Supporting Information

Rotational Spectroscopy Study of Microsolvation Effects on Intramolecular Proton Transfer in Trifluoroacetylacetone-$(H_2O)_{1-3}$

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Details of ring-polymer instanton theory calculations

Instanton theory calculations were performed for the $enol_H$-$1W_{CH}$ to $enol_F$-$1W_{CF}$ transition as an example to evaluate the importance of quantum tunneling for the transition between the $enol_H$ and $enol_F$ conformers. In specific, we performed thermalized microcanonical instanton theory[1, 2] calculations using the instanton program developed by Prof. Jeremy O. Richardson's group, combined with on-the-fly *ab initio* calculations at the B3LYP-D3/def2-TZVP level performed with Gaussian09 [3]. 5 instantons were optimized at 200K, 150K, 120K, 100K, and 80K respectively, and the rates were obtained by combing contributions from all the instantons using the procedure described in Ref.2. 48 beads were used at 200K and an increasing number of beads up to 128 were used for lower temperatures. We have checked that the results are converged with respect to the number of beads. Additionally, we accounted for anharmonicity in the reactive mode (i.e. the stretching of OH bond) using 2nd order vibrational perturbation theory[4].

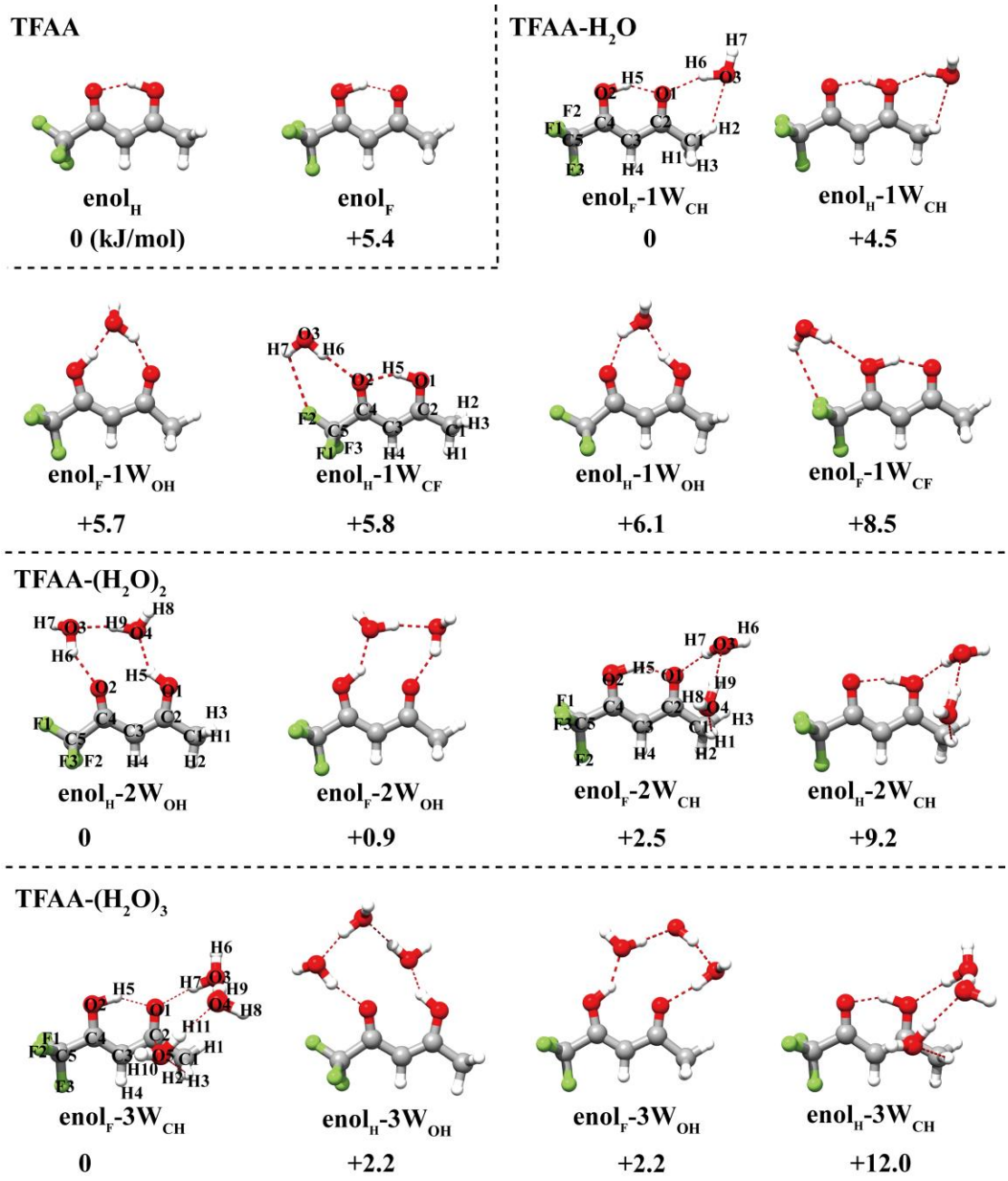

Figure S1. Optimized (B3LYP-D4/def2-TZVP) structures of TFAA-$(H_2O)_n$ (n=0,1,2,3). The relative energies (in kJ mol^{-1}) calculated at DLPNO-CCSD(T)/def2-TZVP// B3LYP-D4/def2-TZVP are also listed.

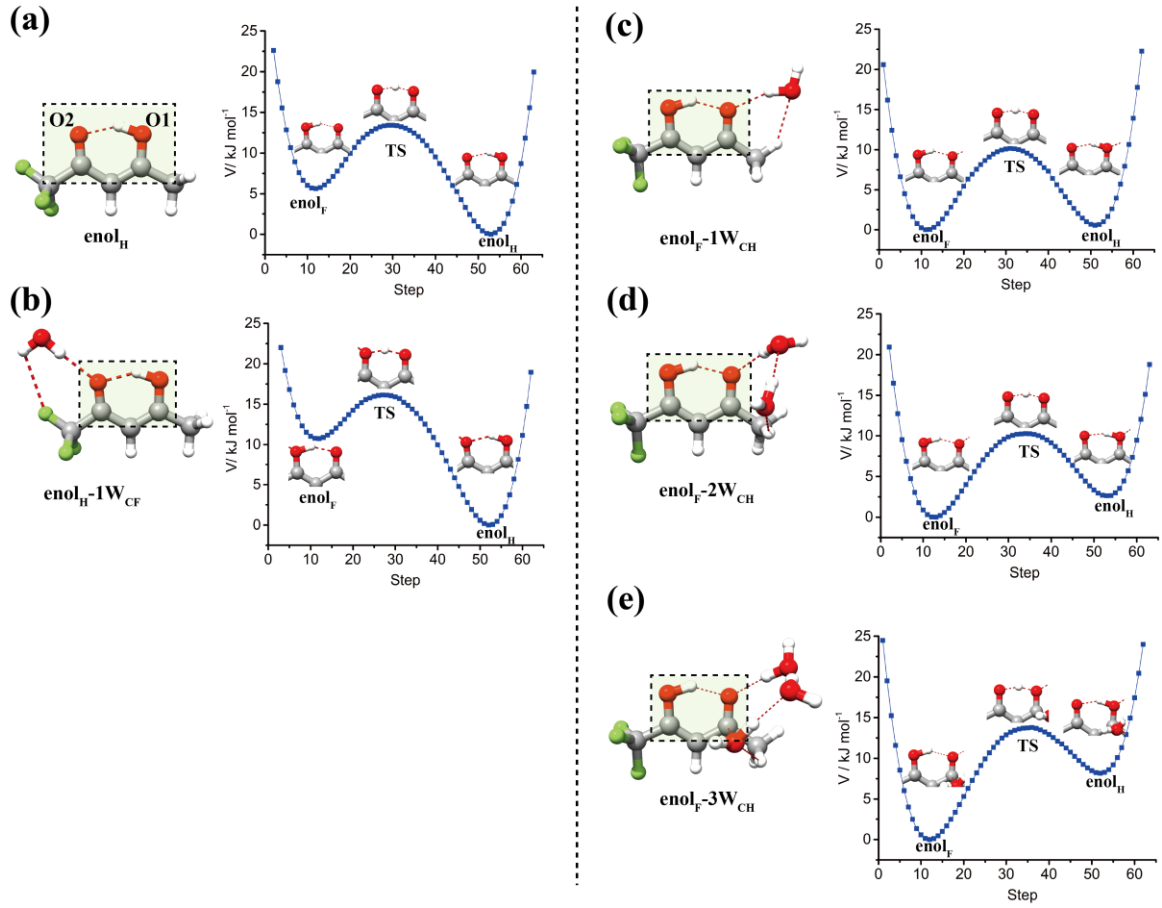

Figure S2. The relaxed potential energy surface analysis for the TFAA monomer and the observed complexes of TFAA-$(H_2O)_{1\text{-}3}$. Relaxed energy scans by simultaneously changing the O-H-O distances in TFAA on a regular grid with a step of 0.01 Å that results in proton transfer process.

Table S1. Calculated spectroscopic parameters, dipole moment components and relative energies for TFAA-$(H_2O)_n$ (n=1,2,3) complexes. The resulting conformers were optimized at the B3LYP-D4/def2-TZVP level of theory and their single-point energies were evaluated at the DLPNO-CCSD(T)/def2-TZVP level.

		$\Delta E_{+ZPE+BSSE}$ kJ mol^{-1}	A / MHz	B / MHz	C / MHz	$\lvert\mu_a\rvert$ /D	$\lvert\mu_b\rvert$ /D	$\lvert\mu_c\rvert$ /D
TFAA-H_2O	$enol_F$-$1W_{CH}$	0.0	2446.2	439.7	400.0	0.4	1.2	0.0
	$enol_H$-$1W_{CH}$	4.5	2243.2	450.6	417.5	2.2	1.1	0.6
	$enol_F$-$1W_{OH}$	5.7	1393.0	667.4	492.8	2.4	1.5	1.1
	$enol_H$-$1W_{CF}$	5.8	1277.8	664.7	475.5	4.6	3.8	0.3
	$enol_H$-$1W_{OH}$	6.1	1389.4	654.3	485.4	2.5	1.3	1.1
	$enol_F$-$1W_{CF}$	8.5	1467.5	637.0	484.2	4.4	3.7	0.8
TFAA-$(H_2O)_2$	$enol_H$-$2W_{OH}$	0.0	809.1	630.1	380.9	1.5	1.6	1.0
	$enol_F$-$2W_{OH}$	0.9	1204.2	451.1	350.4	2.3	2.5	0.3
	$enol_F$-$2W_{CH}$	2.5	1443.6	373.5	365.4	2.0	1.3	1.6
	$enol_H$-$2W_{CH}$	9.2	1530.1	334.0	318.4	2.4	0.8	1.7
TFAA-$(H_2O)_3$	$enol_F$-$3W_{CH}$	0.0	1171.1	304.0	293.3	2.3	1.0	1.2
	$enol_H$-$3W_{OH}$	2.2	607.3	530.2	305.9	0.2	-2.7	0.1
	$enol_F$-$3W_{OH}$	2.2	1026.8	329.6	266.0	1.5	2.3	0.5
	$enol_H$-$3W_{CH}$	12.0	1220.9	280.1	272.7	3.3	1.4	1.6

Table S2. Experimental spectroscopic parameters of the $H_2{}^{18}O$ and deuterated isotopologues of $enol_F$-$1W_{CH}$.

	^{18}O-3	D-5	D-6	D-7
A / MHz	2419.504(6)[a]	2402.884(2)	2419.377(7)	2408.293(1)
B / MHz	418.2496(6)	435.6431(4)	430.464(1)	425.2398(2)
C / MHz	381.5805(7)	395.5708(4)	391.7083(6)	387.1213(2)
D_J / kHz	-0.011(5)	-0.011(3)		
P_{cc} / uÅ^2	46.380(2)	46.40(1)	46.37(2)	46.413(7)
N [b]	26	41	11	54
σ[c] / kHz	2.67	6.08	7.29	8.65

[a] Error in parentheses in units of the last digit.
[b] Number of lines in the fit.
[c] Standard deviation of the fit.

Table S3. Experimental spectroscopic parameters of the $H_2{}^{18}O$ and deuterated isotopologues of $enol_H$-$1W_{CF}$.

	^{18}O-3
A / MHz	1221.42(1) [a]
B / MHz	657.0451(5)
C / MHz	463.677(1)
D_J / kHz	0.031(8)
P_{cc} / uÅ^2	46.496(7)
N [b]	14
σ[c] / kHz	5.03

[a] Error in parentheses in units of the last digit.
[b] Number of lines in the fit.
[c] Standard deviation of the fit.

Table S4. Experimental spectroscopic parameters of the $H_2{}^{18}O$ and deuterated isotopologue of $enol_H$-$2W_{OH}$.

	^{18}O-3	^{18}O-4	D-5	D-6	D-7	D-8	D-9
A / MHz	757.0(3) [a]	779.239(2)	785.88(6)	777.95(4)	765.3(1)	782.3(5)	779.5(2)
B / MHz	639.2(2)	625.65(2)	636.76(3)	640.25(3)	640.4(1)	628.3(3)	635.2(1)
C / MHz	370.4095(8)	370.988(2)	376.3213(8)	375.752(2)	372.952(1)	372.644(1)	374.3797(8)
D_J / kHz		-0.023(7)		-0.015(7)			
P_{cc} / uÅ^2	46.9(3)	47.0(1)	46.90(4)	47.00(4)	47.2(1)	47.1(4)	47.0(1)
N [b]	17	24	18	22	13	16	18
σ[c] / kHz	6.96	6.57	5.10	5.71	5.30	5.29	6.05

[a] Error in parentheses in units of the last digit.
[b] Number of lines in the fit.
[c] Standard deviation of the fit.

Table S5. Equilibrium coordinates (r_e) calculated at the B3LYP-D4/def2-TZVP level of theory and substitution coordinates (r_s) from Kraitchman's equations for single isotopic substitution of $enol_F$-$1W_{CH}$.

		a/Å		b/Å		c/Å	
		r_e	r_s	r_e	r_s	r_e	r_s
1	C1	2.4953		1.6712		0.0165	
2	H1	2.3225		2.2808		0.9076	
3	H2	3.5245		1.3222		0.0031	
4	H3	2.3063		2.3126		-0.8480	
5	C2	1.5341		0.5198		0.0090	
6	C3	0.1144		0.8060		-0.0088	
7	H4	-0.2334		1.8258		-0.0269	
8	C4	-0.7772		-0.2139		-0.0001	
9	C5	-2.2808		0.0104		-0.0071	
10	F1	-2.8511		-0.6259		-1.0397	
11	F2	-2.8342		-0.4580		1.1225	
12	F3	-2.5847		1.3140		-0.1047	
13	O1	1.9387		-0.6575		0.0214	
14	O2	-0.4607		-1.4905		0.0227	
15	H5	0.5428	1.195(1)	-1.5158	-1.504(1)	0.0279	0.16(1)
16	O3	4.8082	5.0062(3)	-0.6808	-0.667(2)	-0.0287	-0.04 (4)
17	H6	3.8668	3.9246(4)	-0.9176	-0.937(2)	-0.0131	0[a]
18	H7	5.2958	5.4524(3)	-1.5095	-1.353(1)	-0.0344	-0.196(8)

[a] Set to zero by imaginary value.

Table S6. Equilibrium coordinates (r_e) calculated at the B3LYP-D4/def2-TZVP level of theory and substitution coordinates (r_s) from Kraitchman's equations for single isotopic substitution of $enol_H$-$1W_{CF}$.

		a/Å		b/Å		c/Å	
		r_e	r_s	r_e	r_s	r_e	r_s
1	C1	3.8793		-0.3258		0.0197	
2	H1	3.8947		-1.4126		0.0463	
3	H2	4.4153		0.0240		-0.8658	
4	H3	4.4058		0.0688		0.8914	
5	C2	2.4885		0.2010		-0.0017	
6	C3	1.3693		-0.5960		-0.0189	
7	H4	1.4747		-1.6690		-0.0180	
8	C4	0.0790		-0.0063		-0.0309	
9	C5	-1.1320		-0.9690		-0.0023	
10	F1	2.4124		1.5156		-0.0028	
11	F2	-0.1445		1.2102		-0.0405	
12	F3	1.4484		1.7658		-0.0199	
13	O1	-1.1892		-1.5994		1.1864	
14	O2	-2.2818		-0.3213		-0.1875	
15	H5	-1.0234		-1.9095		-0.9586	
16	O3	-2.6039	-2.5361(7)	2.8833	2.7881(7)	0.0243	0[a]
17	H6	-1.8204		2.3164		-0.0030	
18	H7	-3.3475		2.2820		-0.0803	

[a] Set to zero by imaginary value.

Table S7. Equilibrium coordinates (r_e) calculated at the B3LYP-D4/def2-TZVP level of theory and substitution coordinates (r_s) from Kraitchman's equations for single isotopic substitution of $enol_H$-$2W_{OH}$.

		a/Å		b/Å		c/Å	
		r_e	r_s	r_e	r_s	r_e	r_s
1	C1	-1.9514		-3.1057		-0.0039	
2	H1	-2.5397		-3.2881		-0.9059	
3	H2	-1.1507		-3.8384		0.0585	
4	H3	-2.6229		-3.2270		0.8489	
5	C2	-1.4241		-1.7075		-0.0294	
6	C3	-0.0771		-1.4555		0.0415	
7	H4	0.5848		-2.3011		0.1468	
8	C4	0.4970		-0.1596		-0.0506	
9	C5	2.0474		-0.1096		0.0273	
10	F1	2.4989		1.1450		0.0703	
11	F2	2.4987		-0.7517		1.1238	
12	F3	2.5936		-0.7134		-1.0474	
13	O1	-0.1061		0.8955		-0.2062	
14	O2	-2.3848		-0.8221		-0.1272	
15	H5	-2.1496	-2.199(8)	0.1423	0.64 (3)	-0.0553	0[a]
16	O3	-0.7527	-0.80(5)	3.5586	3.58(1)	-0.1674	0
17	H6	-0.1959	-0.396(3)	2.7625	2.669(4)	-0.2361	0
18	H7	-0.3741	0	4.0926	4.17 (1)	0.5379	0.53(9)
19	O4	-2.8285	-2.993(1)	1.7717	1.852 (2)	0.2951	0
20	H8	-3.6497	-3.83 (4)	2.0290	1.94 (9)	-0.1344	-0.3(5)
21	H9	-2.1966	-2.48(2)	2.5074	2.46 (2)	0.1561	0.1 (4)

[a] Set to zero by imaginary value.

Table S8. Equilibrium coordinates (r_e) calculated at the B3LYP-D4/def2-TZVP level of theory of $enol_F$-$2W_{CH}$.

		a/Å	b/Å	c/Å
		r_e	r_e	r_e
1	C1	-2.0956	1.6089	-1.0855
2	H1	-2.5325	1.8622	-0.1137
3	H2	-1.5936	2.4912	-1.4823
4	H3	-2.8950	1.2954	-1.7546
5	C2	-1.1378	0.4841	-0.8585
6	C3	0.2200	0.7860	-0.4692
7	H4	0.5426	1.8091	-0.3730
8	C4	1.0844	-0.2247	-0.2095
9	C5	2.5221	0.0158	0.2209
10	O1	-1.5111	-0.7009	-0.9760
11	O2	0.7950	-1.5043	-0.2934
12	H5	-0.1677	-1.5413	-0.5769
13	F1	3.3764	-0.5540	-0.6428
14	F2	2.8068	1.3255	0.2807
15	F3	2.7474	-0.5123	1.4341
16	O3	-3.9732	-1.3593	0.1783
17	H6	-4.7467	-1.3104	-0.3916
18	H7	-3.1948	-1.2475	-0.3984
19	O4	-3.1465	0.7787	1.8075
20	H8	-3.1016	0.5686	2.7446
21	H9	-3.5586	0.0057	1.3768

[a] Set to zero by imaginary value.

Table S9. Equilibrium coordinates (r_e) calculated at the B3LYP-D4/def2-TZVP level of theory of $enol_F$-$3W_{CH}$.

		a/Å	b/Å	c/Å
		r_e	r_e	r_e
1	C1	1.666567	-0.669030	1.998366
2	H1	2.612645	-1.175595	1.820535
3	H2	1.177505	-1.086777	2.880752
4	H3	1.848534	0.392237	2.184066
5	C2	0.772082	-0.775524	0.804602
6	C3	-0.595545	-0.320918	0.922562
7	H4	-0.954706	0.066789	1.861254
8	C4	-1.405639	-0.332552	-0.159807
9	C5	-2.836841	0.175137	-0.122083
10	O1	1.190933	-1.244905	-0.272770
11	O2	-1.060212	-0.756161	-1.359422
12	H5	-0.107944	-1.051039	-1.272980
13	F1	-3.693187	-0.775827	-0.526276
14	F2	-2.982987	1.231398	-0.939574
15	F3	-3.197944	0.556358	1.112820
16	O3	4.145608	1.452328	-0.740066
17	H6	4.891976	1.723981	-0.197245
18	H7	4.173021	0.471336	-0.773494
19	O4	3.917498	-1.290515	-0.694324
20	H8	4.160879	-1.830045	-1.452953
21	H9	2.947620	-1.385377	-0.583680
22	O5	1.653917	2.048220	0.353300
23	H10	1.219021	2.740401	-0.152704
24	H11	2.512812	1.892314	-0.091850

Table S10. The optimized hydrogen bonding parameters r_e at the B3LYP-D4/def2-TZVP level of theory of the TFAA-$(H_2O)_{1-3}$ clusters.

	$enol_H$	$enol_F$-$1W_{CH}$	$enol_H$-$1W_{CF}$	$enol_H$-$2W_{OH}$	$enol_F$-$2W_{CH}$	$enol_F$-$3W_{CH}$
O1-O2	2.57	2.54	2.58	2.85	2.54	2.55
O1-O3	-	2.87	-	2.67	2.80	2.76
O2-O3	-	-	2.98	-	-	-
O2-O4	-	-	-	2.75	-	-
O3-O4	-	-	-	2.78/ 2.79(4)[a]	2.81	2.75
O4-O5	-	-	-	-	-	2.79

[a] Compared with the experimental values r_s.

Table S11. NBO stabilization energy contributions (calculated at the B3LYP-D4/def2-TZVP level of theory) of intramolecular hydrogen bond in observed conformers.

	Donor NBO	Acceptor NBO	E(2) (kJ mol^{-1})
$enol_H$	LP(1)O**2**	BD*(1)O**1**-H5	3.93
	LP(2)O**2**	BD*(1)O**1**-H5	22.17
$enol_F$-$1W_{CH}$	LP(1)O**1**	BD*(1)O**2**-H5	4.42
	LP(2)O**1**	BD*(1)O**2**-H5	25.12
$enol_H$-$1W_{CF}$	LP(1)O**2**	BD*(1)O**1**-H5	3.94
	LP(2)O**2**	BD*(1)O**1**-H5	19.39
$enol_H$-$2W_{OH}$	LP(1)O**2**	BD*(1)O**1**-H5	**0.79**
	LP(2)O**2**	BD*(1)O**1**-H5	**2.18**
$enol_F$-$2W_{CH}$	LP(1)O**1**	BD*(1)O**2**-H5	5.09
	LP(2)O**1**	BD*(1)O**2**-H5	26.33
$enol_F$-$3W_{CH}$	LP(1)O**1**	BD*(1)O**2**-H5	5.34
	LP(2)O**1**	BD*(1)O**2**-H5	21.94

Table S12. NBO stabilization energy contributions in chelated ring and that between TFAA and water at the B3LYP-D4/def2-TZVP level of theory.

		$enol_H$	$enol_F$	$enol_H$-$1W_{CF}$	$enol_F$-$1W_{CH}$	$enol_H$-$2W_{CF}$	$enol_F$-$2W_{CH}$	$enol_H$-$3W_{CF}$	$enol_F$-$3W_{CH}$
Donor NBO	Acceptor NBO	E(2)(kJ mol^{-1})							
In TFAA									
LP O2	BD* C3-C4	60.06	58.87	56.783	58.62	54.74	59.05	55.25	56.35
BD C3-C4	BD* C2-O1	37.73	26.88	39.19	28.15	39.9	28.88	42.19	28.11
LP O1	BD* O2-H5	27.03	33.71	33.77	29.99	37.35	31.24	40	27.28
BD C2-O1	BD* C3-C4	3.45	3.68	3.44	3.49	3.42	3.31	3.31	3.31
From TFAA to water									
LP O1	BD*(1)O3-H6			2.57	5.91	5.63	8.02	7.27	12.31
From water to water									
LP(2)O3	BD*(1)O4-H8					10.92	11.55	14.07	15.78
LP(2)O4	BD*(1)O5-H10							13.6	14.39
From water to TFAA									
LP(2)O3	BD*(1)C1-H2			0.84	1.02				
LP(2)O4	BD*(1)C1-H1					3.94	3.13		
LP(2)O5	BD*(1)C1-H3							0.83	0.78
LP(2)O5	BD*(1)C2-O1								1.38

Table S13. Experimental transition frequencies (ν/MHz) and obs-calc. values ($\Delta\nu$/MHz) of $enol_F$-$1W_{CH}$.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν	$\Delta\nu$
3	0	3	2	0	2	2496.4017	-0.0003
4	0	4	3	0	3	3325.8364	0.0045
5	0	5	4	0	4	4152.9633	0.0011
6	0	6	5	0	5	4977.2609	0.0030
7	0	7	6	0	6	5798.2370	0.0008
8	0	8	7	0	7	6615.4999	0.0016
3	1	3	2	1	2	2439.1527	0.0002
3	1	2	2	1	1	2557.5710	0.0027
3	1	2	2	1	1	2557.5710	0.0027
4	1	4	3	1	3	3251.5379	0.0007
4	1	3	3	1	2	3409.4050	0.0050
5	1	5	4	1	4	4063.3660	-0.0006
5	1	4	4	1	3	4260.6264	0.0033
6	1	6	5	1	5	4874.5233	0.0017
6	1	5	5	1	4	5111.0696	0.0043
7	1	7	6	1	6	5684.8960	0.0006
7	1	6	6	1	5	5960.5357	-0.0045
8	1	8	7	1	7	6494.3959	0.0001
8	1	7	7	1	6	6808.8412	-0.0036
9	1	9	8	1	8	7302.9437	-0.0034
4	2	3	3	2	2	3331.1799	0.0016
5	2	4	4	2	3	4163.2455	0.0002
5	2	3	4	2	2	4174.8160	-0.0020
6	2	5	5	2	4	4994.8267	-0.0008
6	2	4	5	2	3	5015.0050	-0.0026
7	2	6	6	2	5	5825.8291	0.0007
7	2	5	6	2	4	5857.9223	-0.0072
8	2	7	7	2	6	6656.1442	-0.0082
8	2	6	7	2	5	6703.8815	-0.0020
9	2	8	8	2	7	7485.6991	-0.0053
9	2	7	8	2	6	7553.0447	-0.0024
8	3	6	7	3	5	6669.5394	-0.0107
1	1	1	0	0	0	2826.0024	0.0078
2	1	2	1	0	1	3619.4369	0.0082
3	1	3	2	0	2	4393.3517	0.0060
4	1	4	3	0	3	5148.4884	0.0074
5	1	5	4	0	4	5886.0155	-0.0002
6	1	6	5	0	5	6607.5803	0.0052
7	1	7	6	0	6	7315.2114	-0.0012
8	1	8	7	0	7	8011.3670	-0.0053
9	1	9	8	0	8	8698.8071	-0.0139
5	0	5	4	1	4	2330.3082	-0.0049
6	0	6	5	1	5	3244.2040	-0.0004
7	0	7	6	1	6	4167.9231	0.0042
8	0	8	7	1	7	5098.5242	0.0022
2	1	1	2	0	2	2072.6238	0.0094
3	1	2	3	0	3	2133.7901	0.0093
4	1	3	4	0	4	2217.3605	0.0116
5	1	4	5	0	5	2325.0195	0.0096
6	1	5	6	0	6	2458.8165	-0.0008

7	1	6	7	0	7	2621.1291	0.0079
8	1	7	8	0	8	2814.4783	0.0105
9	1	8	9	0	9	3041.4537	-0.0046
10	1	9	10	0	10	3304.5574	-0.0141
11	1	10	11	0	11	3605.9444	-0.0142
11	2	9	11	1	10	5179.6433	0.0020
10	2	8	10	1	9	5263.1496	-0.0037
9	2	7	9	1	8	5358.7396	-0.0079
8	2	6	8	1	7	5461.4485	-0.0091
7	2	5	7	1	6	5566.4142	-0.0047
6	2	4	6	1	5	5669.0230	-0.0066
5	2	3	5	1	4	5765.0879	0.0006
4	2	2	4	1	3	5850.8962	0.0039
3	2	2	3	1	3	6157.2565	0.0052
4	2	3	4	1	4	6236.9005	0.0081
5	2	4	5	1	5	6336.7784	0.0074
6	2	5	6	1	6	6457.0858	0.0090
7	2	6	7	1	7	6598.0178	0.0079
8	2	7	8	1	8	6759.7623	-0.0042
10	2	9	10	1	10	7146.4117	-0.0127
9	0	9	8	1	8	6032.9093	0.0165
10	0	10	9	1	9	6967.8818	0.0159
9	1	8	8	1	7	7655.7614	0.0042
4	2	2	3	2	1	3336.9659	-0.0103

Table S14. Experimental transition frequencies (ν/MHz) and obs-calc. values ($\Delta\nu$/MHz) of ^{18}O-3 isotopologues of enol$_F$-1W$_{CH}$.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν	$\Delta\nu$
3	0	3	2	0	2	2397.4916	-0.0010
4	0	4	3	0	3	3194.3303	0.0001
5	0	5	4	0	4	3989.1902	0.0033
6	0	6	5	0	5	4781.5945	-0.0025
7	0	7	6	0	6	5571.1354	0.0017
8	0	8	7	0	7	6357.4341	0.0011
3	1	3	2	1	2	2344.1782	0.0026
3	1	2	2	1	1	2454.1773	-0.0013
4	1	4	3	1	3	3124.9961	0.0025
4	1	3	3	1	2	3271.6424	-0.0020
5	1	5	4	1	4	3905.3293	-0.0029
5	1	4	4	1	3	4088.5895	0.0011
6	1	6	5	1	5	4685.0817	-0.0055
6	1	5	5	1	4	4904.8644	0.0005
7	1	7	6	1	6	5464.1637	-0.0007
7	1	6	6	1	5	5720.3117	-0.0017
8	1	8	7	1	7	6242.4869	0.0056
8	1	7	7	1	6	6534.7650	-0.0009
1	1	1	0	0	0	2801.0844	0.0002
2	1	2	1	0	1	3564.2441	-0.0008
3	1	3	2	0	2	4309.2583	-0.0016
4	1	4	3	0	3	5036.7623	0.0014
5	1	5	4	0	4	5747.7638	0.0009
6	1	6	5	0	5	6443.6655	0.0023
7	1	7	6	0	6	7126.2345	0.0040
8	1	8	7	0	7	7797.5717	-0.0065

Table S15. Experimental transition frequencies (ν/MHz) and obs-calc. values ($\Delta\nu$/MHz) of D-5 isotopologues of enol$_F$-1W$_{CH}$.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν	$\Delta\nu$
3	0	3	2	0	2	2491.2157	-0.0018
4	0	4	3	0	3	3318.8058	0.0044
5	0	5	4	0	4	4143.9868	0.0006
6	0	6	5	0	5	4966.2154	-0.0011
7	0	7	6	0	6	5785.0064	0.0126
8	0	8	7	0	7	6599.9141	0.0021
9	0	9	8	0	8	7410.6880	-0.0089
5	1	4	4	1	3	4253.5299	-0.0029
3	1	2	2	1	1	2553.3606	-0.0067
4	1	4	3	1	3	3243.5112	-0.0021
4	1	3	3	1	2	3403.7684	0.0004
5	1	5	4	1	4	4053.2884	-0.0033
5	1	4	4	1	3	4253.5299	-0.0029
6	1	6	5	1	5	4862.3585	-0.0092
6	1	5	5	1	4	5102.4849	0.0041
7	1	7	6	1	6	5670.6379	0.0070
7	1	6	6	1	5	5950.4132	-0.0034
8	1	7	7	1	6	6797.1200	-0.0063
9	1	9	8	1	8	7284.3612	0.0033
9	1	8	8	1	7	7642.3728	-0.0034
5	2	3	4	2	2	4166.7915	-0.0034
6	2	5	5	2	4	4984.5457	-0.0018
6	2	4	5	2	3	5005.6104	0.0070
7	2	6	6	2	5	5813.7800	0.0090
7	2	5	6	2	4	5847.2463	-0.0079
8	2	7	7	2	6	6642.2857	-0.0024
8	2	6	7	2	5	6692.0502	0.0000
2	1	2	1	0	1	3589.6024	0.0063
3	1	3	2	0	2	4360.9276	-0.0032
4	1	4	3	0	3	5113.2256	-0.0009
5	1	5	4	0	4	5847.7167	-0.0002
6	1	6	5	0	5	6566.1057	0.0074
7	1	7	6	0	6	7270.5111	-0.0017
8	1	8	7	0	7	7963.5046	-0.0013
5	0	5	4	1	4	2349.5573	-0.0037
6	0	6	5	1	5	3262.4950	0.0091
7	0	7	6	1	6	4185.1178	0.0058
8	0	8	7	1	7	5114.3841	-0.0089
10	0	10	9	1	9	6979.9953	0.0067
2	2	0	1	1	1	7644.9147	0.0140
2	2	1	1	1	0	7604.2092	-0.0133

Table S16. Experimental transition frequencies (ν/MHz) and obs-calc. values ($\Delta\nu$/MHz) of D-6 isotopologues of enol$_F$-1W$_{CH}$.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν	$\Delta\nu$
4	0	4	3	0	3	3283.0875	-0.0010
5	0	5	4	0	4	4099.6862	0.0058
6	0	6	5	0	5	4913.5478	0.0148
7	0	7	6	0	6	5724.1728	-0.0041
8	0	8	7	0	7	6531.2114	-0.0108
1	1	1	0	0	0	2811.0868	0.0020
2	1	2	1	0	1	3594.5082	0.0068
3	1	3	2	0	2	4358.7449	-0.0078
4	1	4	3	0	3	5104.5433	-0.0060
5	1	5	4	0	4	5833.0305	-0.0018
6	1	6	5	0	5	6545.7794	0.0069

Table S17. Experimental transition frequencies (ν/MHz) and obs-calc. values ($\Delta\nu$/MHz) of D-7 isotopologues of enol$_F$-1W$_{CH}$.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν	$\Delta\nu$
4	0	4	3	0	3	3244.0118	0.0033
5	0	5	4	0	4	4050.9568	0.0032
6	0	6	5	0	5	4855.2373	-0.0016
7	0	7	6	0	6	5656.4089	0.0021
8	0	8	7	0	7	6454.0847	0.0099
3	1	2	2	1	1	2493.9205	0.0021
4	1	4	3	1	3	3172.1397	0.0063
4	1	3	3	1	2	3324.5835	0.0053
5	1	5	4	1	4	3964.1864	0.0077
5	1	4	4	1	3	4154.6691	-0.0001
6	1	6	5	1	5	4755.5930	0.0015
6	1	5	5	1	4	4984.0328	0.0022
7	1	7	6	1	6	5546.2788	0.0079
7	1	6	6	1	5	5812.4902	0.0009
8	1	8	7	1	7	6336.1254	-0.0042
4	2	3	3	2	2	3249.0250	0.0039
4	2	2	3	2	1	3254.4524	-0.0047
5	2	4	4	2	3	4060.5943	-0.0018
5	2	3	4	2	2	4071.4380	-0.0098
6	2	5	5	2	4	4871.7134	-0.0044
6	2	4	5	2	3	4890.6453	0.0011
7	2	6	6	2	5	5682.2890	-0.0071
7	2	5	6	2	4	5712.4060	-0.0066
8	2	7	7	2	6	6492.2247	-0.0166
8	2	6	7	2	5	6537.0482	0.0047
9	2	8	8	2	7	7301.4483	-0.0162
1	1	1	0	0	0	2795.4215	0.0065
2	1	2	1	0	1	3569.6714	0.0137
3	1	3	2	0	2	4325.0510	0.0035
4	1	4	3	0	3	5062.2732	-0.0007
5	1	5	4	0	4	5782.4401	-0.0041
6	1	6	5	0	5	6487.0775	-0.0045
7	1	7	6	0	6	7178.1049	-0.0091
8	1	8	7	0	7	7857.8425	0.0057
5	0	5	4	1	4	2232.6957	0.0075
7	0	7	6	1	6	4024.5669	0.0031
8	0	8	7	1	7	4932.3834	0.0158
1	1	0	1	0	1	2021.1790	0.0066
2	1	1	2	0	2	2059.8188	-0.0163
3	1	2	3	0	3	2118.8371	-0.0095
4	1	3	4	0	4	2199.4142	-0.0021
6	1	5	6	0	6	2431.9257	0.0023
7	1	6	7	0	7	2588.0013	-0.0046
8	1	7	8	0	8	2773.7841	-0.0040
9	1	8	9	0	9	2991.7266	-0.0208
2	2	1	2	1	2	6063.5309	0.0138
4	2	2	4	1	3	5824.9127	-0.0134
6	2	4	6	1	5	5648.3056	-0.0128
7	2	5	7	1	6	5548.2355	-0.0062
8	2	6	8	1	7	5445.4208	-0.0075

0	2	8	10	1	9	5249.2210	0.0044
4	2	3	4	1	4	6197.9405	0.0201
5	2	4	5	1	5	6294.3469	0.0091
6	2	5	6	1	6	6410.4770	0.0128

Table S18. Experimental transition frequencies (ν/MHz) and obs-calc. values ($\Delta\nu$/MHz) of enol$_H$-1W$_{CF}$.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν	$\Delta\nu$
2	0	2	1	0	1	2249.6334	0.0079
3	0	3	2	0	2	3285.5315	-0.0061
4	0	4	3	0	3	4254.8129	-0.0007
5	0	5	4	0	4	5191.6363	0.0052
6	0	6	5	0	5	6125.5681	-0.0127
7	0	7	6	0	6	7065.8758	-0.0053
3	1	3	2	1	2	3122.1578	0.0134
4	1	4	3	1	3	4127.1505	0.0029
5	1	5	4	1	4	5113.0618	-0.0044
6	1	6	5	1	5	6084.4308	-0.0063
7	1	7	6	1	6	7046.3962	0.0041
8	1	8	7	1	7	8003.0349	0.0092
3	1	2	2	1	1	3694.8515	0.0000
4	1	3	3	1	2	4867.4357	0.0090
5	1	4	4	1	3	5976.9769	-0.0125
6	1	5	5	1	4	7006.1689	0.0041
5	1	5	4	0	4	5267.1600	0.0043
6	1	6	5	0	5	6159.9484	-0.0132
7	1	7	6	0	6	7080.7721	-0.0008
2	2	1	1	1	0	4276.5866	-0.0081
3	2	2	2	1	1	5228.5208	-0.0036
4	2	3	3	1	2	6080.8804	0.0001
5	2	4	4	1	3	6848.8103	0.0146
4	0	4	3	1	3	3973.0581	0.0000
5	0	5	4	1	4	5037.5458	0.0041
6	0	6	5	1	5	6050.0565	0.0001
7	0	7	6	1	6	7031.4996	-0.0007

Table S19. Experimental transition frequencies (ν/MHz) and obs-calc. values ($\Delta\nu$/MHz) of ^{18}O-3 isotopologues of enol$_H$-1W$_{CF}$.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν	$\Delta\nu$
7	0	7	6	0	6	6884.5071	-0.0024
8	0	8	7	0	7	7806.5414	-0.0039
9	0	9	8	0	8	8731.4012	0.0008
7	1	7	6	1	6	6868.1358	0.0004
8	1	8	7	1	7	7799.5074	0.0020
9	1	9	8	1	8	8728.5039	0.0059
6	1	5	5	1	4	6837.3686	-0.0015
7	1	6	6	1	5	7760.1752	-0.0062
8	1	7	7	1	6	8652.0903	0.0082
7	0	7	6	1	6	6856.3057	0.0062
8	0	8	7	1	7	7794.7105	0.0009
7	1	7	6	0	6	6896.3501	0.0046
8	1	8	7	0	7	7811.3324	-0.0088

9	1	9	8	0	8	8733.2874	-0.0064

Table S20. Experimental transition frequencies (ν/MHz) and obs-calc. values ($\Delta\nu$/MHz) of enol$_H$-2W$_{OH}$.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν	$\Delta\nu$
3	0	3	2	0	2	2613.4853	0.0042
4	0	4	3	0	3	3354.6862	0.0073
5	0	5	4	0	4	4106.6296	0.0092
8	0	8	7	0	7	6372.4148	-0.0017
9	0	9	8	0	8	7127.9730	0.0025
3	1	3	2	1	2	2577.0043	0.0084
3	1	2	2	1	1	3286.1817	-0.0144
4	1	4	3	1	3	3346.6815	0.0076
5	1	4	4	1	3	4791.3303	-0.0034
6	1	5	5	1	4	5525.5099	-0.0178
7	1	7	6	1	6	5616.8415	-0.0138
8	1	8	7	1	7	6372.4147	0.0027
9	1	9	8	1	8	7127.9730	0.0032
4	2	3	3	2	2	3933.5501	0.0078
6	2	5	5	2	4	5513.9026	-0.0068
5	2	3	4	2	2	5538.1303	-0.0134
6	2	4	5	2	3	6267.7445	0.0002
4	3	2	3	3	1	4273.5300	0.0021
4	3	1	3	3	0	4593.5350	0.0051
5	3	2	4	3	1	5854.7611	0.0166
6	3	3	5	3	2	6932.2149	-0.0041
5	4	2	4	4	1	5439.3737	-0.0161
5	4	1	4	4	0	5627.7836	-0.0032
6	4	2	5	4	1	6977.5309	0.0059
7	4	4	6	4	3	7440.3985	-0.0083
3	0	3	2	1	2	2567.3342	0.0097
4	0	4	3	1	3	3345.0075	0.0000
6	0	6	5	1	5	4861.2106	0.0011
7	0	7	6	1	6	5616.8412	-0.0087
8	0	8	7	1	7	6372.4148	0.0035
9	0	9	8	1	8	7127.9730	0.0033
10	0	10	9	1	9	7883.5280	-0.0041
3	1	3	2	0	2	2623.1612	0.0088
4	1	4	3	0	3	3356.3508	0.0055
6	1	6	5	0	5	4861.5134	0.0073
8	1	8	7	0	7	6372.4148	-0.0024
9	1	9	8	0	8	7127.9729	0.0024
3	2	2	2	1	1	3493.0588	0.0131
4	2	3	3	1	2	4140.3995	0.0077
5	2	4	4	1	3	4805.7021	-0.0050
6	2	5	5	1	4	5528.2699	-0.0129
4	1	3	3	2	2	3870.1374	-0.0087
9	1	8	8	2	7	7784.0000	0.0143
6	2	4	5	3	3	6045.6628	0.0092
5	3	3	4	2	2	5760.2396	0.0052
6	3	4	5	2	3	6334.1659	-0.0156
4	4	1	3	3	0	5991.9216	0.0100
5	4	2	4	3	1	6837.7651	-0.0064

5	5	1	4	4	0	7598.1032	-0.0011
5	5	0	4	4	1	7641.0063	0.0064
3	2	1	2	1	2	4884.3817	0.0025
4	3	1	3	2	2	6143.0570	-0.0017

Table S21. Experimental transition frequencies (ν/MHz) and obs-calc. values ($\Delta\nu$/MHz) of ^{18}O-3 isotopologues of enol$_{H}$-2W$_{OH}$.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν	$\Delta\nu$
7	0	7	6	0	6	5508.1702	-0.0048
8	0	8	7	0	7	6248.9633	-0.0001
9	0	9	8	0	8	6989.7668	0.0013
10	0	10	9	0	9	7730.5713	-0.0023
6	0	6	5	0	5	4767.4594	0.0200
5	1	5	4	0	4	4027.0855	-0.0113
6	1	6	5	0	5	4767.4591	0.0082
7	1	7	6	0	6	5508.1701	-0.0062
8	1	8	7	0	7	6248.9632	-0.0003
9	1	9	8	0	8	6989.7666	0.0011
10	1	10	9	0	9	7730.5711	-0.0026
5	0	5	4	1	4	4026.2373	-0.0099
6	0	6	5	1	5	4767.3435	0.0002
7	0	7	6	1	6	5508.1701	0.0067
8	0	8	7	1	7	6248.9632	0.0012
9	0	9	8	1	8	6989.7666	0.0012
10	0	10	9	1	9	7730.5711	-0.0025
7	0	7	6	0	6	5508.1702	-0.0048
8	0	8	7	0	7	6248.9633	-0.0001
9	0	9	8	0	8	6989.7668	0.0013
10	0	10	9	0	9	7730.5713	-0.0023
6	0	6	5	0	5	4767.4594	0.0200
5	1	5	4	0	4	4027.0855	-0.0113
6	1	6	5	0	5	4767.4591	0.0082
7	1	7	6	0	6	5508.1701	-0.0062
8	1	8	7	0	7	6248.9632	-0.0003
9	1	9	8	0	8	6989.7666	0.0011
10	1	10	9	0	9	7730.5711	-0.0026
5	0	5	4	1	4	4026.2373	-0.0099
6	0	6	5	1	5	4767.3435	0.0002
7	0	7	6	1	6	5508.1701	0.0067
8	0	8	7	1	7	6248.9632	0.0012
9	0	9	8	1	8	6989.7666	0.0012
10	0	10	9	1	9	7730.5711	-0.0025

Table S22. Experimental transition frequencies (ν/MHz) and obs-calc. values ($\Delta\nu$/MHz) of ^{18}O-4 isotopologues of enol$_{H}$-2W$_{OH}$.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν	$\Delta\nu$
3	1	3	2	0	2	2580.6026	0.0001
4	1	4	3	0	3	3297.9277	0.0012
5	1	5	4	0	4	4033.9374	-0.0052
6	1	6	5	0	5	4774.7188	0.0007
8	1	8	7	0	7	6258.3189	-0.0026
9	1	9	8	0	8	7000.2454	-0.0009

10	1	10	9	0	9	7742.1739	-0.0051
4	0	4	3	1	3	3284.3271	0.0029
5	0	5	4	1	4	4031.4796	-0.0017
6	0	6	5	1	5	4774.3218	0.0076
8	0	8	7	1	7	6258.3199	0.0076
9	0	9	8	1	8	7000.2413	-0.0037
10	0	10	9	1	9	7742.1819	0.0031
3	0	3	2	0	2	2569.1162	0.0045
4	0	4	3	0	3	3295.8077	-0.0072
5	0	5	4	0	4	4033.5933	0.0004
8	0	8	7	0	7	6258.3198	-0.0006
9	0	9	8	0	8	7000.2413	-0.0048
10	0	10	9	0	9	7742.1819	0.0030
5	1	5	4	1	4	4031.8262	-0.0048
8	1	8	7	1	7	6258.3198	0.0063
9	1	9	8	1	8	7000.2413	-0.0039
10	1	10	9	1	9	7742.1818	0.0030

Table S23. Experimental transition frequencies (ν/MHz) and obs-calc. values ($\Delta\nu$/MHz) of D-5 isotopologues of enol$_{H}$-2W$_{OH}$.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν	$\Delta\nu$
4	0	4	3	1	3	3331.8386	0.0004
5	0	5	4	1	4	4089.1270	-0.0003
6	0	6	5	1	5	4842.5066	0.0022
7	0	7	6	1	6	5595.2071	-0.0068
8	0	8	7	1	7	6347.8401	0.0045
9	0	9	8	1	8	7100.4571	0.0019
7	1	7	6	1	6	5595.2071	-0.0129
8	1	8	7	1	7	6347.8403	0.0038
9	1	9	8	1	8	7100.4568	0.0015
5	0	5	4	0	4	4090.9443	0.0009
7	0	7	6	0	6	5595.2580	0.0011
8	0	8	7	0	7	6347.8403	-0.0015
9	0	9	8	0	8	7100.4568	0.0008
5	1	5	4	0	4	4091.2300	-0.0018
6	1	6	5	0	5	4842.8490	0.0130
7	1	7	6	0	6	5595.2580	-0.0050
8	1	8	7	0	7	6347.8403	-0.0023
9	1	9	8	0	8	7100.4568	0.0006

Table S24. Experimental transition frequencies (ν/MHz) and obs-calc. values ($\Delta\nu$/MHz) of D-6 isotopologues of enol$_{H}$-2W$_{OH}$.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν	$\Delta\nu$
4	1	4	3	0	3	3337.5691	-0.0025
5	1	5	4	0	4	4084.7589	0.0023
6	1	6	5	0	5	4835.4886	0.0171
8	1	8	7	0	7	6338.2507	-0.0036
9	1	9	8	0	8	7089.7260	0.0041
10	1	10	9	0	9	7841.1938	-0.0015
4	0	4	3	1	3	3328.0263	-0.0018
5	0	5	4	1	4	4083.2225	0.0014
6	0	6	5	1	5	4835.2477	0.0004

7	0	7	6	1	6	5586.7678	-0.0102
8	0	8	7	1	7	6338.2507	0.0005
9	0	9	8	1	8	7089.7260	0.0046
10	0	10	9	1	9	7841.1938	-0.0015
7	1	7	6	1	6	5586.7678	-0.0138
8	1	8	7	1	7	6338.2507	0.0001
9	1	9	8	1	8	7089.7255	0.0040
10	1	10	9	1	9	7841.1937	-0.0016
5	0	5	4	0	4	4084.5587	-0.0010
7	0	7	6	0	6	5586.8086	0.0034
8	0	8	7	0	7	6338.2507	-0.0031
9	0	9	8	0	8	7089.7259	0.0040
10	0	10	9	0	9	7841.1941	-0.0012

Table S25. Experimental transition frequencies (ν/MHz) and obs-calc. values ($\Delta\nu$/MHz) of D-7 isotopologues of enol$_{H}$-2W$_{OH}$.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν	$\Delta\nu$
8	1	8	7	0	7	6291.2198	0.0051
9	1	9	8	0	8	7037.0959	-0.0043
6	0	6	5	1	5	4799.4024	-0.0123
7	0	7	6	1	6	5545.3316	0.0022
8	0	8	7	1	7	6291.2194	0.0069
9	0	9	8	1	8	7037.0962	-0.0038
8	0	8	7	0	7	6291.2194	0.0050
9	0	9	8	0	8	7037.0961	-0.0040
5	1	5	4	1	4	4053.2841	0.0022
6	1	5	5	1	4	5452.9600	0.0000
7	1	7	6	1	6	5545.3316	0.0003
8	1	8	7	1	7	6291.2194	0.0067
9	1	9	8	1	8	7037.0961	-0.0038

Table S26. Experimental transition frequencies (ν/MHz) and obs-calc. values ($\Delta\nu$/MHz) of D-8 isotopologues of enol$_{H}$-2W$_{OH}$.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν	$\Delta\nu$
9	1	9	8	0	8	7031.2884	0.0023
8	1	8	7	0	7	6286.0198	-0.0102
7	1	7	6	0	6	5540.8163	0.0027
6	1	6	5	0	5	4795.7689	-0.0074
9	1	9	8	1	8	7031.2883	0.0034
8	1	8	7	1	7	6286.0198	-0.0022
7	1	7	6	1	6	5540.7620	0.0026
6	1	6	5	1	5	4795.4335	0.0063
9	0	9	8	1	8	7031.2884	0.0036
8	0	8	7	1	7	6286.0198	-0.0010
7	0	7	6	1	6	5540.7537	0.0023
6	0	6	5	1	5	4795.3670	-0.0061
6	0	6	5	0	5	4795.7302	0.0080
7	0	7	6	0	6	5540.8079	0.0024
8	0	8	7	0	7	6286.0198	-0.0091
9	0	9	8	0	8	7031.2884	0.0024

Table S27. Experimental transition frequencies (ν/MHz) and obs-calc. values ($\Delta\nu$/MHz) of D-9 isotopologues of enol$_H$-2W$_{OH}$.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν	$\Delta\nu$
5	1	5	4	0	4	4070.1395	-0.0078
7	1	7	6	0	6	5566.5551	0.0164
8	1	8	7	0	7	6315.2336	-0.0073
9	1	9	8	0	8	7063.9745	0.0013
10	1	10	9	0	9	7812.7140	-0.0020
6	0	6	5	1	5	4817.6918	0.0067
7	0	7	6	1	6	5566.5031	0.0057
8	0	8	7	1	7	6315.2337	-0.0015
9	0	9	8	1	8	7063.9749	0.0024
5	0	5	4	0	4	4069.9008	0.0040
8	0	8	7	0	7	6315.2337	-0.0064
9	0	9	8	0	8	7063.9751	0.0019
10	0	10	9	0	9	7812.7145	-0.0015
5	1	5	4	1	4	4068.5160	-0.0105
7	1	7	6	1	6	5566.5041	0.0017
8	1	8	7	1	7	6315.2341	-0.0018
9	1	9	8	1	8	7063.9739	0.0013
10	1	10	9	1	9	7812.7135	-0.0025
5	1	5	4	0	4	4070.1395	-0.0078
7	1	7	6	0	6	5566.5551	0.0164
8	1	8	7	0	7	6315.2336	-0.0073
9	1	9	8	0	8	7063.9745	0.0013
10	1	10	9	0	9	7812.7140	-0.0020
6	0	6	5	1	5	4817.6918	0.0067
7	0	7	6	1	6	5566.5031	0.0057
8	0	8	7	1	7	6315.2337	-0.0015
9	0	9	8	1	8	7063.9749	0.0024
5	0	5	4	0	4	4069.9008	0.0040
8	0	8	7	0	7	6315.2337	-0.0064
9	0	9	8	0	8	7063.9751	0.0019
10	0	10	9	0	9	7812.7145	-0.0015
5	1	5	4	1	4	4068.5160	-0.0105
7	1	7	6	1	6	5566.5041	0.0017
8	1	8	7	1	7	6315.2341	-0.0018
9	1	9	8	1	8	7063.9739	0.0013
10	1	10	9	1	9	7812.7135	-0.0025

Table S28. Experimental transition frequencies (ν/MHz) and obs-calc. values ($\Delta\nu$/MHz) of enol$_F$-2W$_{CH}$.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν	$\Delta\nu$
3	0	3	2	0	2	2280.4668	-0.0040
4	0	4	3	0	3	3040.5575	-0.0007
5	0	5	4	0	4	3800.5880	0.0019
6	0	6	5	0	5	4560.5349	-0.0047
7	0	7	6	0	6	5320.3918	-0.0122
8	0	8	7	0	7	6080.1467	-0.0175
9	0	9	8	0	8	6839.7896	-0.0162
3	1	3	2	1	2	2274.8056	0.0136
3	1	2	2	1	1	2286.2081	-0.0093
4	1	4	3	1	3	3033.0323	0.0105

4	1	3	3	1	2	3048.2473	-0.0083
5	1	5	4	1	4	3791.2360	0.0138
5	1	4	4	1	3	3810.2596	-0.0047
6	1	6	5	1	5	4549.3950	0.0089
6	1	5	5	1	4	4572.2278	-0.0083
7	1	7	6	1	6	5307.5028	-0.0034
7	1	6	6	1	5	5334.1625	-0.0010
8	1	8	7	1	7	6065.5650	-0.0104
8	1	7	7	1	6	6096.0505	0.0115
9	1	9	8	1	8	6823.5673	-0.0192
6	2	5	5	2	4	4560.8538	0.0075
6	2	4	5	2	3	4561.2164	0.0183
7	2	6	6	2	5	5320.8994	0.0108
7	2	5	6	2	4	5321.4570	0.0056
8	2	7	7	2	6	6080.8828	-0.0026
8	2	6	7	2	5	6081.7268	-0.0027
9	2	8	8	2	7	6840.8386	0.0085
9	2	7	8	2	6	6842.0427	0.0073
10	2	9	9	2	8	7600.7252	0.0089
10	2	8	9	2	7	7602.3832	0.0106
2	1	1	1	0	1	2607.9143	0.0122
3	1	2	2	0	2	3373.7874	0.0066
4	1	3	3	0	3	4141.5602	-0.0054
5	1	4	4	0	4	4911.2627	-0.0089
6	1	5	5	0	5	5682.9126	-0.0090
7	1	6	6	0	6	6456.5417	-0.0036
8	1	7	7	0	7	7232.1886	0.0083

Table S29. Experimental transition frequencies (ν/MHz) and obs-calc. values ($\Delta\nu$/MHz) of enol$_F$-3W$_{CH}$.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν	$\Delta\nu$
5	0	5	4	0	4	2902.5370	0.0046
6	0	6	5	0	5	3481.2625	0.0078
7	0	7	6	0	6	4059.0250	0.0004
8	0	8	7	0	7	4635.7250	0.0135
9	0	9	8	0	8	5211.2062	-0.0016
10	0	10	9	0	9	5785.4250	-0.0121
11	0	11	10	0	10	6358.3750	0.0127
12	0	12	11	0	11	6929.9875	-0.0041
13	0	13	12	0	12	7500.3750	-0.0051
4	1	4	3	1	3	2296.3963	0.0013
5	1	5	4	1	4	2870.1910	0.0020
5	1	4	4	1	3	2939.9411	-0.0050
6	1	6	5	1	5	3443.7921	0.0057
6	1	5	5	1	4	3527.4654	0.0069
7	1	7	6	1	6	4017.1534	-0.0008
7	1	6	6	1	5	4114.7097	0.0099
8	1	8	7	1	7	4590.2721	0.0096
8	1	7	7	1	6	4701.6137	-0.0019
9	1	9	8	1	8	5163.0765	-0.0090
9	1	8	8	1	7	5288.1393	-0.0079
10	1	10	9	1	9	5735.5914	-0.0098
10	1	9	9	1	8	5874.2234	-0.0076

11	1	11	10	1	10	6307.7885	-0.0037
11	1	10	10	1	9	6459.7975	-0.0005
12	1	12	11	1	11	6879.6506	0.0051
12	1	11	11	1	10	7044.7739	0.0007
13	1	13	12	1	12	7451.1454	-0.0073
13	1	12	12	1	11	7629.0713	-0.0047
5	2	3	4	2	2	2908.6247	-0.0401
6	2	5	5	2	4	3486.1889	-0.0034
6	2	4	5	2	3	3491.8703	0.0088
7	2	6	6	2	5	4066.7990	0.0010
7	2	5	6	2	4	4075.8286	-0.0069
8	2	7	7	2	6	4647.2074	0.0001
8	2	6	7	2	5	4660.6758	-0.0123
9	2	8	8	2	7	5227.3877	-0.0047
9	2	7	8	2	6	5246.4910	-0.0063
10	2	9	9	2	8	5807.3295	0.0038
10	2	8	9	2	7	5833.3130	0.0037
11	2	10	10	2	9	6386.9702	-0.0101
11	2	9	10	2	8	6421.1215	-0.0094
12	2	11	11	2	10	6966.3285	-0.0008
12	2	10	11	2	9	7009.9197	-0.0030
13	2	12	12	2	11	7545.3461	-0.0007
13	2	11	12	2	10	7599.5956	-0.0019
10	3	8	9	3	7	5814.6451	0.0096
10	3	7	9	3	6	5815.5877	0.0180
11	3	9	10	3	8	6396.6379	0.0303
11	3	8	10	3	7	6398.1186	-0.0035
12	3	10	11	3	9	6978.6898	0.0183
12	3	9	11	3	8	6981.0265	0.0064
13	3	11	12	3	10	7560.8145	0.0013
13	3	10	12	3	9	7564.3172	-0.0048

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