01505   0.10000  0.06431
  3:  7  7  1  6  6  1          12194.86000  12194.85713   0.00287   0.10000  0.09993
  4:  8  5  4  7  4  4          12387.75000  12387.75328  -0.00328   0.10000  0.09967
  5:  8  7  2  7  6  2          13380.26000  13380.21729   0.04271   0.10000  0.05405
  6:  9  8  2  8  7  2          15162.50000  15162.51739  -0.01739   0.10000  0.09414
  7: 11  0 11 10  0 10            10287.48000  10287.48634  -0.00634   0.10000  0.09965  10287.48639  -0.00639 0.5000
  8: 11  1 11 10  0 10            10287.48000  10287.48643  -0.00643   0.10000  0.09965  10287.48639  -0.00639 0.5000
  9: 14  2 12 13  2 11            14289.15000  14289.09977   0.05023   0.10000  0.06426  14289.10204   0.04796 0.5000
 10: 14  3 12 13  2 11             14289.15000  14289.10431   0.04569   0.10000  0.06426  14289.10204   0.04796 0.5000
 11: 15  1 14 14  1 13             14550.83000  14550.86443  -0.03443   0.10000  0.08006  14550.86443  -0.03443 0.5000
 12: 15  2 14 14  1 13             14550.83000  14550.86444  -0.03444   0.10000  0.08006  14550.86443  -0.03443 0.5000
 13: 17  3 14 16  3 13             17650.81000  17650.82052  -0.01052   0.10000  0.09857  17650.82148  -0.01148 0.5000
 14: 17  4 14 16  3 13             17650.81000  17650.82245  -0.01245   0.10000  0.09857  17650.82148  -0.01148 0.5000
 15: 19  0 19 18  0 18             17530.50000  17530.49251   0.00749   0.10000  0.09919  17530.49251   0.00749 0.5000
 16: 19  1 19 18  0 18             17530.50000  17530.49251   0.00749   0.10000  0.09919  17530.49251   0.00749 0.5000
NORMALIZED DIAGONAL:
  1 1.00000E+000   2 6.29442E-001   3 2.60863E-001   4 2.90979E-002   5 7.49267E-001   6 2.60250E-003
  7 1.32050E-001   8 9.98264E-001
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                    NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1       10000         A        893.0982(207)          0.0000
  2       20000         B         685.617( 59)         -0.000
  3       30000         C        453.1270( 94)          0.0000
  4         200    -DeltaJ         -1.692(295)E-03       0.000E-03
  5        2000    -DeltaK        -0.01174( 88)         0.00000
  6        1100   -DeltaJK         0.01313(116)        -0.00000
  7       40100    -deltaJ          2.861(173)E-03       0.000E-03
  8       41000    -deltaK        -0.01926( 84)         0.00000
 MICROWAVE AVG =       -0.000187 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.023956 MHz, IR RMS =        0.00000
```

D2O_wuudu SPFIT Output

```
                    EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  7  5  3  6  4  3          11070.57000   11070.53861    0.03139    0.10000   0.00000
  2:  7  5  3  6  4  3          11070.57000   11070.53861    0.03139    0.10000   0.00000
  3:  8  5  4  7  4  4          12422.21000   12422.23853   -0.02853    0.10000   0.00000
  4:  9  7  3  8  6  3          14511.28000   14511.33349   -0.05349    0.10000   0.00000
  5: 11  8  4 10  7  4           17479.59000   17479.56221    0.02779    0.10000   0.00000
  6: 13  2 11 12  2 10           13334.29000   13334.28483    0.00517    0.10000   0.00000   13334.28842    0.00158 0.5000
  7: 13  3 11 12  2 10           13334.29000   13334.29200   -0.00200    0.10000   0.00000   13334.28842    0.00158 0.5000
  8: 14  3 12 13  2 11           14232.16000   14232.05701    0.10299    0.10000   0.00000
  9: 15  3 12 14  3 11           15790.92000   15791.07577   -0.15577    0.10000   0.00000   15791.08205   -0.16205 0.5000
 10: 15  4 12 14  3 11           15790.92000   15791.08833   -0.16833    0.10000   0.00000   15791.08205   -0.16205 0.5000
 11: 16  4 12 15  4 11           17353.44000   17353.34249    0.09751    0.10000   0.00000   17353.38390    0.05610 0.5000
 12: 16  5 12 15  4 11           17353.44000   17353.42531    0.01469    0.10000   0.00000   17353.38390    0.05610 0.5000
 13: 17  0 17 16  0 16           15608.95000   15608.97472   -0.02472    0.10000   0.00000   15608.97472   -0.02472 0.5000
 14: 17  1 17 16  0 16           15608.95000   15608.97472   -0.02472    0.10000   0.00000   15608.97472   -0.02472 0.5000
 15: 18  1 17 17  1 16           17162.52000   17162.49467    0.02533    0.10000   0.00000   17162.49467    0.02533 0.5000
 16: 18  2 17 17  1 16           17162.52000   17162.49467    0.02533    0.10000   0.00000   17162.49467    0.02533 0.5000
NORMALIZED DIAGONAL:
  1 1.00000E+000   2 3.33326E-001   3 1.67519E-001   4 6.62688E-002   5 6.67432E-001   6 7.54276E-004
  7 1.17272E-001   8 9.99775E-001
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                    NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1       10000         A         884.948( 40)          -0.000
  2       20000         B         697.458( 60)           0.000
  3       30000         C         449.724( 38)          -0.000
  4         200    -DeltaJ          -6.67( 87)E-03       -0.00E-03
  5        2000    -DeltaK          -0.0253( 32)         -0.0000
  6        1100   -DeltaJK           0.0314( 41)          0.0000
  7       40100    -deltaJ           1.374(165)E-03       -0.000E-03
  8       41000    -deltaK          -0.0329( 33)         -0.0000
 MICROWAVE AVG =       0.000708 MHz, IR AVG =       0.00000
 MICROWAVE RMS =       0.065843 MHz, IR RMS =       0.00000
```

D2O_wudud SPFIT Output

```
                    EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  6  6  1  5  5  1          10381.55000   10381.55628   -0.00628    0.10000   0.00000
  2:  6  6  1  5  5  1          10381.55000   10381.55628   -0.00628    0.10000   0.00000
  3:  7  5  2  6  4  2          10840.27000   10840.25856    0.01144    0.10000   0.00000
  4: 10  3  8  9  2  8          15241.84000   15241.85202   -0.01202    0.10000   0.00000
  5: 10 10  1  9  9  1          17501.95000   17501.94891    0.00109    0.10000   0.00000
  6: 11  2  9 10  2  8          11667.18000   11667.13430    0.04570    0.10000   0.00000
  7: 12  1 11 11  1 10          11966.27000   11966.18021    0.08979    0.10000   0.00000   11966.18146    0.08854 0.5000
  8: 12  2 11 11  1 10          11966.27000   11966.18271    0.08729    0.10000   0.00000   11966.18146    0.08854 0.5000
  9: 14  0 14 13  0 13          13194.46000   13194.67774   -0.21774    0.10000   0.00000   13194.67774   -0.21774 0.5000
 10: 14  1 14 13  0 13          13194.46000   13194.67774   -0.21774    0.10000   0.00000   13194.67774   -0.21774 0.5000
 11: 15  1 14 14  1 13          14728.08000   14728.08803   -0.00803    0.10000   0.00000   14728.08804   -0.00804 0.5000
 12: 15  2 14 14  1 13          14728.08000   14728.08805   -0.00805    0.10000   0.00000   14728.08804   -0.00804 0.5000
 13: 16  0 16 15  0 15          15037.50000   15037.36128    0.13872    0.10000   0.00000   15037.36128    0.13872 0.5000
 14: 16  1 16 15  0 15          15037.50000   15037.36128    0.13872    0.10000   0.00000   15037.36128    0.13872 0.5000
 15: 17  2 15 16  2 14          17185.87000   17185.89998   -0.02998    0.10000   0.00000   17185.90000   -0.03000 0.5000
 16: 17  3 15 16  2 14          17185.87000   17185.90002   -0.03002    0.10000   0.00000   17185.90000   -0.03000 0.5000
NORMALIZED DIAGONAL:
  1 1.00000E+000   2 7.96420E-001   3 2.35539E-001   4 3.43229E-002   5 5.97360E-001   6 1.69438E-003
  7 3.85199E-001   8 9.98626E-001
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                    NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1       10000        A       890.2716(151)        -0.0000
  2       20000        B        678.500( 81)         0.000
  3       30000        C       460.1564( 70)        -0.0000
  4         200   -DeltaJ          7.92( 58)E-03      -0.00E-03
  5        2000   -DeltaK        0.01910(157)        -0.00000
  6        1100  -DeltaJK       -0.02651(214)         0.00000
  7       40100   -deltaJ         4.154(293)E-03      -0.001E-03
  8       41000   -deltaK          8.92(121)E-03      -0.00E-03
 MICROWAVE AVG =       0.000466 MHz, IR AVG =       0.00000
 MICROWAVE RMS =       0.084154 MHz, IR RMS =       0.00000
```

D2O_wduud SPFIT Output

```
                    EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  6  6  1  5  5  1          10196.97000  10196.96408   0.00592   0.10000  0.00000
  2:  6  6  1  5  5  1          10196.97000  10196.96408   0.00592   0.10000  0.00000
  3:  7  6  1  6  5  1          11386.19000  11386.25401  -0.06401   0.10000  0.00000
  4:  9  4  5  8  3  5          14012.49000  14012.66948  -0.17948   0.10000  0.00000
  5: 10  4  7  9  3  7          15732.91000  15732.74497   0.16503   0.10000  0.00000
  6: 10  2  8  9  2  7          10537.67000  10537.73617  -0.06617   0.10000  0.00000  10537.76535  -0.09535 0.5000
  7: 10  3  8  9  2  7          10537.67000  10537.79453  -0.12453   0.10000  0.00000  10537.76535  -0.09535 0.5000
  8: 10 10  0  9  9  1          17158.17000  17158.19347  -0.02347   0.10000  0.00000  17158.16295   0.00705 0.5000
  9: 10 10  1  9  9  1          17158.17000  17158.13243   0.03757   0.10000  0.00000  17158.16295   0.00705 0.5000
 10: 11  1 10 10  1  9          10708.08000  10707.93947   0.14053   0.10000  0.00000  10707.93953   0.14047 0.5000
 11: 11  2 10 10  1  9          10708.08000  10707.93959   0.14041   0.10000  0.00000  10707.93953   0.14047 0.5000
 12: 11  6  5 10  5  5          16847.37000  16847.33163   0.03837   0.10000  0.00000
 13: 11  8  4 10  7  4          17476.25000  17476.24431   0.00569   0.10000  0.00000
 14: 13  0 13 12  0 12          11757.49000  11757.54124  -0.05124   0.10000  0.00000  11757.54124  -0.05124 0.5000
 15: 13  1 13 12  0 12          11757.49000  11757.54124  -0.05124   0.10000  0.00000  11757.54124  -0.05124 0.5000
 16: 12  2 10 11  2  9          12291.31000  12291.24261   0.06739   0.10000  0.00000  12291.24325   0.06675 0.5000
 17: 12  3 10 11  2  9          12291.31000  12291.24388   0.06612   0.10000  0.00000  12291.24325   0.06675 0.5000
 18: 14  4 10 13  4  9          15465.46000  15465.53382  -0.07382   0.10000  0.00000
 19: 17  1 17 16  1 16          15265.45000  15265.44391   0.00609   0.10000  0.00000  15265.44391   0.00609 0.5000
 20: 17  0 17 16  1 16          15265.45000  15265.44391   0.00609   0.10000  0.00000  15265.44391   0.00609 0.5000
NORMALIZED DIAGONAL:
  1 1.00000E+000   2 3.21935E-001   3 3.01146E-001   4 1.52053E-001   5 9.98102E-001   6 2.51728E-002
  7 9.23968E-001   8 8.39123E-001
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                    NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1       10000        A       870.1694( 96)         0.0000
  2       20000        B       725.4836(132)        -0.0000
  3       30000        C       438.7370( 66)        -0.0000
  4         200   -DeltaJ         1.577( 44)E-03       0.000E-03
  5        2000   -DeltaK         1.080(139)E-03       0.000E-03
  6        1100   -DeltaJK       -2.873(176)E-03      -0.000E-03
  7       40100    -deltaJ        0.1684(300)E-03      0.0000E-03
  8       41000    -deltaK         0.569(257)E-03       0.000E-03
 MICROWAVE AVG =      -0.001614 MHz, IR AVG =       0.00000
 MICROWAVE RMS =       0.087244 MHz, IR RMS =       0.00000
```

D2O_wuwdu SPFIT Output

```
                          EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  7  3  5  6  2  5              12530.46000   12530.47407   -0.01407    0.10000   0.09765
  2:  8  5  4  7  4  4              14973.30000   14973.30079   -0.00079    0.10000   0.09999
  3: 10  0 10  9  1  9               10598.68000   10598.67935    0.00065    0.10000   0.06692
  4: 10  1  9  9  1  8               11397.00000   11397.00143   -0.00143    0.10000   0.09996
  5: 10  1 10  9  1  9               10598.68000   10598.71048   -0.03048    0.10000   0.06693
  6: 10  4  7  9  3  7               17720.95000   17720.93813    0.01187    0.10000   0.09834
  7: 11  2 10 10  2  9               12412.62000   12412.56993    0.05007    0.10000   0.06425
  8: 11  3  8 10  4  7               13721.76000   13721.76894   -0.00894    0.10000   0.09906
  9: 14  3 11 13  4 10               17061.02000   17061.00504    0.01496    0.10000   0.09734
 10: 14  4 11 13  3 10               17108.54000   17108.56593   -0.02593    0.10000   0.09181
NORMALIZED DIAGONAL:
  1 1.00000E+000   2 6.46371E-001   3 5.68982E-001   4 2.68956E-002   5 1.20171E-001   6 8.48027E-004
  7 1.39626E-001   8 9.78173E-001
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                        NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1       10000        A        1153.38( 36)          -0.00
  2       20000        B         753.831(130)          0.000
  3       30000        C         510.3192(241)        -0.0000
  4         200    -DeltaJ        -0.0203( 33)         0.0000
  5        2000    -DeltaK        -0.0402( 65)         0.0000
  6        1100   -DeltaJK         0.0592( 97)        -0.0000
  7       40100    -deltaJ         0.01312(224)        -0.00000
  8       41000    -deltaK        -0.0351( 57)         0.0000
 MICROWAVE AVG =      -0.000410 MHz, IR AVG =       0.00000
 MICROWAVE RMS =       0.021805 MHz, IR RMS =       0.00000
```

D2O_wwduu SPFIT Output

```
                        EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  6  5  2  5  4  2              11938.32000   11938.32000    0.00000    0.10000   0.10000
  2:  11  0 11 10  1 10               11772.76000   11772.70993    0.05007    0.10000   0.07071
  3:  11  1 11 10  1 10               11772.66000   11772.71007   -0.05007    0.10000   0.07071
  4:  13  4  9 12  5  8              17162.51000   17162.51000   -0.00000    0.10000   0.10000
NORMALIZED DIAGONAL:
  1  1.00000E+000    2  6.60643E-001    3  9.76639E-001
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                    NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1       10000        A       1092.7203(141)        -0.0000
  2       20000        B        814.5854(195)         0.0000
  3       30000        C        516.2677( 37)        -0.0000
 MICROWAVE AVG =       0.000000 MHz, IR AVG =       0.00000
 MICROWAVE RMS =       0.035407 MHz, IR RMS =       0.00000
```

D2O_wuwuu SPFIT Output

```
                    EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  6  2  5  5  1  5          10893.86000   10893.87163   -0.01163    0.10000   0.09941
  2:  9  3  6  8  2  6          15732.90000   15732.89499    0.00501    0.10000   0.09990
  3: 10  2  9  9  1  8           11357.45000   11357.48563   -0.03563    0.10000   0.09446
  4: 11  0 11 10  0 10             11546.44000   11546.44918   -0.00918    0.10000   0.09955   11546.45054   -0.01054 0.5000
  5: 11  1 11 10  0 10             11546.44000   11546.45189   -0.01189    0.10000   0.09955   11546.45054   -0.01054 0.5000
  6: 12  3  9 11  3  8            15091.55000   15091.51461    0.03539    0.10000   0.09444
  7: 13  3 11 12  2 10             15214.14000   15214.06358    0.07642    0.10000   0.07085
  8: 14  3 11 13  3 10             17062.51000   17062.56294   -0.05294    0.10000   0.08679
  9: 14  3 11 13  4 10             17049.37000   17049.38277   -0.01277    0.10000   0.10010
NORMALIZED DIAGONAL:
  1 1.00000E+000   2 6.45859E-001   3 1.49703E-001   4 5.84292E-003   5 7.71266E-001   6 8.31505E-007
  7 9.49613E-002   8 3.59432E-001
MARQUARDT PARAMETER = 9.08602e-009, TRUST EXPANSION = 1.00
                    NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1       10000        A        1139.53(107)         -0.01
  2       20000        B         770.44( 34)          0.00
  3       30000        C         506.478( 60)         0.000
  4         200    -DeltaJ        -0.0201(199)         0.0002
  5        2000    -DeltaK         -0.027( 44)         0.000
  6        1100   -DeltaJK          0.046( 64)        -0.000
  7       40100    -deltaJ         0.0152(123)        -0.0001
  8       41000    -deltaK         -0.025( 41)         0.000
 MICROWAVE AVG =      -0.000837 MHz, IR AVG =       0.00000
 MICROWAVE RMS =       0.038078 MHz, IR RMS =       0.00000
```

D2O_wwuud SPFIT Output

```
                    EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  7  3  4  6  2  4          12651.48000   12651.51809   -0.03809    0.10000   0.09503
  2:  7  4  4  6  3  4          13071.99000   13072.02354   -0.03354    0.10000   0.09617
  3:  8  8  0  7  7  1          16941.23000   16941.28234   -0.05234    0.10000   0.09999   16941.22798    0.00202 0.5000
  4:  8  8  1  7  7  1          16941.23000   16941.17363    0.05637    0.10000   0.09999   16941.22798    0.00202 0.5000
  5:  9  2  7  8  1  7          16789.62000   16789.56197    0.05803    0.10000   0.08804
  6:  9  4  6  8  3  5          12411.50000   12411.50616   -0.00616    0.10000   0.09987
  7: 10  1  9  9  1  8          11490.78000   11490.71651    0.06349    0.10000   0.09053   11490.72804    0.05196 0.5000
  8: 10  2  9  9  1  8          11490.78000   11490.73956    0.04044    0.10000   0.09053   11490.72804    0.05196 0.5000
  9: 11  8  4 10  8  3          15808.85000   15808.84232    0.00768    0.10000   0.09979
 10: 12  4  9 11  3  8          15265.42000   15265.49504   -0.07504    0.10000   0.07906
 11: 13  5  9 12  5  8          17151.97000   17151.94577    0.02423    0.10000   0.09789
NORMALIZED DIAGONAL:
  1 1.00000E+000   2 1.08222E-001   3 5.53102E-001   4 1.55535E-001   5 2.12711E-001   6 1.29948E-002
  7 9.70338E-001   8 8.14517E-001
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                    NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1       10000        A       1083.029( 64)          0.000
  2       20000        B        831.529( 44)         -0.000
  3       30000        C        510.1725(277)         0.0000
  4         200    -DeltaJ         0.152(154)E-03       0.000E-03
  5        2000    -DeltaK          5.47( 90)E-03       0.00E-03
  6        1100   -DeltaJK         -5.50(108)E-03       -0.00E-03
  7       40100    -deltaJ         2.118(280)E-03       0.000E-03
  8       41000    -deltaK          1.90( 96)E-03       0.00E-03
 MICROWAVE AVG =      -0.000990 MHz, IR AVG =       0.00000
 MICROWAVE RMS =       0.040773 MHz, IR RMS =       0.00000
```

D2O_wwdud SPFIT Output

		EXP.FREQ.	- CALC.FREQ.	- DIFF.	- EXP.ERR.	- EST.ERR.	-AVG. CALC.FREQ.	- DIFF.	- WT.
1:	7 3 4 6 2 4		12562.03000	12562.07628	-0.04628	0.10000			0.09820
2:	8 2 6 7 3 5		10670.29000	10670.08713	0.20287	0.10000			0.05674
3:	9 1 9 8 0 8		10318.42000	10318.55124	-0.13124	0.10000			0.08463
4:	9 8 2 8 7 2		17508.18000	17508.19305	-0.01305	0.10000			0.09986

NORMALIZED DIAGONAL:

1 1.00000E+000 2 9.38376E-001 3 9.93248E-001

MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00

			NEW PARAMETER (EST. ERROR)	-- CHANGE THIS ITERATION
1	10000	A	1021.4800(72)	-0.0000
2	20000	B	838.8022(76)	0.0000
3	30000	C	552.9136(50)	0.0000

MICROWAVE AVG = 0.003076 MHz, IR AVG = 0.00000

MICROWAVE RMS = 0.123177 MHz, IR RMS = 0.00000

D2O_wwudu SPFIT Output

```
                        EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  8  2  7  7  1  7              14653.17000   14652.86267    0.30733    0.10000   0.07084
  2:  8  4  5  7  3  5              14550.80000   14551.06178   -0.26178    0.10000   0.06897
  3: 10  4  7  9  3  6              13527.60000   13527.40895    0.19105    0.10000   0.06402
  4: 10  5  6  9  4  5              14686.63000   14686.75974   -0.12974    0.10000   0.08627
  5: 12  5  7 11  6  6              16855.37000   16855.45141   -0.08141    0.10000   0.09324
NORMALIZED DIAGONAL:
  1  1.00000E+000    2  9.83032E-001    3  8.14042E-001
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                    NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1       10000        A       1040.1180( 91)        -0.0000
  2       20000        B        826.1940( 43)         0.0000
  3       30000        C        540.7627( 58)         0.0000
 MICROWAVE AVG =       0.005091 MHz, IR AVG =       0.00000
 MICROWAVE RMS =       0.211158 MHz, IR RMS =       0.00000
```

D2O_wuwud SPFIT Output

```
                        EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  9  2  7  8  1  7              15808.85000   15808.62664    0.22336    0.10000   0.08631
  2:  10  2  9  9  1  9              17888.73000   17888.92577   -0.19577    0.10000   0.08956
  3:  12  3  9 11  3  8              15053.12000   15052.89176    0.22824    0.10000   0.08556
  4:  12  4  9 11  4  8              14889.22000   14889.45241   -0.23241    0.10000   0.08499
NORMALIZED DIAGONAL:
  1  1.00000E+000    2  3.18339E-001    3  9.58917E-001
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                    NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1       10000        A       1160.514( 44)         -0.000
  2       20000        B       744.3230(118)          0.0000
  3       30000        C       505.7563( 53)         0.0000
 MICROWAVE AVG =       0.005855 MHz, IR AVG =       0.00000
 MICROWAVE RMS =       0.220408 MHz, IR RMS =       0.00000
```

D2O_wwwdu SPFIT Output

```
                    EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  6  4  3  5  3  2          11310.52000   11310.52073   -0.00073    0.10000   0.09723
  2:  7  5  3  6  5  2          13012.87000   13012.87167   -0.00167    0.10000   0.09405
  3:  7  6  2  6  6  1          13306.18000   13306.17961    0.00039    0.10000   0.09987
  4:  7  7  1  6  6  0          16279.02000   16279.01996    0.00004    0.10000   0.10000
  5:  8  3  5  7  3  4          13527.60000   13527.59011    0.00989    0.10000   0.05349
  6:  8  4  5  7  3  4          13529.70000   13529.70641   -0.00641    0.10000   0.05287
  7:  9  2  7  8  2  6          13739.83000   13739.83030   -0.00030    0.10000   0.07975   13739.83216   -0.00216 0.5000
  8:  9  3  7  8  2  6          13739.83000   13739.83403   -0.00403    0.10000   0.07975   13739.83216   -0.00216 0.5000
  9:  9  6  4  8  6  3          16667.62000   16667.61948    0.00052    0.10000   0.09886
 10: 17  5 12 17  4 13             12641.72000   12641.72025   -0.00025    0.10000   0.09974   12641.72025   -0.00025 0.5000
 11: 17  5 12 17  5 13             12641.72000   12641.72025   -0.00025    0.10000   0.09974   12641.72025   -0.00025 0.5000
 12: 18  7 12 18  6 13             12626.97000   12626.96990    0.00010    0.10000   0.09995
NORMALIZED DIAGONAL:
  1 1.00000E+000   2 3.69807E-001   3 1.73616E-001   4 9.21532E-001   5 8.82758E-002   6 1.44566E-002
  7 9.69919E-001   8 2.81731E-001
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                    NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1       10000        A       1183.0933(253)         -0.0000
  2       20000        B       1081.6496(154)          0.0000
  3       30000        C        622.563( 32)           0.000
  4         200    -DeltaJ        -0.831(108)E-03       0.000E-03
  5        2000    -DeltaK         0.75( 43)E-03        0.00E-03
  6        1100   -DeltaJK         -1.63( 59)E-03       -0.00E-03
  7       40100    -deltaJ        -0.041(133)E-03       -0.000E-03
  8       41000    -deltaK         2.64(177)E-03        0.00E-03
 MICROWAVE AVG =      -0.000028 MHz, IR AVG =       0.00000
 MICROWAVE RMS =       0.003840 MHz, IR RMS =       0.00000
```

D2O_wwwud SPFIT Output

```
                        EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  5  4  2  4  3  2              11306.15000   11306.16582  -0.01582    0.10000   0.09063
  2:  6  3  4  5  2  4              13492.19000   13492.22664  -0.03664    0.10000   0.06446
  3:  6  5  2  5  4  2              13588.95000   13588.92191   0.02809    0.10000   0.07647
  4:  7  3  4  6  2  4              15720.95000   15720.96541  -0.01541    0.10000   0.08588
  5:  7  3  5  6  2  5              15744.73000   15744.69388   0.03612    0.10000   0.08095
  6:  8  4  5  7  3  4              13607.72000   13607.71416   0.00584    0.10000   0.09883
  7:  8  7  2  7  7  1              15368.90000   15368.89917   0.00083    0.10000   0.09999
  8:  9  4  6  8  4  5              14866.67000   14866.66565   0.00435    0.10000   0.09499
  9:  9  6  4  8  5  3              17131.25000   17131.25493  -0.00493    0.10000   0.09926
 10: 10  5  6  9  5  5               17122.14000   17122.14627  -0.00627    0.10000   0.09598
NORMALIZED DIAGONAL:
  1 1.00000E+000   2 9.70756E-001   3 7.31932E-001   4 1.64318E-001   5 1.39172E-001   6 1.68451E-002
  7 5.93207E-002   8 9.93737E-001
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                        NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1       10000        A       1173.543(108)         -0.000
  2       20000        B       1082.289( 91)          0.000
  3       30000        C        634.443( 42)          0.000
  4         200   -DeltaJ         -4.41( 60)E-03       0.00E-03
  5        2000   -DeltaK         -6.03(180)E-03       0.00E-03
  6        1100  -DeltaJK        0.01573(229)        -0.00000
  7       40100   -deltaJ          3.08(102)E-03       -0.00E-03
  8       41000   -deltaK        -0.0372( 53)          0.0000
 MICROWAVE AVG =      -0.000384 MHz, IR AVG =       0.00000
 MICROWAVE RMS =       0.020103 MHz, IR RMS =       0.00000
```

D2O_wwuwd SPFIT Output

```
                        EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  5  3  2  4  2  2              11178.25000   11178.18122    0.06878    0.10000   0.04782
  2:  7  5  3  6  4  3              17693.38000   17693.41710   -0.03710    0.10000   0.08757
  3:  8  1  7  7  1  6              11013.60000   11013.60971   -0.00971    0.10000   0.04154
  4:  8  1  7  7  2  6              10720.68000   10720.68679   -0.00679    0.10000   0.08944
  5: 10  1  9  9  2  8              13231.82000   13231.81126    0.00874    0.10000   0.05428
  6: 11  0 11 10  0 10                13428.63000   13428.63357   -0.00357    0.10000   0.08583
NORMALIZED DIAGONAL:
  1  1.00000E+000    2  5.97641E-001    3  9.82898E-001
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                    NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1       10000        A       1560.5497(118)         -0.0000
  2       20000        B        850.2716(208)          0.0000
  3       30000        C        587.3559( 47)         -0.0000
 MICROWAVE AVG =       0.003391 MHz, IR AVG =       0.00000
 MICROWAVE RMS =       0.032499 MHz, IR RMS =       0.00000
```

D2O_wwwdd SPFIT Output

		EXP.FREQ.	- CALC.FREQ.	- DIFF.	- EXP.ERR.	- EST.ERR.	-AVG. CALC.FREQ.	- DIFF.	- WT.
1:	6 6 0 5 5 1		14317.78000	14317.73173	0.04827	0.10000			0.09266
2:	7 5 2 6 3 3		17708.24000	17708.31046	-0.07046	0.10000			0.08359
3:	8 3 5 7 4 4		13409.81000	13409.86928	-0.05928	0.10000			0.08870
4:	9 6 3 8 6 2		17945.29000	17945.21469	0.07531	0.10000			0.08098

NORMALIZED DIAGONAL:

1 1.00000E+000 2 9.73228E-001 3 9.99177E-001

MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00

			NEW PARAMETER (EST. ERROR)	-- CHANGE THIS ITERATION
1	10000	A	1212.9260(94)	0.0000
2	20000	B	1076.7211(44)	-0.0000
3	30000	C	603.7366(97)	0.0000

MICROWAVE AVG = -0.001538 MHz, IR AVG = 0.00000

MICROWAVE RMS = 0.064187 MHz, IR RMS = 0.00000

D2O_wwuwu SPFIT Output

		EXP.FREQ.	CALC.FREQ.	DIFF.	EXP.ERR.	EST.ERR.-AVG.	CALC.FREQ. - DIFF.	WT.
1:	5 3 3 4 2 3	11484.15000	11484.49164	-0.34164	0.10000			0.07150
2:	5 4 2 4 3 2	12753.26000	12753.00837	0.25163	0.10000			0.08569
3:	8 3 6 7 3 5	11645.70000	11645.84033	-0.14033	0.10000			0.09583
4:	8 5 4 7 5 3	11943.55000	11943.35340	0.19660	0.10000			0.09156

NORMALIZED DIAGONAL:

1 1.00000E+000 2 4.46745E-001 3 9.92512E-001

MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00

			NEW PARAMETER (EST. ERROR)	-- CHANGE THIS ITERATION
1	10000	A	1502.6606(133)	-0.0000
2	20000	B	859.9598(165)	-0.0000
3	30000	C	591.7598(201)	0.0000

MICROWAVE AVG = -0.008436 MHz, IR AVG = 0.00000

MICROWAVE RMS = 0.244120 MHz, IR RMS = 0.00000

D2O_wwwwu SPFIT Output

```
                        EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  4  4  1  3  3  1          13209.81000   13209.81000   -0.00000    0.10000   0.10000
  2:  8  1  7  7  1  6          13466.53000   13466.58042   -0.05042    0.10000   0.07933
  3:  8  6  3  7  6  2          15467.91000   15467.91057   -0.00057    0.10000   0.10000
  4:  9  2  8  8  1  7          14886.66000   14886.59645    0.06355    0.10000   0.06412
  5: 10  0 10  9  1  9           14973.30000   14973.28674    0.01326    0.10000   0.09998   14973.29822    0.00178 0.5000
  6: 10  1 10  9  1  9           14973.30000   14973.30969   -0.00969    0.10000   0.09998   14973.29822    0.00178 0.5000
  7: 11  1 10 10  2  9           17730.48000   17730.49653   -0.01653    0.10000   0.09798
  8: 13  4  9 13  3 10           11265.24000   11265.23968    0.00032    0.10000   0.10000
  9: 14  3 11 14  2 12           14585.75000   14585.74897    0.00103    0.10000   0.09998
 10: 17  4 13 17  4 14           16985.83000   16985.83061   -0.00061    0.10000   0.10000
NORMALIZED DIAGONAL:
  1 1.00000E+000   2 2.48725E-001   3 1.70831E-001   4 9.90207E-001   5 4.60502E-001   6 1.17002E-003
  7 1.12541E-001   8 8.12936E-001
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                    NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1      10000        A       1748.683(105)         0.000
  2      20000        B       1139.579( 45)        -0.000
  3      30000        C       715.9006(182)        -0.0000
  4        200   -DeltaJ          0.72(188)E-03      -0.00E-03
  5       2000   -DeltaK           1.6( 45)E-03      -0.0E-03
  6       1100  -DeltaJK          -4.1( 64)E-03       0.0E-03
  7      40100    -deltaJ         -0.66(113)E-03       0.00E-03
  8      41000    -deltaK           1.7( 39)E-03      -0.0E-03
 MICROWAVE AVG =      -0.000162 MHz, IR AVG =       0.00000
 MICROWAVE RMS =       0.027609 MHz, IR RMS =       0.00000
```

D2O_wwwwd SPFIT Output

```
                        EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  5  4  1  4  3  1          14866.67000   14866.66557    0.00443    0.10000   0.09987
  2:  6  2  5  5  1  5          16451.83000   16451.80194    0.02806    0.10000   0.09478
  3:  6  3  4  5  2  4          16512.95000   16513.00516   -0.05516    0.10000   0.07792
  4:  9  2  7  8  2  6          16497.45000   16497.39885    0.05115    0.10000   0.08137
  5: 10  3  8  9  3  7          17840.27000   17840.30199   -0.03199    0.10000   0.09317
  6: 11  3  8 11  3  9          10374.06000   10374.05779    0.00221    0.10000   0.09999
  7: 11  4  8 11  3  9          10517.87000   10517.85454    0.01546    0.10000   0.09843
  8: 16  4 13 16  2 14          17146.90000   17146.91083   -0.01083    0.10000   0.09993   17146.90336   -0.00336 0.5000
  9: 16  4 13 16  3 14          17146.90000   17146.89590    0.00410    0.10000   0.09993   17146.90336   -0.00336 0.5000
 10: 16  5 11 16  4 12          13739.83000   13739.83128   -0.00128    0.10000   0.09998
NORMALIZED DIAGONAL:
  1 1.00000E+000   2 2.82814E-001   3 1.12323E-001   4 8.73705E-001   5 6.65377E-001   6 4.71991E-004
  7 3.89129E-002   8 9.99021E-001
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                    NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1      10000       A       1723.002(284)         0.000
  2      20000       B       1158.257(133)        -0.000
  3      30000       C        728.868(109)        -0.000
  4        200   -DeltaJ        0.0107( 51)       -0.0000
  5       2000   -DeltaK        0.0238(119)       -0.0000
  6       1100   -DeltaJK      -0.0371(173)        0.0000
  7      40100   -deltaJ         -7.1( 32)E-03      0.0E-03
  8      41000   -deltaK        0.0203(104)       -0.0000
 MICROWAVE AVG =       0.001057 MHz, IR AVG =       0.00000
 MICROWAVE RMS =       0.029338 MHz, IR RMS =       0.00000
```

D2O_wwwwd' SPFIT Output

```
                    EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  8  2  6  7  3  5          14864.82000   14864.96484   -0.14484    0.10000   0.08545
  2:  11  0 11 10  0 10           17010.49000   17010.38711    0.10289    0.10000   0.09259   17010.38466    0.10534 0.2500
  3:  11  0 11 10  1 10           17010.49000   17010.38079    0.10921    0.10000   0.09259   17010.38466    0.10534 0.2500
  4:  11  1 11 10  0 10           17010.49000   17010.38852    0.10148    0.10000   0.09259   17010.38466    0.10534 0.2500
  5:  11  1 11 10  1 10           17010.49000   17010.38221    0.10779    0.10000   0.09259   17010.38466    0.10534 0.2500
  6:  13  5  9 13  4 10          11306.16000   11305.97359    0.18641    0.10000   0.07437
  7:  16  3 13 16  2 14           16710.09000   16710.09702   -0.00702    0.10000   0.09271   16710.19450   -0.10450 0.5000
  8:  16  4 13 16  3 14           16710.09000   16710.29199   -0.20199    0.10000   0.09271   16710.19450   -0.10450 0.5000
NORMALIZED DIAGONAL:
  1 1.00000E+000   2 2.76370E-001   3 5.70266E-001
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                    NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1       10000       A       1683.208( 47)         -0.000
  2       20000       B       1173.5501(125)         0.0000
  3       30000       C        744.3310( 41)        -0.0000
 MICROWAVE AVG =       0.010600 MHz, IR AVG =       0.00000
 MICROWAVE RMS =       0.139414 MHz, IR RMS =       0.00000
```

HDO1_wduud SPFIT Output

```
                        EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  6  6  1  5  5  1              10378.35000   10378.34958    0.00042    0.10000   0.10000
  2:  9  4  6  8  3  5              10518.43000   10518.43291   -0.00291    0.10000   0.09998
  3: 10  4  7  9  4  6              11347.28000   11347.20650    0.07350    0.10000   0.08494
  4: 10  5  6  9  4  6              15844.39000   15844.45962   -0.06962    0.10000   0.08661
  5: 11  3  8 10  4  7              12229.35000   12229.35199   -0.00199    0.10000   0.09999
  6: 11  4  7 10  3  7              17438.08000   17438.01068    0.06932    0.10000   0.08673
  7: 11  4  7 10  5  6              12937.53000   12937.59571   -0.06571    0.10000   0.08817
  8: 11  5  7 10  4  6              13005.76000   13005.76296   -0.00296    0.10000   0.09998
  9: 13  6  7 12  6  6              16395.73000   16395.73003   -0.00003    0.10000   0.10000
NORMALIZED DIAGONAL:
  1 1.00000E+000   2 2.67165E-002   3 1.64167E-001   4 1.91871E-001   5 7.95603E-001   6 6.16026E-003
  7 8.68043E-001   8 1.22055E-001
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                    NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1       10000        A        886.788(133)          0.000
  2       20000        B        729.407(159)         -0.000
  3       30000        C        441.763( 51)          0.000
  4         200    -DeltaJ          -0.23( 70)E-03       -0.00E-03
  5        2000    -DeltaK           1.33(220)E-03        0.00E-03
  6        1100   -DeltaJK          -0.38(259)E-03       -0.00E-03
  7       40100    -deltaJ           1.45( 88)E-03        0.00E-03
  8       41000    -deltaK          -8.40(242)E-03       -0.00E-03
 MICROWAVE AVG =       0.000002 MHz, IR AVG =       0.00000
 MICROWAVE RMS =       0.046420 MHz, IR RMS =       0.00000
```

HDO1_wuduu SPFIT Output

```
                    EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  7  2  5  6  1  5          10748.19000   10748.20022   -0.01022    0.10000   0.09994
  2:  7  6  2  6  5  1          11770.65000   11770.57738    0.07262    0.10000   0.09696
  3:  7  7  0  6  6  1          12427.27000   12427.28201   -0.01201    0.10000   0.09992
  4:  8  6  3  7  5  2          12864.72000   12864.78078   -0.06078    0.10000   0.09788
  5: 10  3  7  9  3  6          11488.80000   11488.80172   -0.00172    0.10000   0.10000
  6: 14  4 11 13  3 10          15065.48000   15065.29303    0.18697    0.10000   0.07765
  7: 15  2 13 14  2 12          15319.69000   15319.89426   -0.20426    0.10000   0.07346   15319.89129   -0.20129 0.2500
  8: 15  2 13 14  3 12          15319.69000   15319.88667   -0.19667    0.10000   0.07346   15319.89129   -0.20129 0.2500
  9: 15  3 13 14  2 12          15319.69000   15319.89591   -0.20591    0.10000   0.07346   15319.89129   -0.20129 0.2500
 10: 15  3 13 14  3 12          15319.69000   15319.88832   -0.19832    0.10000   0.07346   15319.89129   -0.20129 0.2500
 11: 15  5 10 14  6  9          17277.23000   17277.25311   -0.02311    0.10000   0.09969
 12: 17  1 16 16  1 15          16492.74000   16492.68711    0.05289    0.10000   0.09840   16492.68711    0.05289 0.2500
 13: 17  1 16 16  2 15          16492.74000   16492.68711    0.05289    0.10000   0.09840   16492.68711    0.05289 0.2500
 14: 17  2 16 16  1 15          16492.74000   16492.68711    0.05289    0.10000   0.09840   16492.68711    0.05289 0.2500
 15: 17  2 16 16  2 15          16492.74000   16492.68711    0.05289    0.10000   0.09840   16492.68711    0.05289 0.2500
NORMALIZED DIAGONAL:
  1 1.00000E+000   2 5.65989E-001   3 2.22021E-001   4 1.62530E-002   5 8.29973E-001   6 5.24002E-003
  7 9.95313E-001   8 1.37604E-001
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                    NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1       10000         A        910.567( 99)          0.000
  2       20000         B       688.5752(277)         -0.0000
  3       30000         C       456.6607(207)         -0.0000
  4         200    -DeltaJ         -1.33( 45)E-03       -0.00E-03
  5        2000    -DeltaK         -0.60( 50)E-03        0.00E-03
  6        1100   -DeltaJK          1.48( 87)E-03        0.00E-03
  7       40100    -deltaJ         0.616(313)E-03       0.000E-03
  8       41000    -deltaK          0.81( 49)E-03        0.00E-03
 MICROWAVE AVG =       0.000372 MHz, IR AVG =       0.00000
 MICROWAVE RMS =       0.098897 MHz, IR RMS =       0.00000
```

HDO1_wdudu SPFIT Output

```
                              EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  7  5  2  6  4  2              10968.19000   10967.90735    0.28265    0.10000   0.07727
  2:  9  4  5  8  3  5              13252.90000   13252.76131    0.13869    0.10000   0.06770
  3: 11  4  8 10  3  8               16830.20000   16830.49077   -0.29077    0.10000   0.07212
  4: 13  5  8 12  6  7               15244.43000   15244.28369    0.14631    0.10000   0.08113
  5: 14  6  9 13  6  8               16497.45000   16497.58788   -0.13788    0.10000   0.08753
NORMALIZED DIAGONAL:
  1 1.00000E+000    2 8.95165E-001    3 9.91106E-001
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                     NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1       10000        A       900.6808( 87)         0.0000
  2       20000        B       684.1236( 32)        -0.0000
  3       30000        C       469.0249( 59)         0.0000
 MICROWAVE AVG =       0.027801 MHz, IR AVG =       0.00000
 MICROWAVE RMS =       0.211705 MHz, IR RMS =       0.00000
```

HDO1_wudud SPFIT Output

```
                          EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  10  3  7  9  3  6              11558.26000   11557.89802    0.36198    0.10000   0.07905
  2:  14  3 11 13  3 10               15180.98000   15180.51107    0.46893    0.10000   0.05131
  3:  14  5 10 13  4  9              15844.39000   15844.92438   -0.53438    0.10000   0.06336
  4:  15  2 13 14  2 12               15479.43000   15479.58633   -0.15633    0.10000   0.08864
  5:  15  6 10 14  6  9              17369.22000   17369.24391   -0.02391    0.10000   0.09615
NORMALIZED DIAGONAL:
  1  1.00000E+000    2  3.22828E-001    3  4.15294E-001
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                    NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1       10000        A       908.057( 41)         0.000
  2       20000        B       680.4086(263)        -0.0000
  3       30000        C       464.2687( 62)        0.0000
 MICROWAVE AVG =       0.023260 MHz, IR AVG =       0.00000
 MICROWAVE RMS =       0.363732 MHz, IR RMS =       0.00000
```

HDO1_wuudu SPFIT Output

```
                    EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  11  3  9 10  2  9          17201.05000  17202.15095   -1.10095    0.10000   0.09377
  2:  11  4  7 10  3  7          16977.39000  16977.28756    0.10244    0.10000   0.09682
  3:  11  5  7 10  5  6          12943.82000  12942.90852    0.91148    0.10000   0.03882
  4:  13  1 12 12  1 11           12776.11000  12777.14896  -1.03896   0.10000   0.05615  12777.14857  -1.03857 0.2500
  5:  13  1 12 12  2 11           12776.11000  12777.14800  -1.03800   0.10000   0.05615  12777.14857  -1.03857 0.2500
  6:  13  2 12 12  1 11           12776.11000  12777.14914  -1.03914   0.10000   0.05615  12777.14857  -1.03857 0.2500
  7:  13  2 12 12  2 11           12776.11000  12777.14818  -1.03818   0.10000   0.05615  12777.14857  -1.03857 0.2500
  8:  14  1 13 13  1 12           13681.55000  13683.03080  -1.48080   0.10000   0.06136  13683.03073  -1.48073 0.2500
  9:  14  1 13 13  2 12           13681.55000  13683.03062  -1.48062   0.10000   0.06136  13683.03073  -1.48073 0.2500
 10:  14  2 13 13  1 12           13681.55000  13683.03083  -1.48083   0.10000   0.06136  13683.03073  -1.48073 0.2500
 11:  14  2 13 13  2 12           13681.55000  13683.03065  -1.48065   0.10000   0.06136  13683.03073  -1.48073 0.2500
 12:  15  5 11 14  5 10           16606.61000  16604.25982   2.35018   0.10000   0.05905
NORMALIZED DIAGONAL:
  1  1.00000E+000   2  3.08827E-001   3  9.45450E-001
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                    NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1       10000       A       902.591( 34)        -0.001
  2       20000       B       699.4352(119)        0.0005
  3       30000       C       452.99646(269)       0.00003
 MICROWAVE AVG =      -0.042691 MHz, IR AVG =       0.00000
 MICROWAVE RMS =       1.344613 MHz, IR RMS =       0.00000
```

HDO1_wwdud SPFIT Output

```
                        EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  7  5  3  6  4  3              13438.73000   13438.74566   -0.01566    0.10000   0.07125
  2:  8  1  7  7  0  7              15105.54000   15105.54324   -0.00324    0.10000   0.09894
  3:  9  6  4  8  5  4              17087.03000   17087.01444    0.01556    0.10000   0.07168
  4: 11  4  7 10  5  6               15861.09000   15861.09041   -0.00041    0.10000   0.09998
NORMALIZED DIAGONAL:
  1  1.00000E+000    2  3.69874E-001    3  9.88347E-001
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                    NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1       10000        A       1065.7455(173)        -0.0000
  2       20000        B        855.9642(155)         0.0000
  3       30000        C        569.8553(133)        -0.0000
 MICROWAVE AVG =      -0.000937 MHz, IR AVG =       0.00000
 MICROWAVE RMS =       0.011160 MHz, IR RMS =       0.00000
```

HDO1_wuwud SPFIT Output

```
                        EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  9  2  8  8  1  8              16455.31000   16455.29287    0.01713    0.10000   0.09926
  2:  9  6  4  8  6  3              11759.02000   11759.05190   -0.03190    0.10000   0.09741
  3:  12  3 10 11  3  9               14401.81000   14401.70485    0.10515    0.10000   0.06668
  4:  13  3 10 12  3  9               16365.20000   16365.28683   -0.08683    0.10000   0.07882
NORMALIZED DIAGONAL:
  1  1.00000E+000    2  6.95698E-001    3  9.17561E-001
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                    NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1       10000        A       1217.6054(259)        -0.0000
  2       20000        B        751.8418( 67)         0.0000
  3       30000        C        514.6696( 40)        -0.0000
 MICROWAVE AVG =       0.000886 MHz, IR AVG =       0.00000
 MICROWAVE RMS =       0.070548 MHz, IR RMS =       0.00000
```

HDO1_wwduu SPFIT Output

```
                    EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  8  1  7  7  0  7          15262.51000  15262.69215  -0.18215   0.10000  0.08658
  2:  8  5  4  7  4  4          15447.45000  15447.14852   0.30148   0.10000  0.05613
  3:  8  8  0  7  7  1          17867.76000  17867.86359  -0.10359   0.10000  0.09680  17867.85142  -0.09142 0.5000
  4:  8  8  1  7  7  1          17867.76000  17867.83924  -0.07924   0.10000  0.09680  17867.85142  -0.09142 0.5000
  5: 14  0 14 13  1 13             15265.43000  15265.44594  -0.01594   0.10000  0.09990  15265.44595  -0.01595 0.5000
  6: 14  1 14 13  1 13             15265.43000  15265.44595  -0.01595   0.10000  0.09990  15265.44595  -0.01595 0.5000
NORMALIZED DIAGONAL:
  1  1.00000E+000   2  8.53586E-001   3  9.99543E-001
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                    NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1       10000        A       1144.2509( 67)        -0.0000
  2       20000        B        829.2658( 82)         0.0000
  3       30000        C        529.8739( 37)        -0.0000
 MICROWAVE AVG =       0.002991 MHz, IR AVG =       0.00000
 MICROWAVE RMS =       0.182126 MHz, IR RMS =       0.00000
```

HDO1_wwudu SPFIT Output

```
                        EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  8  2  6  7  3  5              10813.32000   10812.93599    0.38401    0.10000   0.05089
  2:  9  1  8  8  1  7              11191.29000   11191.45277   -0.16277    0.10000   0.09311
  3: 10  5  6  9  4  5              15319.69000   15319.69245   -0.00245    0.10000   0.09999
  4: 10  5  6  9  5  5              14489.13000   14489.28827   -0.15827    0.10000   0.09348
NORMALIZED DIAGONAL:
  1  1.00000E+000    2  9.58730E-001    3  4.56030E-001
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                     NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1       10000        A       1085.7237(200)        -0.0000
  2       20000        B        841.0634(135)         0.0000
  3       30000        C        557.0169( 88)         0.0000
 MICROWAVE AVG =       0.015130 MHz, IR AVG =       0.00000
 MICROWAVE RMS =       0.223055 MHz, IR RMS =       0.00000
```

HDO1_wuwdu SPFIT Output

```
                        EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  6  2  5  5  1  5              11035.70000   11035.20076    0.49924    0.10000   0.06971
  2:  8  4  5  7  3  5              14794.44000   14794.83965   -0.39965    0.10000   0.08189
  3: 12  4  9 11  3  8               15677.86000   15677.64379    0.21621    0.10000   0.09506
  4: 14  3 11 13  3 10               17471.55000   17471.72091   -0.17091    0.10000   0.09694
NORMALIZED DIAGONAL:
  1  1.00000E+000    2  5.49425E-001    3  8.12874E-001
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                    NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1       10000        A       1209.1670(251)         -0.0000
  2       20000        B        761.6147(121)          0.0000
  3       30000        C        519.5340( 51)          0.0000
 MICROWAVE AVG =       0.036222 MHz, IR AVG =       0.00000
 MICROWAVE RMS =       0.348181 MHz, IR RMS =       0.00000
```

HDO1_wuwuu SPFIT Output

```
                        EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  7  2  5  6  1  5              12537.47000   12538.63399   -1.16399    0.10000   0.09201
  2: 10  4  7  9  4  6              13145.21000   13142.66661    2.54339    0.10000   0.05175
  3: 14  1 14 13  1 13              14886.66000   14887.62937   -0.96937    0.10000   0.09453
  4: 14  3 12 13  2 11              16583.86000   16584.12534   -0.26534    0.10000   0.09960
NORMALIZED DIAGONAL:
  1  1.00000E+000    2  3.52860E-001    3  8.45927E-001
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                    NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1       10000        A       1194.235(129)         -0.000
  2       20000        B       778.9241(155)         0.0000
  3       30000        C       516.6388( 43)         0.0000
 MICROWAVE AVG =       0.036173 MHz, IR AVG =       0.00000
 MICROWAVE RMS =       1.486087 MHz, IR RMS =       0.00000
```

HDO1_wwdwd SPFIT Output

```
                        EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  8  3  6  7  2  6              17910.85000   17910.82839    0.02161    0.10000   0.08063
  2:  11  1 10 10  2  9              15334.25000   15334.26571   -0.01571    0.10000   0.09027
  3:  13  3 11 13  2 12              11151.15000   11151.17272   -0.02272    0.10000   0.07830
  4:  14  3 11 14  2 12              10518.48000   10518.46979    0.01021    0.10000   0.09602
NORMALIZED DIAGONAL:
  1  1.00000E+000    2  3.00783E-001    3  7.52088E-001
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                    NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1       10000        A       1605.513( 34)        -0.000
  2       20000        B       895.2822( 81)        0.0000
  3       30000        C       627.6455( 44)        -0.0000
 MICROWAVE AVG =      -0.001656 MHz, IR AVG =       0.00000
 MICROWAVE RMS =       0.018263 MHz, IR RMS =       0.00000
```

HDO1_wwwud SPFIT Output

```
                    EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  5 5 0 4 4 1          12322.81000  12322.81856  -0.00856   0.10000  0.09985
  2:  6 3 4 5 3 3          10628.52000  10628.53105  -0.01105   0.10000  0.09975
  3:  7 3 5 6 2 4          11972.55000  11972.42413   0.12587   0.10000  0.06124
  4:  8 2 6 7 2 5          13306.15000  13306.23989  -0.08989   0.10000  0.07954  13306.24650  -0.09650 0.5000
  5:  8 3 6 7 2 5          13306.15000  13306.25311  -0.10311   0.10000  0.07954  13306.24650  -0.09650 0.5000
NORMALIZED DIAGONAL:
  1 1.00000E+000   2 1.09172E-001   3 8.69464E-001
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                    NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1       10000       A       1235.389(100)         0.000
  2       20000       B       1150.776(145)        -0.000
  3       30000       C       667.9763(191)         0.0000
 MICROWAVE AVG =       0.002440 MHz, IR AVG =       0.00000
 MICROWAVE RMS =       0.079608 MHz, IR RMS =       0.00000
```

HDO2_wwwwu SPFIT Output

```
                        EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  8  2  6  7  2  5          16267.10000   16267.08586    0.01414    0.10000   0.09817
  2:  9  1  8  8  2  7          15974.20000   15974.27427   -0.07427    0.10000   0.05420
  3:  9  1  9  8  1  8          14550.80000   14550.79369    0.00631    0.10000   0.05499
  4:  9  3  7  8  3  6          17331.00000   17330.94460    0.05540    0.10000   0.06790
  5: 14  4 11 14  2 12             15666.59000   15666.59609   -0.00609    0.10000   0.09895
NORMALIZED DIAGONAL:
  1  1.00000E+000    2  1.92701E-001    3  9.10797E-001
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                    NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1       10000        A       1975.782( 89)         -0.000
  2       20000        B       1199.1085(221)         0.0000
  3       30000        C        768.2722( 33)         0.0000
 MICROWAVE AVG =      -0.000904 MHz, IR AVG =       0.00000
 MICROWAVE RMS =       0.042099 MHz, IR RMS =       0.00000
```

HDO1_wwwwd' SPFIT Output

```
                        EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  3  3  1  2  2  1            10343.11000   10343.08323    0.02677    0.10000   0.09898
  2:  5  2  4  4  1  3            10565.61000   10565.72810   -0.11810    0.10000   0.08114
  3:  5  3  2  4  3  1            11191.28000   11191.32074   -0.04074    0.10000   0.09042
  4:  5  3  3  4  2  2            13296.43000   13296.47269   -0.04269    0.10000   0.09542
  5:  5  3  3  4  3  2            10520.78000   10520.74243    0.03757    0.10000   0.07884
  6:  6  2  5  5  1  4            11889.28000   11889.07595    0.20405    0.10000   0.06141
  7:  8  0  8  7  0  7            13466.56000   13466.55660    0.00340    0.10000   0.08523   13466.67008   -0.11008 0.5000
  8:  8  1  8  7  0  7            13466.56000   13466.78355   -0.22355    0.10000   0.08523   13466.67008   -0.11008 0.5000
  9:  9  1  9  8  0  8            15062.47000   15062.42603    0.04397    0.10000   0.09542
 10: 11  3  8 11  2  9              10910.24000   10910.23200    0.00800    0.10000   0.09993
 11: 14  3 12 14  2 13               16847.37000   16847.37559   -0.00559    0.10000   0.09998
NORMALIZED DIAGONAL:
  1 1.00000E+000   2 7.85043E-001   3 2.88522E-001   4 9.84698E-001   5 2.46418E-002   6 1.04899E-003
  7 1.23672E-001   8 8.27073E-001
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                    NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1       10000        A       1844.405(111)         -0.000
  2       20000        B       1250.2226(142)        -0.0000
  3       30000        C        798.883( 42)          0.000
  4         200    -DeltaJ          6.2( 41)E-03        0.0E-03
  5        2000    -DeltaK         0.0103( 90)          0.0000
  6        1100   -DeltaJK        -0.0181(132)         -0.0000
  7       40100    -deltaJ         -5.13(238)E-03       -0.00E-03
  8       41000    -deltaK          6.0( 80)E-03         0.0E-03
 MICROWAVE AVG =       0.000318 MHz, IR AVG =       0.00000
 MICROWAVE RMS =       0.086799 MHz, IR RMS =       0.00000
```

HDO2_wwwwd' SPFIT Output

```
                        EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  5  3  2  4  2  2            14289.13000   14289.53617   -0.40617    0.10000   0.06224
  2:  5  5  0  4  4  0            17912.50000   17912.17408    0.32592    0.10000   0.05889
  3:  5  5  1  4  4  0            17910.86000   17910.77981    0.08019    0.10000   0.05890
  4:  8  7  2  8  6  3            10670.29000   10670.43745   -0.14745    0.10000   0.09587
  5: 13  2 11 13  1 12               15368.90000   15368.89322    0.00678    0.10000   0.10000
NORMALIZED DIAGONAL:
  1  1.00000E+000    2  9.98387E-001    3  5.00738E-001
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                    NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1       10000        A       1875.1602( 61)        -0.0000
  2       20000        B       1229.7763( 83)        -0.0000
  3       30000        C        794.7908( 75)        -0.0000
 MICROWAVE AVG =      -0.028146 MHz, IR AVG =       0.00000
 MICROWAVE RMS =       0.244709 MHz, IR RMS =       0.00000
```

HDO2_wwwwd SPFIT Output

```
                        EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  6  1  5  5  1  4            11711.55000   11710.43678    1.11322    0.10000   0.04308
  2:  6  3  4  5  2  3            14951.57000   14951.72668   -0.15668    0.10000   0.09919
  3:  7  1  7  6  1  6            11673.86000   11674.11715   -0.25715    0.10000   0.09780
  4:  9  3  7  8  3  6            17573.40000   17573.83714   -0.43714    0.10000   0.09355
NORMALIZED DIAGONAL:
  1  1.00000E+000   2  9.94376E-001   3  4.95432E-001
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                    NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1       10000        A       1945.3595(290)         0.0000
  2       20000        B       1218.3171(275)         0.0001
  3       30000        C        783.1562( 94)        -0.0000
 MICROWAVE AVG =       0.065561 MHz, IR AVG =       0.00000
 MICROWAVE RMS =       0.616652 MHz, IR RMS =       0.00000
```

HDO1_wwwwd SPFIT Output

```
                        EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
  1:  4  4  0  3  3  1              14491.76000   14491.22850    0.53150    0.10000   0.09618
  2:  8  2  6  7  3  5              15569.14000   15567.84499    1.29501    0.10000   0.07450
  3: 10  1  9  9  2  8               17840.27000   17841.51817   -1.24817    0.10000   0.07660
  4: 11  3  8 11  2  9               11087.17000   11087.67312   -0.50312    0.10000   0.09655
NORMALIZED DIAGONAL:
  1  1.00000E+000    2  8.55651E-001    3  9.85012E-001
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                     NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1       10000        A       1919.0414(140)         0.0000
  2       20000        B       1233.9826( 53)         0.0000
  3       30000        C        784.9006( 41)         0.0000
 MICROWAVE AVG =       0.018806 MHz, IR AVG =       0.00000
 MICROWAVE RMS =       0.970902 MHz, IR RMS =       0.00000
```

Section 5: Double Resonance Connections

The list of connected lines below has been confirmed with double resonance techniques. Power at a frequency corresponding to one of the transitions was added to the circuit and both transitions were monitored for modulation after processing the data.

uduud $13_{13,1} - 12_{12,1} \longleftrightarrow 12_{12,1} - 11_{11,1}$

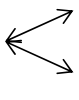
wduud $9_{3,6} - 8_{4,5} \longleftrightarrow 8_{4,5} - 7_{3,5}$

wudud $8_{3,6} - 7_{2,6} \longleftrightarrow 7_{2,6} - 6_{1,6}$

wwuwd $8_{8,1} - 8_{5,3} \longleftrightarrow 8_{5,3} - 8_{4,5}$

wwwdd $22_{13,10} - 22_{11,11} \longleftrightarrow 22_{11,11} - 22_{11,12}$

hdo_wduud $10_{4,7} - 9_{4,6} \longleftrightarrow 9_{4,6} - 8_{3,5}$

hdo1_wuwud $10_{3,8} - 9_{2,7}$  $10_{3,8} - 9_{3,7}$, $9_{2,7} - 8_{2,6}$

$14_{4,11} - 13_{4,10} \longleftrightarrow 13_{4,10} - 12_{3,9}$

hdo1_wuwuu $14_{4,11} - 13_{3,10} \longleftrightarrow 13_{3,10} - 12_{4,9}$