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

Supporting Information for :

Disentangling the complex network of non-covalent interactions in fenchone hydrates via rotational spectroscopy and quantum chemistry

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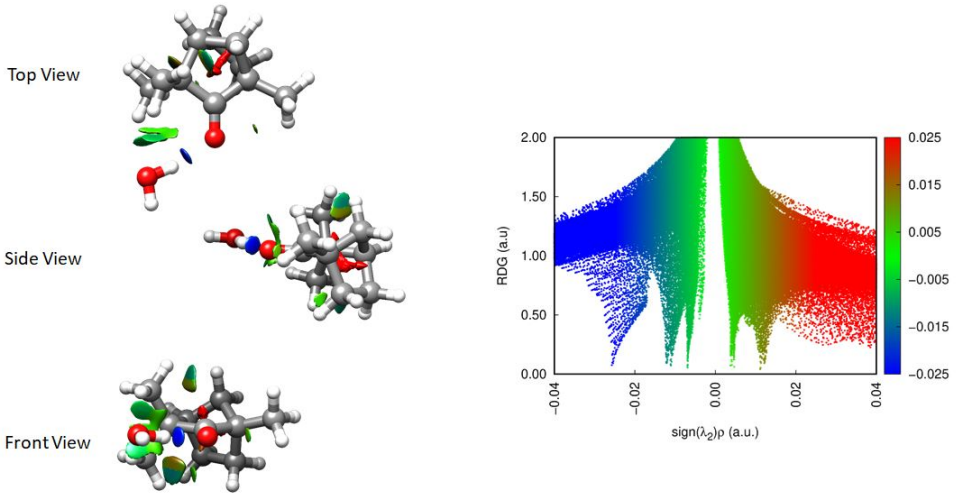

Figure S1: The three different views of the fenchone monohydrate 1w-I.

Table S1: Experimental rotational and quartic centrifugal distortion constants of the normal and of the $H_2^{18}O$ substituted species of the monohydrate of fenchone 1w-I.

	Normal	$^{18}O_1$
A/MHz	1288.791 91(18)	1285.928 058(93)
B/MHz	739.998 659(45)	709.272 048(39)
C/MHz	608.776 708(32)	587.402 628(36)
Δ_J/kHz	0.051 99(20)	0.052 58(46)
Δ_{JK}/kHz	0.250 89(93)	0.2541(44)
Δ_K/kHz	−0.1799(86)	*b*
δ_J/kHz	0.006 28(10)	*b*
δ_K/kHz	0.0444(25)	*b*
N_{lines} [a]	91	29
σ_{fit}/kHz	1.99	0.57
P_a/u Å^2	560.4835(1)	589.9435(1)
P_b/u Å^2	269.6715(1)	270.4187(1)
P_c/u Å^2	122.4624(1)	122.5885(1)

[a] The number of fitted lines ; [b] Fixed at the value of the normal species.

Table S2: Experimental coordinates (in Å) in the principal axis frame of the water oxygen atom O_1 of the 1w-I monohydrate of fenchone, along with those obtained by *ab initio* and DFT calculations.

	a	b	c
r_s	3.8509(4)	−0.6443(23)	0.2613(57)
r_0	3.8497(11)	−0.650 31(3)	0.2791(3)
MP2 [a]	3.820	−0.655	0.250
DFT [b]	3.758	−0.670	0.266

[a] MP2 / 6-311++G(d,p) ; [b] B3LYP-D3BJ / def2-TZVP.

Table S3: The effective structural parameters of the fenchone monohydrate 1w-I along with those optimized by quantum chemistry.

Parameters [a]	r_0 [b]	B3LYP [c]	MP2 [d]
$r(\mathrm{OfO_1})$ /Å	2.845(1)	2.830	2.868
$\angle(\mathrm{O_1OfC_1})$ /°	122.544(9)	118.1	119.4
$\tau(\mathrm{O_1OfC_1C_2})$ /°	176.067(23)	174.3	173.7
$\sigma_{\mathrm{fit}}/\mathrm{uÅ}^2$	0.016	-	-

[a] The numbering scheme is shown in Fig. S1; [b] Parameters involving the H atoms taken from MP2/6-311++G(d,p) ; [c] B3LYP-D3BJ / def2-TZVP ; [d] MP2/6-311++G(d,p).

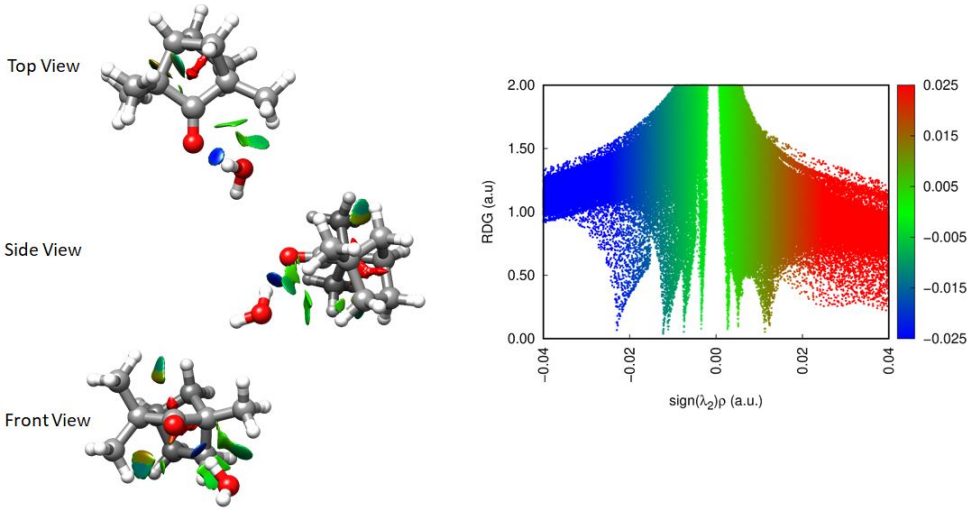

Figure S2: The three different views of the structure of the fenchone monohydrate 1w-II.

Table S4: Experimental rotational and quartic centrifugal distortion constants of the normal and of the $H_2^{18}O$ substituted species of the monohydrate of fenchone 1w-II.

	Normal	$^{18}O_1$
A/MHz	1150.183 15(30)	1144.0485(14)
B/MHz	793.033 620(63)	763.247 84(26)
C/MHz	672.035 636(34)	650.091 78(13)
Δ_J/kHz	0.543 48(34)	0.5668(12)
Δ_{JK}/kHz	−0.7295(25)	−0.815(16)
Δ_K/kHz	0.632(12)	[b]
δ_J/kHz	−0.039 48(18)	−0.0270(10)
δ_K/kHz	0.0961(23)	[b]
N_{lines} [a]	74	27
σ_{fit}/kHz	8.01	1.37
P_a/u Å^2	474.9476(2)	498.8965(8)
P_b/u Å^2	277.0646(2)	278.4999(8)
P_c/u Å^2	162.3255(2)	163.2462(8)

[a,b] See Table S1

Table S5: Experimental coordinates (in Å) in the principal axis frame of the water oxygen atom O_1 of the monohydrate of fenchone 1w-II, along with those obtained by *ab initio* and DFT calculations.

	a	*b*	*c*
r_s	3.4593(4)	−0.8976(17)	−0.7118(21)
r_0	3.4592(19)	−0.9104(2)	−0.6968(8)
MP2 [a]	3.461	−0.918	−0.683
DFT [b]	3.373	−0.966	−0.689

[a,b] See Table S2.

Table S6: The effective structural parameters of the fenchone monohydrate 1w-II along with those optimized by quantum chemistry.

Parameters [a]	r_0 [b]	B3LYP [c]	MP2 [d]
$r(\mathrm{OfO_1})$ / Å	2.8719(27)	2.839	2.881
$\angle(\mathrm{O_1OfC_1})$ / °	110.062(16)	108.3	109.6
$\tau(\mathrm{O_1OfC_1C_2})$ / °	−47.181(23)	−43.9	−44.1
σ_{fit} / u$\mathrm{Å}^2$	0.028	-	-

[a] The numbering scheme is shown in Fig. S2; [b,c,d] See Table S3.

Table S7: Experimental rotational and quartic centrifugal distortion constants of the two monohydrates of fenchone, along with the computational constants, dipole moments and difference of energy including ZPE corrections.

	1w-I					1w-II				
	Exp.	MP2	()[a]	DFT	()[a]	Exp.	MP2	()[a]	DFT	()[a]
A/MHz	1288.791 91(18)	1297.63	(0.69)	1301.86	(1.01)	1150.183 15(30)	1163.78	(1.18)	1167.13	(1.47)
B/MHz	739.998 659(45)	746.79	(0.92)	754.88	(2.01)	793.033 620(63)	796.24	(0.40)	805.31	(1.55)
C/MHz	608.776 708(32)	614.12	(0.88)	620.67	(1.95)	672.035 636(34)	675.12	(0.46)	685.32	(1.98)
Δ_J/kHz	0.051 99(20)	0.0450		0.0406		0.543 48(34)	0.5744		0.2158	
Δ_{JK}/kHz	0.250 89(93)	0.2054		0.1615		−0.7295(25)	−0.5760		−0.1874	
Δ_K/kHz	−0.1799(86)	−0.1423		−0.0994		0.632(12)	0.3260		0.2086	
δ_J/kHz	0.006 28(10)	0.0055		0.0050		−0.039 48(18)	−0.0599		−0.0155	
δ_K/kHz	0.0444(25)	0.0378		0.0324		0.0961(23)	0.2216		0.0654	
σ_{fit}/kHz	1.99	-		-		8.01	-		-	
N_{lines}	91	-		-		74	-		-	
κ	−0.614	−0.612		−0.606		−0.494	−0.504		−0.502	
$\lvert \mu_a \rvert$/D	-	2.96		3.02		-	2.57		2.54	
$\lvert \mu_b \rvert$/D	-	0.30		0.44		-	0.50		0.68	
$\lvert \mu_c \rvert$/D	-	0.21		0.32		-	0.006		0.04	
ΔE/kJ mol^{-1}	-	0.0		0.0		-	1.58		2.68	

[a] Deviation = (calc. − exp.)/exp. in % .

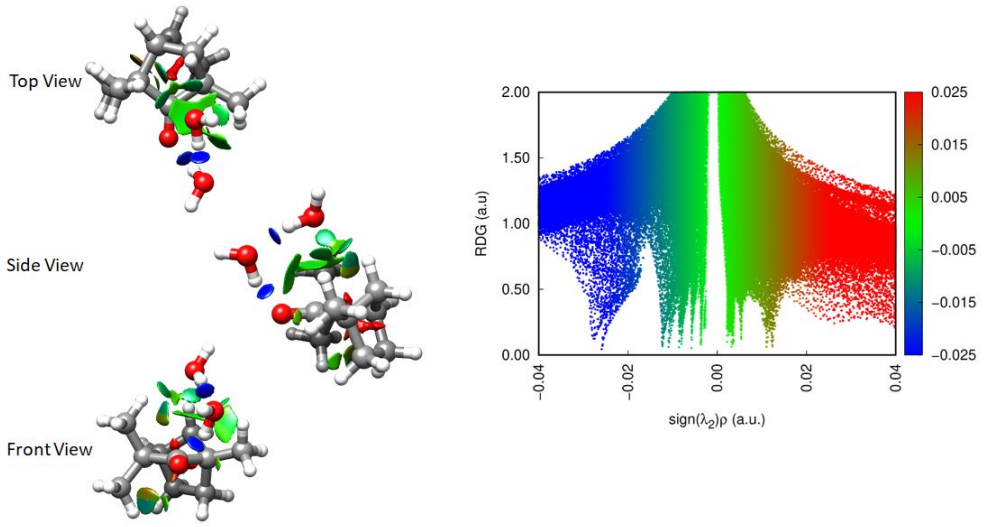

Figure S3: The three different views of the structure of the fenchone dihydrate 2w-I.

Table S8: Calculated equilibrium rotational constants, dipole moments and relative energies of the four dihydrates of fenchone.

Parameter	DFT [a]	MP2 [b]	DFT [a]	MP2 [b]
	2w-I		2w-II	
A / MHz	990.66	988.73	899.37	898.93
B / MHz	608.92	602.86	614.65	602.46
C / MHz	536.11	532.21	568.65	561.1
$\mid \mu_a \mid$ / D	1.38	0.83	1.23	0.72
$\mid \mu_b \mid$ / D	0.38	0.21	1.03	0.37
$\mid \mu_c \mid$ / D	0.38	0.26	0.23	0.1
ΔE [c] / kJ mol^{-1}	0.0	0.0	1.51	2.05
	2w-III		2w-IV	
A / MHz	1137.14	1128.42	1147.03	1136.34
B / MHz	490.46	480.06	490.74	482.18
C / MHz	423.55	418.62	419.27	408.33
$\mid \mu_a \mid$ / D	3.49	2.97	3.44	3.06
$\mid \mu_b \mid$ / D	0.38	0.11	0.27	0.28
$\mid \mu_c \mid$ / D	0.69	0.88	0.25	1.1
ΔE [c] / kJ mol^{-1}	3.72	6.40	3.82	6.88

[a] B3LYP-D3BJ/def2TZVP ; [b] MP2 / 6-311++G(d,p) ; [c] Energy gap relative to conformer 2w-I (including ZPE correction).

Table S9: Experimental rotational and quartic centrifugal distortion constants of the two dihydrates of fenchone, along with the computational constants.

	2w-I					2w-II				
	Exp.	MP2	()[a]	DFT	()[a]	Exp.	MP2	()[a]	DFT	()[a]
A/MHz	983.2739(21)	988.73	(0.55)	990.66	(0.75)	882.5076(36)	898.93	(1.86)	899.36	(1.91)
B/MHz	591.320 83(20)	602.86	(1.95)	608.92	(2.98)	591.877 33(21)	602.46	(1.79)	614.65	(3.85)
C/MHz	523.534 13(14)	532.21	(1.66)	536.11	(2.40)	549.006 20(16)	561.10	(2.20)	568.65	(3.58)
Δ_J/kHz	0.056 32(49)	0.0407		0.0425		0.071 47(97)	0.0918		0.0841	
Δ_{JK}/kHz	0.2722(75)	0.2088		0.1747		0.320(14)	0.0918		0.0936	
Δ_K/kHz	-	−0.1640		−0.1401		-	−0.0882		−0.0570	
δ_J/kHz	0.005 46(44)	0.0035		0.0042		0.006 72(72)	0.0213		0.0189	
δ_K/kHz	-	−0.0363		−0.0558		-	−0.0443		0.0015	
σ_{fit}/kHz	3.89	-		-		4.09	-		-	
N_{lines}	60	-		-		40	-		-	
κ	−0.705	−0.690		−0.679		−0.743	−0.755		−0.722	
P_{aa}/u^{2}Å	653.0037(6)	638.37		631.25		600.8647(12)	588.68		574.51	
P_{bb}/u^{2}Å	312.3183(6)	311.21		311.43		319.6695(12)	312.02		314.22	
P_{cc}/u^{2}Å	201.6575(6)	199.93		198.71		252.9930(12)	250.18		247.71	

[a] See Table S7.

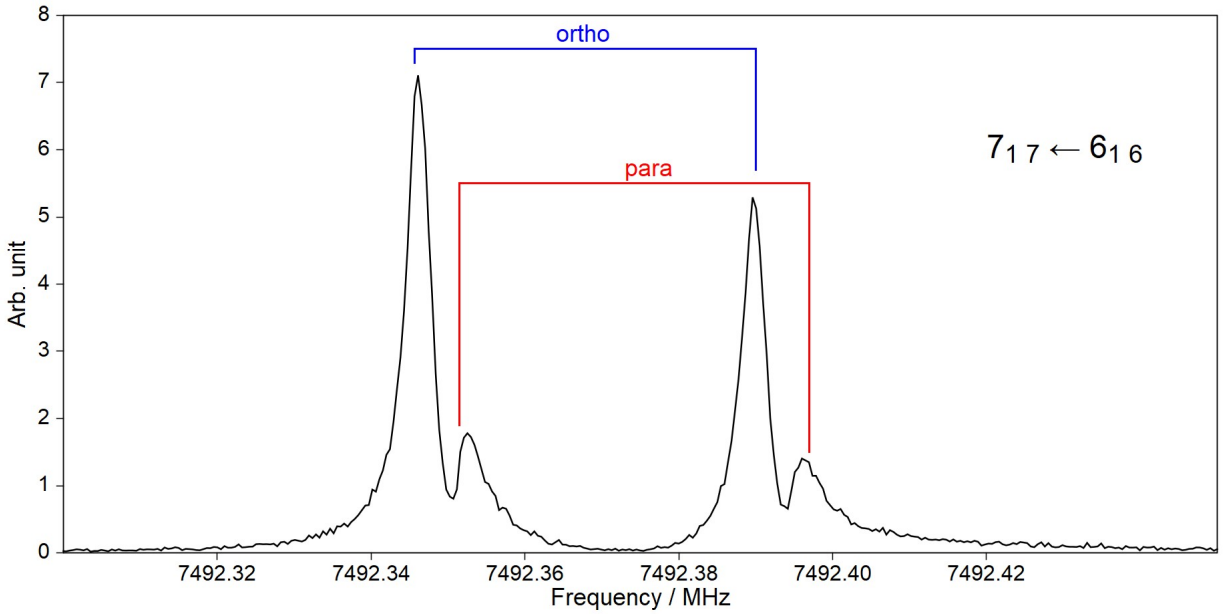

Figure S4: The $7_{17} \leftarrow 6_{06}$ transition of the hydrate 2w-I, showing a splitting of 6 kHz.

Table S10: Experimental rotational and quartic centrifugal distortion constants of the normal and of the $H_2^{18}O$ substituted species of the dihydrate of fenchone 2w-I.

	Normal	$^{18}O_1$-$^{18}O_2$	$^{18}O_1$-$^{16}O_2$	$^{16}O_1$-$^{18}O_2$
A / MHz	983.2739(21)	968.1931(19)	979.9318(40)	972.1031(17)
B / MHz	591.320 83(20)	560.621 12(16)	573.158 24(13)	577.772 233(68)
C / MHz	523.534 13(14)	503.123 34(10)	510.155 87(18)	515.777 209(65)
Δ_J / kHz	0.056 32(49)	0.053 99(97)	0.0575(18)	0.056 40(81)
Δ_{JK} / kHz	0.2722(75)	0.2514(47)	0.277(24)	0.271(11)
Δ_K / kHz	-	-	-	-
δ_J / kHz	0.005 46(44)	0.004 82(79)	[b]	[b]
δ_K / kHz	-	-	-	-
N_{lines} [a]	60	34	24	24
σ_{fit}/kHz	3.89	2.38	2.67	1.90
P_a/u Å^2	653.0037(6)	691.9822(5)	678.3260(11)	667.3302(5)
P_b/u Å^2	312.3183(6)	312.5011(5)	312.3105(11)	312.5095(5)
P_c/u Å^2	201.6575(6)	209.4805(5)	203.4183(11)	207.3726(5)

[a,b] See Table S1.

Table S11: Experimental coordinates (in Å) in the principal axis frame of the water oxygen atoms of the dihydrate of fenchone 2w-I, along with those obtained by *ab initio* and DFT calculations.

	a	*b*	*c*
		O_1	
r_s	3.5664(4)	i	−0.9683(16)
r_0	3.5665(23)	−0.091(15)	−0.9593(78)
MP2 [a]	3.554	−0.044	−0.923
DFT [b]	3.499	−0.067	−0.948
		O_2	
r_s	2.6700(6)	−0.3087(49)	1.7258(9)
r_0	2.6667(31)	−0.319(26)	1.7352(26)
MP2 [a]	2.598	−0.339	1.722
DFT [b]	2.619	−0.342	1.708

[a,b] See Table S2.

Table S12: The substitution and effective structural parameters of the dihydrate of fenchone 2w-I along with those optimized by quantum chemistry.

Parameters [a]	r_s	r_0 [b]	B3LYP[c]	MP2[d]
$r(OfO_1)$ / Å	-	2.823(27)	2.762	2.805
$r(O_2O_1)$ / Å	2.8561(31)	2.859(20)	2.812	2.828
$\angle(O_1OfC_1)$ / °	-	120.4(13)	118.5	119.0
$\angle(O_2O_1Of)$ / °	-	81.40(63)	82.3	81.2
$\tau(O_1OfC_1C_2)$ / °	-	60.9(12)	61.1	62.6
$\tau(O_2O_1OfC_1)$ / °	-	24.8(16)	25.2	24.2
σ_{fit}/uÅ^2	-	0.084	-	-

[a] Numbering scheme is shown in Fig. S3 ; [b,c,d] See Table S3.

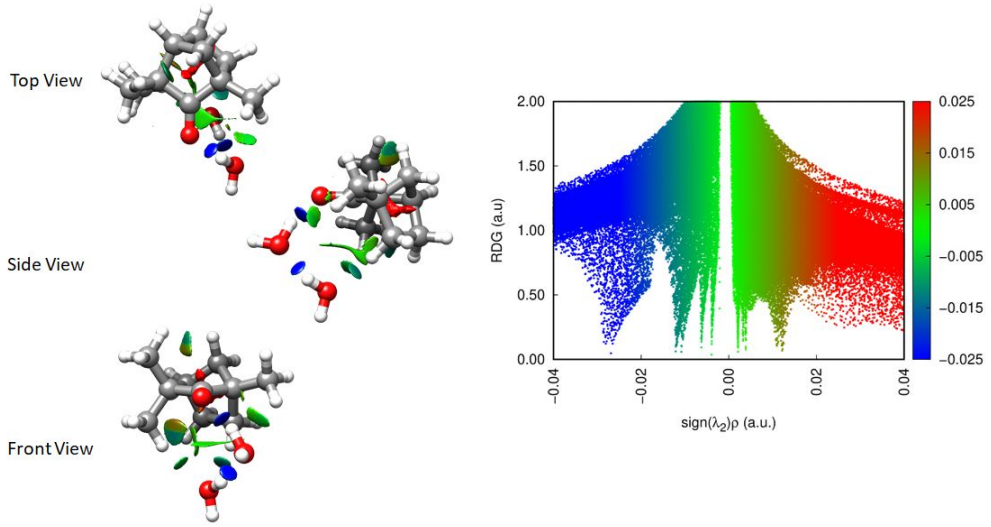

Figure S5: The three different views of the structure of the fenchone dihydrate 2w-II.

Table S13: Experimental rotational and quartic centrifugal distortion constants of the normal and of the $H_2^{18}O$ substituted species of the dihydrate of fenchone 2w-II.

	Normal	$^{18}O_1$-$^{18}O_2$	$^{18}O_1$-$^{16}O_2$	$^{16}O_1$-$^{18}O_2$
A / MHz	882.5076(36)	869.2273(40)	880.3906(29)	871.9281(42)
B / MHz	591.877 33(21)	562.949 41(21)	574.396 35(12)	579.372 17(18)
C / MHz	549.006 20(16)	524.792 75(10)	534.520 910(90)	538.435 30(14)
Δ_J / kHz	0.071 47(97)	0.0700(15)	0.0688(12)	0.0723(17)
Δ_{JK} / kHz	0.320(14)	0.277(26)	0.313(16)	0.217(41)
Δ_K / kHz	-	-	-	-
δ_J / kHz	0.006 72(72)	0.006 71(97)	*b*	*b*
δ_K / kHz	-	-	-	-
N_{lines} [a]	40	29	27	23
σ_{fit}/kHz	4.09	2.91	1.71	1.99
P_a / u Å^2	600.8647(12)	639.6647(14)	625.6422(10)	615.6416(14)
P_b / u Å^2	319.6695(12)	323.3422(14)	319.8381(10)	322.9651(14)
P_c / u Å^2	252.9930(12)	258.0696(14)	254.2017(10)	256.6457(14)

[a,b] See Table S1.

Table S14: Experimental coordinates (in Å) in the principal axis frame of the water oxygen atoms of the dihydrate of fenchone 2w-II, along with those obtained by *ab initio* and DFT calculations.

	a	*b*	*c*
		O_1	
r_s	3.527 51(44)	0.3013(52)	0.8089(19)
r_0	3.5287(12)	0.2758(13)	0.8060(86)
MP2 [a]	3.477	0.149	0.805
DFT [b]	3.401	0.185	0.789
		O_2	
r_s	2.699 38(58)	−1.2858(12)	−1.4196(11)
r_0	2.6950(20)	−1.2885(40)	−1.4200(39)
MP2 [a]	2.600	−1.198	−1.531
DFT [b]	2.582	−1.332	−1.447

[a,b] See Table S2.

Table S15: The substitution and effective structural parameters of the dihydrate of fenchone 2w-II along with those optimized by quantum chemistry.

Parameters [a]	r_s	r_0 [b]	B3LYP[c]	MP2[d]
$r(OfO_1)$ / Å	-	2.902(10)	2.741	2.782
$r(O_2O_1)$ / Å	2.8585(34)	2.854(8)	2.823	2.836
$\angle(O_1OfC_1)$ / °	-	120.53(37)	118.9	121.1
$\angle(O_2O_1Of)$ / °	-	82.09(17)	81.3	80.9
$\tau(O_1OfC_1C_2)$ / °	-	−55.29(38)	−49.1	−50.5
$\tau(O_2O_1OfC_1)$ / °	-	−46.37(33)	−53.3	−49.5
σ_{fit}/uÅ^2	-	0.047	-	-

[a] Numbering scheme is shown in Fig. S5 ; [b,c,d] See Table S3.

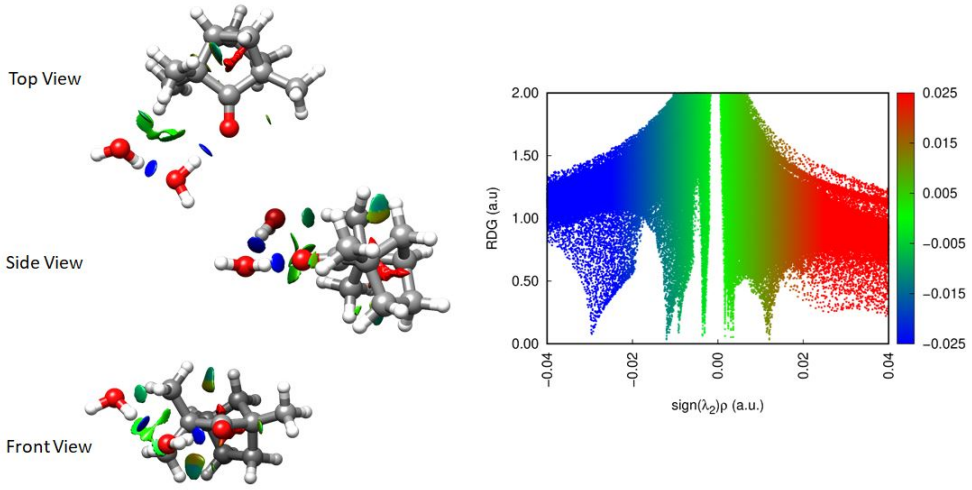

Figure S6: The three different views of the structure of the fenchone dihydrate 2w-IV.

Table S16: Experimental rotational and quartic centrifugal distortion constants of the dihydrates of fenchone 2w-IV, along with the computational constants and dipole moments.

	2w-IV				
	Exp.	MP2	()[a]	DFT	()[a]
A/MHz	1153.237(12)	1128.42	(-2.16)	1137.14	(1.40)
B/MHz	479.537 21(25)	480.06	(0.11)	490.46	(2.28)
C/MHz	407.800 26(27)	418.62	(2.65)	423.55	(3.86)
Δ_J/kHz	0.0437(15)	0.0749		0.0525	
Δ_{JK}/kHz	0.284(10)	0.3345		0.1134	
Δ_K/kHz	-	−0.1575		0.0653	
δ_J/kHz	-	0.0149		0.0013	
δ_K/kHz	-	0.3211		0.3053	
σ_{fit}/kHz	4.51	-		-	
N_{lines}	51	-		-	
κ	−0.808	−0.827		−0.812	
P_a/u Å^2	927.4716(23)	906.06		889.59	
P_b/u Å^2	311.8091(23)	301.19		303.60	
P_c/u Å^2	126.4174(23)	146.68		140.83	

[a] See Table S7.

Table S17: Experimental rotational and quartic centrifugal distortion constants of the normal and of the $H_2^{18}O$ substituted species of the dihydrate of fenchone 2w-IV.

	Normal	$^{18}O_1$-$^{18}O_2$	$^{18}O_1$-$^{16}O_2$	$^{16}O_1$-$^{18}O_2$
A (MHz)	1153.237(12)	1133.504(12)	1137.885(15)	1149.544(15)
B (MHz)	479.537 21(25)	454.768 84(21)	470.194 72(32)	463.154 27(40)
C (MHz)	407.800 26(27)	387.710 12(28)	399.364 68(32)	395.496 59(37)
Δ_J (kHz)	0.0437(15)	0.0372(13)	0.0387(21)	0.0435(23)
Δ_{JK} (kHz)	0.284(10)	0.316(15)	0.355(39)	0.327(46)
N_{lines}	51	30	30	30
σ_{fit} (kHz)	4.51	4.44	4.39	5.39

Table S18: Experimental coordinates in Å of the water oxygen atoms of the dihydrates of fenchone 2w-III and 2w-IV, along with those obtained by *ab initio* and DFT calculations.

	a	b	c
		O_1	
r_s	3.207 86(55)	−1.7029(11)	0.4243(43)
r_0(2w-III)	3.2174(87)	−1.715(17)	0.451(27)
r_0(2w-IV)	3.236(11)	−1.7150(73)	0.0878(9)
MP2 (2w-III)	3.264	−1.522	0.828
MP2(2w-IV)	3.267	−1.683	−0.109
DFT (2w-III)	3.195	−1.601	0.732
DFT (2w-IV)	3.215	−1.696	0.494
		O_2	
r_s	4.326 89(41)	0.8467(21)	−0.1882(96)
r_0(2w-III)	4.335(7)	0.844(16)	−0.265(11)
r_0(2w-IV)	4.3249(88)	0.9018(93)	−0.4438(19)
MP2 (2w-III)	4.262	0.648	−0.651
MP2 (2w-IV)	4.325	0.857	−0.482
DFT (2w-III)	4.225	0.681	−0.496
DFT (2w-IV)	4.229	0.793	−0.249

[a,b] See Table S2.

Table S19: The substitution and effective structural parameters of the dihydrate of fenchone 2w-IV along with those optimized by quantum chemistry.

Parameters [a]	r_0(2w-III)	r_0(2w-IV)	B3LYP(III)	MP2(III)	B3LYP(IV)	MP2(IV)
$r(OfO_1)$ / Å	2.821(18)	2.895(15)	2.769	2.809	2.777	2.810
$r(O_2O_1)$ / Å	2.882(40)	2.884(15)	2.788	2.809	2.789	2.814
$\angle(O_1OfC_1)$ / °	131.4(10)	126.19(48)	132.65	133.83	132.73	131.06
$\angle(O_2O_1Of)$ / °	108.72(22)	107.09(33)	102.82	100.93	106.05	106.23
σ_{fit}/uÅ^2	0.16	0.27	-	-		

[a] Numbering scheme is shown Fig. S6; [b,c,d] See Table S3.

Table S20: Calculated rotational constants, dipole moments and relative energies (including ZPE corrections) of the five optimized trihydrates of fenchone.

Parameter	DFT [a]	MP2 [b]	DFT [a]	MP2 [b]	DFT [a]	MP2 [b]
	3w-I		3w-II		3w-II	
A / MHz	822.89	835.94	776.73	774.67	828.90	826.30
B / MHz	423.34	412.76	447.19	435.91	462.79	448.16
C / MHz	410.57	401.37	412.32	402.9	399.05	390.21
$\lvert \mu_a \rvert$ / D	1.30	1.07	1.51	1.20	1.85	1.36
$\lvert \mu_b \rvert$ / D	0.39	0.52	0.86	0.95	1.01	1.07
$\lvert \mu_c \rvert$ / D	0.01	0.06	0.38	0.40	1.10	0.86
ΔE [c] / kJ mol^{-1}	0.0	0.0	0.95	1.66	1.98	2.02
	3w-IV		3w-V			
A / MHz	751.92	746.09	917.83	913.89		
B / MHz	439.21	424.62	390.93	387.36		
C / MHz	407.55	396.86	318.74	314.55		
$\lvert \mu_a \rvert$ / D	2.00	1.80	2.24	1.75		
$\lvert \mu_b \rvert$ / D	1.25	0.96	0.20	0.51		
$\lvert \mu_c \rvert$ / D	1.27	0.87	0.56	0.13		
ΔE [c] / kJ mol^{-1}	4.12	4.58	5.61	7.27		

[a,b] See Table S8 ; [c] Energy gap relative to the lowest energy conformer 3w-I (including ZPE correction).

Table S21: Experimental rotational and quartic centrifugal distortion constants of the three observed trihydrates of fenchone, along with the computational constants and dipole moments.

	3w-I		3w-II		3w-III	
Parameters	exp.	MP2 [a]	exp.	MP2 [a]	exp.	MP2 [a]
A / MHz	825.2745(94)	835.94	756.3620(34)	774.67	820.5228(14)	826.30
B / MHz	406.893833(93)	412.76	431.82218(20)	435.91	449.00647(12)	448.16
C / MHz	396.499381(82)	401.37	396.89694(11)	402.9	393.456862(81)	390.21
Δ_J / kHz	0.04150(21)	0.0319	0.05504(57)	0.0411	0.05590(45)	0.0569
Δ_{JK} / kHz	0.0208(35)	0.0386	0.1442(65)	0.0784	-	0.1449
Δ_K / kHz	-	0.2678	-	0.0094	-	−0.0516
δ_J / kHz	0.00397(29)	0.0011	0.01016(52)	0.0068	0.01313(40)	0.0111
δ_k / kHz	-	0.0601	-	−0.0308	-	0.0889
σ_{fit}/kHz	2.99	-	1.55	-	1.42	-
N_{lines}	45	-	37	-	37	-
κ	-0.951	−0.948	-0.806	−0.822	-0.740	−0.734

[a] MP2 / 6-311++G(d,p).

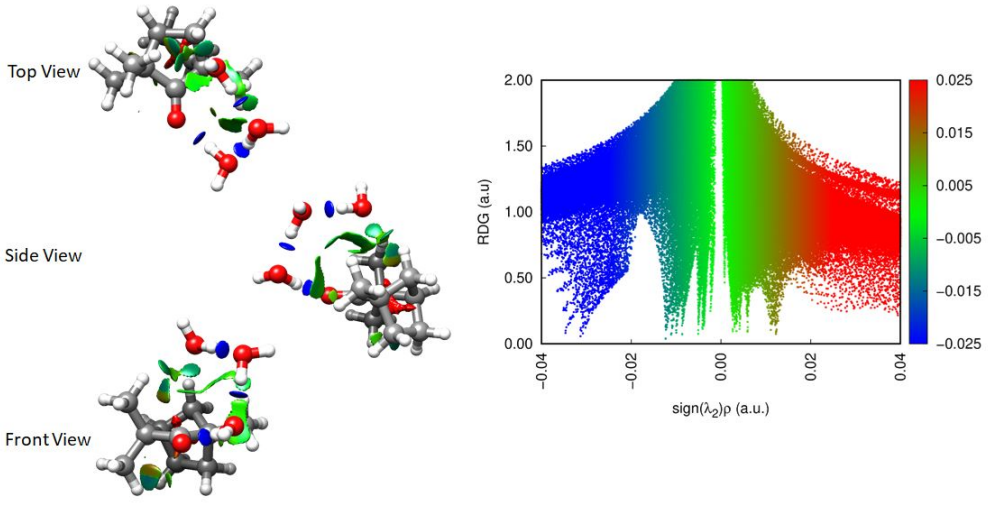

Figure S7: The three different views of the structure of the fenchone trihydrate 3w-I.

Table S22: Experimental rotational and quartic centrifugal distortion constants of the normal and of the $H_2^{18}O$ substituted species of the trihydrate of fenchone 3w-I.

	Normal	$^{18}O_1$-$^{18}O_2$-$^{18}O_3$	$^{18}O_1$-$^{18}O_2$-$^{16}O_3$	$^{18}O_1$-$^{16}O_2$-$^{18}O_3$
A / MHz	825.2745(94)	799.20(18)	813.66(11)	800.00(14)
B / MHz	406.893 833(93)	386.249 83(72)	388.977 76(22)	396.281 58(45)
C / MHz	396.499 381(82)	375.345 17(77)	379.994 16(25)	384.803 57(52)
Δ_J / kHz	0.041 50(21)	0.0379(50)	0.0362(17)	0.0342(37)
Δ_{JK} / kHz	0.0208(35)	*b*	*b*	*b*
Δ_K / kHz	-	-	-	-
δ_J / kHz	0.003 97(29)	*b*	*b*	*b*
δ_K / kHz	-	-	-	-
N_{lines} [a]	45	26	18	17
σ_{fit}/kHz	2.99	3.29	2.88	5.98
P_a/u Å^2	952.1334(35)	1011.254(71)	1004.048(42)	978.461(55)
P_b/u Å^2	322.4688(35)	335.184(71)	325.917(42)	334.882(55)
P_c/u Å^2	289.9080(35)	297.172(71)	295.201(42)	296.842(55)
	$^{16}O_1$-$^{18}O_2$-$^{18}O_3$	$^{18}O_1$-$^{16}O_2$-$^{16}O_3$	$^{16}O_1$-$^{18}O_2$-$^{16}O_3$	$^{16}O_1$-$^{16}O_2$-$^{18}O_3$
A / MHz	810.64(21)	814.75(11)	824.59(12)	810.752(87)
B / MHz	392.753 64(48)	399.257 10(23)	396.037 08(27)	403.318 68(31)
C / MHz	381.714 12(50)	389.755 26(28)	386.256 43(29)	391.644 74(36)
Δ_J / kHz	0.0447(31)	0.0418(19)	0.0432(20)	0.0446(21)
Δ_{JK} / kHz	*b*	*b*	*b*	*b*
Δ_K / kHz	-	-	-	-
δ_J / kHz	*b*	*b*	*b*	*b*
δ_K / kHz	-	-	-	-
N_{lines} [a]	17	19	21	22
σ_{fit}/kHz	6.09	3.32	4.13	4.92
P_a/u Å^2	993.649(81)	971.084(42)	985.804(45)	1027.9201(11)
P_b/u Å^2	330.323(81)	325.573(42)	322.599(45)	471.1235(11)
P_c/u Å^2	293.109(81)	294.714(42)	290.286(45)	184.2327(11)

[a] The number of fitted lines ; [b] Fixed at the value of the normal species; [c] Fixed at the value of the fully substituted species.

Table S23: Experimental coordinates (in Å) in the principal axis frame of the water oxygen atoms of the trihydrate of fenchone 3w-I, along with those obtained by *ab initio* and DFT calculations.

	a	*b*	*c*
		O_1	
r_s	−3.0714(32)	1.1712(75)	1.6507(68)
r_0	−3.074(6)	1.177(14)	1.666(13)
MP2 [a]	−3.080	1.072	1.667
DFT [b]	−3.017	1.299	1.531
		O_2	
r_s	−4.1170(30)	−0.262(49)	−0.448(29)
r_0	−4.118(4)	−0.339(12)	−0.477(14)
MP2 [a]	−4.101	−0.330	−0.474
DFT [b]	−3.982	−0.383	−0.394
		O_3	
r_s	−1.9808(78)	−1.9071(78)	−1.398(14)
r_0	−1.999(8)	−1.905(11)	−1.393(17)
MP2 [a]	−1.933	−1.796	−1.482
DFT [b]	−1.926	−2.018	−1.325

[a,b] See Table S2.

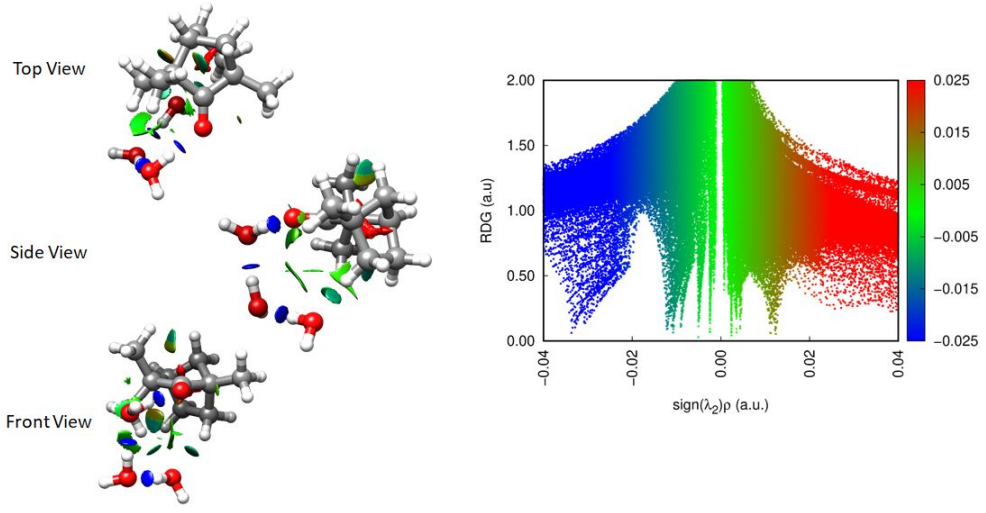

Figure S8: The three different views of the structure of the fenchone trihydrate 3w-II.

Table S24: The substitution and effective structural parameters of the fenchone trihydrate 3w-I along with those optimized by quantum chemistry.

Parameters [a]	r_s	r_0 [b]	B3LYP[c]	MP2[d]
$r(OfO_1)$ / Å	-	2.795(13)	2.734	2.779
$r(O_2O_1)$ / Å	2.748(35)	2.825(15)	2.733	2.755
$r(O_3O_2)$ / Å	2.859(31)	2.790(19)	2.786	2.805
$\angle(O_1OfC_1)$ / °	-	134.33(94)	131.3	132.5
$\angle(O_2O_1Of)$ / °	-	98.15(80)	98.0	99.3
$\angle(O_3O_2O_1)$ / °	105.64(43)	105.65(36)	109.6	105.0
$\tau(O_1OfC_1C_2)$ / °	-	27.6(19)	30.1	29.9
$\tau(O_2O_1OfC_1)$ / °	-	47.4(19)	47.2	47.3
$\tau(O_3O_2O_1Of)$ [e] / °	-	2.79(80)	−0.3	0.7
σ_{fit}/uÅ^2	-	0.128	-	-

[a] Numbering scheme is shown in Fig. S7 ; [b,c,d] See Table S3 ; [e] r_0 value calculated using the ouput coordinates of the fit.

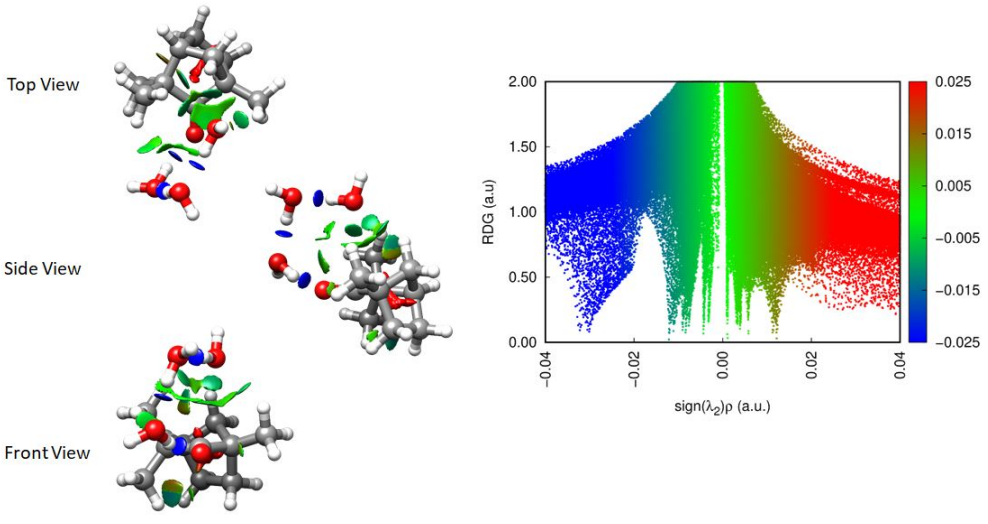

Figure S9: The three different views of the structure of the fenchone trihydrate 3w-III.

Table S25: Experimental rotational and quartic centrifugal distortion constants of the normal and the $H_2^{18}O$ substituted species of the trihydrate of fenchone 3w-II.

	Normal	$^{18}O_1$-$^{18}O_2$-$^{18}O_3$	$^{18}O_1$-$^{18}O_2$-$^{16}O_3$	$^{18}O_1$-$^{16}O_2$-$^{18}O_3$
A / MHz	756.3620(34)	733.0349(37)	733.774(20)	741.463(69)
B / MHz	431.822 18(20)	411.286 22(23)	422.337 70(39)	417.312 49(93)
C / MHz	396.896 94(11)	374.162 98(14)	383.501 18(41)	380.791 73(48)
Δ_J / kHz	0.055 04(57)	0.051 62(73)	0.0667(27)	[c]
Δ_{JK} / kHz	0.1442(65)	0.130(10)	[c]	[c]
Δ_K / kHz	-	-	-	-
δ_J / kHz	0.010 16(52)	0.009 98(66)	[c]	[c]
δ_K / kHz	-	-	-	-
N_{lines}[a]	37	21	15	9
σ_{fit}/kHz	1.55	1.06	3.55	5.47
P_a/u Å^2	887.7476(15)	945.0176(18)	912.8433(94)	928.307(32)
P_b/u Å^2	385.5779(15)	405.6745(18)	404.9597(94)	398.872(32)
P_c/u Å^2	282.5929(15)	283.7592(18)	283.7797(94)	282.725(32)
	$^{16}O_1$-$^{18}O_2$-$^{18}O_3$	$^{18}O_1$-$^{16}O_2$-$^{16}O_3$	$^{16}O_1$-$^{18}O_2$-$^{16}O_3$	$^{16}O_1$-$^{16}O_2$-$^{18}O_3$
A / MHz	747.159(36)	742.327(39)	748.341(28)	755.348(49)
B / MHz	413.690 53(69)	428.928 53(73)	424.905 63(51)	420.004 55(96)
C / MHz	379.834 48(46)	390.590 36(57)	389.567 46(47)	386.676 48(75)
Δ_J / kHz	0.0510(46)	0.0560(52)	0.0589(44)	0.0650(56)
Δ_{JK} / kHz	[c]	[b]	[b]	[b]
Δ_K / kHz	-	-	-	-
δ_J / kHz	[c]	[b]	[b]	[b]
δ_K / kHz	-	-	-	-
N_{lines}[a]	15	14	15	17
σ_{fit}/kHz	5.98	6.03	5.04	9.77
P_a/u Å^2	937.879(16)	895.658(18)	905.670(13)	920.592(22)
P_b/u Å^2	392.645(16)	398.226(18)	391.619(13)	386.389(22)
P_c/u Å^2	283.756(16)	282.577(18)	283.721(13)	282.678(22)

[a,b,c] See Table S22 .

Table S26: Experimental coordinates (in Å) in the principal axis frame of the water oxygen atoms of the trihydrate of fenchone 3w-II, along with those obtained by *ab initio* and DFT calculations.

	a	*b*	*c*
		O_1	
r_s	−2.9841(12)	1.7645(21)	0.7866(50)
r_0	−2.985(3)	1.763(5)	0.786(11)
MP2 [a]	−3.019	1.643	0.852
DFT [b]	−2.963	1.649	0.813
		O_2	
r_s	−4.0643(14)	−0.6594(90)	−0.213(28)
r_0	−4.067(2)	−0.649(10)	−0.104(27)
MP2 [a]	−4.064	−0.715	−0.151
DFT [b]	−3.980	−0.740	−0.082
		O_3	
r_s	−1.9712(24)	−2.5443(19)	i
r_0	−1.964(4)	−2.547(4)	−0.169(55)
MP2 [a]	−1.871	−2.463	−0.286
DFT [b]	−1.812	−2.482	−0.267

[a,b] See Table S2.

Table S27: The substitution and effective structural parameters of fenchone trihydrate 3w-II along with those optimized by quantum chemistry.

Parameters [a]	r_s	r_0 [b]	B3LYP[c]	MP2[d]
$r(\mathrm{OfO_1})$Å	-	2.739(18)	2.718	2.765
$r(\mathrm{O_2O_1})$Å	2.836(13)	2.789(12)	2.746	2.767
$r(\mathrm{O_3O_2})$Å	2.817(6)	2.835(8)	2.787	2.808
$\angle(\mathrm{O_1OfC_1})$ / °	-	133.02(72)	128.2	130.3
$\angle(\mathrm{O_2O_1Of})$ / °	-	100.6(12)	97.8	98.9
$\angle(\mathrm{O_3O_2O_1})$ / °	107.22(79)	107.3(3)	106.1	104.6
$\tau(\mathrm{O_1OfC_1C_2})$ / °	-	−1556(21)	−1632	−1609
$\tau(\mathrm{O_2O_1OfC_1})$ / °	-	62.7(32)	72.7	70.5
$\tau(\mathrm{O_3O_2O_1Of})$ / °	-	-	−8.3	−5.2
σ_{fit} / u$\mathrm{Å}^2$	-	0.054	-	-

[a] Numbering scheme is shown in Fig. S8 ; [b,c,d] See Table S3.

Table S28: Experimental rotational and quartic centrifugal distortion constants of the normal and of the $H_2^{18}O$ substituted species of the trihydrate of fenchone 3w-III.

	Normal	$^{18}O_1$-$^{18}O_2$-$^{18}O_3$	$^{18}O_1$-$^{18}O_2$-$^{16}O_3$	$^{18}O_1$-$^{16}O_2$-$^{18}O_3$
A / MHz	820.5228(14)	794.549(12)	809.568(17)	795.694(11)
B / MHz	449.006 47(12)	426.333 20(36)	429.007 08(59)	437.848 15(63)
C / MHz	393.456 862(81)	373.134 21(32)	377.520 67(44)	381.950 11(38)
Δ_J / kHz	0.055 90(45)	0.0558(17)	0.0578(33)	0.0624(23)
Δ_{JK} / kHz	-	-	-	-
Δ_K / kHz	-	-	-	-
δ_J / kHz	0.013 13(40)	[b]	[b]	[b]
δ_K / kHz	-	-	-	-
N_{lines}[a]	37	22	18	19
σ_{fit}/kHz	1.42	4.22	5.48	5.25
P_a/u Å^2	897.0424(6)	951.8835(49)	946.2208(66)	921.1228(45)
P_b/u Å^2	387.4161(6)	402.5327(49)	392.4582(66)	402.0317(45)
P_c/u Å^2	228.5071(6)	233.5250(49)	231.7994(66)	233.1107(45)
	$^{16}O_1$-$^{18}O_2$-$^{18}O_3$	$^{18}O_1$-$^{16}O_2$-$^{16}O_3$	$^{16}O_1$-$^{18}O_2$-$^{16}O_3$	$^{16}O_1$-$^{16}O_2$-$^{18}O_3$
A / MHz	804.7051(90)	810.9967(99)	819.411(11)	805.544(12)
B / MHz	433.615 43(38)	440.738 80(35)	436.610 37(42)	445.757 78(41)
C / MHz	379.377 73(26)	386.620 81(27)	383.894 27(31)	388.635 20(33)
Δ_J / kHz	0.0563(16)	0.0545(20)	0.0554(19)	0.0596(26)
Δ_{JK} / kHz	-	-	-	-
Δ_K / kHz	-	-	-	-
δ_J / kHz	[b]	[b]	[b]	[b]
δ_K / kHz	-	-	-	-
N_{lines}[a]	22	19	21	17
σ_{fit}/kHz	3.94	3.57	4.51	3.83
P_a/u Å^2	934.7983(36)	915.3375(38)	928.6002(42)	903.3854(47)
P_b/u Å^2	397.3278(36)	391.8321(38)	387.8534(42)	397.0089(47)
$P_c(u.\text{Å}^2)$	230.7022(36)	231.3257(38)	228.9055(42)	230.3671(47)

[a,b,c] See Table S22.

Table S29: Experimental coordinates (in Å) in the principal axis frame of the water oxygen atoms of the trihydrate of fenchone 3w-III, along with those obtained by *ab initio* and DFT calculations.

	a	*b*	*c*
		O_1	
r_s	3.016 38(59)	−1.5046(12)	−1.2245(15)
r_0	3.029(10)	−1.554(14)	−1.1541(5)
MP2 [a]	3.104	−1.561	−1.146
DFT [b]	3.018	−1.584	−1.092
		O_2	
r_s	3.984 40(46)	0.4831(39)	0.4591(41)
r_0	3.990(7)	0.601(22)	0.369(10)
MP2 [a]	4.037	0.553	0.382
DFT [b]	3.957	0.592	0.301
		O_3	
r_s	1.7682(11)	2.199 02(87)	1.0015(20)
r_0	1.776(16)	2.198(17)	1.056(26)
MP2 [a]	1.765	2.036	1.136
DFT [b]	1.733	2.033	1.161

[a,b] See Table S2.

Table S30: The substitution and effective structural parameters of the fenchone trihydrate 3w-III along with those optimized by quantum chemistry.

Parameters [a]	r_s	r_0 [b]	B3LYP[c]	MP2[d]
$r(\mathrm{OfO_1})$ / Å	-	2.825(26)	2.719	2.763
$r(\mathrm{O_2O_1})$ Å	2.7789(39)	2.809(32)	2.749	2.770
$r(\mathrm{O_3O_2})$ Å	2.8548(27)	2.815(27)	2.786	2.816
$\angle(\mathrm{O_1OfC_1})$	-	125.8(12)	129.7	133.2
$\angle(\mathrm{O_2O_1Of})$ / °	-	92.32(40)	89.1	90.8
$\angle(\mathrm{O_3O_2O_1})$ / °	105.940(58)	107.38(44)	107.1	106.1
$\tau(\mathrm{O_1OfC_1C_2})^e$ / °	-	152.43(89)	150.7	147.5
$\tau(\mathrm{O_2O_1OfC_1})^e$ / °	-	−69.31(94)	−75.2	−69.3
$\tau(\mathrm{O_3O_2O_1Of})^e$ / °	-	12.82(78)	18.7	12.8
$\sigma_{\mathrm{fit}}/\mathrm{u\AA}^2$	-	0.240	-	-

[a] Numbering scheme is shown in Fig. S9 ; [b,c,d,e] See Table S24.

Table S31: Measured frequencies ($\nu_{\text{obs.}}$) and residuals ($\nu_{\text{obs.}} - \nu_{\text{calc.}}$) in MHz of the monohydrate of fenchone 1w-I.

J'	K'_a	K'_c	$\leftarrow$	J''	K''_a	K''_c	$\nu_{\text{obs.}}$	$\nu_{\text{obs.}} - \nu_{\text{calc.}}$	exp. error [a]
2	1	2	$\leftarrow$	1	1	1	2566.3279	0.0014	0.010
6	1	5	$\leftarrow$	6	1	6	2595.5496	−0.0021	0.010
2	0	2	$\leftarrow$	1	0	1	2676.7063	−0.0003	0.010
2	1	1	$\leftarrow$	1	1	0	2828.7700	0.0004	0.010
3	1	3	$\leftarrow$	2	1	2	3837.3529	0.0009	0.010
3	0	3	$\leftarrow$	2	0	2	3966.2137	0.0004	0.010
3	2	2	$\leftarrow$	2	2	1	4046.3126	−0.0019	0.010
3	2	1	$\leftarrow$	2	2	0	4126.4285	0.0069	0.010
3	1	2	$\leftarrow$	2	1	1	4228.9158	0.0007	0.010
4	0	4	$\leftarrow$	3	1	3	4902.6107	−0.0003	0.002
4	1	4	$\leftarrow$	3	1	3	5096.5199	−0.0001	0.002
4	0	4	$\leftarrow$	3	0	3	5212.1627	0.0001	0.002
4	2	3	$\leftarrow$	3	2	2	5378.7723	0.0040	0.010
4	1	4	$\leftarrow$	3	0	3	5406.0706	−0.0009	0.002
4	3	2	$\leftarrow$	3	3	1	5431.1835	−0.0109	0.010
4	2	2	$\leftarrow$	3	2	1	5561.5187	0.0000	0.010
4	1	3	$\leftarrow$	3	1	2	5609.0138	0.0000	0.001
5	1	5	$\leftarrow$	4	1	4	6343.6750	−0.0005	0.002
5	0	5	$\leftarrow$	4	0	4	6427.6774	−0.0003	0.002
5	1	5	$\leftarrow$	4	0	4	6537.5842	−0.0003	0.002
5	2	4	$\leftarrow$	4	2	3	6697.6282	0.0015	0.010
5	3	3	$\leftarrow$	4	3	2	6796.1961	0.0035	0.010
5	3	2	$\leftarrow$	4	3	1	6837.9621	−0.0008	0.010
5	1	4	$\leftarrow$	4	1	3	6957.9945	−0.0002	0.002
5	2	3	$\leftarrow$	4	2	2	7012.4136	0.0001	0.002
3	3	1	$\leftarrow$	2	2	0	7109.6247	−0.0001	0.002
6	0	6	$\leftarrow$	5	1	5	7522.6201	−0.0003	0.002
6	1	6	$\leftarrow$	5	1	5	7580.4865	−0.0003	0.010
6	0	6	$\leftarrow$	5	0	5	7632.5269	−0.0003	0.010

[a] The expected accuracy is respectively 10 kHz and 1 to 2 kHz for the transitions respectively measured with the chirped-pulse and the cavity-based spectrometers.

J'	K'_a	K'_c	$\leftarrow$	J''	K''_a	K''_c	$\nu_{\text{obs.}}$	$\nu_{\text{obs.}} - \nu_{\text{calc.}}$	exp. error [a]
6	1	6	$\leftarrow$	5	0	5	7690.3932	−0.0003	0.002
6	2	5	$\leftarrow$	5	2	4	8000.4255	−0.0002	0.002
6	3	4	$\leftarrow$	5	3	3	8158.3749	0.0015	0.002
6	3	3	$\leftarrow$	5	3	2	8262.0526	0.0009	0.001
4	3	1	$\leftarrow$	3	2	1	8428.8853	−0.0030	0.005
4	3	2	$\leftarrow$	3	2	2	8515.3460	−0.0012	0.002
5	2	3	$\leftarrow$	4	1	3	8529.6459	0.0001	0.002
7	0	7	$\leftarrow$	6	0	6	8838.4812	−0.0004	0.001
5	3	2	$\leftarrow$	4	2	2	9705.3312	−0.0013	0.002
7	2	6	$\leftarrow$	6	1	5	9995.4405	0.0010	0.002
8	0	8	$\leftarrow$	7	1	7	10 019.5123	−0.0002	0.002
6	2	4	$\leftarrow$	5	1	4	10 026.0416	0.0004	0.002
8	1	7	$\leftarrow$	7	2	6	10 262.3636	−0.0007	0.002
8	4	4	$\leftarrow$	7	4	3	10 967.6072	0.0001	0.001
8	2	7	$\leftarrow$	7	1	6	11 028.5741	0.0003	0.002
5	4	2	$\leftarrow$	4	3	1	11 044.4113	−0.0011	0.002
8	3	5	$\leftarrow$	7	3	4	11 197.5444	−0.0004	0.001
6	3	3	$\leftarrow$	5	2	4	11 553.4575	0.0001	0.002
9	1	8	$\leftarrow$	8	2	7	11 639.9033	−0.0001	0.002
9	2	8	$\leftarrow$	8	1	7	12 098.6679	0.0003	0.002
9	3	7	$\leftarrow$	8	3	6	12 178.5716	−0.0005	0.001
9	7	2	$\leftarrow$	8	7	1	12 223.6484	−0.0005	0.005
9	7	3	$\leftarrow$	8	7	2	12 223.6489	0.0065	0.005
9	6	4	$\leftarrow$	8	6	3	12 243.6307	0.0023	0.002
9	6	3	$\leftarrow$	8	6	2	12 243.9580	0.0011	0.001
9	5	5	$\leftarrow$	8	5	4	12 274.3738	−0.0005	0.001
9	5	4	$\leftarrow$	8	5	3	12 283.1247	−0.0002	0.001
9	4	6	$\leftarrow$	8	4	5	12 293.3885	−0.0007	0.001
6	4	3	$\leftarrow$	5	3	2	12 367.9912	0.0001	0.002

[a] see Table S31

J'	K'_a	K'_c	←	J''	K''_a	K''_c	$\nu_{\text{obs.}}$	$\nu_{\text{obs.}} - \nu_{\text{calc.}}$	exp. error [a]
9	4	5	←	8	4	4	12 406.1741	0.0032	0.005
6	4	2	←	5	3	3	12 431.9296	0.0011	0.002
10	0	10	←	9	1	9	12 470.3620	0.0002	0.002
10	1	10	←	9	1	9	12 473.3666	−0.0002	0.002
10	1	10	←	9	0	9	12 479.9074	−0.0003	0.002
10	2	8	←	9	3	7	12 641.2645	−0.0017	0.002
9	3	6	←	8	3	5	12 673.4091	−0.0003	0.001
10	8	2	←	9	8	1	13 578.1648	0.0001	0.002
10	8	3	←	9	8	2	13 578.1652	0.0010	0.002
10	6	5	←	9	6	4	13 623.1588	0.0011	0.001
10	6	4	←	9	6	3	13 624.3615	−0.0009	0.002
7	4	4	←	6	3	3	13 643.7013	0.0003	0.002
10	5	6	←	9	5	5	13 661.3814	−0.0004	0.001
10	4	7	←	9	4	6	13 663.9090	−0.0002	0.001
10	5	5	←	9	5	4	13 684.7748	0.0005	0.001
9	3	7	←	8	2	6	13 772.3615	0.0058	0.005
10	4	6	←	9	4	5	13 877.9801	0.0009	0.002
12	1	12	←	11	1	11	14 909.3444	0.0003	0.001
12	0	12	←	11	0	11	14 910.0960	−0.0006	0.001
11	6	6	←	10	6	5	15 008.4732	−0.0003	0.002
11	5	7	←	10	5	6	15 051.2284	−0.0005	0.002
13	1	13	←	12	1	12	16 126.9086	0.0018	0.002
13	0	13	←	12	0	12	16 127.2455	0.0002	0.002
12	2	10	←	11	2	9	16 252.0992	−0.0005	0.002
12	11	1	←	11	11	0	16 276.9400	−0.0032	0.002
12	11	2	←	11	11	1	16 276.9400	−0.0032	0.002
12	9	4	←	11	9	3	16 302.6051	−0.0009	0.002
12	9	3	←	11	9	2	16 302.6051	−0.0012	0.002
12	7	6	←	11	7	5	16 354.2358	0.0024	0.002

[a] see Table S31

J'	K'_a	K'_c	$\leftarrow$	J''	K''_a	K''_c	$\nu_{\text{obs.}}$	$\nu_{\text{obs.}} - \nu_{\text{calc.}}$	exp. error [a]
12	7	5	$\leftarrow$	11	7	4	16 354.7404	0.0012	0.002
13	1	12	$\leftarrow$	12	1	11	16 736.7472	0.0005	0.002
14	1	14	$\leftarrow$	13	1	13	17 344.3739	0.0002	0.002
14	0	14	$\leftarrow$	13	0	13	17 344.5231	−0.0010	0.002

[a] see Table S31

Table S32: Measured frequencies ($\nu_{\text{obs.}}$) and residuals ($\nu_{\text{obs.}} - \nu_{\text{calc.}}$) in MHz of the monohydrate of fenchone 1w-I(18).

J'	K'_a	K'_c	←	J''	K''_a	K''_c	$\nu_{\text{obs.}}$	$\nu_{\text{obs.}} - \nu_{\text{calc.}}$	exp. error [a]
2	0	2	←	1	0	1	2575.9956	0.0004	0.002
3	1	3	←	2	1	2	3697.0431	−0.0008	0.002
3	0	3	←	2	0	2	3822.8224	0.0012	0.002
3	1	2	←	2	1	1	4061.0861	−0.0010	0.001
4	0	4	←	3	1	3	4684.5303	0.0021	0.002
4	1	4	←	3	1	3	4912.4397	−0.0004	0.001
4	0	4	←	3	0	3	5030.8890	−0.0002	0.001
4	1	3	←	3	1	2	5390.6619	−0.0001	0.001
5	0	5	←	4	1	4	5980.7607	−0.0002	0.001
5	1	5	←	4	1	4	6117.2032	0.0001	0.001
5	0	5	←	4	0	4	6208.6732	0.0004	0.001
5	1	5	←	4	0	4	6345.1148	−0.0002	0.001
3	3	1	←	2	2	0	7070.7793	−0.0003	0.001
3	3	0	←	2	2	1	7089.6956	0.0004	0.001
6	0	6	←	5	1	5	7236.4484	0.0000	0.001
6	1	6	←	5	1	5	7312.4113	0.0007	0.001
6	0	6	←	5	0	5	7372.8907	0.0001	0.001
6	1	6	←	5	0	5	7448.8525	−0.0003	0.002
6	2	5	←	5	2	4	7702.9968	0.0002	0.001
6	3	4	←	5	3	3	7838.2048	0.0004	0.001
6	3	3	←	5	3	2	7917.4249	−0.0006	0.001
6	1	5	←	5	1	4	7964.3161	−0.0001	0.001
6	2	4	←	5	2	3	8106.0140	0.0004	0.001
7	0	7	←	6	1	6	8459.9345	0.0001	0.002
7	1	7	←	6	1	6	8500.0740	−0.0001	0.001
7	0	7	←	6	0	6	8535.8963	−0.0004	0.001
7	1	7	←	6	0	6	8576.0360	−0.0004	0.002
7	2	6	←	6	2	5	8946.1600	−0.0002	0.001
7	3	5	←	6	3	4	9142.4893	0.0001	0.001

[a] see Table S31

Table S33: Measured frequencies ($\nu_{\text{obs.}}$) and residuals ($\nu_{\text{obs.}} - \nu_{\text{calc.}}$) in MHz of the monohydrate of fenchone 1w-II.

J'	K'_a	K'_c	$\leftarrow$	J''	K''_a	K''_c	$\nu_{\text{obs.}}$	$\nu_{\text{obs.}} - \nu_{\text{calc.}}$	exp. error [a]
2	1	2	$\leftarrow$	1	1	1	2809.1263	0.0011	0.010
2	0	2	$\leftarrow$	1	0	1	2904.2294	−0.0020	0.010
2	1	1	$\leftarrow$	1	1	0	3051.1184	−0.0045	0.010
3	1	3	$\leftarrow$	2	1	2	4198.8893	−0.0008	0.002
3	0	3	$\leftarrow$	2	0	2	4298.5627	0.0003	0.002
3	2	2	$\leftarrow$	2	2	1	4395.1735	0.0069	0.010
3	2	1	$\leftarrow$	2	2	0	4491.7554	0.0022	0.010
3	1	2	$\leftarrow$	2	1	1	4558.3325	0.0002	0.002
4	1	4	$\leftarrow$	3	1	3	5575.3078	−0.0005	0.001
4	0	4	$\leftarrow$	3	0	3	5651.1217	−0.0001	0.002
4	2	3	$\leftarrow$	3	2	2	5839.7966	0.0008	0.002
4	1	3	$\leftarrow$	3	1	2	6038.6437	−0.0009	0.002
4	2	2	$\leftarrow$	3	2	1	6048.4106	0.0027	0.010
5	1	5	$\leftarrow$	4	1	4	6939.5918	0.0017	0.002
5	0	5	$\leftarrow$	4	0	4	6984.8363	−0.0009	0.002
5	2	4	$\leftarrow$	4	2	3	7267.8002	−0.0003	0.002
5	3	3	$\leftarrow$	4	3	2	7383.3553	0.0004	0.002
5	3	2	$\leftarrow$	4	3	1	7450.6984	−0.0029	0.002
5	1	4	$\leftarrow$	4	1	3	7477.2300	0.0002	0.002
5	2	3	$\leftarrow$	4	2	2	7604.8716	0.0009	0.002
6	0	6	$\leftarrow$	5	1	5	8276.4909	−0.0006	0.002
6	1	6	$\leftarrow$	5	1	5	8294.8083	−0.0003	0.001
6	0	6	$\leftarrow$	5	0	5	8317.8022	−0.0006	0.002
6	1	6	$\leftarrow$	5	0	5	8336.1198	−0.0001	0.002
6	2	5	$\leftarrow$	5	2	4	8677.0390	0.0007	0.002
6	3	4	$\leftarrow$	5	3	3	8856.1935	−0.0006	0.002
6	1	5	$\leftarrow$	5	1	4	8863.7376	−0.0012	0.002
6	2	4	$\leftarrow$	5	2	3	9135.4559	−0.0019	0.002
7	0	7	$\leftarrow$	6	1	6	9636.5518	0.0003	0.002

[a] see Table S31

J'	K'_a	K'_c	←	J''	K''_a	K''_c	$\nu_{\text{obs.}}$	$\nu_{\text{obs.}} - \nu_{\text{calc.}}$	exp. error [a]
5	3	2	←	4	2	3	9641.1678	0.0003	0.002
7	1	7	←	6	1	6	9644.2822	0.0002	0.002
7	0	7	←	6	0	6	9654.8688	0.0003	0.001
7	1	7	←	6	0	6	9662.5990	0.0000	0.002
7	1	6	←	6	2	5	9892.3805	0.0006	0.002
7	2	6	←	6	2	5	10 067.5093	0.0001	0.002
7	1	6	←	6	1	5	10 205.6868	−0.0001	0.002
5	4	2	←	4	3	1	10 244.5639	−0.0009	0.002
5	4	1	←	4	3	2	10 272.3712	0.0018	0.002
7	3	5	←	6	3	4	10 315.2347	0.0005	0.002
7	4	4	←	6	4	3	10 368.1453	0.0011	0.002
7	2	6	←	6	1	5	10 380.8170	0.0008	0.002
7	4	3	←	6	4	2	10 410.9287	0.0005	0.002
7	3	4	←	6	3	3	10 598.7360	0.0007	0.002
7	2	5	←	6	2	4	10 624.5486	−0.0001	0.001
8	0	8	←	7	1	7	10 987.4019	−0.0006	0.001
8	1	8	←	7	1	7	10 990.5536	0.0004	0.001
8	0	8	←	7	0	7	10 995.1332	0.0002	0.001
8	1	8	←	7	0	7	10 998.2847	0.0010	0.002
8	1	7	←	7	2	6	11 352.3190	0.0002	0.002
8	2	7	←	7	2	6	11 441.4974	0.0001	0.001
8	1	7	←	7	1	6	11 527.4482	0.0000	0.001
8	2	7	←	7	1	6	11 616.6269	0.0002	0.002
6	4	3	←	5	3	2	11 667.8164	−0.0017	0.002
8	3	6	←	7	3	5	11 755.6325	0.0001	0.001
6	4	2	←	5	3	3	11 776.6893	0.0008	0.002
8	2	6	←	7	2	5	12 060.3168	0.0001	0.002
9	0	9	←	8	1	8	12 333.9357	−0.0005	0.002
9	1	9	←	8	1	8	12 335.1891	0.0017	0.002

[a] see Table S31

J'	K'_a	K'_c	$\leftarrow$	J''	K''_a	K''_c	$\nu_{\text{obs.}}$	$\nu_{\text{obs.}} - \nu_{\text{calc.}}$	exp. error [a]
9	0	9	$\leftarrow$	8	0	8	12 337.0190	−0.0679	0.102
9	1	9	$\leftarrow$	8	0	8	12 338.3395	0.0014	0.002
9	2	8	$\leftarrow$	8	2	7	12 802.8331	0.0004	0.001
9	1	8	$\leftarrow$	8	1	7	12 849.6049	−0.0004	0.002
9	2	8	$\leftarrow$	8	1	7	12 892.0108	−0.0005	0.002
9	3	7	$\leftarrow$	8	3	6	13 174.8234	0.0002	0.002
9	5	4	$\leftarrow$	8	5	3	13 374.7685	−0.0003	0.002
9	2	7	$\leftarrow$	8	2	6	13 437.2990	0.0003	0.002
9	4	5	$\leftarrow$	8	4	4	13 554.4696	0.0002	0.002
10	1	10	$\leftarrow$	9	1	9	13 679.0093	0.0009	0.001
10	0	10	$\leftarrow$	9	0	9	13 679.7712	−0.0015	0.001
9	3	6	$\leftarrow$	8	3	5	13 723.9546	−0.0002	0.002
10	2	9	$\leftarrow$	9	2	8	14 155.6461	−0.0007	0.002
10	3	8	$\leftarrow$	9	3	7	14 572.8468	0.0001	0.001
10	2	8	$\leftarrow$	9	2	7	14 767.0244	−0.0012	0.002
10	4	7	$\leftarrow$	9	4	6	14 811.4846	−0.0003	0.002

[a] see Table S31

Table S34: Measured frequencies ($\nu_{\text{obs.}}$) and residuals ($\nu_{\text{obs.}} - \nu_{\text{calc.}}$) in MHz of the monohydrate of fenchone 1w-II(18).

J'	K'_a	K'_c	$\leftarrow$	J''	K''_a	K''_c	$\nu_{\text{obs.}}$	$\nu_{\text{obs.}} - \nu_{\text{calc.}}$	exp. error [a]
2	0	2	$\leftarrow$	1	0	1	2804.9726	−0.0012	0.002
3	1	3	$\leftarrow$	2	1	2	4057.7564	−0.0014	0.002
3	0	3	$\leftarrow$	2	0	2	4158.0033	−0.0005	0.002
4	1	4	$\leftarrow$	3	1	3	5390.3485	−0.0005	0.002
4	0	4	$\leftarrow$	3	0	3	5471.9145	0.0003	0.001
4	2	3	$\leftarrow$	3	2	2	5636.2183	0.0001	0.002
4	1	3	$\leftarrow$	3	1	2	5827.4507	−0.0010	0.002
5	1	5	$\leftarrow$	4	1	4	6711.8508	−0.0006	0.001
5	0	5	$\leftarrow$	4	0	4	6764.4675	0.0006	0.001
5	2	4	$\leftarrow$	4	2	3	7018.4076	−0.0010	0.001
5	3	3	$\leftarrow$	4	3	2	7117.4999	0.0046	0.002
5	3	2	$\leftarrow$	4	3	1	7168.8835	−0.0002	0.002
5	1	4	$\leftarrow$	4	1	3	7226.2437	−0.0001	0.002
5	2	3	$\leftarrow$	4	2	2	7318.2392	−0.0010	0.002
6	0	6	$\leftarrow$	5	0	5	8053.4413	0.0005	0.001
6	2	5	$\leftarrow$	5	2	4	8384.4158	−0.0010	0.002
6	1	5	$\leftarrow$	5	1	4	8580.2726	0.0012	0.002
7	1	7	$\leftarrow$	6	1	6	9331.3179	0.0003	0.002
7	0	7	$\leftarrow$	6	0	6	9345.6147	0.0011	0.002
7	2	6	$\leftarrow$	6	2	5	9733.6717	−0.0026	0.002
7	1	6	$\leftarrow$	6	1	5	9890.4830	0.0005	0.001
7	3	4	$\leftarrow$	6	3	3	10 183.8839	0.0015	0.002
7	2	5	$\leftarrow$	6	2	4	10 251.3838	0.0006	0.002
8	1	8	$\leftarrow$	7	1	7	10 634.4858	0.0005	0.002
8	0	8	$\leftarrow$	7	0	7	10 641.1173	0.0009	0.002
8	2	7	$\leftarrow$	7	2	6	11 067.4485	−0.0032	0.002
8	1	7	$\leftarrow$	7	1	6	11 174.0896	−0.0006	0.002

[a] see Table S31

Table S35: Measured frequencies ($\nu_{\text{obs.}}$) and residuals ($\nu_{\text{obs.}} - \nu_{\text{calc.}}$) in MHz of the dihydrate of fenchone 2w-I.

J'	K'_a	K'_c	←	J''	K''_a	K''_c	$\nu_{\text{obs.}}$	$\nu_{\text{obs.}} - \nu_{\text{calc.}}$	exp. error [a]
3	1	3	←	2	1	2	3238.1062	−0.0048	0.002
3	0	3	←	2	0	2	3313.0651	−0.0026	0.002
3	2	2	←	2	2	1	3344.5507	−0.0016	0.010
3	1	2	←	2	1	1	3440.8662	−0.0004	0.002
4	1	4	←	3	1	3	4309.3778	0.0024	0.002
4	0	4	←	3	0	3	4384.8913	0.0044	0.002
4	2	3	←	3	2	2	4453.1081	−0.0020	0.010
4	3	2	←	3	3	1	4473.8234	−0.0183	0.010
4	2	2	←	3	2	1	4527.5890	−0.0022	0.002
4	1	3	←	3	1	2	4576.9330	−0.0005	0.002
5	1	5	←	4	1	4	5375.2560	−0.0006	0.002
5	0	5	←	4	0	4	5438.9913	0.0043	0.002
5	2	4	←	4	2	3	5556.3569	−0.0015	0.010
5	3	2	←	4	3	1	5608.4373	−0.0093	0.010
5	2	3	←	4	2	2	5691.3186	−0.0018	0.010
5	1	4	←	4	1	3	5701.8830	0.0001	0.010
6	1	6	←	5	1	5	6435.9977	−0.0017	0.002
6	0	6	←	5	0	5	6482.5053	−0.0002	0.002
6	2	5	←	5	2	4	6653.1744	−0.0026	0.010
6	4	3	←	5	4	2	6716.0094	0.0061	0.010
6	4	2	←	5	4	1	6717.3175	−0.0107	0.010
6	3	4	←	5	3	3	6718.5096	−0.0045	0.010
6	3	3	←	5	3	2	6750.0819	−0.0014	0.010
6	1	5	←	5	1	4	6811.1202	0.0002	0.002
6	2	4	←	5	2	3	6858.4261	−0.0015	0.002
7	1	7	←	6	1	6	7492.3684	−0.0007	0.002
7	0	7	←	6	0	6	7522.7589	0.0001	0.002
7	2	6	←	6	2	5	7742.7182	−0.0017	0.002
7	3	5	←	6	3	4	7839.1739	0.0002	0.002
7	4	4	←	6	4	3	7842.3215	0.0023	0.002

[a] see Table S31

J'	K'_a	K'_c	←	J''	K''_a	K''_c	$\nu_{\text{obs.}}$	$\nu_{\text{obs.}} - \nu_{\text{calc.}}$	exp. error [a]
7	4	3	←	6	4	2	7846.6571	0.0018	0.002
7	1	6	←	6	1	5	7900.2529	0.0006	0.002
7	3	4	←	6	3	3	7905.6750	0.0067	0.002
7	2	5	←	6	2	4	8019.5299	−0.0013	0.002
8	1	8	←	7	1	7	8545.3736	−0.0003	0.002
8	0	8	←	7	0	7	8563.7409	−0.0005	0.002
8	2	7	←	7	2	6	8824.5479	−0.0031	0.002
8	3	6	←	7	3	5	8956.1442	−0.0023	0.002
8	1	7	←	7	1	6	8967.4048	0.0035	0.002
8	3	5	←	7	3	4	9075.9376	−0.0019	0.002
8	2	6	←	7	2	5	9167.9408	−0.0007	0.002
9	1	9	←	8	1	8	9596.0084	0.0008	0.002
9	0	9	←	8	0	8	9606.5268	0.0007	0.002
9	2	8	←	8	2	7	9898.7420	−0.0037	0.002
9	1	8	←	8	1	7	10 015.6383	0.0003	0.002
9	3	7	←	8	3	6	10 067.5482	0.0007	0.002
9	4	5	←	8	4	4	10 126.6782	0.0016	0.002
9	3	6	←	8	3	5	10 256.5235	−0.0014	0.002
9	2	7	←	8	2	6	10 299.1115	0.0009	0.002
10	1	10	←	9	1	9	10 645.0923	0.0012	0.002
10	0	10	←	9	0	9	10 650.8920	0.0020	0.002
10	2	9	←	9	2	8	10 965.8981	−0.0044	0.002
10	1	9	←	9	1	8	11 052.4841	−0.0012	0.002
10	2	8	←	9	2	7	11 409.2338	0.0024	0.002
10	3	7	←	9	3	6	11 438.3110	−0.0001	0.002
11	1	11	←	10	1	10	11 693.2249	0.0031	0.002
11	0	11	←	10	0	10	11 696.3330	0.0021	0.002
11	2	10	←	10	2	9	12 027.0327	−0.0059	0.002
11	1	10	←	10	1	9	12 085.9030	−0.0023	0.002
11	2	9	←	10	2	8	12 495.3179	0.0034	0.002

[a] see Table S31

Table S36: Measured frequencies ($\nu_{\text{obs.}}$) and residuals ($\nu_{\text{obs.}} - \nu_{\text{calc.}}$) in MHz of the dihydrate of fenchone 2w-I with the O_1 and O_2 atoms substituted by ^{18}O atoms.

J'	K'_a	K'_c	←	J''	K''_a	K''_c	$\nu_{\text{obs.}}$	$\nu_{\text{obs.}} - \nu_{\text{calc.}}$	exp. error [a]
3	1	3	←	2	1	2	3101.5993	0.0008	0.002
3	0	3	←	2	0	2	3168.9262	−0.0002	0.002
3	1	2	←	2	1	1	3273.7400	−0.0001	0.010
4	1	4	←	3	1	3	4129.6181	0.0012	0.010
4	0	4	←	3	0	3	4201.3546	0.0057	0.010
4	2	3	←	3	2	2	4250.5381	−0.0017	0.010
4	3	2	←	3	3	1	4265.2996	0.0029	0.010
4	2	2	←	3	2	1	4304.1366	−0.0003	0.010
4	1	3	←	3	1	2	4357.5161	0.0020	0.010
5	1	5	←	4	1	4	5153.5563	−0.0057	0.010
5	0	5	←	4	0	4	5218.9309	0.0016	0.002
5	2	4	←	4	2	3	5306.1072	−0.0012	0.002
5	3	3	←	4	3	2	5334.7289	0.0006	0.010
5	2	3	←	4	2	2	5405.7299	−0.0011	0.002
5	1	4	←	4	1	3	5433.8249	0.0003	0.001
6	1	6	←	5	1	5	6173.4162	−0.0005	0.001
6	0	6	←	5	0	5	6225.5943	0.0005	0.001
6	2	5	←	5	2	4	6357.0904	−0.0007	0.001
6	4	3	←	5	4	2	6401.4278	−0.0030	0.010
6	4	2	←	5	4	1	6402.0804	0.0088	0.010
6	3	4	←	5	3	3	6404.6836	0.0009	0.002
6	3	3	←	5	3	2	6423.4517	0.0006	0.002
6	1	5	←	5	1	4	6499.6181	−0.0003	0.001
6	2	4	←	5	2	3	6513.2770	0.0003	0.001
7	1	7	←	6	1	6	7189.5597	−0.0001	0.001
7	0	7	←	6	0	6	7226.9821	0.0002	0.001
7	2	6	←	6	2	5	7402.7872	−0.0024	0.002
7	4	4	←	6	4	3	7473.4836	0.0001	0.002
7	3	5	←	6	3	4	7474.0682	−0.0029	0.010

[a] see Table S31

J'	K'_a	K'_c	$\leftarrow$	J''	K''_a	K''_c	$\nu_{\text{obs.}}$	$\nu_{\text{obs.}} - \nu_{\text{calc.}}$	exp. error [a]
7	4	3	$\leftarrow$	6	4	2	7475.5925	−0.0006	0.002
7	3	4	$\leftarrow$	6	3	3	7514.4834	0.0005	0.001
7	2	5	$\leftarrow$	6	2	4	7619.8339	−0.0010	0.010
8	1	8	$\leftarrow$	7	1	7	8202.6229	0.0002	0.002
8	0	8	$\leftarrow$	7	0	7	8227.3885	0.0005	0.002

[a] see Table S31

Table S37: Measured frequencies ($\nu_{\text{obs.}}$) and residuals ($\nu_{\text{obs.}} - \nu_{\text{calc.}}$) in MHz of the dihydrate of fenchone 2w-I with the O_1 atom substituted by a ^{18}O atom.

J'	K'_a	K'_c	←	J''	K''_a	K''_c	$\nu_{\text{obs.}}$	$\nu_{\text{obs.}} - \nu_{\text{calc.}}$	exp. error [a]
3	1	3	←	2	1	2	3151.4084	0.0007	0.010
3	0	3	←	2	0	2	3223.3727	−0.0010	0.010
3	1	2	←	2	1	1	3339.9555	−0.0008	0.010
4	1	4	←	3	1	3	4194.9692	0.0002	0.010
4	0	4	←	3	0	3	4269.8066	−0.0019	0.010
4	2	3	←	3	2	2	4327.9556	0.0005	0.010
4	2	2	←	3	2	1	4391.3635	0.0007	0.010
4	1	3	←	3	1	2	4444.2489	−0.0036	0.010
5	1	5	←	4	1	4	5233.8195	0.0024	0.010
5	0	5	←	4	0	4	5299.7695	−0.0009	0.002
5	2	4	←	4	2	3	5401.5112	0.0018	0.002
5	3	3	←	4	3	2	5435.3617	0.0020	0.010
5	2	3	←	4	2	2	5518.0753	−0.0016	0.002
5	1	4	←	4	1	3	5539.4457	0.0003	0.002
6	1	6	←	5	1	5	6268.0357	0.0003	0.002
6	0	6	←	5	0	5	6318.6323	0.0019	0.002
6	2	5	←	5	2	4	6469.6157	−0.0019	0.002
6	1	5	←	5	1	4	6621.7789	−0.0012	0.002
6	2	4	←	5	2	3	6649.9141	0.0016	0.002
7	1	7	←	6	1	6	7298.1670	−0.0014	0.002
7	0	7	←	6	0	6	7332.9727	0.0005	0.002
7	2	6	←	6	2	5	7531.4975	0.0002	0.002
7	3	5	←	6	3	4	7614.8096	−0.0014	0.010
7	2	5	←	6	2	4	7778.6682	0.0110	0.010

[a] see Table S31

Table S38: Measured frequencies ($\nu_{\text{obs.}}$) and residuals ($\nu_{\text{obs.}} - \nu_{\text{calc.}}$) in MHz of the dihydrate of fenchone 2w-I with the O_2 atom substituted by a ^{18}O atom.

J'	K'_a	K'_c	$\leftarrow$	J''	K''_a	K''_c	$\nu_{\text{obs.}}$	$\nu_{\text{obs.}} - \nu_{\text{calc.}}$	exp. error [a]
3	1	3	$\leftarrow$	2	1	2	3183.6374	0.0002	0.010
3	0	3	$\leftarrow$	2	0	2	3254.1561	−0.0003	0.010
3	1	2	$\leftarrow$	2	1	1	3369.1559	−0.0026	0.010
4	1	4	$\leftarrow$	3	1	3	4237.9707	−0.0001	0.002
4	0	4	$\leftarrow$	3	0	3	4311.0052	−0.0003	0.010
4	2	3	$\leftarrow$	3	2	2	4368.9029	−0.0060	0.010
4	2	2	$\leftarrow$	3	2	1	4432.0642	0.0033	0.010
4	1	3	$\leftarrow$	3	1	2	4483.1971	0.0034	0.010
5	1	5	$\leftarrow$	4	1	4	5287.6274	0.0002	0.002
5	0	5	$\leftarrow$	4	0	4	5351.6285	−0.0006	0.002
5	2	4	$\leftarrow$	4	2	3	5452.7226	0.0002	0.002
5	3	3	$\leftarrow$	4	3	2	5486.4385	0.0022	0.010
5	2	3	$\leftarrow$	4	2	2	5568.6031	−0.0005	0.002
5	1	4	$\leftarrow$	4	1	3	5588.1160	0.0001	0.002
6	1	6	$\leftarrow$	5	1	5	6332.7057	−0.0006	0.002
6	0	6	$\leftarrow$	5	0	5	6381.4823	0.0001	0.002
6	2	5	$\leftarrow$	5	2	4	6531.1091	0.0010	0.002
6	3	4	$\leftarrow$	5	3	3	6586.8135	0.0021	0.010
6	1	5	$\leftarrow$	5	1	4	6680.1630	−0.0001	0.002
6	2	4	$\leftarrow$	5	2	3	6709.9417	0.0004	0.002
7	1	7	$\leftarrow$	6	1	6	7373.7680	0.0026	0.010
7	0	7	$\leftarrow$	6	0	6	7407.0899	0.0007	0.002
7	2	6	$\leftarrow$	6	2	5	7603.2933	−0.0011	0.010
7	3	5	$\leftarrow$	6	3	4	7686.1083	−0.0007	0.010

[a] see Table S31

Table S39: Measured frequencies ($\nu_{\text{obs.}}$) and residuals ($\nu_{\text{obs.}} - \nu_{\text{calc.}}$) in MHz of the dihydrate of fenchone 2w-II.

J'	K'_a	K'_c	$\leftarrow$	J''	K''_a	K''_c	$\nu_{\text{obs.}}$	$\nu_{\text{obs.}} - \nu_{\text{calc.}}$	exp. error [a]
3	0	3	$\leftarrow$	2	0	2	3405.3359	−0.0002	0.002
3	1	2	$\leftarrow$	2	1	1	3484.0416	0.0021	0.002
4	1	4	$\leftarrow$	3	1	3	4469.7400	−0.0190	0.010
4	0	4	$\leftarrow$	3	0	3	4522.0361	−0.0004	0.002
4	1	3	$\leftarrow$	3	1	2	4639.5467	0.0005	0.002
5	1	5	$\leftarrow$	4	1	4	5580.6865	0.0017	0.002
5	0	5	$\leftarrow$	4	0	4	5627.5835	−0.0005	0.002
5	2	4	$\leftarrow$	4	2	3	5694.5967	0.0003	0.002
5	2	3	$\leftarrow$	4	2	2	5771.2745	0.0015	0.002
5	1	4	$\leftarrow$	4	1	3	5789.1929	0.0003	0.002
6	1	6	$\leftarrow$	5	1	5	6688.5089	0.0013	0.002
6	0	6	$\leftarrow$	5	0	5	6725.2483	−0.0024	0.002
6	2	5	$\leftarrow$	5	2	4	6825.5640	0.0019	0.002
6	3	4	$\leftarrow$	5	3	3	6862.2679	−0.0017	0.002
6	3	3	$\leftarrow$	5	3	2	6877.4126	−0.0019	0.002
6	1	5	$\leftarrow$	5	1	4	6930.5712	0.0006	0.002
6	2	4	$\leftarrow$	5	2	3	6945.0112	0.0012	0.002
7	1	7	$\leftarrow$	6	1	6	7793.5505	0.0001	0.002
7	0	7	$\leftarrow$	6	0	6	7819.3861	−0.0018	0.002
7	2	6	$\leftarrow$	6	2	5	7952.4456	0.0034	0.002
7	3	4	$\leftarrow$	6	3	3	8039.7301	−0.0064	0.005
7	1	6	$\leftarrow$	6	1	5	8061.1140	−0.0002	0.002
7	2	5	$\leftarrow$	6	2	4	8117.3616	−0.0008	0.002
8	1	8	$\leftarrow$	7	1	7	8896.3208	0.0005	0.002
8	0	8	$\leftarrow$	7	0	7	8913.0886	−0.0014	0.002
8	2	7	$\leftarrow$	7	2	6	9074.8939	0.0054	0.002
8	3	6	$\leftarrow$	7	3	5	9150.6490	−0.0012	0.002

[a] see Table S31

J'	K'_a	K'_c	$\leftarrow$	J''	K''_a	K''_c	$\nu_{\text{obs.}}$	$\nu_{\text{obs.}} - \nu_{\text{calc.}}$	exp. error [a]
8	1	7	$\leftarrow$	7	1	6	9178.9574	−0.0007	0.002
8	3	5	$\leftarrow$	7	3	4	9210.7910	−0.0045	0.005
8	2	6	$\leftarrow$	7	2	5	9283.9270	−0.0030	0.002
9	1	9	$\leftarrow$	8	1	8	9997.3764	0.0003	0.002
9	0	9	$\leftarrow$	8	0	8	10 007.6554	−0.0016	0.002
9	2	8	$\leftarrow$	8	2	7	10 192.7985	0.0075	0.005
9	1	8	$\leftarrow$	8	1	7	10 284.2427	−0.0016	0.002
9	3	7	$\leftarrow$	8	3	6	10 291.3651	0.0006	0.002
10	1	10	$\leftarrow$	9	1	9	11 097.2279	0.0011	0.002
10	0	10	$\leftarrow$	9	0	9	11 103.2779	−0.0011	0.002
10	2	9	$\leftarrow$	9	2	8	11 306.3176	0.0090	0.005
11	1	11	$\leftarrow$	10	1	10	12 196.2768	−0.0014	0.005
11	0	11	$\leftarrow$	10	0	10	12 199.7346	−0.0023	0.005

[a] see Table S31

Table S40: Measured frequencies ($\nu_{\text{obs.}}$) and residuals ($\nu_{\text{obs.}} - \nu_{\text{calc.}}$) in MHz of the dihydrate of fenchone 2w-II with the O_1 and O_2 atoms substituted by ^{18}O atoms.

J'	K'_a	K'_c	←	J''	K''_a	K''_c	$\nu_{\text{obs.}}$	$\nu_{\text{obs.}} - \nu_{\text{calc.}}$	exp. error [a]
3	1	3	←	2	1	2	3203.9758	0.0006	0.010
4	1	4	←	3	1	3	4268.4614	0.0010	0.002
4	0	4	←	3	0	3	4318.9207	−0.0003	0.002
4	2	3	←	3	2	2	4348.3318	−0.0015	0.010
4	3	3	←	3	3	2	4380.3541	−0.0004	0.010
4	1	3	←	3	1	2	4419.9829	0.0001	0.002
5	1	5	←	4	1	4	5330.4427	0.0010	0.002
5	0	5	←	4	0	4	5378.3146	−0.0004	0.002
5	3	3	←	4	3	2	5448.3524	0.0075	0.010
5	2	3	←	4	2	2	5491.5234	−0.0010	0.010
5	3	4	←	4	3	3	5491.5234	−0.0010	0.010
5	1	4	←	4	1	3	5517.4064	0.0002	0.001
6	1	6	←	5	1	5	6389.8410	0.0004	0.001
6	0	6	←	5	0	5	6429.9719	−0.0003	0.001
6	2	5	←	5	2	4	6511.3968	0.0001	0.002
6	3	5	←	5	3	4	6607.5125	−0.0041	0.010
6	2	4	←	5	2	3	6607.5133	−0.0033	0.002
6	1	5	←	5	1	4	6608.8030	0.0005	0.001
7	1	7	←	6	1	6	7446.8153	0.0001	0.002
7	0	7	←	6	0	6	7477.1582	−0.0012	0.001
7	2	6	←	6	2	5	7588.3906	0.0020	0.002
7	3	5	←	6	3	4	7631.6322	−0.0093	0.010
7	1	6	←	6	1	5	7692.2136	0.0009	0.002
7	2	5	←	6	2	4	7724.3311	−0.0055	0.010
7	3	6	←	6	3	5	7724.3311	−0.0055	0.010
8	1	8	←	7	1	7	8501.6951	0.0009	0.002
9	1	9	←	8	1	8	9554.8915	0.0012	0.002
9	0	9	←	8	0	8	9568.7998	−0.0010	0.002
10	0	10	←	9	0	9	10 615.5736	0.0002	0.002

[a] see Table S31

Table S41: Measured frequencies ($\nu_{\text{obs.}}$) and residuals ($\nu_{\text{obs.}} - \nu_{\text{calc.}}$) in MHz of the dihydrate of fenchone 2w-II with the O_1 atom substituted by a ^{18}O atom.

J'	K'_a	K'_c	←	J''	K''_a	K''_c	$\nu_{\text{obs.}}$	$\nu_{\text{obs.}} - \nu_{\text{calc.}}$	exp. error [a]
3	1	3	←	2	1	2	3264.7447	−0.0007	0.010
3	0	3	←	2	0	2	3312.3483	−0.0002	0.010
3	1	2	←	2	1	1	3384.1617	0.0014	0.010
4	1	4	←	3	1	3	4349.1909	0.0004	0.010
4	0	4	←	3	0	3	4400.8689	0.0004	0.010
4	2	3	←	3	2	2	4432.7974	−0.0003	0.010
4	3	3	←	3	3	2	4467.5703	−0.0003	0.010
4	1	3	←	3	1	2	4507.4372	−0.0001	0.010
5	1	5	←	4	1	4	5430.9432	0.0001	0.002
5	0	5	←	4	0	4	5479.2890	0.0004	0.002
5	3	3	←	4	3	2	5555.0116	0.0007	0.010
5	2	3	←	4	2	2	5601.6212	0.0003	0.010
5	3	4	←	4	3	3	5601.6212	0.0003	0.010
6	1	6	←	5	1	5	6509.9446	0.0004	0.002
6	0	6	←	5	0	5	6549.7793	−0.0009	0.002
6	2	5	←	5	2	4	6637.1062	−0.0004	0.010
6	3	4	←	5	3	3	6668.1269	−0.0039	0.010
6	1	5	←	5	1	4	6737.8930	0.0053	0.010
6	3	5	←	5	3	4	6740.4129	−0.0015	0.010
6	2	4	←	5	2	3	6740.4140	−0.0004	0.002
7	1	7	←	6	1	6	7586.3932	0.0008	0.010
7	0	7	←	6	0	6	7615.9532	−0.0008	0.010
7	2	6	←	6	2	5	7734.3354	0.0010	0.010
7	3	5	←	6	3	4	7781.0437	0.0041	0.010
7	1	6	←	6	1	5	7841.0069	0.0027	0.010
7	2	5	←	6	2	4	7879.5328	0.0006	0.010
7	3	6	←	6	3	5	7879.5328	0.0006	0.010

[a] see Table S31

Table S42: Measured frequencies ($\nu_{\text{obs.}}$) and residuals ($\nu_{\text{obs.}} - \nu_{\text{calc.}}$) in MHz of the dihydrate of fenchone 2w-II with the O_2 atom substituted by a ^{18}O atom.

J'	K'_a	K'_c	←	J''	K''_a	K''_c	$\nu_{\text{obs.}}$	$\nu_{\text{obs.}} - \nu_{\text{calc.}}$	exp. error [a]
3	1	3	←	2	1	2	3289.6204	0.0016	0.010
3	0	3	←	2	0	2	3337.6545	0.0016	0.010
3	1	2	←	2	1	1	3412.1778	−0.0039	0.010
4	1	4	←	3	1	3	4382.0223	0.0033	0.010
4	0	4	←	3	0	3	4433.2985	0.0007	0.002
4	2	3	←	3	2	2	4468.0831	−0.0009	0.010
4	2	2	←	3	2	1	4505.9851	0.0001	0.010
4	1	3	←	3	1	2	4544.2984	0.0023	0.010
5	1	5	←	4	1	4	5471.5324	0.0018	0.002
5	0	5	←	4	0	4	5518.3900	0.0000	0.002
5	2	4	←	4	2	3	5580.1049	−0.0008	0.010
5	2	3	←	4	2	2	5650.6174	0.0004	0.010
5	1	4	←	4	1	3	5671.1428	0.0000	0.010
6	1	6	←	5	1	5	6558.1362	0.0007	0.010
6	0	6	←	5	0	5	6595.6631	−0.0017	0.002
6	2	5	←	5	2	4	6688.8817	0.0001	0.002
6	1	5	←	5	1	4	6790.5676	−0.0020	0.002
6	2	4	←	5	2	3	6799.5525	−0.0007	0.002
7	1	7	←	6	1	6	7642.0966	0.0009	0.002
7	0	7	←	6	0	6	7669.1067	−0.0016	0.002
7	2	6	←	6	2	5	7793.9098	−0.0053	0.010
7	1	6	←	6	1	5	7900.2302	0.0029	0.002
7	2	5	←	6	2	4	7947.8901	−0.0011	0.010

[a] see Table S31

Table S43: Measured frequencies ($\nu_{\text{obs.}}$) and residuals ($\nu_{\text{obs.}} - \nu_{\text{calc.}}$) in MHz of the dihydrate of fenchone 2w-III.

J'	K'_a	K'_c	←	J''	K''_a	K''_c	$\nu_{\text{obs.}}$	$\nu_{\text{obs.}} - \nu_{\text{calc.}}$	exp. error [a]
3	1	3	←	2	1	2	2551.1203	−0.0066	0.010
3	0	3	←	2	0	2	2640.4932	−0.0020	0.010
3	1	2	←	2	1	1	2766.0857	0.0056	0.010
3	2	2	←	2	2	1	2661.9980	−0.0029	0.010
3	2	1	←	2	2	0	2683.5153	0.0020	0.010
4	1	4	←	3	1	3	3395.7313	−0.0047	0.010
4	0	4	←	3	0	3	3496.8229	−0.0014	0.010
4	1	3	←	3	1	2	3681.1478	0.0044	0.010
4	2	3	←	3	2	2	3545.1025	0.0015	0.010
4	2	2	←	3	2	1	3597.6063	0.0011	0.010
4	3	2	←	3	3	1	3559.4555	0.0107	0.010
4	3	1	←	3	3	0	3560.9849	−0.0003	0.010
5	1	5	←	4	1	4	4236.1182	0.0032	0.010
5	0	5	←	4	0	4	4336.3591	−0.0022	0.010
5	1	4	←	4	1	3	4589.4513	0.0005	0.010
5	2	4	←	4	2	3	4424.5956	0.0002	0.010
5	2	3	←	4	2	2	4524.8214	0.0027	0.010
5	3	3	←	4	3	2	4452.7440	0.0015	0.010
5	3	2	←	4	3	1	4458.0907	−0.0004	0.010
6	1	6	←	5	1	5	5072.0015	−0.0030	0.010
6	0	6	←	5	0	5	5160.8232	−0.0013	0.010
6	1	5	←	5	1	4	5488.3678	−0.0000	0.010
6	2	5	←	5	2	4	5299.6417	0.0013	0.010
6	2	4	←	5	2	3	5462.4430	0.0027	0.010
6	3	4	←	5	3	3	5347.1174	0.0003	0.010
6	3	3	←	5	3	2	5361.1696	−0.0023	0.010
6	4	2	←	5	4	1	5342.6404	−0.0005	0.010
6	5	1	←	5	5	0	5337.5089	−0.0043	0.010
6	5	2	←	5	5	1	5337.5089	−0.0007	0.010

[a] see Table S31

J'	K'_a	K'_c	$\leftarrow$	J''	K''_a	K''_c	$\nu_{\text{obs.}}$	$\nu_{\text{obs.}} - \nu_{\text{calc.}}$	exp. error [a]
7	1	7	$\leftarrow$	6	1	6	5903.52	−0.0016	0.010
7	0	7	$\leftarrow$	6	0	6	5974.9524	−0.0022	0.010
7	1	6	$\leftarrow$	6	1	5	6374.8129	−0.0037	0.010
7	2	6	$\leftarrow$	6	2	5	6169.4727	−0.0002	0.010
7	2	5	$\leftarrow$	6	2	4	6404.6205	0.0000	0.010
7	3	5	$\leftarrow$	6	3	4	6241.7699	0.0005	0.010
7	3	4	$\leftarrow$	6	3	3	6272.6125	−0.0008	0.010
7	4	4	$\leftarrow$	6	4	3	6237.8280	0.0173	0.010
7	4	3	$\leftarrow$	6	4	2	6239.0055	−0.0053	0.010
7	5	2	$\leftarrow$	6	5	1	6230.5241	−0.0139	0.010
7	5	3	$\leftarrow$	6	5	2	6230.5241	0.0059	0.010
8	1	8	$\leftarrow$	7	1	7	6731.0924	0.0043	0.010
8	0	8	$\leftarrow$	7	0	7	6784.1660	−0.0017	0.010
8	1	7	$\leftarrow$	7	1	6	7245.6278	0.0020	0.010
8	2	7	$\leftarrow$	7	2	6	7033.4497	−0.0125	0.010
8	2	6	$\leftarrow$	7	2	5	7344.6357	−0.0048	0.010
8	3	6	$\leftarrow$	7	3	5	7135.6015	0.0022	0.010
8	3	5	$\leftarrow$	7	3	4	7194.8754	−0.0032	0.010
8	4	5	$\leftarrow$	7	4	4	7135.3609	0.0029	0.010
8	4	4	$\leftarrow$	7	4	3	7138.6159	−0.0055	0.010
9	0	9	$\leftarrow$	8	0	8	7592.4271	0.0072	0.010
9	2	8	$\leftarrow$	8	2	7	7891.1728	0.0039	0.010

[a] see Table S31

Table S44: Measured frequencies ($\nu_{\text{obs.}}$) and residuals ($\nu_{\text{obs.}} - \nu_{\text{calc.}}$) in MHz of the dihydrate of fenchone 2w-III with the O_1 and O_2 atoms substituted by ^{18}O atoms.

J'	K'_a	K'_c	←	J''	K''_a	K''_c	$\nu_{\text{obs.}}$	$\nu_{\text{obs.}} - \nu_{\text{calc.}}$	exp. error [a]
4	1	4	←	3	1	3	3226.9263	−0.0010	0.010
4	0	4	←	3	0	3	3323.9822	−0.0027	0.010
4	2	3	←	3	2	2	3366.2199	0.0050	0.010
4	1	3	←	3	1	2	3493.9196	0.0069	0.010
5	1	5	←	4	1	4	4026.1155	−0.0034	0.010
5	0	5	←	4	0	4	4124.1839	−0.0008	0.010
5	2	4	←	4	2	3	4201.865	0.0021	0.010
5	1	4	←	4	1	3	4357.0715	0.0022	0.010
6	1	6	←	5	1	5	4821.2674	−0.0141	1.01
6	0	6	←	5	0	5	4910.2674	−0.0007	0.010
6	2	5	←	5	2	4	5033.6288	0.0013	0.010
6	2	4	←	5	2	3	5177.9285	0.0015	0.010
7	1	7	←	6	1	6	5612.454	−0.0035	0.010
7	0	7	←	6	0	6	5686.0022	−0.0038	0.010
7	3	5	←	6	3	4	5924.5966	0.0019	0.010
7	3	4	←	6	3	3	5949.7765	−0.0015	0.010
7	1	6	←	6	1	5	6056.6722	0.0009	0.010
7	2	5	←	6	2	4	6071.2164	0.0001	0.010
8	1	8	←	7	1	7	6399.9631	0.0011	0.010
8	0	8	←	7	0	7	6456.2053	0.0047	0.010
8	2	7	←	7	2	6	6682.8943	0.0078	0.010
8	4	5	←	7	4	4	6771.8845	0.0023	0.010
8	3	6	←	7	3	5	6773.359	−0.0030	0.010
8	4	4	←	7	4	3	6774.351	−0.0031	0.010
8	1	7	←	7	1	6	6887.6979	−0.0036	0.010
8	2	6	←	7	2	5	6963.9631	−0.0059	0.010
9	1	9	←	8	1	8	7184.2959	−0.0002	0.010
9	0	9	←	8	0	8	7224.7286	−0.0085	0.010
10	1	10	←	9	1	9	7966.0515	0.0039	0.010
10	0	10	←	9	0	9	7993.8059	0.0034	0.010

[a] see Table S31

Table S45: Measured frequencies ($\nu_{\text{obs.}}$) and residuals ($\nu_{\text{obs.}} - \nu_{\text{calc.}}$) in MHz of the dihydrate of fenchone 2w-III with the O_1 atom substituted by a ^{18}O atom.

J'	K'_a	K'_c	←	J''	K''_a	K''_c	$\nu_{\text{obs.}}$	$\nu_{\text{obs.}} - \nu_{\text{calc.}}$	exp. error [a]
3	1	3	←	2	1	2	2499.2039	0.0007	0.010
4	1	4	←	3	1	3	3326.5977	0.0016	0.010
4	0	4	←	3	0	3	3426.5518	0.0023	0.010
4	2	3	←	3	2	2	3474.0613	0.0030	0.010
4	1	3	←	3	1	2	3608.4149	−0.0004	0.010
5	1	5	←	4	1	4	4149.8276	0.0034	0.010
5	0	5	←	4	0	4	4249.0418	0.0007	0.010
5	2	4	←	4	2	3	4335.8992	−0.0018	0.010
5	2	3	←	4	2	2	4434.5651	0.0060	0.010
5	1	4	←	4	1	3	4498.737	−0.0014	0.010
6	1	6	←	5	1	5	4968.6264	−0.0029	0.010
6	0	6	←	5	0	5	5056.6437	−0.0021	0.010
6	2	5	←	5	2	4	5193.3656	0.0002	0.010
6	3	4	←	5	3	3	5240.1004	0.0052	0.010
6	3	3	←	5	3	2	5253.8747	−0.0015	0.010
6	1	5	←	5	1	4	5379.8254	−0.0051	0.010
7	1	7	←	6	1	6	5783.1204	−0.0033	0.010
7	0	7	←	6	0	6	5854.0071	−0.0029	0.010
7	2	6	←	6	2	5	6045.7028	0.0025	0.010
7	3	5	←	6	3	4	6116.865	−0.0081	0.010
7	3	4	←	6	3	3	6147.1204	−0.0007	0.010
7	1	6	←	6	1	5	6248.6686	0.0017	0.010
7	2	5	←	6	2	4	6277.3754	−0.0016	0.010
8	1	8	←	7	1	7	6593.7157	−0.0044	0.010
8	0	8	←	7	0	7	6646.4767	0.0059	0.010
8	2	7	←	7	2	6	6892.2874	0.0038	0.010
8	1	7	←	7	1	6	7102.1253	−0.0002	0.010
9	1	9	←	8	1	8	7401.024	0.0025	0.010
9	0	9	←	8	0	8	7437.9436	−0.0031	0.010
9	2	8	←	8	2	7	7732.6833	0.0028	0.010

[a] see Table S31

Table S46: Measured frequencies ($\nu_{\text{obs.}}$) and residuals ($\nu_{\text{obs.}} - \nu_{\text{calc.}}$) in MHz of the dihydrate of fenchone 2w-III with the O_2 atom substituted by a ^{18}O atom.

J'	K'_a	K'_c	←	J''	K''_a	K''_c	$\nu_{\text{obs.}}$	$\nu_{\text{obs.}} - \nu_{\text{calc.}}$	exp. error [a]
3	0	3	←	2	0	2	2557.0662	0.0006	0.010
3	1	2	←	2	1	1	2674.351	−0.0007	0.010
4	1	4	←	3	1	3	3290.3514	0.0029	0.010
4	0	4	←	3	0	3	3388.3514	−0.0033	0.010
4	1	3	←	3	1	2	3559.7346	−0.0016	0.010
5	0	5	←	4	0	4	4204.4229	0.0026	0.010
5	2	4	←	4	2	3	4282.6511	0.0023	0.010
5	3	2	←	4	3	1	4311.8303	−0.0034	0.010
5	2	3	←	4	2	2	4371.4034	0.0034	0.010
5	1	4	←	4	1	3	4439.2723	−0.0069	0.010
6	1	6	←	5	1	5	4916.2723	−0.0044	0.010
6	0	6	←	5	0	5	5006.2528	0.0077	0.010
6	2	5	←	5	2	4	5130.5162	0.0058	0.010
7	1	7	←	6	1	6	5723.1942	0.0011	0.010
7	0	7	←	6	0	6	5797.6066	−0.0073	0.010
7	2	6	←	6	2	5	5973.7759	−0.0003	0.010
7	3	5	←	6	3	4	6037.9973	0.0008	0.010
7	3	4	←	6	3	3	6063.2972	−0.0007	0.010
7	1	6	←	6	1	5	6171.4887	0.0035	0.010
7	2	5	←	6	2	4	6185.7492	0.0011	0.010
8	1	8	←	7	1	7	6526.4043	−0.0031	0.010
8	0	8	←	7	0	7	6583.3581	−0.0043	0.010
8	2	7	←	7	2	6	6811.865	0.0021	0.010
8	3	5	←	7	3	4	6951.8992	−0.0022	0.010
8	1	7	←	7	1	6	7018.6979	−0.0013	0.010
8	2	6	←	7	2	5	7095.1399	0.0015	0.010
9	1	9	←	8	1	8	7326.4247	0.0015	0.010
9	2	8	←	8	2	7	7644.3461	0.0098	0.010
9	1	8	←	8	1	7	7849.973	−0.0031	0.010
9	3	6	←	8	3	5	7851.5802	−0.0044	0.010

[a] see Table S31

Table S47: Measured frequencies ($\nu_{\text{obs.}}$) and residuals ($\nu_{\text{obs.}} - \nu_{\text{calc.}}$) in MHz of the trihydrate of fenchone 3w-I.

J'	K'_a	K'_c	←	J''	K''_a	K''_c	$\nu_{\text{obs.}}$	$\nu_{\text{obs.}} - \nu_{\text{calc.}}$	exp. error [a]
3	1	3	←	2	1	2	2394.4677	0.0024	0.010
3	0	3	←	2	0	2	2409.4131	0.0026	0.010
3	2	2	←	2	2	1	2410.1828	0.0081	0.010
3	2	1	←	2	2	0	2410.9361	−0.0033	0.010
3	1	2	←	2	1	1	2425.6420	−0.0036	0.010
4	1	4	←	3	1	3	3192.3984	0.0002	0.002
4	0	4	←	3	0	3	3211.6547	0.0013	0.010
4	2	3	←	3	2	2	3213.4076	−0.0052	0.010
4	3	2	←	3	3	1	3213.9330	−0.0038	0.010
4	2	2	←	3	2	1	3215.3165	−0.0051	0.010
5	1	5	←	4	1	4	3990.1471	0.0001	0.002
5	0	5	←	4	0	4	4013.1463	0.0068	0.010
5	2	4	←	4	2	3	4016.5324	0.0129	0.010
5	3	3	←	4	3	2	4017.5751	−0.0030	0.010
5	2	3	←	4	2	2	4020.3265	0.0014	0.010
5	1	4	←	4	1	3	4042.0692	0.0001	0.002
6	1	6	←	5	1	5	4787.6734	−0.0005	0.002
6	0	6	←	5	0	5	4813.6998	−0.0003	0.002
6	2	5	←	5	2	4	4819.4615	−0.0005	0.002
6	3	3	←	5	3	2	4821.4326	−0.0028	0.002
6	2	4	←	5	2	3	4826.0839	−0.0007	0.002
6	1	5	←	5	1	4	4849.9099	−0.0008	0.003
7	1	7	←	6	1	6	5584.9460	0.0001	0.001
7	0	7	←	6	0	6	5613.1933	0.0009	0.003
7	2	6	←	6	2	5	5622.2093	0.0015	0.003
7	4	3	←	6	4	2	5624.6448	0.0004	0.003
7	1	6	←	6	1	5	5657.4201	0.0004	0.001
8	1	8	←	7	1	7	6381.9368	0.0008	0.002

[a] see Table S31

J'	K'_a	K'_c	$\leftarrow$	J''	K''_a	K''_c	$\nu_{\text{obs.}}$	$\nu_{\text{obs.}} - \nu_{\text{calc.}}$	exp. error [a]
8	0	8	$\leftarrow$	7	0	7	6411.5141	−0.0004	0.001
8	2	7	$\leftarrow$	7	2	6	6424.7255	0.0008	0.001
8	1	7	$\leftarrow$	7	1	6	6464.5238	0.0001	0.001
9	1	9	$\leftarrow$	8	1	8	7178.6233	−0.0003	0.001
9	0	9	$\leftarrow$	8	0	8	7208.6197	−0.0001	0.001
9	2	8	$\leftarrow$	8	2	7	7226.9822	0.0011	0.002
9	3	7	$\leftarrow$	8	3	6	7233.1140	−0.0001	0.002
9	3	6	$\leftarrow$	8	3	5	7234.1225	0.0004	0.002
9	2	7	$\leftarrow$	8	2	6	7248.7622	−0.0004	0.002
9	1	8	$\leftarrow$	8	1	7	7271.1417	−0.0007	0.002
10	1	10	$\leftarrow$	9	1	9	7974.9946	−0.0001	0.002
10	0	10	$\leftarrow$	9	0	9	8004.5279	−0.0004	0.002
10	2	9	$\leftarrow$	9	2	8	8028.9472	0.0013	0.002
10	3	8	$\leftarrow$	9	3	7	8037.2303	0.0001	0.002
10	3	7	$\leftarrow$	9	3	6	8038.9501	−0.0004	0.002
10	2	8	$\leftarrow$	9	2	7	8058.1473	−0.0006	0.002
10	1	9	$\leftarrow$	9	1	8	8077.1864	−0.0004	0.002

[a] see Table S31

Table S48: Measured frequencies ($\nu_{\text{obs.}}$) and residuals ($\nu_{\text{obs.}} - \nu_{\text{calc.}}$) in MHz of the trihydrate of fenchone 3w-I with all oxygen atoms of water substituted by ^{18}O atoms.

J'	K'_a	K'_c	$\leftarrow$	J''	K''_a	K''_c	$\nu_{\text{obs.}}$	$\nu_{\text{obs.}} - \nu_{\text{calc.}}$	exp. error [a]
4	1	4	$\leftarrow$	3	1	3	3024.1424	−0.0009	0.002
4	0	4	$\leftarrow$	3	0	3	3044.2446	0.0005	0.002
4	1	3	$\leftarrow$	3	1	2	3067.7386	−0.0057	0.010
5	1	5	$\leftarrow$	4	1	4	3779.7896	−0.0013	0.002
5	0	5	$\leftarrow$	4	0	4	3803.7177	−0.0008	0.002
5	2	4	$\leftarrow$	4	2	3	3807.4788	−0.0029	0.005
5	1	4	$\leftarrow$	4	1	3	3834.2571	0.0016	0.002
6	1	6	$\leftarrow$	5	1	5	4535.1933	−0.0002	0.001
6	0	6	$\leftarrow$	5	0	5	4562.1668	−0.0008	0.002
6	1	5	$\leftarrow$	5	1	4	4600.4696	0.0006	0.001
7	1	7	$\leftarrow$	6	1	6	5290.3158	0.0001	0.002
7	0	7	$\leftarrow$	6	0	6	5319.4390	0.0000	0.002
7	2	6	$\leftarrow$	6	2	5	5329.4560	0.0003	0.002
7	2	5	$\leftarrow$	6	2	4	5341.1265	0.0000	0.002
7	1	6	$\leftarrow$	6	1	5	5366.3108	0.0003	0.002
8	1	8	$\leftarrow$	7	1	7	6045.1296	0.0006	0.002
8	0	8	$\leftarrow$	7	0	7	6075.4298	−0.0008	0.002
8	2	7	$\leftarrow$	7	2	6	6090.0810	0.0008	0.002
8	2	6	$\leftarrow$	7	2	5	6107.3228	−0.0006	0.002
8	1	7	$\leftarrow$	7	1	6	6131.6960	−0.0017	0.002
9	1	9	$\leftarrow$	8	1	8	6799.6135	0.0012	0.002
9	0	9	$\leftarrow$	8	0	8	6830.1085	0.0018	0.002
9	1	8	$\leftarrow$	8	1	7	6896.5259	−0.0135	0.010
10	1	10	$\leftarrow$	9	1	9	7553.7538	0.0016	0.010
10	0	10	$\leftarrow$	9	0	9	7583.5088	−0.0010	0.002
10	1	9	$\leftarrow$	9	1	8	7660.7278	−0.0063	0.010

[a] see Table S31

Table S49: Measured frequencies ($\nu_{\text{obs.}}$) and residuals ($\nu_{\text{obs.}} - \nu_{\text{calc.}}$) in MHz of the trihydrate of fenchone 3w-I with the O_1 atom substituted by a ^{18}O atom.

J'	K'_a	K'_c	←	J''	K''_a	K''_c	$\nu_{\text{obs.}}$	$\nu_{\text{obs.}} - \nu_{\text{calc.}}$	exp. error [a]
3	1	3	←	2	1	2	2352.6838	0.0035	0.010
3	0	3	←	2	0	2	2366.3881	−0.0004	0.010
3	1	2	←	2	1	1	2381.1847	0.0015	0.010
4	0	4	←	3	0	3	3154.4311	0.0006	0.010
4	1	3	←	3	1	2	3174.7166	0.0027	0.010
5	1	5	←	4	1	4	3920.5957	−0.0053	0.010
5	0	5	←	4	0	4	3941.8341	0.0011	0.010
5	1	4	←	4	1	3	3968.0738	0.0034	0.010
6	1	6	←	5	1	5	4704.2907	−0.0035	0.010
6	0	6	←	5	0	5	4728.4515	0.0008	0.010
6	1	5	←	5	1	4	4761.2083	0.0054	0.010
7	1	7	←	6	1	6	5487.7704	0.0010	0.010
7	0	7	←	6	0	6	5514.1561	−0.0012	0.010
7	1	6	←	6	1	5	5554.0534	−0.0034	0.010
8	1	8	←	7	1	7	6270.9991	−0.0033	0.010
8	0	8	←	7	0	7	6298.8536	−0.0030	0.010
8	1	7	←	7	1	6	6346.5673	−0.0053	0.010
9	1	9	←	8	1	8	7053.9800	0.0059	0.010
9	0	9	←	8	0	8	7082.4967	0.0028	0.010

[a] see Table S31

Table S50: Measured frequencies ($\nu_{\text{obs.}}$) and residuals ($\nu_{\text{obs.}} - \nu_{\text{calc.}}$) in MHz of the trihydrate of fenchone 3w-I with the O_2 atom substituted by a ^{18}O atom.

J'	K'_a	K'_c	$\leftarrow$	J''	K''_a	K''_c	$\nu_{\text{obs.}}$	$\nu_{\text{obs.}} - \nu_{\text{calc.}}$	exp. error [a]
3	1	3	$\leftarrow$	2	1	2	2332.1036	0.0010	0.010
3	0	3	$\leftarrow$	2	0	2	2346.2162	0.0020	0.010
3	1	2	$\leftarrow$	2	1	1	2361.4414	−0.0006	0.010
4	1	4	$\leftarrow$	3	1	3	3109.2783	0.0016	0.010
4	0	4	$\leftarrow$	3	0	3	3127.5135	0.0026	0.010
4	1	3	$\leftarrow$	3	1	2	3148.3864	−0.0004	0.010
5	0	5	$\leftarrow$	4	0	4	3908.1486	−0.0018	0.010
5	1	4	$\leftarrow$	4	1	3	3935.1537	0.0009	0.010
6	1	6	$\leftarrow$	5	1	5	4663.1175	0.0081	0.010
6	0	6	$\leftarrow$	5	0	5	4687.9843	0.0007	0.010
6	1	5	$\leftarrow$	5	1	4	4721.6830	−0.0056	0.010
7	1	7	$\leftarrow$	6	1	6	5439.6970	−0.0076	0.010
7	0	7	$\leftarrow$	6	0	6	5466.8799	−0.0008	0.010
7	1	6	$\leftarrow$	6	1	5	5507.9322	−0.0061	0.010
8	1	8	$\leftarrow$	7	1	7	6216.0488	−0.0020	0.010
8	0	8	$\leftarrow$	7	0	7	6244.7500	0.0076	0.010
8	1	7	$\leftarrow$	7	1	6	6293.8393	−0.0013	0.010
9	1	9	$\leftarrow$	8	1	8	6992.1288	0.0005	0.010
9	0	9	$\leftarrow$	8	0	8	7021.5096	−0.0026	0.010
9	1	8	$\leftarrow$	8	1	7	7079.3364	0.0084	0.010
10	0	10	$\leftarrow$	9	0	9	7797.1836	−0.0027	0.010

[a] see Table S31

Table S51: Measured frequencies ($\nu_{\text{obs.}}$) and residuals ($\nu_{\text{obs.}} - \nu_{\text{calc.}}$) in MHz of the trihydrate of fenchone 3w-I with the O_3 atom substituted by a ^{18}O atom.

J'	K'_a	K'_c	$\leftarrow$	J''	K''_a	K''_c	$\nu_{\text{obs.}}$	$\nu_{\text{obs.}} - \nu_{\text{calc.}}$	exp. error [a]
3	1	3	$\leftarrow$	2	1	2	2367.2284	0.0065	0.010
3	0	3	$\leftarrow$	2	0	2	2383.8968	−0.0003	0.010
3	1	2	$\leftarrow$	2	1	1	2402.2386	−0.0010	0.010
4	1	4	$\leftarrow$	3	1	3	3156.0164	0.0060	0.010
4	0	4	$\leftarrow$	3	0	3	3177.3704	−0.0058	0.010
4	1	3	$\leftarrow$	3	1	2	3202.6862	0.0018	0.010
5	1	5	$\leftarrow$	4	1	4	3944.5677	0.0039	0.010
5	0	5	$\leftarrow$	4	0	4	3969.8795	−0.0034	0.010
5	1	4	$\leftarrow$	4	1	3	4002.8573	−0.0035	0.010
6	1	6	$\leftarrow$	5	1	5	4732.8458	0.0105	0.010
6	0	6	$\leftarrow$	5	0	5	4761.2083	−0.0001	0.010
6	1	5	$\leftarrow$	5	1	4	4802.6885	−0.0006	0.010
7	1	7	$\leftarrow$	6	1	6	5520.7742	−0.0113	0.010
7	0	7	$\leftarrow$	6	0	6	5551.1848	−0.0028	0.010
7	1	6	$\leftarrow$	6	1	5	5602.0791	−0.0021	0.010
8	1	8	$\leftarrow$	7	1	7	6308.3822	−0.0011	0.010
8	0	8	$\leftarrow$	7	0	7	6339.7191	−0.0017	0.010
8	1	7	$\leftarrow$	7	1	6	6400.9453	0.0063	0.010
9	1	9	$\leftarrow$	8	1	8	7095.6011	−0.0059	0.010
9	0	9	$\leftarrow$	8	0	8	7126.7995	0.0059	0.010
10	1	10	$\leftarrow$	9	1	9	7882.4474	0.0034	0.010
10	0	10	$\leftarrow$	9	0	9	7912.4855	−0.0017	0.010

[a] see Table S31

Table S52: Measured frequencies ($\nu_{\text{obs.}}$) and residuals ($\nu_{\text{obs.}} - \nu_{\text{calc.}}$) in MHz of the trihydrate of fenchone 3w-I with the O_{1-2} atoms substituted by ^{18}O atoms.

J'	K'_a	K'_c	$\leftarrow$	J''	K''_a	K''_c	$\nu_{\text{obs.}}$	$\nu_{\text{obs.}} - \nu_{\text{calc.}}$	exp. error [a]
3	1	3	$\leftarrow$	2	1	2	2293.3402	−0.0091	0.010
3	0	3	$\leftarrow$	2	0	2	2306.3488	0.0008	0.010
3	1	2	$\leftarrow$	2	1	1	2320.3013	0.0035	0.010
4	1	4	$\leftarrow$	3	1	3	3057.6385	0.0044	0.010
4	0	4	$\leftarrow$	3	0	3	3074.4715	0.0011	0.010
4	1	3	$\leftarrow$	3	1	2	3093.5561	−0.0021	0.010
5	0	5	$\leftarrow$	4	0	4	3842.0335	0.0017	0.010
5	1	4	$\leftarrow$	4	1	3	3866.6685	0.0018	0.010
6	1	6	$\leftarrow$	5	1	5	4585.7637	0.0009	0.010
6	0	6	$\leftarrow$	5	0	5	4608.9031	−0.0002	0.010
7	1	7	$\leftarrow$	6	1	6	5349.5484	−0.0031	0.010
7	0	7	$\leftarrow$	6	0	6	5374.9689	−0.0012	0.010
7	1	6	$\leftarrow$	6	1	5	5412.2509	−0.0010	0.010
8	1	8	$\leftarrow$	7	1	7	6113.1261	0.0006	0.010
8	0	8	$\leftarrow$	7	0	7	6140.1424	0.0020	0.010
8	1	7	$\leftarrow$	7	1	6	6184.6295	−0.0012	0.010
9	1	9	$\leftarrow$	8	1	8	6876.4685	0.0018	0.010
9	0	9	$\leftarrow$	8	0	8	6904.3538	−0.0012	0.010

[a] see Table S31

Table S53: Measured frequencies ($\nu_{\text{obs.}}$) and residuals ($\nu_{\text{obs.}} - \nu_{\text{calc.}}$) in MHz of the trihydrate of fenchone 3w-I with the O_{1-3} atoms substituted by ^{18}O atoms.

J'	K'_a	K'_c	$\leftarrow$	J''	K''_a	K''_c	$\nu_{\text{obs.}}$	$\nu_{\text{obs.}} - \nu_{\text{calc.}}$	exp. error [a]
3	0	3	$\leftarrow$	2	0	2	2342.2853	−0.0021	0.010
4	1	4	$\leftarrow$	3	1	3	3100.9016	−0.0019	0.010
4	0	4	$\leftarrow$	3	0	3	3121.9280	0.0024	0.010
4	1	3	$\leftarrow$	3	1	2	3146.8033	0.0088	0.010
5	1	5	$\leftarrow$	4	1	4	3875.6892	−0.0035	0.010
5	0	5	$\leftarrow$	4	0	4	3900.6153	−0.0002	0.010
5	1	4	$\leftarrow$	4	1	3	3932.9997	−0.0125	0.010
6	1	6	$\leftarrow$	5	1	5	4650.2109	0.0032	0.010
6	1	5	$\leftarrow$	5	1	4	4718.8995	0.0078	0.010
7	1	7	$\leftarrow$	6	1	6	5424.4073	−0.0028	0.010
7	0	7	$\leftarrow$	6	0	6	5454.3727	−0.0041	0.010
7	1	6	$\leftarrow$	6	1	5	5504.3491	0.0018	0.010
8	1	8	$\leftarrow$	7	1	7	6198.2818	0.0121	0.010
8	0	8	$\leftarrow$	7	0	7	6229.1835	−0.0035	0.010
8	1	7	$\leftarrow$	7	1	6	6289.2806	−0.0033	0.010
9	1	9	$\leftarrow$	8	1	8	6971.7577	−0.0074	0.010
9	0	9	$\leftarrow$	8	0	8	7002.5727	0.0049	0.010

[a] see Table S31

Table S54: Measured frequencies ($\nu_{\text{obs.}}$) and residuals ($\nu_{\text{obs.}} - \nu_{\text{calc.}}$) in MHz of the trihydrate of fenchone 3w-I with the O_{2-3} atoms substituted by ^{18}O atoms.

J'	K'_a	K'_c	$\leftarrow$	J''	K''_a	K''_c	$\nu_{\text{obs.}}$	$\nu_{\text{obs.}} - \nu_{\text{calc.}}$	exp. error [a]
3	1	3	$\leftarrow$	2	1	2	2306.6962	−0.0097	0.010
3	0	3	$\leftarrow$	2	0	2	2322.5364	0.0008	0.010
3	1	2	$\leftarrow$	2	1	1	2339.8183	−0.0026	0.010
4	1	4	$\leftarrow$	3	1	3	3075.3595	0.0020	0.010
4	0	4	$\leftarrow$	3	0	3	3095.7058	−0.0004	0.010
4	1	3	$\leftarrow$	3	1	2	3119.4974	−0.0004	0.010
5	0	5	$\leftarrow$	4	0	4	3868.0177	−0.0071	0.010
5	1	4	$\leftarrow$	4	1	3	3898.9416	0.0008	0.010
6	1	6	$\leftarrow$	5	1	5	4611.9963	−0.0024	0.010
6	0	6	$\leftarrow$	5	0	5	4639.3033	−0.0008	0.010
7	0	7	$\leftarrow$	6	0	6	5409.4031	0.0131	0.010
7	1	6	$\leftarrow$	6	1	5	5456.8473	0.0028	0.010
8	1	8	$\leftarrow$	7	1	7	6147.5126	0.0052	0.010
8	0	8	$\leftarrow$	7	0	7	6178.1724	−0.0063	0.010
8	1	7	$\leftarrow$	7	1	6	6235.1567	0.0103	0.010
9	1	9	$\leftarrow$	8	1	8	6914.7685	−0.0008	0.010
9	1	8	$\leftarrow$	8	1	7	7012.8837	−0.0108	0.010

[a] see Table S31

Table S55: Measured frequencies ($\nu_{\text{obs.}}$) and residuals ($\nu_{\text{obs.}} - \nu_{\text{calc.}}$) in MHz of the trihydrate of fenchone 3w-II.

J'	K'_a	K'_c	$\leftarrow$	J''	K''_a	K''_c	$\nu_{\text{obs.}}$	$\nu_{\text{obs.}} - \nu_{\text{calc.}}$	exp. error [a]
4	1	4	$\leftarrow$	3	1	3	3240.0363	−0.0010	0.001
4	0	4	$\leftarrow$	3	0	3	3289.0569	0.0002	0.001
5	1	5	$\leftarrow$	4	1	4	4045.8432	−0.0004	0.002
5	0	5	$\leftarrow$	4	0	4	4094.3197	−0.0004	0.002
5	2	4	$\leftarrow$	4	2	3	4137.6319	−0.0011	0.002
5	1	4	$\leftarrow$	4	1	3	4217.8036	−0.0001	0.002
6	1	6	$\leftarrow$	5	1	5	4849.4492	−0.0006	0.001
6	0	6	$\leftarrow$	5	0	5	4892.2516	0.0011	0.001
6	2	5	$\leftarrow$	5	2	4	4960.2951	−0.0018	0.002
6	3	4	$\leftarrow$	5	3	3	4983.6090	−0.0001	0.002
6	3	3	$\leftarrow$	5	3	2	4990.5854	−0.0001	0.002
6	1	5	$\leftarrow$	5	1	4	5052.0058	0.0003	0.002
7	1	7	$\leftarrow$	6	1	6	5650.9178	−0.0002	0.002
7	0	7	$\leftarrow$	6	0	6	5685.2042	0.0002	0.001
7	2	6	$\leftarrow$	6	2	5	5780.3932	−0.0027	0.002
7	3	5	$\leftarrow$	6	3	4	5815.8745	0.0003	0.002
7	3	4	$\leftarrow$	6	3	3	5831.1755	0.0003	0.002
7	1	6	$\leftarrow$	6	1	5	5880.0566	0.0007	0.002
7	2	5	$\leftarrow$	6	2	4	5895.5488	0.0005	0.002
8	1	8	$\leftarrow$	7	1	7	6450.4596	0.0001	0.001
8	0	8	$\leftarrow$	7	0	7	6475.8334	0.0015	0.001
8	2	7	$\leftarrow$	7	2	6	6597.6186	−0.0035	0.002
8	3	5	$\leftarrow$	7	3	4	6677.0901	−0.0002	0.002
8	1	7	$\leftarrow$	7	1	6	6700.3999	−0.0004	0.002
8	2	6	$\leftarrow$	7	2	5	6749.7950	0.0010	0.002
9	1	9	$\leftarrow$	8	1	8	7248.3786	0.0002	0.001
9	0	9	$\leftarrow$	8	0	8	7266.0422	0.0004	0.001
9	2	8	$\leftarrow$	8	2	7	7411.7596	−0.0037	0.002

[a] see Table S31

J'	K'_a	K'_c	$\leftarrow$	J''	K''_a	K''_c	$\nu_{\text{obs.}}$	$\nu_{\text{obs.}} - \nu_{\text{calc.}}$	exp. error [a]
9	3	7	$\leftarrow$	8	3	6	7478.4837	−0.0021	0.002
9	4	6	$\leftarrow$	8	4	5	7482.3216	0.0017	0.002
9	4	5	$\leftarrow$	8	4	4	7486.1819	0.0019	0.002
9	1	8	$\leftarrow$	8	1	7	7511.8714	0.0006	0.002
9	3	6	$\leftarrow$	8	3	5	7529.1348	0.0019	0.002
9	2	7	$\leftarrow$	8	2	6	7600.1724	0.0017	0.002
10	1	10	$\leftarrow$	9	1	9	8045.0115	−0.0002	0.002
10	0	10	$\leftarrow$	9	0	9	8056.7615	0.0011	0.002
10	2	9	$\leftarrow$	9	2	8	8222.7243	−0.0050	0.002

[a] see Table S31

Table S56: Measured frequencies ($\nu_{\text{obs.}}$) and residuals ($\nu_{\text{obs.}} - \nu_{\text{calc.}}$) in MHz of the trihydrate of fenchone 3w-II with all oxygen atoms of water substituted by ^{18}O atoms.

J'	K'_a	K'_c	$\leftarrow$	J''	K''_a	K''_c	$\nu_{\text{obs.}}$	$\nu_{\text{obs.}} - \nu_{\text{calc.}}$	exp. error [a]
4	1	4	$\leftarrow$	3	1	3	3061.9168	0.0003	0.002
4	0	4	$\leftarrow$	3	0	3	3112.6239	0.0002	0.002
4	1	3	$\leftarrow$	3	1	2	3209.4771	0.0001	0.002
5	0	5	$\leftarrow$	4	0	4	3871.8870	−0.0001	0.001
6	2	5	$\leftarrow$	5	2	4	4699.0706	−0.0014	0.002
6	3	4	$\leftarrow$	5	3	3	4725.2976	0.0015	0.002
6	3	3	$\leftarrow$	5	3	2	4733.7247	0.0004	0.002
6	1	5	$\leftarrow$	5	1	4	4795.3217	−0.0001	0.002
7	1	7	$\leftarrow$	6	1	6	5337.0604	−0.0005	0.002
7	0	7	$\leftarrow$	6	0	6	5370.1413	0.0019	0.002
7	2	6	$\leftarrow$	6	2	5	5474.7647	−0.0018	0.002
7	1	6	$\leftarrow$	6	1	5	5578.4678	−0.0003	0.002
8	1	8	$\leftarrow$	7	1	7	6091.0455	0.0006	0.002
8	0	8	$\leftarrow$	7	0	7	6114.8563	0.0003	0.002
8	2	7	$\leftarrow$	7	2	6	6247.2361	−0.0031	0.002
8	3	6	$\leftarrow$	7	3	5	6303.1303	−0.0002	0.002
8	3	5	$\leftarrow$	7	3	4	6338.2702	0.0010	0.002
8	1	7	$\leftarrow$	7	1	6	6352.7973	0.0012	0.002
8	2	6	$\leftarrow$	7	2	5	6413.7587	0.0004	0.002
9	1	9	$\leftarrow$	8	1	8	6843.3433	−0.0001	0.001
9	0	9	$\leftarrow$	8	0	8	6859.4766	0.0001	0.001

[a] see Table S31

Table S57: Measured frequencies ($\nu_{\text{obs.}}$) and residuals ($\nu_{\text{obs.}} - \nu_{\text{calc.}}$) in MHz of the trihydrate of fenchone 3w-II with the O_1 atom substituted by a ^{18}O atom.

J'	K'_a	K'_c	$\leftarrow$	J''	K''_a	K''_c	$\nu_{\text{obs.}}$	$\nu_{\text{obs.}} - \nu_{\text{calc.}}$	exp. error [a]
3	1	3	$\leftarrow$	2	1	2	2399.0604	0.0012	0.010
3	0	3	$\leftarrow$	2	0	2	2445.4828	−0.0026	0.010
4	1	4	$\leftarrow$	3	1	3	3195.2869	0.0093	0.010
4	0	4	$\leftarrow$	3	0	3	3246.3748	−0.0058	0.010
4	1	3	$\leftarrow$	3	1	2	3347.5600	0.0038	0.010
5	1	5	$\leftarrow$	4	1	4	3989.0131	0.0014	0.010
5	0	5	$\leftarrow$	4	0	4	4037.7680	0.0056	0.010
5	1	4	$\leftarrow$	4	1	3	4176.9832	−0.0065	0.010
6	1	6	$\leftarrow$	5	1	5	4780.1734	−0.0015	0.010
7	1	6	$\leftarrow$	6	1	5	5816.1615	0.0058	0.010
8	1	8	$\leftarrow$	7	1	7	6355.5395	−0.0079	0.010
8	0	8	$\leftarrow$	7	0	7	6377.5704	−0.0088	0.010
8	1	7	$\leftarrow$	7	1	6	6622.1500	−0.0024	0.010
9	0	9	$\leftarrow$	8	0	8	7155.0756	0.0105	0.010

[a] see Table S31

Table S58: Measured frequencies ($\nu_{\text{obs.}}$) and residuals ($\nu_{\text{obs.}} - \nu_{\text{calc.}}$) in MHz of the trihydrate of fenchone 3w-II with the O_2 atom substituted by a ^{18}O atom.

J'	K'_a	K'_c	$\leftarrow$	J''	K''_a	K''_c	$\nu_{\text{obs.}}$	$\nu_{\text{obs.}} - \nu_{\text{calc.}}$	exp. error [a]
4	1	4	$\leftarrow$	3	1	3	3182.1127	0.0128	0.010
4	0	4	$\leftarrow$	3	0	3	3231.4127	−0.0021	0.010
4	1	3	$\leftarrow$	3	1	2	3322.6455	−0.0054	0.010
5	1	5	$\leftarrow$	4	1	4	3973.3220	0.0005	0.010
5	0	5	$\leftarrow$	4	0	4	4021.8981	0.0033	0.010
5	1	4	$\leftarrow$	4	1	3	4147.2299	−0.0075	0.010
6	1	6	$\leftarrow$	5	1	5	4762.2939	−0.0052	0.010
6	0	6	$\leftarrow$	5	0	5	4804.9645	−0.0035	0.010
6	1	5	$\leftarrow$	5	1	4	4967.0527	0.0031	0.010
7	1	7	$\leftarrow$	6	1	6	5549.1048	0.0016	0.010
7	0	7	$\leftarrow$	6	0	6	5583.0900	0.0020	0.010
7	1	6	$\leftarrow$	6	1	5	5780.5263	0.0026	0.010
8	1	8	$\leftarrow$	7	1	7	6333.9574	0.0008	0.010
8	0	8	$\leftarrow$	7	0	7	6358.9506	−0.0064	0.010
8	1	7	$\leftarrow$	7	1	6	6586.0753	0.0040	0.010

[a] see Table S31

Table S59: Measured frequencies ($\nu_{\text{obs.}}$) and residuals ($\nu_{\text{obs.}} - \nu_{\text{calc.}}$) in MHz of the trihydrate of fenchone 3w-II with the O_3 atom substituted by a ^{18}O atom.

J'	K'_a	K'_c	$\leftarrow$	J''	K''_a	K''_c	$\nu_{\text{obs.}}$	$\nu_{\text{obs.}} - \nu_{\text{calc.}}$	exp. error [a]
3	1	3	$\leftarrow$	2	1	2	2368.6045	−0.0120	0.010
3	0	3	$\leftarrow$	2	0	2	2410.6668	0.0032	0.010
3	1	2	$\leftarrow$	2	1	1	2468.5032	0.0097	0.010
4	1	4	$\leftarrow$	3	1	3	3155.6189	−0.0080	0.010
4	0	4	$\leftarrow$	3	0	3	3203.7578	−0.0070	0.010
4	1	3	$\leftarrow$	3	1	2	3288.3025	−0.0036	0.010
5	1	5	$\leftarrow$	4	1	4	3940.7522	−0.0103	0.010
5	0	5	$\leftarrow$	4	0	4	3989.3341	0.0032	0.010
6	0	6	$\leftarrow$	5	0	5	4767.8813	0.0046	0.010
6	1	5	$\leftarrow$	5	1	4	4918.1053	0.0155	0.010
7	1	7	$\leftarrow$	6	1	6	5505.0045	−0.0140	0.010
7	0	7	$\leftarrow$	6	0	6	5541.3110	0.0093	0.010
7	1	6	$\leftarrow$	6	1	5	5725.6357	0.0037	0.010
8	1	8	$\leftarrow$	7	1	7	6284.3214	0.0005	0.010
8	0	8	$\leftarrow$	7	0	7	6312.0138	0.0101	0.010
9	1	9	$\leftarrow$	8	1	8	7062.0535	0.0096	0.010
9	1	8	$\leftarrow$	8	1	7	7319.3151	−0.0196	0.010

[a] see Table S31

Table S60: Measured frequencies ($\nu_{\text{obs.}}$) and residuals ($\nu_{\text{obs.}} - \nu_{\text{calc.}}$) in MHz of the trihydrate of fenchone 3w-II with the O_{1-2} atoms substituted by ^{18}O atoms.

J'	K'_a	K'_c	$\leftarrow$	J''	K''_a	K''_c	$\nu_{\text{obs.}}$	$\nu_{\text{obs.}} - \nu_{\text{calc.}}$	exp. error [a]
3	1	3	$\leftarrow$	2	1	2	2357.2068	−0.0029	0.010
3	0	3	$\leftarrow$	2	0	2	2404.0445	0.0044	0.010
4	0	4	$\leftarrow$	3	0	3	3190.7090	−0.0031	0.010
4	1	3	$\leftarrow$	3	1	2	3293.5910	−0.0029	0.010
5	1	5	$\leftarrow$	4	1	4	3918.9939	0.0021	0.010
5	0	5	$\leftarrow$	4	0	4	3967.6790	−0.0032	0.010
5	1	4	$\leftarrow$	4	1	3	4109.2767	−0.0011	0.010
6	1	6	$\leftarrow$	5	1	5	4695.9740	−0.0061	0.010
6	0	6	$\leftarrow$	5	0	5	4736.7857	0.0036	0.010
6	1	5	$\leftarrow$	5	1	4	4918.8243	0.0031	0.010
7	1	7	$\leftarrow$	6	1	6	5470.5099	0.0078	0.010
7	0	7	$\leftarrow$	6	0	6	5501.3414	0.0000	0.010
8	1	8	$\leftarrow$	7	1	7	6242.8930	−0.0002	0.010
8	0	8	$\leftarrow$	7	0	7	6264.3981	−0.0002	0.010
9	0	9	$\leftarrow$	8	0	8	7027.6990	−0.0027	0.010

[a] see Table S31

Table S61: Measured frequencies ($\nu_{\text{obs.}}$) and residuals ($\nu_{\text{obs.}} - \nu_{\text{calc.}}$) in MHz of the trihydrate of fenchone 3w-II with the O_{1-3} atoms substituted by ^{18}O atoms.

J'	K'_a	K'_c	$\leftarrow$	J''	K''_a	K''_c	$\nu_{\text{obs.}}$	$\nu_{\text{obs.}} - \nu_{\text{calc.}}$	exp. error [a]
4	1	4	$\leftarrow$	3	1	3	3113.9477	0.0011	0.010
4	0	4	$\leftarrow$	3	0	3	3164.3122	0.0046	0.010
4	1	3	$\leftarrow$	3	1	2	3259.1565	0.0043	0.010
5	1	5	$\leftarrow$	4	1	4	3887.8743	−0.0070	0.010
5	1	4	$\leftarrow$	4	1	3	4067.4517	0.0028	0.010
6	1	6	$\leftarrow$	5	1	5	4659.4542	−0.0075	0.010
6	1	5	$\leftarrow$	5	1	4	4870.6238	−0.0054	0.010
7	1	7	$\leftarrow$	6	1	6	5428.7872	0.0093	0.010
7	1	6	$\leftarrow$	6	1	5	5667.0163	−0.0009	0.010

[a] see Table S31

Table S62: Measured frequencies ($\nu_{\text{obs.}}$) and residuals ($\nu_{\text{obs.}} - \nu_{\text{calc.}}$) in MHz of the trihydrate of fenchone 3w-II with the O_{2-3} atoms substituted by ^{18}O atoms.

J'	K'_a	K'_c	$\leftarrow$	J''	K''_a	K''_c	$\nu_{\text{obs.}}$	$\nu_{\text{obs.}} - \nu_{\text{calc.}}$	exp. error [a]
3	1	3	$\leftarrow$	2	1	2	2328.2982	−0.0086	0.010
3	0	3	$\leftarrow$	2	0	2	2370.8644	0.0071	0.010
4	1	4	$\leftarrow$	3	1	3	3101.7960	0.0015	0.010
4	0	4	$\leftarrow$	3	0	3	3150.3346	0.0024	0.010
4	1	3	$\leftarrow$	3	1	2	3236.5499	0.0005	0.010
5	0	5	$\leftarrow$	4	0	4	3922.0731	0.0055	0.010
5	1	4	$\leftarrow$	4	1	3	4040.3081	−0.0044	0.010
6	1	6	$\leftarrow$	5	1	5	4642.8480	0.0094	0.010
6	0	6	$\leftarrow$	5	0	5	4686.6736	0.0018	0.010
7	1	7	$\leftarrow$	6	1	6	5410.2813	−0.0117	0.010
7	0	7	$\leftarrow$	6	0	6	5446.1608	−0.0089	0.010
7	1	6	$\leftarrow$	6	1	5	5633.8937	−0.0015	0.010
8	1	8	$\leftarrow$	7	1	7	6175.8926	0.0062	0.010
8	1	7	$\leftarrow$	7	1	6	6420.9018	−0.0005	0.010
9	1	8	$\leftarrow$	8	1	7	7199.7193	0.0025	0.010

[a] see Table S31

Table S63: Measured frequencies ($\nu_{\text{obs.}}$) and residuals ($\nu_{\text{obs.}} - \nu_{\text{calc.}}$) in MHz of the trihydrate of fenchone 3w-III.

J'	K'_a	K'_c	←	J''	K''_a	K''_c	$\nu_{\text{obs.}}$	$\nu_{\text{obs.}} - \nu_{\text{calc.}}$	exp. error [a]
3	0	3	←	2	0	2	2504.6872	0.0002	0.001
4	1	4	←	3	1	3	3248.2411	−0.0003	0.002
4	0	4	←	3	0	3	3315.4942	−0.0004	0.002
4	1	3	←	3	1	2	3468.1824	−0.0007	0.002
5	1	5	←	4	1	4	4051.7891	−0.0002	0.001
5	0	5	←	4	0	4	4111.8319	0.0014	0.002
5	1	4	←	4	1	3	4321.7681	0.0001	0.001
6	0	6	←	5	1	5	4767.6939	0.0039	0.004
6	1	6	←	5	1	5	4851.3034	−0.0002	0.001
6	0	6	←	5	0	5	4898.0717	−0.0009	0.001
6	3	4	←	5	3	3	5077.0190	0.0020	0.002
6	1	5	←	5	1	4	5164.4745	0.0006	0.002
6	2	4	←	5	2	3	5184.8730	−0.0002	0.001
7	1	7	←	6	1	6	5647.2209	0.0005	0.001
7	0	7	←	6	0	6	5679.9095	−0.0008	0.001
7	1	7	←	6	0	6	5730.8337	−0.0004	0.002
7	2	6	←	6	2	5	5853.0732	0.0015	0.001
7	3	5	←	6	3	4	5924.7905	−0.0001	0.002
7	3	4	←	6	3	3	5967.8201	−0.0018	0.002
7	1	6	←	6	1	5	5992.9463	0.0005	0.002
7	2	5	←	6	2	4	6067.9352	−0.0014	0.002
8	0	8	←	7	1	7	6410.3831	0.0017	0.002
8	1	8	←	7	1	7	6440.2127	0.0001	0.001
8	0	8	←	7	0	7	6461.3040	−0.0012	0.002
8	1	8	←	7	0	7	6491.1349	−0.0015	0.002
8	2	7	←	7	2	6	6671.4166	0.0020	0.002
8	3	6	←	7	3	5	6770.4222	0.0010	0.002
8	1	7	←	7	1	6	6804.8148	0.0009	0.002
8	3	5	←	7	3	4	6849.9451	−0.0014	0.002

[a] see Table S31

J'	K'_a	K'_c	$\leftarrow$	J''	K''_a	K''_c	$\nu_{\text{obs.}}$	$\nu_{\text{obs.}} - \nu_{\text{calc.}}$	exp. error [a]
8	2	6	$\leftarrow$	7	2	5	6943.2630	−0.0016	0.002
9	0	9	$\leftarrow$	8	1	8	7214.0421	0.0004	0.002
9	1	9	$\leftarrow$	8	1	8	7231.0144	0.0001	0.002
9	0	9	$\leftarrow$	8	0	8	7243.8726	−0.0003	0.002
9	1	9	$\leftarrow$	8	0	8	7260.8433	−0.0022	0.002
9	2	8	$\leftarrow$	8	2	7	7483.8468	0.0036	0.004
9	1	8	$\leftarrow$	8	1	7	7600.4293	0.0024	0.002
9	2	7	$\leftarrow$	8	2	6	7807.0183	−0.0016	0.002

[a] see Table S31

Table S64: Measured frequencies ($\nu_{\text{obs.}}$) and residuals ($\nu_{\text{obs.}} - \nu_{\text{calc.}}$) in MHz of the trihydrate of fenchone 3w-III with all oxygen atoms of water substituted by ^{18}O atoms.

J'	K'_a	K'_c	$\leftarrow$	J''	K''_a	K''_c	$\nu_{\text{obs.}}$	$\nu_{\text{obs.}} - \nu_{\text{calc.}}$	exp. error [a]
4	1	4	$\leftarrow$	3	1	3	3081.6841	−0.0053	0.010
4	0	4	$\leftarrow$	3	0	3	3147.2534	−0.0065	0.010
4	2	3	$\leftarrow$	3	2	2	3193.6773	−0.0004	0.010
4	1	3	$\leftarrow$	3	1	2	3292.4560	−0.0003	0.010
5	1	5	$\leftarrow$	4	1	4	3844.1538	0.0008	0.010
5	0	5	$\leftarrow$	4	0	4	3903.4108	−0.0020	0.010
5	1	4	$\leftarrow$	4	1	3	4103.1509	−0.0057	0.010
6	1	6	$\leftarrow$	5	1	5	4602.8024	0.0026	0.010
6	0	6	$\leftarrow$	5	0	5	4649.6374	0.0013	0.010
6	2	5	$\leftarrow$	5	2	4	4772.8239	0.0058	0.010
6	1	5	$\leftarrow$	5	1	4	4903.8503	0.0007	0.010
7	1	7	$\leftarrow$	6	1	6	5358.0068	−0.0008	0.010
7	0	7	$\leftarrow$	6	0	6	5391.2476	−0.0017	0.010
7	2	6	$\leftarrow$	6	2	5	5555.2436	0.0029	0.010
8	1	8	$\leftarrow$	7	1	7	6110.3868	0.0014	0.010
8	0	8	$\leftarrow$	7	0	7	6132.1602	0.0015	0.010
8	2	7	$\leftarrow$	7	2	6	6332.2467	0.0031	0.010
8	1	7	$\leftarrow$	7	1	6	6463.4496	−0.0010	0.010
9	1	9	$\leftarrow$	8	1	8	6860.6177	0.0031	0.010
9	0	9	$\leftarrow$	8	0	8	6874.0841	0.0034	0.010
10	1	10	$\leftarrow$	9	1	9	7609.3102	−0.0131	0.010
10	0	10	$\leftarrow$	9	0	9	7617.3228	0.0050	0.010

[a] see Table S31

Table S65: Measured frequencies ($\nu_{\text{obs.}}$) and residuals ($\nu_{\text{obs.}} - \nu_{\text{calc.}}$) in MHz of the trihydrate of fenchone 3w-III with the O_1 atom substituted by a ^{18}O atom.

J'	K'_a	K'_c	$\leftarrow$	J''	K''_a	K''_c	$\nu_{\text{obs.}}$	$\nu_{\text{obs.}} - \nu_{\text{calc.}}$	exp. error [a]
3	1	3	$\leftarrow$	2	1	2	2397.6104	−0.0029	0.010
3	0	3	$\leftarrow$	2	0	2	2460.4049	−0.0002	0.010
3	1	2	$\leftarrow$	2	1	1	2559.6100	−0.0017	0.010
4	0	4	$\leftarrow$	3	0	3	3257.4636	0.0039	0.010
4	1	3	$\leftarrow$	3	1	2	3405.5204	0.0030	0.010
5	1	5	$\leftarrow$	4	1	4	3980.7816	0.0013	0.010
5	0	5	$\leftarrow$	4	0	4	4040.4650	0.0053	0.010
5	1	4	$\leftarrow$	4	1	3	4244.1085	0.0017	0.010
6	1	6	$\leftarrow$	5	1	5	4766.5078	−0.0001	0.010
6	0	6	$\leftarrow$	5	0	5	4813.4406	−0.0058	0.010
6	1	5	$\leftarrow$	5	1	4	5072.3767	0.0003	0.010
7	1	7	$\leftarrow$	6	1	6	5548.7325	−0.0023	0.010
7	0	7	$\leftarrow$	6	0	6	5581.8830	0.0050	0.010
7	1	6	$\leftarrow$	6	1	5	5887.1052	−0.0065	0.010
8	1	8	$\leftarrow$	7	1	7	6328.0911	−0.0014	0.010
8	0	8	$\leftarrow$	7	0	7	6349.6877	−0.0040	0.010
9	1	9	$\leftarrow$	8	1	8	7105.2880	0.0060	0.010
9	0	9	$\leftarrow$	8	0	8	7118.5727	−0.0031	0.010
9	1	8	$\leftarrow$	8	1	7	7468.9246	0.0025	0.010

[a] see Table S31

Table S66: Measured frequencies ($\nu_{\text{obs.}}$) and residuals ($\nu_{\text{obs.}} - \nu_{\text{calc.}}$) in MHz of the trihydrate of fenchone 3w-III with the O_2 atom substituted by a ^{18}O atom.

J'	K'_a	K'_c	$\leftarrow$	J''	K''_a	K''_c	$\nu_{\text{obs.}}$	$\nu_{\text{obs.}} - \nu_{\text{calc.}}$	exp. error [a]
3	0	3	$\leftarrow$	2	0	2	2441.5040	0.0027	0.010
3	1	2	$\leftarrow$	2	1	1	2537.2364	−0.0026	0.010
4	1	4	$\leftarrow$	3	1	3	3167.2805	0.0024	0.010
4	1	3	$\leftarrow$	3	1	2	3376.3006	−0.0018	0.010
5	1	5	$\leftarrow$	4	1	4	3951.4858	0.0100	0.010
5	0	5	$\leftarrow$	4	0	4	4012.6229	0.0011	0.010
5	1	4	$\leftarrow$	4	1	3	4208.7110	0.0020	0.010
6	1	6	$\leftarrow$	5	1	5	4731.9614	0.0024	0.010
6	0	6	$\leftarrow$	5	0	5	4781.2449	−0.0056	0.010
6	1	5	$\leftarrow$	5	1	4	5031.7394	−0.0052	0.010
7	1	7	$\leftarrow$	6	1	6	5509.0486	−0.0006	0.010
7	0	7	$\leftarrow$	6	0	6	5544.7749	−0.0009	0.010
7	1	6	$\leftarrow$	6	1	5	5842.4329	0.0047	0.010
8	1	8	$\leftarrow$	7	1	7	6283.2967	−0.0043	0.010
8	0	8	$\leftarrow$	7	0	7	6307.1909	−0.0014	0.010
8	1	7	$\leftarrow$	7	1	6	6638.3195	−0.0034	0.010
9	1	9	$\leftarrow$	8	1	8	7055.3482	−0.0097	0.010
9	0	9	$\leftarrow$	8	0	8	7070.4340	0.0028	0.010
9	1	8	$\leftarrow$	8	1	7	7418.9239	0.0039	0.010
10	1	10	$\leftarrow$	9	1	9	7825.8380	0.0076	0.010
10	0	10	$\leftarrow$	9	0	9	7834.9500	−0.0018	0.010

[a] see Table S31

Table S67: Measured frequencies ($\nu_{\text{obs.}}$) and residuals ($\nu_{\text{obs.}} - \nu_{\text{calc.}}$) in MHz of the trihydrate of fenchone 3w-III with the O_3 atom substituted by a ^{18}O atom.

J'	K'_a	K'_c	$\leftarrow$	J''	K''_a	K''_c	$\nu_{\text{obs.}}$	$\nu_{\text{obs.}} - \nu_{\text{calc.}}$	exp. error [a]
3	0	3	$\leftarrow$	2	0	2	2478.5509	−0.0045	0.010
3	1	2	$\leftarrow$	2	1	1	2584.6914	−0.0011	0.010
4	1	4	$\leftarrow$	3	1	3	3211.9631	0.0015	0.010
4	0	4	$\leftarrow$	3	0	3	3278.8863	0.0028	0.010
4	1	3	$\leftarrow$	3	1	2	3437.8650	0.0038	0.010
5	1	5	$\leftarrow$	4	1	4	4005.8302	0.0012	0.010
5	0	5	$\leftarrow$	4	0	4	4064.2563	0.0006	0.010
5	1	4	$\leftarrow$	4	1	3	4282.5264	−0.0112	0.010
6	1	6	$\leftarrow$	5	1	5	4795.4697	0.0024	0.010
6	0	6	$\leftarrow$	5	0	5	4839.8010	−0.0002	0.010
6	1	5	$\leftarrow$	5	1	4	5115.2225	0.0073	0.010
7	0	7	$\leftarrow$	6	0	6	5611.5530	−0.0038	0.010
7	1	6	$\leftarrow$	6	1	5	5932.3141	0.0009	0.010
8	1	8	$\leftarrow$	7	1	7	6364.3946	−0.0001	0.010
8	0	8	$\leftarrow$	7	0	7	6383.3381	−0.0015	0.010
8	1	7	$\leftarrow$	7	1	6	6731.6599	−0.0001	0.010
9	0	9	$\leftarrow$	8	0	8	7156.4935	0.0008	0.010

[a] see Table S31

Table S68: Measured frequencies ($\nu_{\text{obs.}}$) and residuals ($\nu_{\text{obs.}} - \nu_{\text{calc.}}$) in MHz of the trihydrate of fenchone 3w-III with the O_{1-2} atoms substituted by ^{18}O atoms.

J'	K'_a	K'_c	$\leftarrow$	J''	K''_a	K''_c	$\nu_{\text{obs.}}$	$\nu_{\text{obs.}} - \nu_{\text{calc.}}$	exp. error [a]
3	1	3	$\leftarrow$	2	1	2	2339.4343	0.0024	0.010
3	0	3	$\leftarrow$	2	0	2	2400.3482	0.0006	0.010
3	1	2	$\leftarrow$	2	1	1	2493.5996	0.0018	0.010
4	1	4	$\leftarrow$	3	1	3	3114.1808	−0.0014	0.010
4	0	4	$\leftarrow$	3	0	3	3179.7469	0.0056	0.010
5	0	5	$\leftarrow$	4	0	4	3945.9701	0.0022	0.010
5	1	4	$\leftarrow$	4	1	3	4136.8018	−0.0064	0.010
6	1	6	$\leftarrow$	5	1	5	4652.9684	−0.0017	0.010
6	0	6	$\leftarrow$	5	0	5	4702.1532	−0.0104	0.010
6	1	5	$\leftarrow$	5	1	4	4946.2641	−0.0010	0.010
7	1	7	$\leftarrow$	6	1	6	5417.2531	−0.0021	0.010
7	1	6	$\leftarrow$	6	1	5	5743.8933	−0.0005	0.010
8	1	8	$\leftarrow$	7	1	7	6178.7584	0.0013	0.010
8	0	8	$\leftarrow$	7	0	7	6202.9774	0.0104	0.010
8	1	7	$\leftarrow$	7	1	6	6527.3050	0.0117	0.010
9	1	9	$\leftarrow$	8	1	8	6938.0940	0.0018	0.010
9	0	9	$\leftarrow$	8	0	8	6953.4724	−0.0060	0.010
9	1	8	$\leftarrow$	8	1	7	7295.8131	−0.0069	0.010

[a] see Table S31

Table S69: Measured frequencies ($\nu_{\text{obs.}}$) and residuals ($\nu_{\text{obs.}} - \nu_{\text{calc.}}$) in MHz of the trihydrate of fenchone 3w-III with the O_{1-3} atoms substituted by ^{18}O atoms.

J'	K'_a	K'_c	$\leftarrow$	J''	K''_a	K''_c	$\nu_{\text{obs.}}$	$\nu_{\text{obs.}} - \nu_{\text{calc.}}$	exp. error [a]
3	1	3	$\leftarrow$	2	1	2	2371.9425	−0.0030	0.010
3	0	3	$\leftarrow$	2	0	2	2435.6472	0.0044	0.010
3	1	2	$\leftarrow$	2	1	1	2539.2258	0.0011	0.010
4	1	4	$\leftarrow$	3	1	3	3156.4145	−0.0088	0.010
4	0	4	$\leftarrow$	3	0	3	3222.5094	−0.0002	0.010
4	1	3	$\leftarrow$	3	1	2	3377.5519	−0.0030	0.010
5	1	5	$\leftarrow$	4	1	4	3936.7089	0.0093	0.010
5	0	5	$\leftarrow$	4	0	4	3994.7575	0.0040	0.010
6	1	6	$\leftarrow$	5	1	5	4712.8589	0.0012	0.010
6	1	5	$\leftarrow$	5	1	4	5026.3816	0.0022	0.010
7	1	7	$\leftarrow$	6	1	6	5485.3955	0.0036	0.010
7	0	7	$\leftarrow$	6	0	6	5515.7854	−0.0101	0.010
7	1	6	$\leftarrow$	6	1	5	5830.0287	−0.0073	0.010
8	1	8	$\leftarrow$	7	1	7	6255.0286	0.0023	0.010
8	0	8	$\leftarrow$	7	0	7	6274.2681	0.0007	0.010
8	1	7	$\leftarrow$	7	1	6	6616.4989	0.0072	0.010
9	1	8	$\leftarrow$	8	1	7	7386.6727	−0.0016	0.010
10	1	10	$\leftarrow$	9	1	9	7788.5594	−0.0068	0.010
10	0	10	$\leftarrow$	9	0	9	7795.1942	0.0050	0.010

[a] see Table S31

Table S70: Measured frequencies ($\nu_{\text{obs.}}$) and residuals ($\nu_{\text{obs.}} - \nu_{\text{calc.}}$) in MHz of the trihydrate of fenchone 3w-III with the O_{2-3} atoms substituted by ^{18}O atoms.

J'	K'_a	K'_c	$\leftarrow$	J''	K''_a	K''_c	$\nu_{\text{obs.}}$	$\nu_{\text{obs.}} - \nu_{\text{calc.}}$	exp. error [a]
3	1	3	$\leftarrow$	2	1	2	2354.3299	0.0029	0.010
3	0	3	$\leftarrow$	2	0	2	2417.2565	−0.0019	0.010
3	1	2	$\leftarrow$	2	1	1	2516.6918	0.0080	0.010
4	1	4	$\leftarrow$	3	1	3	3133.4244	−0.0021	0.010
4	0	4	$\leftarrow$	3	0	3	3199.8744	−0.0056	0.010
4	1	3	$\leftarrow$	3	1	2	3348.2638	−0.0004	0.010
5	1	5	$\leftarrow$	4	1	4	3908.5981	−0.0046	0.010
5	0	5	$\leftarrow$	4	0	4	3968.4242	0.0083	0.010
5	1	4	$\leftarrow$	4	1	3	4172.5115	−0.0006	0.010
6	1	6	$\leftarrow$	5	1	5	4679.8737	0.0022	0.010
6	0	6	$\leftarrow$	5	0	5	4726.9116	−0.0043	0.010
6	1	5	$\leftarrow$	5	1	4	4986.4172	−0.0005	0.010
7	1	7	$\leftarrow$	6	1	6	5447.6264	−0.0051	0.010
7	0	7	$\leftarrow$	6	0	6	5480.8516	0.0016	0.010
7	1	6	$\leftarrow$	6	1	5	5786.7568	−0.0025	0.010
8	1	8	$\leftarrow$	7	1	7	6212.5167	0.0009	0.010
8	0	8	$\leftarrow$	7	0	7	6234.1673	0.0029	0.010
8	1	7	$\leftarrow$	7	1	6	6571.1535	0.0001	0.010
9	1	9	$\leftarrow$	8	1	8	6975.2337	0.0070	0.010
9	0	9	$\leftarrow$	8	0	8	6988.5512	0.0001	0.010
9	1	8	$\leftarrow$	8	1	7	7339.6770	0.0001	0.010
10	1	10	$\leftarrow$	9	1	9	7736.4023	−0.0046	0.010

[a] see Table S31