Supplementary information:

Probing the structure and dynamics of the heterocyclic PAH xanthene and its water complexes with infrared and microwave spectroscopy

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1 Supplementary theoretical and experimental results

1.1 Monomer

Table S1: Experimental spectroscopic parameters for the parent species and seven ^{13}C singly-substituted isotopologues of xanthene, including rotational constants (A, B, and C), centrifugal distortion constants (D_J, D_{JK}, and D_K), number of lines in total (N), and root-mean-square (RMS) deviation. 0^+ and 0^- denote the two tunneling states. The fittings were performed with Watson's S-reduced Hamiltonian in its I^r representation using Pickett's SPFIT program. Note that limited by number of observed transitions, the 0^+ state of $^{13}C_1$ and $^{13}C_7$ were excluded from the fit.

		parent		$^{13}C_1$	
Parameters	Units	0^+	0^-	0^+	0^-
A	MHz	2031.0404(12)	2032.1108(11)		2017.0066(10)
B	MHz	466.05932(60)	465.95043(44)		463.30596(36)
C	MHz	385.25282(60)	385.12537(40)		382.78050(24)
D_J	kHz	0.1180(49)	0.0192(29)		[0.0192]
D_{JK}	kHz	-0.258(23)	-0.298(18)		[-0.298]
D_K	kHz	1.17(15)	1.38(14)		[1.38]
N		68			18
RMS	kHz	7.3			9.4

		$^{13}C_2$		$^{13}C_3$	
Parameters	Units	0^+	0^-	0^+	0^-
A	MHz	2026.0773(10)	2027.13468(83)	2027.7780(17)	2028.8402(11)
B	MHz	465.40538(60)	465.29873(36)	465.46580(90)	465.35884(45)
C	MHz	384.64404(62)	384.51648(24)	384.74787(70)	384.61783(29)
D_J	kHz	[0.1180]	[0.0192]	[0.1180]	[0.0192]
D_{JK}	kHz	[-0.258]	[-0.298]	[-0.258]	[-0.298]
D_K	kHz	[1.17]	[1.38]	[1.17]	[1.38]

N		36		31	
RMS	kHz	8.5		9.6	
		$^{13}C_4$		$^{13}C_5$	
Parameters	Units	0^+	0^-	0^+	0^-
A	MHz	2015.2048(36)	2016.2135(11)	2025.6235(11)	2026.68632(88)
B	MHz	463.7431(11)	463.65542(58)	460.69034(39)	460.58401(38)
C	MHz	383.06776(92)	382.98255(42)	381.41548(44)	381.28854(25)
D_J	kHz	[0.1180]	[0.0192]	[0.1180]	[0.0192]
D_{JK}	kHz	[-0.258]	[-0.298]	[-0.258]	[-0.298]
D_K	kHz	[1.17]	[1.38]	[1.17]	[1.38]
N		23		42	
RMS	kHz	9.1		8.3	
		$^{13}C_6$		$^{13}C_7$	
Parameters	Units	0^+	0^-	0^+	0^-
A	MHz	2027.5799(13)	2028.6343(10)		2010.5640(15)
B	MHz	460.41980(49)	460.31357(33)		465.92388(45)
C	MHz	381.31012(55)	381.18595(22)		384.42183(29)
D_J	kHz	[0.1180]	[0.0192]		[0.0192(34)]
D_{JK}	kHz	[-0.258]	[-0.298]		[-0.298(21)]
D_K	kHz	[1.17]	[1.38]		[1.38(16)]
N		31		19	
RMS	kHz	7.6		9.8	

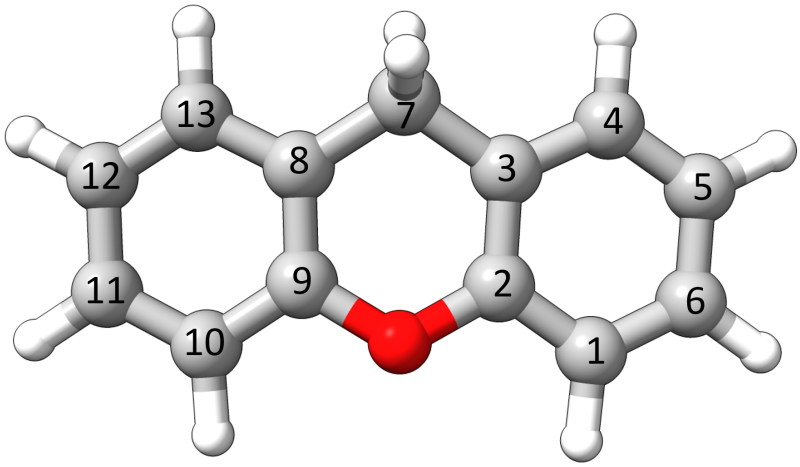

Figure S1: Theoretical structure of the xanthene monomer calculated at the B3LYP-D3BJ/def2-TZVP level of theory. The numbering of the carbon atoms, which was used for the identification of the ^{13}C isotopologues, is provided.

Table S2: Kraitchman coordinates (in Å) and the estimated uncertainties for the substituted structure (r_s) of the xanthene monomer, obtained with rotational constants of the parent species and seven ^{13}C isotopologues in the 0^- state.

Atoms	a(Δa)	b(Δb)	c(Δc)
C_1/C_{10}	2.48657(65)	1.3685(12)	0.086(19)
C_2/C_9	1.2231(13)	0.7657(21)	0.1638(99)
C_3/C_8	1.1640(14)	0.6158(26)	0.150(10)
C_4/C_{13}	2.31810(69)	1.4082(11)	0.0
C_5/C_{12}	3.55040(45)	0.7916(20)	0.2248(72)
C_6/C_{11}	3.63745(44)	0.5982(27)	0.2756(59)
C_7	0.0	1.5830(10)	0.4060(40)

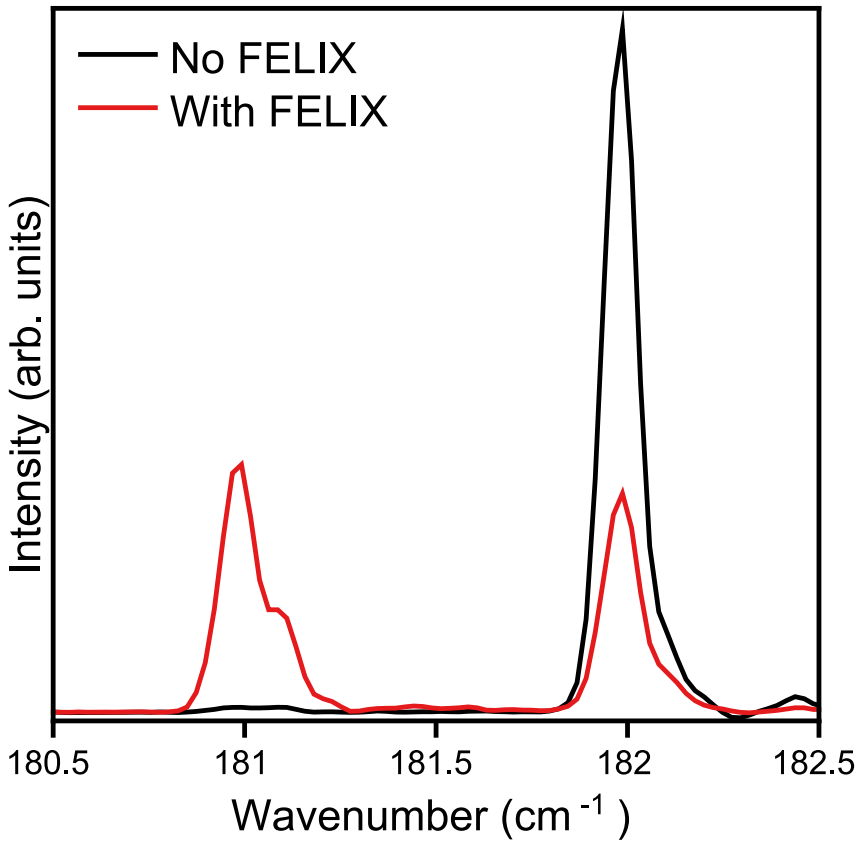

Figure S2: Mass spectra of xanthene (m/z = 182) recorded with (red trace) and without (black trace) FELIX. The comparison between the two mass spectra shows the depletion in the signal of xanthene and signal in-growth in its dissociation channel induced by FELIX.

1.2 Xanthene-H_2O

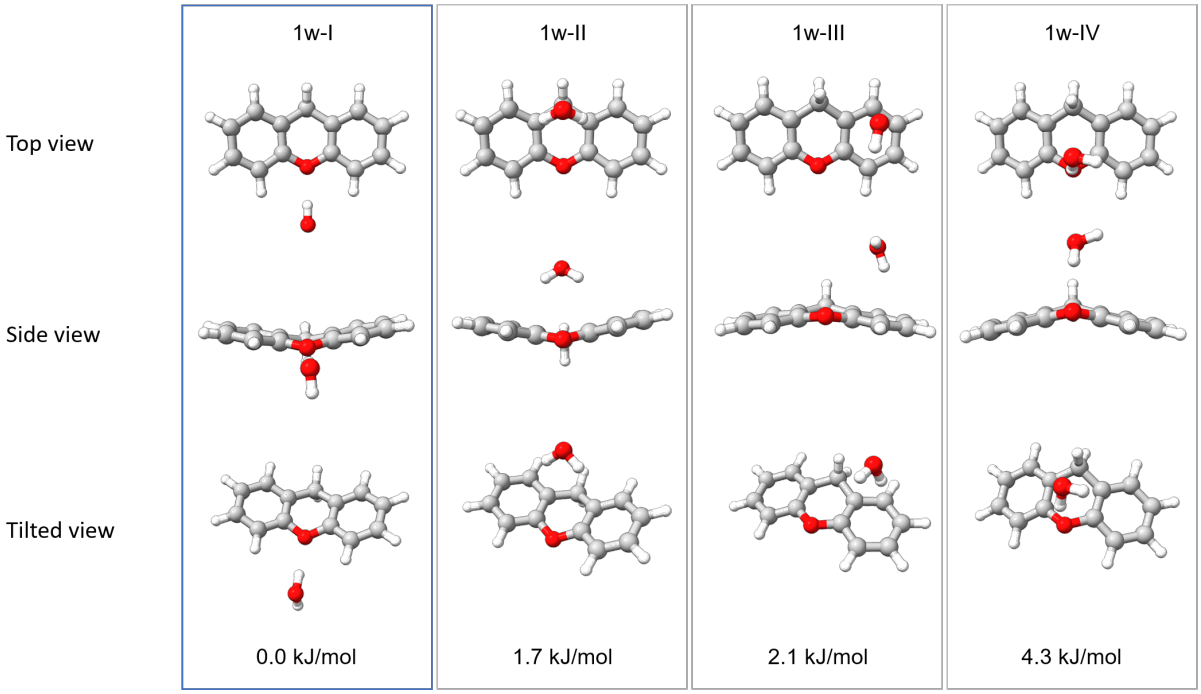

Figure S3: Molecular geometries of the energetically low-lying isomers of the xanthene-H_2O complexes within an energy window of 5.0 kJ/mol, calculated at the B3LYP-D4/def2-QZVP level of theory. Each isomer is shown from three different perspectives: top view, side view, and tilted view. The relative energies (in kJ/mol), corrected with zero-point energies (ZPE), are provided, with the energy of 1w-I set to 0 kJ/mol. The molecular geometry of the experimentally observed isomer is highlighted by a blue box. The corresponding Cartesian coordinates are available in Tables S14–S17 in Section 2.2. Rendered using UCSF ChimeraX software.[1]

Table S3: Theoretical spectroscopic constants for the xanthene-H_2O complexes, calculated at the B3LYP-D4/def2-QZVP level of theory. The relative energies (ΔE_0 in kJ mol^{-1}) with vibrational zero-point energy corrections.

Isomers	ΔE_0	A/MHz	B/MHz	C/MHz	μ_a/D	μ_b/D	μ_c/D
1w-I	0.0	934.3	465.8	318.4	0.0	2.6	-1.3
1w-II	1.7	1227.8	425.3	377.2	0.0	-0.8	1.7
1w-III	2.1	1239.7	379.7	351.4	0.3	0.9	1.2
1w-IV	2.3	1148.6	408.0	386.2	-1.1	0.9	0.9

Table S4: Experimental spectroscopic constants for the xanthene-H_2O, 1w-I, fitted with Watson's A-reduced Hamiltonian in its I^r representation using Pickett's SPFIT program.

Parameters	Units	Calc.	Expt. (average)
A	MHz	934.3	913.47858(16)
B	MHz	465.8	464.72514(10)
C	MHz	318.4	317.02967(11)
Δ_J	kHz		0.01419(62)
Δ_{JK}	kHz		0.5924(12)
Δ_K	kHz		-0.3894(23)
δ_K	kHz		0.3378(15)
N (a|b|c)			226 (0|193|33)
RMS	kHz		7.0

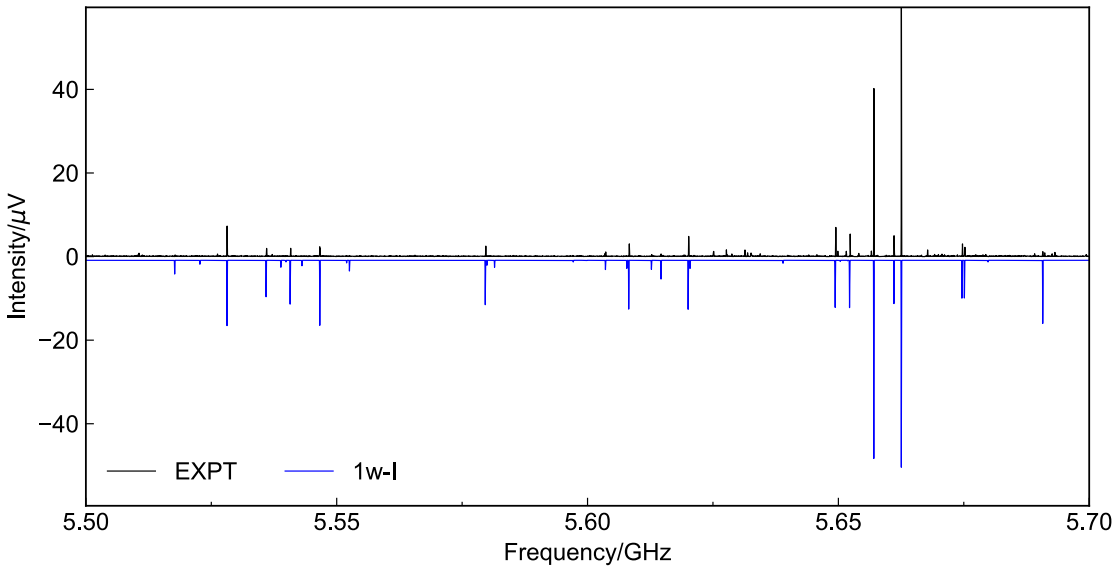

Figure S4: Portion of the microwave spectrum highlighting the transitions arising from the 1w-I complex.

Table S5: Experimental spectroscopic constants for ^{13}C singly substituted isotopologues of 1w-I, including rotational constants (A, B, and C), number of lines in total (N), and root-mean-square (RMS) deviation. The centrifugal distortion constants were fixed to those for the parent species (see Table S4). The fittings were performed with Watson's A-reduction Hamiltonian in its I^r representation using Pickett's SPFIT program.

Parameters	Units	$^{13}C_1/^{13}C_{13}$	$^{13}C_2/^{13}C_{12}$	$^{13}C_3/^{13}C_{11}$	$^{13}C_4/^{13}C_{10}$
A	MHz	913.37507(26)	911.69772(38)	912.96821(39)	911.66649(48)
B	MHz	464.13978(15)	462.42283(41)	459.38403(30)	459.16642(36)
C	MHz	316.748151(89)	315.77515(11)	314.54398(12)	314.24891(17)
N		47	43	36	36
RMS	kHz	6.1	8.1	7.8	9.5
Parameters	Unit	$^{13}C_5/^{13}C_9$	$^{13}C_6/^{13}C_8$	$^{13}C_7$	
A	MHz	908.48592(39)	911.32408(29)	907.04529(45)	
B	MHz	462.11299(45)	464.06271(22)	464.58472(71)	
C	MHz	315.21282(13)	316.48392(10)	316.34505(16)	
N		32	42	19	
RMS	kHz	6.7	5.9	6.2	

Since no c-type transitions were observed for any of the singly-substituted ^{13}C isotopologues, to determine the substitution structure of xanthene in the 1w-I complex, we considered the rotational constants of the monomer obtained from an average fit that did not account for the tunneling splitting of the c-type transitions; instead, only the center frequencies were considered.

Table S6: Kraitchman coordinates (in Å) and the estimated uncertainties for the substituted structure (r_s) of xanthene in the 1w-I complex, obtained with rotational constants of the parent species and seven ^{13}C isotopologues.

Atoms	a(Δa)	b(Δb)	c(Δc)
C_1/C_{13}	-3.61682(43)	-1.0232(15)	-0.2840(54)
C_2/C_{12}	-2.47438(62)	-1.75523(88)	0.0
C_3/C_{11}	-1.2229(12)	-1.1215(14)	0.2367(64)
C_4/C_{10}	-1.1704(13)	0.2432(63)	0.062(25)
C_5/C_9	-2.30906(66)	1.0056(15)	-0.2858(54)
C_6/C_8	-3.53289(43)	0.3671(42)	-0.4246(36)
C_7	0.0	-1.87753(84)	-0.6362(25)

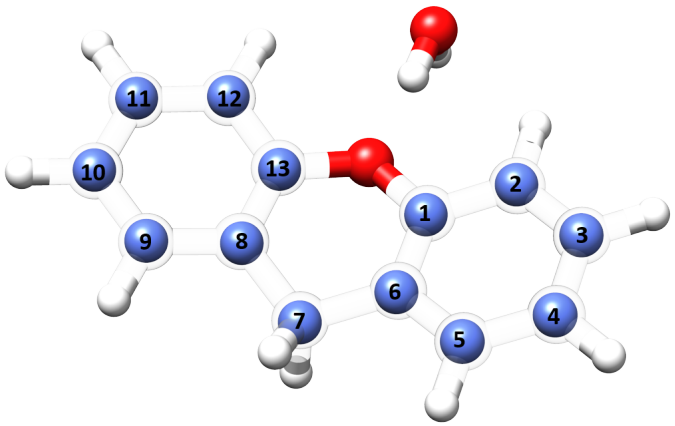

Figure S5: Comparison of the Kraitchman substitution coordinates (r_s, orange solid spheres) of 1w-I with the equlibrium structure (r_e, ball and stick model) calculated at the B3LYP-D4/def2-QZVP level of theory. Rendered using UCSF ChimeraX software.[1]

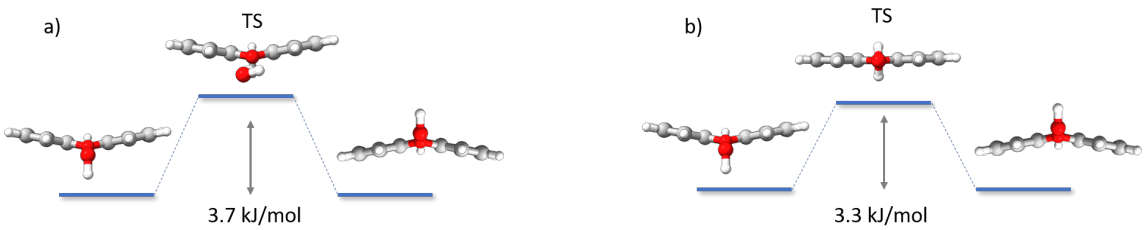

Figure S6: Tunneling pathways for the 1w-I complex. (a) The pathway involves a swinging motion of the water molecule, causing a switch of the water's hydrogen atom involved in the O-H$\cdots$O interaction, while xanthene undergoes a butterfly-like motion to tunnel between its two equivalent geometries. (b) The pathway involves a simple flip of the water's dangling hydrogen atom above and below xanthene's plane, alongside the butterfly-like motion of xanthene. The reported energy barriers are single-point energies calculated at the DLPNO-CCSD(T)/cc-pVTZ//B3LYP-D3(BJ)/def2-TZVP level of theory.

1.3 Xanthene-$(H_2O)_2$

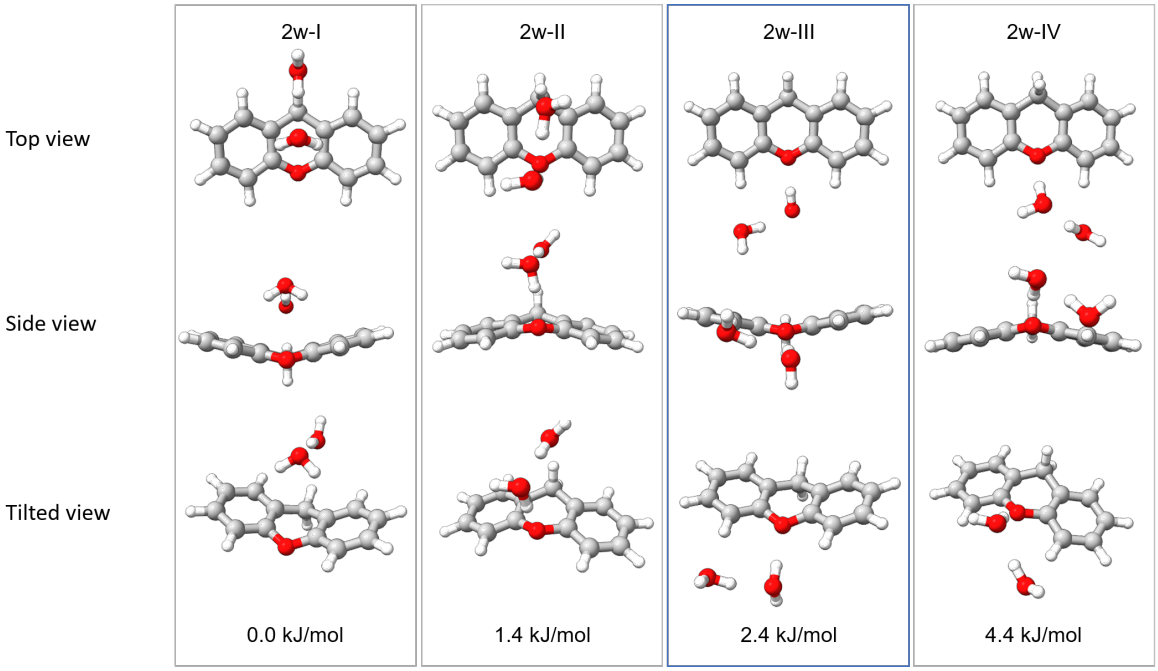

Figure S7: Molecular geometries of the energetically low-lying isomers of the xanthene-$(H_2O)_2$ complexes within an energy window of 5.0 kJ/mol, calculated at the B3LYP-D4/def2-QZVP level of theory. Each isomer is shown from three different perspectives: top view, side view, and tilted view. The relative energies (in kJ/mol), corrected with zero-point energies (ZPE), are provided, with the energy of 2w-I set to 0 kJ/mol. The molecular geometry of the experimentally observed isomer is highlighted by a blue box. The corresponding Cartesian coordinates are available in Tables S18–S21 in Section 2.3. Rendered using UCSF ChimeraX software.[1]

Table S7: Theoretical spectroscopic constants for the xanthene-$(H_2O)_2$ complexes, calculated at the B3LYP-D4/def2-QZVP level of theory. The relative energies (ΔE_0 in kJ mol^{-1}) with vibrational zero-point energy corrections.

Isomers	ΔE_0	A/MHz	B/MHz	C/MHz	μ_a/D	μ_b/D	μ_c/D
2w-I	0.0	770.6	425.9	325.6	0.0	0.3	0.3
2w-II	1.4	738.0	371.2	346.9	-0.4	0.7	-0.5
2w-III	2.4	625.7	406.1	255.6	-2.3	1.2	0.7
2w-IV	4.4	632.3	400.5	260.9	-2.4	1.3	1.4

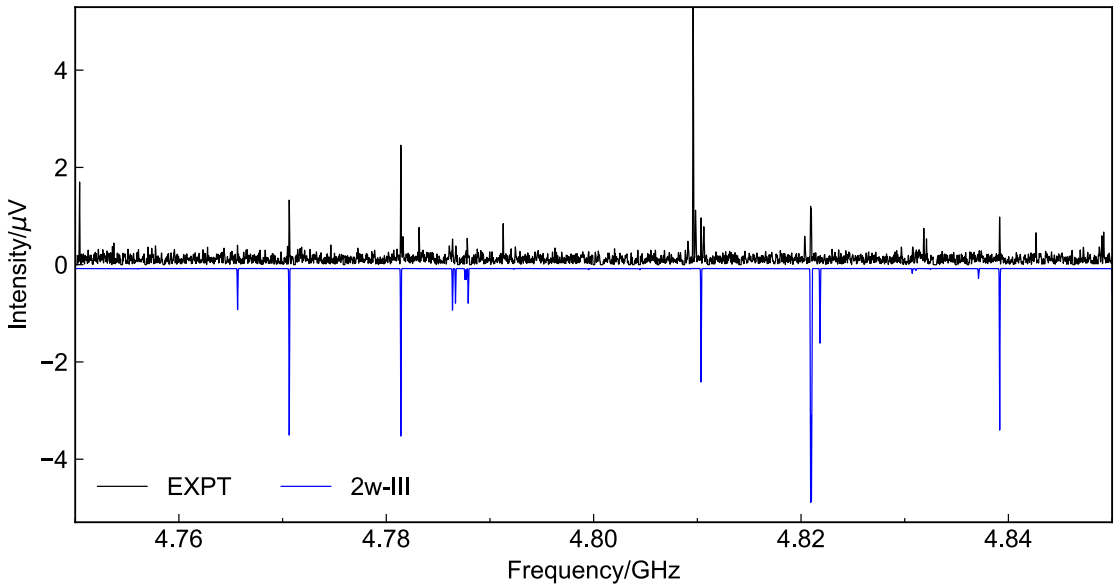

Figure S8: Portion of the microwave spectrum highlighting the transitions arising from the 2w-III complex.

Table S8: Experimental spectroscopic constants for the xanthene-$(H_2O)_2$ complex, 2w-III, fitted with Watson's A-reduced Hamiltonian in its I^r representation using Pickett's SPFIT program. The spectrum is assigned to 2w-III due to its lower energy compared to 2w-IV, and its smaller dipole-moment component along the principal c-axis, which is in consistency with the observed line intensities.

Parameters	Units	Calc.		Expt.
		2w-III	2w-IV	
A	MHz	625.7	632.3	610.66041(75)
B	MHz	406.1	400.5	404.52319(18)
C	MHz	255.6	260.9	255.01107(21)
Δ_J	kHz			0.0150(10)
Δ_{JK}	kHz			0.0832(76)
Δ_K	kHz			0.126(27)
N (a|b|c)				107 (72|23|12)

RMS	kHz		9.0

1.4 Xanthene-$(H_2O)_3$

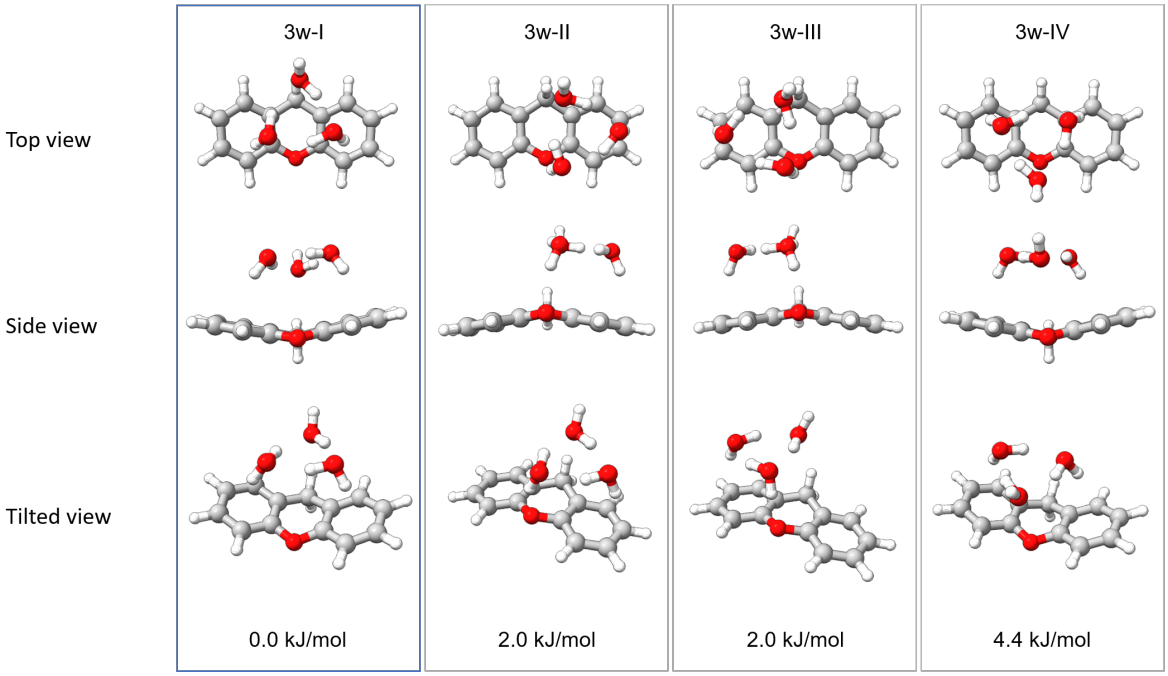

Figure S9: Molecular geometries of the energetically low-lying isomers of the xanthene-$(H_2O)_3$ complexes within an energy window of 5.0 kJ/mol, calculated at the B3LYP-D4/def2-QZVP level of theory. Each isomer is shown from three different perspectives: top view, side view, and tilted view. The relative energies (in kJ/mol), corrected with zero-point energies (ZPE), are provided, with the energy of 3w-I set to 0 kJ/mol. The molecular geometry of the experimentally observed isomer is highlighted by a blue box. The corresponding Cartesian coordinates are available in Tables S22–S25 in Section 2.4. Rendered using UCSF ChimeraX software.[1]

Table S9: Theoretical spectroscopic constants for the xanthene-$(H_2O)_3$ complexes, calculated at the B3LYP-D4/def2-QZVP level of theory. The relative energies (ΔE_0 in kJ mol^{-1}) with vibrational zero-point energy corrections.

Isomers	ΔE_0	A/MHz	B/MHz	C/MHz	μ_a/D	μ_b/D	μ_c/D
3w-I	0.0	690.8	356.4	319.4	0.3	-0.8	-1.7
3w-II	2.0	674.9	320.0	295.6	0.9	1.9	1.7
3w-III	2.0	674.3	322.8	295.8	1.0	-1.7	-1.7
3w-IV	4.5	685.4	357.1	319.5	0.2	-1.9	0.4

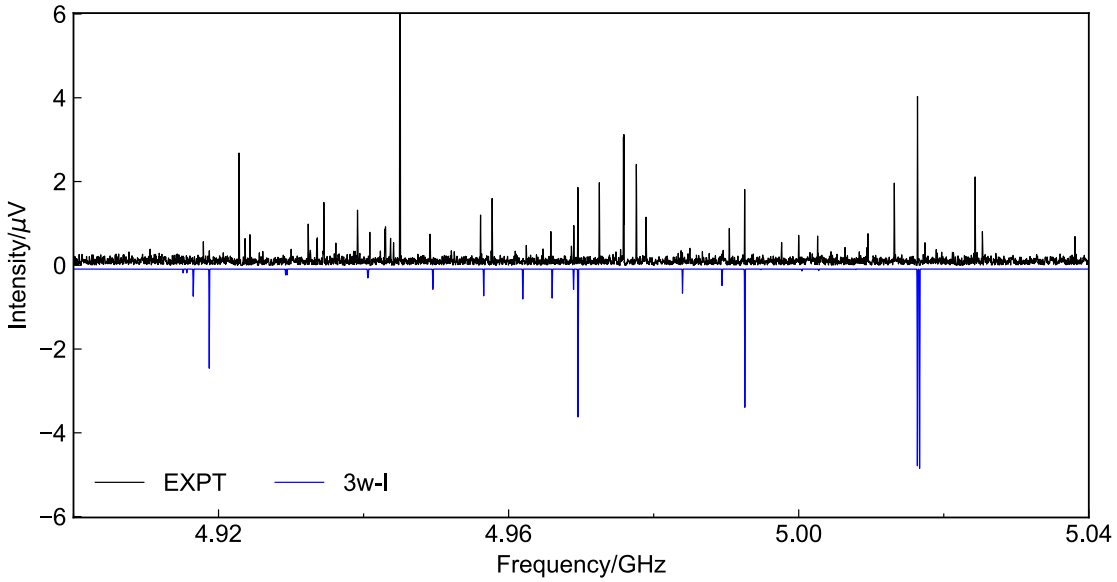

Figure S10: Portion of the microwave spectrum highlighting the transitions arising from the 3w-I complex.

Table S10: Experimental spectroscopic constants for the xanthene-$(H_2O)_3$ complex, 3w-I, fitted with Watson's A-reduced Hamiltonian in its I^r representation using Pickett's SPFIT program.

Parameters	Units	Calc.	Expt.
A	MHz	690.8	668.50669(85)

B	MHz	356.4	359.35148(40)
C	MHz	319.4	313.21931(45)
Δ_J	kHz		0.0530(25)
Δ_{JK}	kHz		0.176(13)
N (a|b|c)			52 (0|0|49)
RMS	kHz		10.6

1.5 Xanthene-$(H_2O)_4$

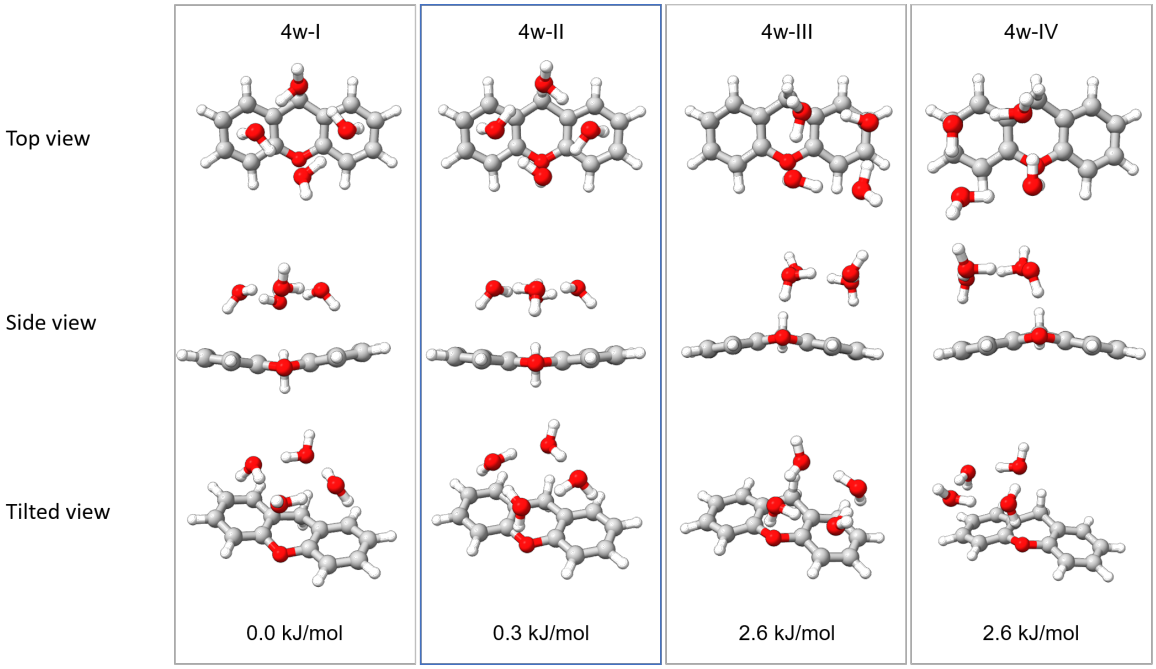

Figure S11: Molecular geometries of the energetically low-lying isomers of the xanthene-$(H_2O)_4$ complexes within an energy window of 5.0 kJ/mol, calculated at the B3LYP-D4/def2-QZVP level of theory. Each isomer is shown from three different perspectives: top view, side view, and tilted view. The relative energies (in kJ/mol), corrected with zero-point energies (ZPE), are provided, with the energy of 4w-I set to 0 kJ/mol. The molecular geometry of the experimentally observed isomer is highlighted by a blue box. The corresponding Cartesian coordinates are available in Tables S26–S29 in Section 2.5. Rendered using UCSF ChimeraX software.[1]

Table S11: Theoretical spectroscopic constants for the xanthene-$(H_2O)_4$ complexes, calculated at the B3LYP-D4/def2-QZVP level of theory. The relative energies (ΔE_0 in kJ mol^{-1}) with vibrational zero-point energy corrections.

Isomers	ΔE_0	A/MHz	B/MHz	C/MHz	μ_a/D	μ_b/D	μ_c/D
4w-I	0.0	559.8	320.4	290.7	-0.1	-0.4	-0.9
4w-II	0.3	569.3	317.3	289.7	-0.1	-2.7	-2.4
4w-III	2.6	582.7	279.5	247.7	-0.6	1.2	0.7
4w-IV	2.6	582.0	277.0	246.0	-0.6	1.2	-0.6

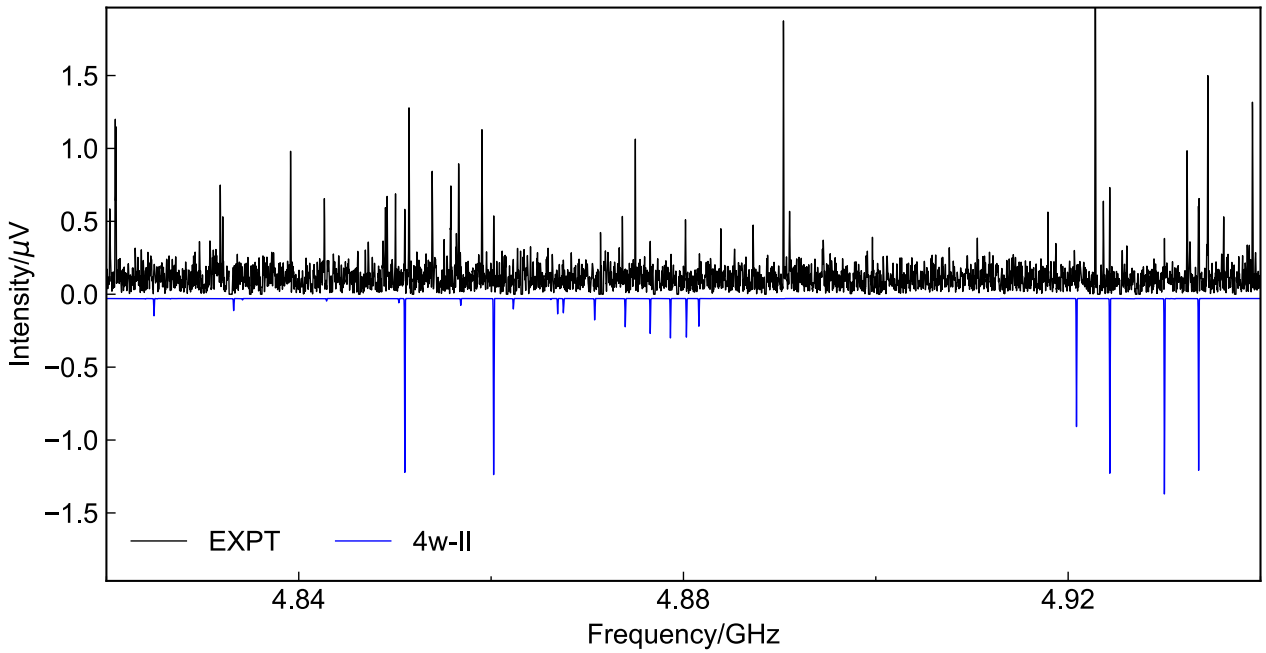

Figure S12: Portion of the microwave spectrum highlighting the transitions arising from the 4w-II complex.

Table S12: Experimental spectroscopic constants for the xanthene-$(H_2O)_4$ complex, 4w-II, fitted with Watson's A-reduced Hamiltonian in its I^r representation using Pickett's SPFIT program. The spectrum is assigned to 4w-II due to its larger dipole-moment components compared to 4w-I.

Parameters	Units	Calc.		Expt.
		4w-I	4w-II	
A	MHz	559.8	569.3	558.1509(10)
B	MHz	320.4	317.3	314.64302(37)
C	MHz	290.7	289.7	286.93462(51)
Δ_K	kHz			0.136(24)
δ_K	kHz			1.682(98)
N (a|b|c)				44 (0|24|20)
RMS	kHz			10.6

1.6 Non-Covalent interactions analysis

To visualize the non-covalent interactions at play in the observed xanthene-$(H_2O)_{n=1-4}$ complexes, we applied the non-covalent interaction method (NCI) using the Multiwfn program.[2,3] This method is based on the analysis of the electron density and its derivatives to reveal the non-covalent interactions within a molecular system.

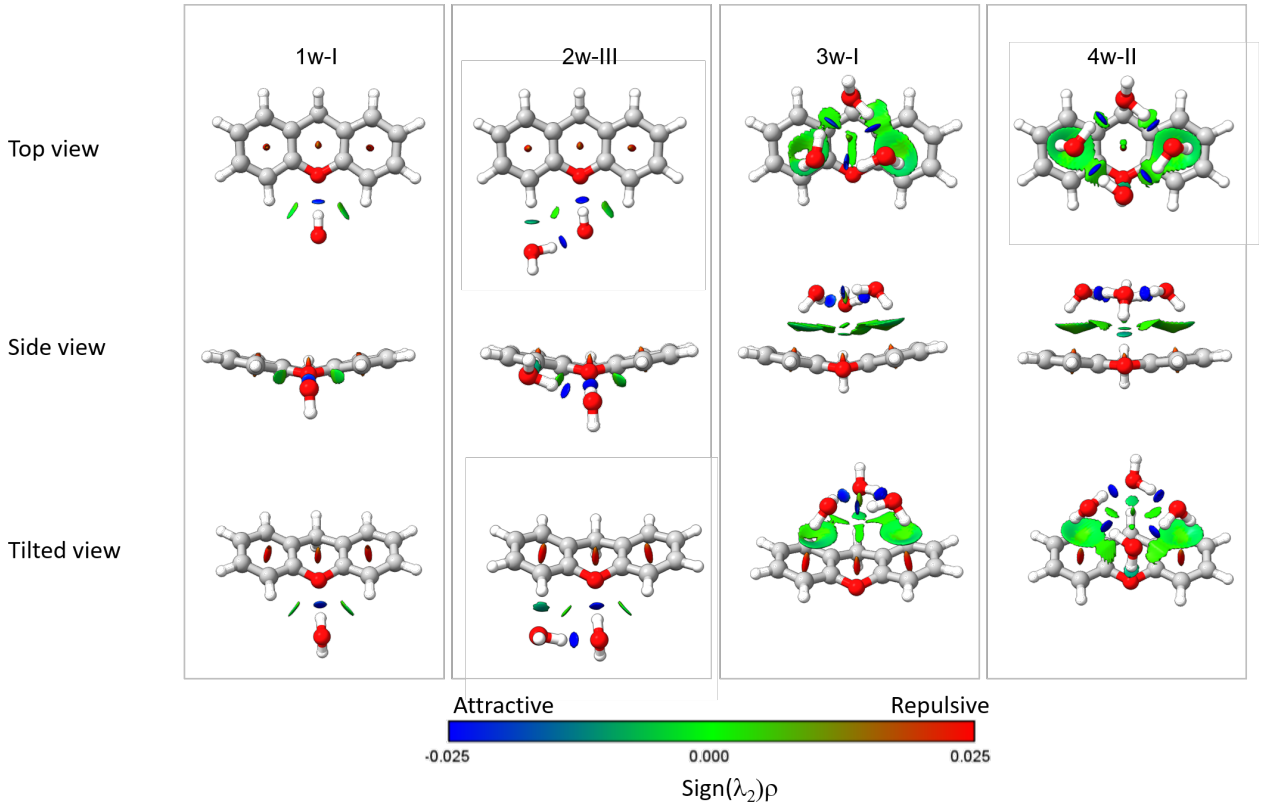

Figure S13: NCI plots of the observed xanthene-$(H_2O)_{n=1-4}$ complexes. The presented structures were optimized at the B3LYP-D4/def2-QZVP level of theory. The isourfaces are displayed with a cut-off of 0.5. Attractive and repulsive interactions are defined by the sign of sign$(\lambda_2)\rho$, where λ_2 is the second eigenvalue of the electron density Hessian and ρ is the electron density.

2 Cartesian coordinates of molecular geometries

2.1 Cartesian coordinates of the xanthene monomer

Table S13: Cartesian coordinates for the equilibrium structure of the xanthene monomer.

Atoms	X	Y	Z
C	-3.638007	-0.599538	0.245328
C	-2.489632	-1.361750	0.091187
C	-1.245418	-0.768434	-0.106602
C	-1.181905	0.621213	-0.125197
C	-2.321923	1.401731	0.026865
C	-3.550899	0.788714	0.206818
C	1.181900	0.621222	-0.125175
C	1.245422	-0.768429	-0.106600
C	2.489636	-1.361749	0.091166
H	2.552983	-2.442310	0.116487
C	3.638011	-0.599539	0.245312
C	3.550895	0.788713	0.206825
C	2.321919	1.401735	0.026892
H	-4.593187	-1.082509	0.393899
H	-2.552973	-2.442313	0.116528
H	-2.223805	2.477481	0.005670
H	-4.438573	1.394091	0.325077
H	4.593196	-1.082505	0.393872
H	4.438567	1.394095	0.325088
H	2.223810	2.477486	0.005706

Atoms	X	Y	Z
O	-0.000001	1.299124	-0.297253
C	0.000002	-1.581950	-0.334063
H	-0.000011	-1.967113	-1.360474
H	-0.000005	-2.459814	0.314618

2.2 Cartesian coordinates of the xanthene-H_2O complexes

Table S14: Cartesian coordinates for the equilibrium structure of the xanthene-H_2O complex, 1w-I.

Atoms	X	Y	Z
C	-3.618844	1.010983	-0.266521
C	-2.477462	1.744610	0.022110
C	-1.243612	1.123096	0.194594
C	-1.186722	-0.257593	0.046148
C	-2.315356	-1.012091	-0.244926
C	-3.535451	-0.371830	-0.394231
C	1.186722	-0.257594	0.046148
C	1.243613	1.123096	0.194594
C	2.477462	1.744610	0.022110
H	2.538816	2.820509	0.124186
C	3.618844	1.010983	-0.266521
C	3.535451	-0.371830	-0.394231
C	2.315356	-1.012091	-0.244926
H	-4.567330	1.513010	-0.392468

Atoms	X	Y	Z
H	-2.538816	2.820509	0.124186
H	-2.221737	-2.082891	-0.356775
H	-4.418376	-0.952301	-0.621008
H	4.567330	1.513010	-0.392468
H	4.418376	-0.952301	-0.621008
H	2.221737	-2.082892	-0.356774
O	0.000000	-0.948734	0.188481
C	0.000000	1.885260	0.564999
H	0.000000	2.865014	0.085497
H	0.000000	2.077150	1.644497
O	0.000000	-3.853581	0.301716
H	0.000000	-4.156519	1.212207
H	0.000000	-2.888845	0.350855

Table S15: Cartesian coordinates for the equilibrium structure of the xanthene-H_2O complex, 1w-II.

Atoms	X	Y	Z
C	-3.605560	-0.487620	0.126265
C	-2.467512	-1.101458	0.629701
C	-1.239515	-0.444437	0.645008
C	-1.178575	0.840653	0.112547
C	-2.307887	1.471493	-0.393668
C	-3.523561	0.806315	-0.378782
C	1.178575	0.840652	0.112547
C	1.239515	-0.444437	0.645008
C	2.467512	-1.101458	0.629701

Atoms	X	Y	Z
H	2.526178	-2.106775	1.026032
C	3.605561	-0.487620	0.126265
C	3.523561	0.806315	-0.378782
C	2.307887	1.471493	-0.393669
H	-4.549244	-1.013642	0.126925
H	-2.526178	-2.106775	1.026032
H	-2.213274	2.469038	-0.797347
H	-4.404108	1.293433	-0.772917
H	4.549244	-1.013641	0.126926
H	4.404108	1.293433	-0.772917
H	2.213274	2.469038	-0.797348
O	0.000000	1.546792	0.058541
C	0.000000	-1.057056	1.238670
H	0.000000	-0.897252	2.323282
H	0.000000	-2.136264	1.086289
O	0.000000	-2.072536	-2.044635
H	-0.760838	-1.578498	-1.725214
H	0.760838	-1.578498	-1.725214

Table S16: Cartesian coordinates for the equilibrium structure of the xanthene-H_2O complex, 1w-III.

Atoms	X	Y	Z
C	-3.348589	-0.060961	-1.043776
C	-2.250652	-0.910979	-1.053117
C	-1.021648	-0.515560	-0.529590
C	-0.914850	0.775323	-0.019764

Atoms	X	Y	Z
C	-2.003098	1.640761	-0.003838
C	-3.221852	1.218211	-0.509711
C	1.427660	0.593486	0.231737
C	1.442121	-0.710018	-0.252883
C	2.678582	-1.292909	-0.516951
H	2.706161	-2.304337	-0.901686
C	3.863141	-0.608858	-0.286775
C	3.822006	0.688604	0.213673
C	2.602765	1.295126	0.468889
H	-4.294094	-0.392843	-1.447556
H	-2.346441	-1.910224	-1.458002
H	-1.873872	2.633003	0.403665
H	-4.069279	1.888701	-0.495052
H	4.811493	-1.083060	-0.494741
H	4.738489	1.231146	0.397630
H	2.541226	2.305861	0.845443
O	0.254570	1.258461	0.507359
C	0.148297	-1.455388	-0.437579
H	0.198046	-2.087487	-1.325551
H	-0.009165	-2.130792	0.410989
O	-2.507449	-1.514493	2.287928
H	-2.332011	-0.734971	2.820245
H	-2.701937	-1.172400	1.409166

Table S17: Cartesian coordinates for the equilibrium structure of the xanthene-H_2O complex, 1w-IV.

Atoms	X	Y	Z
C	-3.564565	0.917559	0.323836
C	-2.431494	1.472689	-0.255544
C	-1.214729	0.798519	-0.248575
C	-1.161364	-0.439485	0.382539
C	-2.280678	-1.012855	0.967487
C	-3.488437	-0.331438	0.930427
C	1.200461	-0.461637	0.354235
C	1.261090	0.775506	-0.276438
C	2.488685	1.429106	-0.308720
H	2.553366	2.397249	-0.788178
C	3.623211	0.853933	0.246895
C	3.538365	-0.394309	0.853977
C	2.320696	-1.055231	0.915530
H	-4.501409	1.455609	0.302143
H	-2.489479	2.441960	-0.733660
H	-2.188722	-1.976313	1.447818
H	-4.365064	-0.770945	1.384825
H	4.568975	1.374888	0.205113
H	4.417129	-0.850044	1.287649
H	2.222966	-2.019170	1.393446
O	0.012437	-1.167894	0.431380
C	0.020605	1.326266	-0.924726
H	0.030998	2.416263	-0.909545
H	0.005913	1.021830	-1.976973

Atoms	X	Y	Z
O	-0.187604	-1.833961	-2.488696
H	-0.093585	-1.947330	-1.536256
H	-1.094147	-2.084476	-2.680485

2.3 Cartesian coordinates of the xanthene-$(H_2O)_2$ complexes

Table S18: Cartesian coordinates for the equilibrium structure of the xanthene-$(H_2O)_2$ complex, 2w-I.

Atoms	X	Y	Z
C	-3.571893	-0.231584	-0.111305
C	-2.442898	-0.800362	-0.685566
C	-1.234039	-0.110743	-0.725978
C	-1.178143	1.151063	-0.138609
C	-2.297193	1.735954	0.439150
C	-3.498714	1.042935	0.442154
C	1.173432	1.154252	-0.138589
C	1.232768	-0.107469	-0.725810
C	2.443426	-0.793896	-0.685188
H	2.491601	-1.787158	-1.110376
C	3.570835	-0.221954	-0.110986
C	3.494251	1.052477	0.442234
C	2.290909	1.742312	0.439038
H	-4.503328	-0.778908	-0.094378
H	-2.488573	-1.793569	-1.111207

Atoms	X	Y	Z
H	-2.208113	2.717428	0.881682
H	-4.373555	1.492766	0.889779
H	4.503720	-0.766806	-0.093819
H	4.367888	1.504719	0.889790
H	2.199202	2.723647	0.881337
O	-0.003358	1.869595	-0.098456
C	0.000160	-0.658756	-1.388413
H	-0.000090	-0.365660	-2.445174
H	0.001567	-1.746429	-1.360617
O	0.015346	-3.584087	0.126511
H	0.011303	-2.963516	0.875492
H	0.028241	-4.460943	0.514312
O	-0.000628	-1.487643	2.042870
H	0.759002	-0.967887	1.758746
H	-0.765541	-0.976627	1.757108

Table S19: Cartesian coordinates for the equilibrium structure of the xanthene-$(H_2O)_2$ complex, 2w-II.

Atoms	X	Y	Z
C	-3.565360	1.157604	0.335640
C	-2.412571	1.232097	1.105247
C	-1.197019	0.742010	0.637172
C	-1.170846	0.195664	-0.640397
C	-2.309342	0.113871	-1.429078
C	-3.513474	0.591808	-0.933632
C	1.199432	0.139796	-0.672814

Atoms	X	Y	Z
C	1.283071	0.692702	0.599027
C	2.529600	1.136959	1.029468
H	2.614425	1.576887	2.014569
C	3.655932	1.010822	0.228250
C	3.545624	0.436487	-1.033513
C	2.310289	0.004050	-1.491466
H	-4.499236	1.538572	0.723289
H	-2.452324	1.666861	2.095413
H	-2.234600	-0.310079	-2.420465
H	-4.404705	0.532864	-1.542022
H	4.614968	1.357148	0.585954
H	4.416854	0.333508	-1.664516
H	2.192042	-0.431764	-2.473085
O	-0.005432	-0.319958	-1.180612
C	0.056644	0.744865	1.467540
H	0.054040	-0.136672	2.116459
H	0.082799	1.623205	2.113263
O	-0.414861	-3.106602	-0.582973
H	-0.215329	-2.238766	-0.964218
H	-1.365220	-3.211131	-0.674269
O	0.138813	-2.496382	2.132747
H	-0.010259	-2.809760	1.223909
H	0.768444	-3.110458	2.515139

Table S20: Cartesian coordinates for the equilibrium structure of the xanthene-$(H_2O)_2$ complex, 2w-III.

Atoms	X	Y	Z
C	-4.014902	-0.139219	-0.349148
C	-3.234386	0.957698	-0.014026
C	-1.861600	0.834909	0.181184
C	-1.290611	-0.420071	0.005015
C	-2.051895	-1.531288	-0.331529
C	-3.420131	-1.387358	-0.501316
C	0.913542	0.470917	0.045198
C	0.442463	1.765605	0.226808
C	1.347435	2.812735	0.077314
H	0.996677	3.828832	0.204686
C	2.680895	2.571436	-0.219652
C	3.125409	1.263353	-0.380674
C	2.240762	0.202412	-0.257330
H	-5.079589	-0.022461	-0.491658
H	-3.693934	1.930059	0.108110
H	-1.566051	-2.487866	-0.459211
H	-4.018931	-2.248066	-0.763164
H	3.368920	3.397931	-0.326249
H	4.161464	1.062764	-0.613285
H	2.574586	-0.816284	-0.400244
O	0.066443	-0.620957	0.167651
C	-0.996685	1.990722	0.604202
H	-1.072182	2.120757	1.690351
H	-1.363078	2.918713	0.163638

Atoms	X	Y	Z
O	0.921016	-3.249149	0.836119
H	0.640743	-2.332032	0.687676
H	0.925193	-3.374177	1.787801
O	3.470372	-2.993753	-0.354229
H	2.613797	-3.237665	0.036324
H	3.629631	-3.633259	-1.051150

Table S21: Cartesian coordinates for the equilibrium structure of the xanthene-$(H_2O)_2$ complex, 2w-IV.

Atoms	X	Y	Z
C	-4.028370	-0.135324	-0.311432
C	-3.235768	0.928617	0.095236
C	-1.856857	0.793559	0.228024
C	-1.292572	-0.438418	-0.082394
C	-2.065969	-1.513571	-0.498226
C	-3.439803	-1.360913	-0.604392
C	0.909868	0.447413	-0.045360
C	0.447958	1.721380	0.261308
C	1.347384	2.778989	0.160511
H	1.004208	3.780826	0.384557
C	2.666979	2.564218	-0.209999
C	3.103519	1.273937	-0.492156
C	2.223534	0.204570	-0.418493
H	-5.097529	-0.009376	-0.403298
H	-3.690796	1.883932	0.322970
H	-1.581606	-2.446477	-0.749225

Atoms	X	Y	Z
H	-4.047280	-2.193680	-0.929068
H	3.351252	3.397840	-0.278446
H	4.129607	1.096788	-0.781568
H	2.545195	-0.803052	-0.644894
O	0.066444	-0.652495	0.016645
C	-0.973888	1.908823	0.717882
H	-1.002722	1.938944	1.813516
H	-1.357522	2.871846	0.379047
O	3.313390	-3.077676	-0.504257
H	4.133310	-3.250120	-0.037094
H	2.611097	-3.180804	0.160010
O	1.132125	-2.977396	1.290809
H	0.456218	-3.649979	1.396737
H	0.689193	-2.207431	0.901584

2.4 Cartesian coordinates of the xanthene-$(H_2O)_3$ complexes

Table S22: Cartesian coordinates for the equilibrium structure of the xanthene-$(H_2O)_3$ complex, 3w-I.

Atoms	X	Y	Z
C	-3.541436	-0.268923	0.613034
C	-2.406930	-0.034206	1.376361
C	-1.157419	-0.499082	0.978192
C	-1.072164	-1.192539	-0.224587

Atoms	X	Y	Z
C	-2.195660	-1.437176	-1.005297
C	-3.433910	-0.977677	-0.580289
C	1.281775	-1.085059	-0.242701
C	1.320180	-0.380179	0.956026
C	2.525774	0.206668	1.328965
H	2.563866	0.776298	2.248062
C	3.664585	0.078002	0.546647
C	3.606059	-0.646661	-0.639822
C	2.410950	-1.225811	-1.041061
H	-4.501604	0.102048	0.940995
H	-2.482869	0.527471	2.297732
H	-2.080643	-1.977260	-1.933866
H	-4.310430	-1.165780	-1.183976
H	4.589716	0.542316	0.855969
H	4.486056	-0.752733	-1.258162
H	2.332689	-1.780342	-1.964996
O	0.125239	-1.661520	-0.709818
C	0.081191	-0.279631	1.802007
H	0.124402	-1.027751	2.602077
H	0.036806	0.697183	2.281500
O	-1.706870	2.057926	-1.439337
H	-0.818727	1.868875	-1.789752
H	-2.154904	1.209002	-1.373074
O	-0.276382	2.838405	0.791911
H	-0.309993	3.789329	0.916519
H	-0.972580	2.632440	0.134038

Atoms	X	Y	Z
O	1.098140	2.007485	-1.580437
H	0.957555	2.282843	-0.659609
H	1.705353	1.262951	-1.539696

Table S23: Cartesian coordinates for the equilibrium structure of the xanthene-$(H_2O)_3$ complex, 3w-II.

Atoms	X	Y	Z
C	-4.098186	-0.137228	-0.586689
C	-2.953003	-0.304123	-1.351882
C	-1.688924	-0.322161	-0.768832
C	-1.613098	-0.189162	0.612271
C	-2.744722	-0.021342	1.397393
C	-3.991284	0.010360	0.792198
C	0.684594	-0.766055	0.639864
C	0.723474	-0.918878	-0.741923
C	1.870926	-1.473991	-1.300454
H	1.918453	-1.600959	-2.374051
C	2.951828	-1.846021	-0.512289
C	2.889283	-1.675419	0.868236
C	1.749567	-1.139341	1.448311
H	-5.068399	-0.121237	-1.061980
H	-3.032919	-0.413740	-2.425652
H	-2.632620	0.076917	2.467443
H	-4.876938	0.141610	1.397308
H	3.834498	-2.270141	-0.968914
H	3.722493	-1.965174	1.492374

Atoms	X	Y	Z
H	1.672093	-0.999681	2.516736
O	-0.400230	-0.203530	1.277392
C	-0.427918	-0.437115	-1.580308
H	-0.173107	0.544755	-1.991882
H	-0.583074	-1.105346	-2.428544
O	3.186328	1.704427	-0.078357
H	2.585352	1.894273	0.665580
H	3.329397	0.753046	-0.056888
O	0.892484	2.496228	1.367223
H	0.650472	2.748385	0.461847
H	0.319050	1.751330	1.579580
O	1.010468	2.600938	-1.501059
H	1.887990	2.262879	-1.226102
H	1.178847	3.373660	-2.044113

Table S24: Cartesian coordinates for the equilibrium structure of the xanthene-$(H_2O)_3$ complex, 3w-III.

Atoms	X	Y	Z
C	-3.018170	-1.707799	-0.683355
C	-1.932794	-1.265799	-1.428404
C	-0.763782	-0.823078	-0.815837
C	-0.708785	-0.856700	0.573466
C	-1.778864	-1.302444	1.337691
C	-2.938929	-1.723266	0.706701
C	1.598173	-0.312733	0.596817
C	1.659840	-0.262679	-0.790403

Atoms	X	Y	Z
C	2.918150	-0.164259	-1.378444
H	2.986914	-0.130661	-2.458069
C	4.071209	-0.096972	-0.610251
C	3.978627	-0.133395	0.777179
C	2.738565	-0.247519	1.385137
H	-3.916676	-2.042530	-1.181551
H	-1.992819	-1.248709	-2.508805
H	-1.688502	-1.307857	2.414191
H	-3.775937	-2.067205	1.297286
H	5.036263	-0.015713	-1.089359
H	4.870415	-0.081035	1.385269
H	2.637489	-0.291298	2.459923
O	0.394945	-0.415335	1.269897
C	0.393763	-0.273117	-1.602313
H	0.155257	0.749219	-1.911864
H	0.536618	-0.852635	-2.515817
O	-0.867607	2.820114	-1.216765
H	-0.605504	2.787873	-0.273129
H	-0.786126	3.736974	-1.487222
O	-3.151910	1.755455	0.123665
H	-3.308203	0.826390	-0.072281
H	-2.596363	2.086535	-0.600780
O	-0.762342	2.355600	1.492088
H	-0.278237	1.560450	1.739323
H	-1.675863	2.061942	1.320645

Table S25: Cartesian coordinates for the equilibrium structure of the xanthene-$(H_2O)_3$ complex, 3w-IV.

Atoms	X	Y	Z
C	-3.485900	-0.854566	-0.451862
C	-2.326750	-1.343139	-1.041743
C	-1.097876	-1.259107	-0.392848
C	-1.057598	-0.649173	0.857490
C	-2.205781	-0.157706	1.464243
C	-3.421612	-0.267800	0.809589
C	1.288077	-0.505102	0.829323
C	1.374581	-1.112548	-0.420178
C	2.588570	-1.044592	-1.099606
H	2.667514	-1.502567	-2.077212
C	3.690053	-0.409294	-0.541082
C	3.582531	0.174714	0.717414
C	2.378773	0.134432	1.402866
H	-4.431288	-0.933263	-0.969048
H	-2.372295	-1.805143	-2.019573
H	-2.121198	0.321634	2.427955
H	-4.316996	0.118919	1.274874
H	4.623272	-0.367617	-1.083779
H	4.432068	0.676734	1.157940
H	2.258528	0.606128	2.366733
O	0.118734	-0.499393	1.547734
C	0.169918	-1.822340	-0.975350
H	0.153793	-1.752361	-2.063489
H	0.235228	-2.890966	-0.738763

Atoms	X	Y	Z
O	-1.835142	2.105577	-1.346517
H	-0.950611	1.936150	-1.716102
H	-2.267244	1.247881	-1.284013
O	0.974458	2.046029	-1.563072
H	0.842226	2.392616	-0.663659
H	1.544781	1.278497	-1.460695
O	-0.294506	2.827463	0.840314
H	-0.395001	3.746038	1.098501
H	-1.039683	2.635434	0.236409

2.5 Cartesian coordinates of the xanthene-$(H_2O)_4$ complexes

Table S26: Cartesian coordinates for the equilibrium structure of the xanthene-$(H_2O)_4$ complex, 4w-I.

Atoms	X	Y	Z
C	-3.612773	0.583326	0.633710
C	-2.467894	0.616203	1.417641
C	-1.221576	0.904916	0.869642
C	-1.150900	1.146463	-0.498647
C	-2.284910	1.116725	-1.301590
C	-3.517591	0.839638	-0.732532
C	1.207322	1.117551	-0.494176
C	1.266257	0.873293	0.874273
C	2.503701	0.554433	1.426908

Atoms	X	Y	Z
H	2.561979	0.349011	2.487802
C	3.650425	0.492212	0.646387
C	3.566204	0.750890	-0.720037
C	2.343419	1.059592	-1.292631
H	-4.570468	0.360004	1.081295
H	-2.534290	0.408805	2.477478
H	-2.177618	1.297725	-2.360735
H	-4.401202	0.814400	-1.354308
H	4.601023	0.246891	1.097755
H	4.450890	0.702700	-1.338814
H	2.244570	1.243646	-2.352067
O	0.033106	1.421863	-1.132379
C	0.021646	0.965966	1.713477
H	0.008722	0.156507	2.443648
H	0.032547	1.903773	2.280584
O	-1.980910	-2.336954	-0.292905
H	-1.369870	-2.197840	-1.047565
H	-2.551188	-1.562329	-0.269345
O	-0.145894	-2.402007	1.693677
H	-0.890555	-2.389013	1.044764
H	-0.250810	-3.212394	2.196343
O	0.009773	-1.912541	-2.128696
H	0.771972	-2.067276	-1.524401
H	0.135486	-2.503246	-2.873594
O	1.869000	-2.376495	-0.206370
H	1.258586	-2.407563	0.558377

Atoms	X	Y	Z
H	2.479540	-1.656552	-0.019814

Table S27: Cartesian coordinates for the equilibrium structure of the xanthene-$(H_2O)_4$ complex, 4w-II.

Atoms	X	Y	Z
C	-3.672860	0.587350	0.693746
C	-2.516735	0.568899	1.460543
C	-1.264899	0.810326	0.899055
C	-1.207788	1.064139	-0.466065
C	-2.354412	1.095394	-1.251199
C	-3.588503	0.857099	-0.669952
C	1.166802	1.083061	-0.468728
C	1.231157	0.834978	0.897142
C	2.487770	0.618635	1.457434
H	2.553265	0.408908	2.516978
C	3.641992	0.654290	0.688771
C	3.550475	0.915895	-0.676225
C	2.311252	1.129868	-1.256445
H	-4.631518	0.395521	1.153567
H	-2.576775	0.354956	2.519634
H	-2.259417	1.295488	-2.308657
H	-4.480556	0.875603	-1.279398
H	4.604791	0.481899	1.147701
H	4.441053	0.947543	-1.287372
H	2.210715	1.323433	-2.314577
O	-0.022826	1.271845	-1.133563

Atoms	X	Y	Z
C	-0.015951	0.790141	1.735750
H	-0.006176	-0.112332	2.348830
H	-0.024034	1.639973	2.426174
O	0.044179	-1.682420	-2.187207
H	-0.030994	-0.730852	-2.297328
H	-0.731604	-1.941384	-1.644291
O	1.974607	-2.351784	-0.345250
H	2.597903	-1.625674	-0.252141
H	1.397790	-2.116234	-1.104789
O	-1.911917	-2.387975	-0.366527
H	-2.531582	-1.683335	-0.156750
H	-1.326843	-2.468749	0.413112
O	0.076103	-2.552868	1.570951
H	0.176804	-3.404179	2.002050
H	0.834365	-2.480265	0.942257

Table S28: Cartesian coordinates for the equilibrium structure of the xanthene-$(H_2O)_4$ complex, 4w-III.

Atoms	X	Y	Z
C	-4.382454	0.015360	0.387042
C	-3.342825	0.695548	1.004630
C	-2.035360	0.598786	0.536705
C	-1.807474	-0.185693	-0.587401
C	-2.831954	-0.874469	-1.221176
C	-4.122892	-0.776879	-0.726251
C	0.415477	0.607267	-0.812783

Atoms	X	Y	Z
C	0.291427	1.435344	0.297699
C	1.303026	2.362797	0.530817
H	1.218473	3.022673	1.384484
C	2.414803	2.443021	-0.298645
C	2.524815	1.583074	-1.388008
C	1.520539	0.665773	-1.650385
H	-5.388683	0.101274	0.771288
H	-3.540768	1.308743	1.874305
H	-2.604423	-1.471201	-2.092653
H	-4.925059	-1.311707	-1.214423
H	3.188124	3.170874	-0.098376
H	3.390037	1.627242	-2.033425
H	1.584284	-0.012719	-2.487898
O	-0.543963	-0.331703	-1.127852
C	-0.879992	1.271234	1.225225
H	-0.565460	0.657442	2.075149
H	-1.186799	2.238496	1.625321
O	0.732514	-2.774183	-0.121342
H	1.665002	-2.690308	-0.409124
H	0.237266	-2.174528	-0.691602
O	0.865456	-1.441639	2.226001
H	0.740027	-1.996464	1.417919
H	0.779559	-2.034021	2.975454
O	3.360238	-2.164421	-0.692338
H	3.461309	-1.508839	0.034975
H	4.087287	-2.783275	-0.600781

Atoms	X	Y	Z
O	3.301358	-0.412856	1.401234
H	2.470935	-0.717888	1.820008
H	3.112441	0.472940	1.074644

Table S29: Cartesian coordinates for the equilibrium structure of the xanthene-$(H_2O)_4$ complex, 4w-IV.

Atoms	X	Y	Z
C	-4.405609	-0.003983	-0.389730
C	-3.368173	0.684990	-1.001868
C	-2.058411	0.575246	-0.544089
C	-1.825844	-0.229430	0.564846
C	-2.847629	-0.926651	1.192953
C	-4.141365	-0.816988	0.707241
C	0.387002	0.579421	0.811608
C	0.256118	1.429783	-0.281231
C	1.246735	2.386267	-0.481329
H	1.156699	3.063201	-1.320883
C	2.346448	2.473700	0.363537
C	2.465329	1.590837	1.433615
C	1.480849	0.642942	1.662697
H	-5.414036	0.091348	-0.765936
H	-3.570115	1.314381	-1.858928
H	-2.616685	-1.538832	2.052754
H	-4.942087	-1.358407	1.190540
H	3.103594	3.225204	0.190383
H	3.321777	1.640897	2.090311

Atoms	X	Y	Z
H	1.551262	-0.053095	2.485109
O	-0.557202	-0.386735	1.091386
C	-0.901098	1.253019	-1.224086
H	-1.209902	2.215240	-1.634068
H	-0.569767	0.636577	-2.066145
O	3.349665	-0.319717	-1.345583
H	3.505030	-0.947675	-0.608611
H	3.213078	0.536358	-0.926872
O	1.027708	-1.337058	-2.289893
H	1.884233	-0.914499	-2.040084
H	1.176501	-1.767468	-3.134163
O	3.387349	-2.158724	0.692390
H	2.465226	-2.480090	0.560995
H	3.946864	-2.937562	0.708293
O	0.813909	-2.784498	0.074945
H	0.794720	-2.394020	-0.821733
H	0.226530	-2.218812	0.589625

3 Measured rotational transitions

3.1 Frequency lists of the xanthene monomer

Table S30: Assigned rotational transitions for the monomer of xanthene.

J'	K_a'	K_c'	v'	J"	K_a"	K_c"	v"	ν_{obs}/MHz	ν_{calc}/MHz	$\Delta\nu$/kHz
4	1	3	1	4	0	4	1	2046.611	2046.607	3.8
4	1	3	0	4	0	4	0	2047.879	2047.879	-0.2
5	1	4	1	5	0	5	1	2294.234	2294.224	10.0
5	1	4	0	5	0	5	0	2295.528	2295.531	-3.8
1	1	1	1	0	0	0	1	2416.288	2416.292	-4.4
1	1	1	0	0	0	0	0	2417.235	2417.235	-0.7
6	1	5	0	6	0	6	0	2613.765	2613.773	-8.5
5	0	5	0	4	1	4	0	2955.548	2955.544	3.9
5	0	5	1	4	1	4	1	2957.739	2957.747	-7.8
7	1	6	0	7	0	7	0	3010.105	3010.129	-23.9
2	1	2	1	1	0	1	1	3186.790	3186.795	-5.5
2	1	2	0	1	0	1	0	3187.485	3187.487	-2.0
3	1	3	1	2	0	2	1	3918.073	3918.069	4.1
3	1	3	0	2	0	2	0	3918.502	3918.503	-1.3
6	0	6	0	5	1	5	0	3919.075	3919.068	6.6
6	0	6	1	5	1	5	1	3921.402	3921.404	-2.2
6	2	4	1	6	1	5	1	4200.993	4200.995	-2.1
6	2	4	0	6	1	5	0	4204.315	4204.306	8.5
5	2	3	1	5	1	4	1	4328.484	4328.482	1.7
5	2	3	0	5	1	4	0	4331.879	4331.877	2.5
4	2	2	1	4	1	3	1	4463.460	4463.456	4.6
4	2	2	0	4	1	3	0	4466.910	4466.914	-3.1
3	2	1	1	3	1	2	1	4590.885	4590.885	0.2
3	2	1	0	3	1	2	0	4594.387	4594.388	-1.3

J'	K_a'	K_c'	v'	J"	K_a"	K_c"	v"	ν_{obs}/MHz	ν_{calc}/MHz	$\Delta\nu$/kHz
4	1	4	0	3	0	3	0	4614.206	4614.206	-0.3
2	2	0	1	2	1	1	1	4697.981	4697.980	1.7
2	2	0	0	2	1	1	0	4701.513	4701.514	-1.1
7	0	7	0	6	1	6	0	4876.953	4876.948	5.2
7	0	7	1	6	1	6	1	4879.390	4879.387	2.9
2	2	1	1	2	1	2	1	4937.351	4937.350	0.9
2	2	1	0	2	1	2	0	4940.950	4940.941	9.1
3	2	2	1	3	1	3	1	5060.431	5060.435	-3.8
3	2	2	0	3	1	3	0	5064.063	5064.054	8.8
4	2	3	1	4	1	4	1	5225.558	5225.570	-12.2
4	2	3	0	4	1	4	0	5229.241	5229.226	14.6
5	1	5	0	4	0	4	0	5280.838	5280.840	-2.3
8	0	8	0	7	1	7	0	5820.403	5820.390	12.7
8	0	8	1	7	1	7	1	5822.910	5822.903	6.4
6	1	6	0	5	0	5	0	5926.679	5926.690	-10.5
2	2	1	1	1	1	0	1	6478.351	6478.359	-7.8
2	2	1	0	1	1	0	0	6481.442	6481.443	-1.4
7	1	7	0	6	0	6	0	6561.381	6561.395	-13.9
2	2	0	0	1	1	1	0	6565.318	6565.316	2.0
9	0	9	0	8	1	8	0	6743.230	6743.222	8.5
9	0	9	1	8	1	8	1	6745.779	6745.784	-4.8
8	1	8	0	7	0	7	0	7194.797	7194.811	-14.0
10	3	7	1	10	2	8	1	7239.904	7239.903	0.5
10	3	7	0	10	2	8	0	7245.893	7245.876	17.0
3	2	2	1	2	1	1	1	7248.859	7248.860	-1.3
3	2	2	0	2	1	1	0	7251.700	7251.698	1.5

J'	K_a'	K_c'	v'	J"	K_a"	K_c"	v"	ν_{obs}/MHz	ν_{calc}/MHz	$\Delta\nu$/kHz
9	3	6	1	9	2	7	1	7452.803	7452.806	-2.6
9	3	6	0	9	2	7	0	7458.806	7458.807	-1.1
3	2	1	1	2	1	2	1	7506.497	7506.496	0.6
3	2	1	0	2	1	2	0	7509.396	7509.386	10.0
8	3	5	1	8	2	6	1	7633.595	7633.593	1.5
8	3	5	0	8	2	6	0	7639.585	7639.596	-10.6
10	0	10	0	9	1	9	0	7642.391	7642.385	5.7
7	3	4	1	7	2	5	1	7776.445	7776.442	2.8
7	3	4	0	7	2	5	0	7782.434	7782.431	2.4
9	1	9	0	8	0	8	0	7835.620	7835.632	-11.4
6	3	3	1	6	2	4	1	7880.760	7880.766	-6.1
6	3	3	0	6	2	4	0	7886.728	7886.737	-9.4
5	3	2	1	5	2	3	1	7950.400	7950.400	-0.3
5	3	2	0	5	2	3	0	7956.349	7956.354	-5.7
4	2	3	1	3	1	2	1	7978.534	7978.523	11.1
4	2	3	0	3	1	2	0	7981.120	7981.112	7.5
4	3	1	1	4	2	2	1	7992.064	7992.059	5.4
4	3	1	0	4	2	2	0	7997.997	7998.001	-4.2

Table S31: Assigned rotational transitions for the $^{13}C_1$ isotopologue of the monomer of xanthene.

J'	K_a'	K_c'	v'	J"	K_a"	K_c"	v"	ν_{obs}/MHz	ν_{calc}/MHz	$\Delta\nu$/kHz
4	1	3	0	4	0	4	0	2033.777	2033.785	-7.8
5	1	4	0	5	0	5	0	2280.679	2280.695	-16.4

J'	K_a'	K_c'	v'	J"	K_a"	K_c"	v"	ν_{obs}/MHz	ν_{calc}/MHz	$\Delta\nu$/kHz
1	1	1	0	0	0	0	0	2399.780	2399.786	-6.3
2	1	2	0	1	0	1	0	3165.347	3165.348	-0.6
3	1	3	0	2	0	2	0	3891.823	3891.825	-1.8
6	0	6	0	5	1	5	0	3899.449	3899.455	-5.9
6	0	6	1	5	1	5	1	3901.753	3901.746	7.5
4	2	2	0	4	1	3	0	4430.604	4430.605	-0.7
3	2	1	0	3	1	2	0	4557.458	4557.466	-8.1
7	0	7	0	6	1	6	0	4851.477	4851.470	6.8
5	1	5	0	4	0	4	0	5245.545	5245.544	1.3
5	1	5	1	4	0	4	1	5246.240	5246.237	2.4
5	2	4	1	5	1	5	1	5393.370	5393.370	0.1
5	2	4	0	5	1	5	0	5397.076	5397.052	24.6
8	0	8	0	7	1	7	0	5788.977	5788.977	0.1
6	1	6	0	5	0	5	0	5887.325	5887.317	7.4
2	2	1	0	1	1	0	0	6433.783	6433.786	-3.0
7	1	7	0	6	0	6	0	6518.101	6518.094	7.2
9	0	9	0	8	1	8	0	6705.860	6705.862	-2.1
9	0	9	1	8	1	8	1	6708.596	6708.603	-6.4
8	1	8	0	7	0	7	0	7147.696	7147.705	-9.3
3	2	2	0	2	1	1	0	7199.350	7199.351	-0.7
7	3	4	0	7	2	5	0	7719.443	7719.446	-2.4

Table S32: Assigned rotational transitions for the $^{13}C_2$ isotopologue of the monomer of xanthene.

J'	K_a'	K_c'	v'	J"	K_a"	K_c"	v"	ν_{obs}/MHz	ν_{calc}/MHz	$\Delta\nu$/kHz
4	1	3	1	4	0	4	1	2042.120	2042.107	13.14
4	1	3	0	4	0	4	0	2043.377	2043.379	-2.21
1	1	1	0	0	0	0	0	2411.640	2411.650	-10.15
6	1	5	0	6	0	6	0	2609.194	2609.207	-13.24
5	0	5	0	4	1	4	0	2953.227	2953.218	8.68
2	1	2	1	1	0	1	1	3180.011	3180.006	4.71
2	1	2	0	1	0	1	0	3180.681	3180.684	-2.74
3	1	3	1	2	0	2	1	3910.077	3910.086	-8.67
3	1	3	0	2	0	2	0	3910.504	3910.506	-2.22
6	0	6	0	5	1	5	0	3915.252	3915.244	8.02
6	0	6	1	5	1	5	1	3917.546	3917.547	-1.33
6	2	4	1	6	1	5	1	4188.817	4188.825	-8.48
6	2	4	0	6	1	5	0	4192.093	4192.085	8.11
5	2	3	1	5	1	4	1	4316.005	4316.009	-3.22
5	2	3	0	5	1	4	0	4319.353	4319.351	1.99
4	2	2	1	4	1	3	1	4450.774	4450.767	6.58
4	1	4	1	3	0	3	1	4604.899	4604.887	12.13
4	1	4	0	3	0	3	0	4605.042	4605.044	-2.82
7	0	7	0	6	1	6	0	4871.563	4871.555	7.13
4	2	3	0	4	1	4	0	5215.990	5215.983	6.52
5	1	5	0	4	0	4	0	5270.551	5270.554	-3.12
5	2	4	1	5	1	5	1	5420.103	5420.105	-2.2
8	0	8	0	7	1	7	0	5813.366	5813.371	-5.45
6	1	6	0	5	0	5	0	5915.321	5915.332	-11.81

J'	K_a'	K_c'	v'	J"	K_a"	K_c"	v"	ν_{obs}/MHz	ν_{calc}/MHz	$\Delta\nu$/kHz
2	2	0	1	1	1	1	1	6546.652	6546.676	-24.02
7	1	7	0	6	0	6	0	6549.042	6549.027	14.77
8	1	8	0	7	0	7	0	7181.482	7181.496	-13.64
3	2	2	1	2	1	1	1	7232.144	7232.145	-0.71
3	2	2	0	2	1	1	0	7234.946	7234.943	2.28
3	2	1	1	2	1	2	1	7489.678	7489.669	8.73
3	2	1	0	2	1	2	0	7492.524	7492.527	-3.21
7	3	4	1	7	2	5	1	7754.485	7754.476	9.09
7	3	4	0	7	2	5	0	7760.375	7760.381	-5.97
5	3	2	0	5	2	3	0	7934.510	7934.508	1.68
4	2	3	0	3	1	2	0	7963.168	7963.160	7.68
4	3	1	0	4	2	2	0	7976.220	7976.217	3.03

Table S33: Assigned rotational transitions for the $^{13}C_3$ isotopologue of the monomer of xanthene.

J'	K_a'	K_c'	v'	J"	K_a"	K_c"	v"	ν_{obs}/MHz	ν_{calc}/MHz	$\Delta\nu$/kHz
4	1	3	0	4	0	4	0	2044.729	2044.723	5.8
1	1	1	1	0	0	0	1	2412.518	2412.525	-6.5
1	1	1	0	0	0	0	0	2413.454	2413.457	-3.2
6	1	5	0	6	0	6	0	2610.097	2610.099	-1.3
2	1	2	1	1	0	1	1	3182.010	3182.018	-8.4
2	1	2	0	1	0	1	0	3182.697	3182.694	3.8
3	1	3	1	2	0	2	1	3912.312	3912.325	-13.5
3	1	3	0	2	0	2	0	3912.739	3912.736	2.3

J'	K_a'	K_c'	v'	J"	K_a"	K_c"	v"	ν_{obs}/MHz	ν_{calc}/MHz	$\Delta\nu$/kHz
6	0	6	0	5	1	5	0	3914.653	3914.643	9.4
6	0	6	1	5	1	5	1	3916.960	3916.962	-2.4
6	2	4	1	6	1	5	1	4193.656	4193.663	-6.8
6	2	4	0	6	1	5	0	4196.949	4196.931	18.7
4	1	4	1	3	0	3	1	4607.355	4607.364	-8.9
4	1	4	0	3	0	3	0	4607.509	4607.506	2.5
7	0	7	0	6	1	6	0	4871.260	4871.237	22.8
5	1	5	0	4	0	4	0	5273.245	5273.244	0.4
5	1	5	1	4	0	4	1	5273.394	5273.375	18.2
8	0	8	0	7	1	7	0	5813.366	5813.389	-23.2
6	1	6	0	5	0	5	0	5918.228	5918.233	-5.0
2	2	1	1	1	1	0	1	6468.058	6468.066	-8.6
2	2	1	0	1	1	0	0	6471.123	6471.124	-0.8
2	2	0	1	1	1	1	1	6551.846	6551.832	14.7
7	1	7	0	6	0	6	0	6552.100	6552.104	-3.9
8	1	8	0	7	0	7	0	7184.712	7184.707	4.9
3	2	2	1	2	1	1	1	7237.563	7237.558	4.8
3	2	2	0	2	1	1	0	7240.353	7240.364	-11.3
7	3	4	0	7	2	5	0	7763.028	7768.950	-3.2
7	3	4	1	7	2	5	1	7768.947	7763.026	1.4
5	3	2	0	5	2	3	0	7942.785	7942.782	3.2
4	2	3	1	3	1	2	1	7966.254	7966.255	-1.1
4	3	1	0	4	2	2	0	7984.408	7984.410	-2.5

Table S34: Assigned rotational transitions for the $^{13}C_4$ isotopologue of the monomer of xanthene.

J'	K_a'	K_c'	v'	J"	K_a"	K_c"	v"	ν_{obs}/MHz	ν_{calc}/MHz	$\Delta\nu$/kHz
1	1	1	0	0	0	0	0	2399.191	2399.195	-4.69
1	1	1	1	0	0	0	1	2398.255	2398.271	-16
2	1	2	0	1	0	1	0	3165.151	3165.161	-9.71
3	1	3	1	2	0	2	1	3891.404	3891.380	24.14
3	1	3	0	2	0	2	0	3891.975	3891.974	1.66
6	0	6	0	5	1	5	0	3904.154	3904.154	0.72
6	0	6	1	5	1	5	1	3906.085	3906.087	-1.71
5	2	3	0	5	1	4	0	4292.540	4292.536	4.02
4	2	2	0	4	1	3	0	4426.886	4426.883	2.44
4	1	4	1	3	0	3	1	4583.140	4583.138	1.95
4	2	3	0	4	1	4	0	5187.451	5187.455	-3.55
5	1	5	0	4	0	4	0	5246.240	5246.236	3.45
5	2	4	0	5	1	5	0	5395.010	5394.997	13.18
8	0	8	0	7	1	7	0	5794.491	5794.489	1.89
6	1	6	0	5	0	5	0	5888.287	5888.280	7.19
2	2	1	0	1	1	0	0	6431.602	6431.608	-6.42
2	2	0	0	1	1	1	0	6515.335	6515.344	-9.31
7	1	7	0	6	0	6	0	6519.373	6519.369	4.39
7	1	7	1	6	0	6	1	6519.373	6519.406	-32.27
3	2	2	1	2	1	1	1	7194.797	7194.798	-1.72
3	2	2	0	2	1	1	0	7197.584	7197.578	6.03
3	2	1	0	2	1	2	0	7454.869	7454.881	-12.14
4	2	3	0	3	1	2	0	7922.790	7922.780	9.46

Table S35: Assigned rotational transitions for the $^{13}C_5$ isotopologue of the monomer of xanthene.

J'	K_a'	K_c'	v'	J"	K_a"	K_c"	v"	ν_{obs}/MHz	ν_{calc}/MHz	$\Delta\nu$/kHz
4	1	3	0	4	0	4	0	2038.041	2038.048	-7.0
1	1	1	1	0	0	0	1	2407.031	2407.038	-6.6
1	1	1	0	0	0	0	0	2407.975	2407.974	0.9
6	1	5	0	6	0	6	0	2591.266	2591.283	-16.7
5	0	5	0	4	1	4	0	2906.263	2906.255	8.4
5	0	5	1	4	1	4	1	2908.423	2908.430	-6.9
2	1	2	1	1	0	1	1	3169.869	3169.867	2.6
2	1	2	0	1	0	1	0	3170.550	3170.552	-1.9
6	0	6	0	5	1	5	0	3859.936	3859.931	5.0
6	0	6	1	5	1	5	1	3862.231	3862.237	-5.7
3	1	3	1	2	0	2	1	3894.179	3894.187	-7.9
3	1	3	0	2	0	2	0	3894.614	3894.615	-0.9
8	2	6	1	8	1	7	1	4034.260	4034.265	-5.3
7	2	5	1	7	1	6	1	4101.326	4101.333	-7.0
6	2	4	1	6	1	5	1	4206.137	4206.141	-3.7
6	2	4	0	6	1	5	0	4209.425	4209.420	4.8
5	2	3	1	5	1	4	1	4333.175	4333.178	-2.8
5	2	3	0	5	1	4	0	4336.537	4336.539	-2.0
4	2	2	1	4	1	3	1	4466.783	4466.776	6.8
4	2	2	0	4	1	3	0	4470.198	4470.200	-2.1
4	1	4	0	3	0	3	0	4583.936	4583.939	-3.3
3	2	1	1	3	1	2	1	4592.412	4592.403	8.3

J'	K_a'	K_c'	v'	J"	K_a"	K_c"	v"	ν_{obs}/MHz	ν_{calc}/MHz	$\Delta\nu$/kHz
3	2	1	0	3	1	2	0	4595.874	4595.875	-1.0
7	0	7	0	6	1	6	0	4808.673	4808.675	-1.9
7	0	7	1	6	1	6	1	4811.079	4811.083	-4.2
3	2	2	0	3	1	3	0	5056.918	5056.929	-10.7
5	1	5	0	4	0	4	0	5244.539	5244.538	0.8
5	1	5	1	4	0	4	1	5244.648	5244.635	13.3
5	2	4	1	5	1	5	1	5419.103	5419.097	6.5
5	2	4	0	5	1	5	0	5422.814	5422.788	25.5
8	0	8	1	7	1	7	1	5746.308	5746.293	14.8
6	1	6	0	5	0	5	0	5884.413	5884.406	6.5
2	2	1	0	1	1	0	0	6461.315	6461.333	-18.1
7	1	7	0	6	0	6	0	6512.865	6512.876	-11.1
2	2	0	0	1	1	1	0	6543.568	6543.564	4.0
9	0	9	1	8	1	8	1	6661.651	6661.656	-4.8
8	1	8	0	7	0	7	0	7139.550	7139.554	-4.1
3	2	2	1	2	1	1	1	7221.091	7221.098	-6.9
3	2	2	0	2	1	1	0	7223.923	7223.914	8.8
3	2	1	0	2	1	2	0	7476.446	7476.452	-5.1
4	2	3	1	3	1	2	1	7943.866	7943.866	0.2
4	2	3	0	3	1	2	0	7946.446	7946.435	11.0

Table S36: Assigned rotational transitions for the $^{13}C_6$ isotopologue of the monomer of xanthene.

J'	K_a'	K_c'	v'	J"	K_a"	K_c"	v"	ν_{obs}/MHz	ν_{calc}/MHz	$\Delta\nu$/kHz
4	1	3	1	4	0	4	1	2037.898	2037.897	0.7
4	1	3	0	4	0	4	0	2039.139	2039.148	-8.4
5	1	4	1	5	0	5	1	2279.410	2279.408	1.3
5	1	4	0	5	0	5	0	2280.679	2280.694	-15.1
1	1	1	1	0	0	0	1	2408.879	2408.889	-9.6
1	1	1	0	0	0	0	0	2409.817	2409.819	-2.2
5	0	5	0	4	1	4	0	2901.932	2901.927	4.8
5	0	5	1	4	1	4	1	2904.074	2904.086	-12.2
2	1	2	1	1	0	1	1	3171.500	3171.507	-6.7
2	1	2	0	1	0	1	0	3172.192	3172.192	0.0
6	0	6	0	5	1	5	0	3855.262	3855.266	-4.1
3	1	3	1	2	0	2	1	3895.695	3895.692	2.8
3	1	3	0	2	0	2	0	3896.124	3896.128	-3.3
6	2	4	0	6	1	5	0	4216.374	4216.365	9.1
4	2	2	1	4	1	3	1	4473.762	4473.765	-2.6
4	2	2	0	4	1	3	0	4477.164	4477.170	-5.4
2	2	0	1	2	1	1	1	4704.389	4704.387	1.5
2	2	0	0	2	1	1	0	4707.863	4707.866	-3.6
7	0	7	0	6	1	6	0	4803.801	4803.795	5.6
7	0	7	1	6	1	6	1	4806.192	4806.184	7.8
4	2	3	0	4	1	4	0	5224.455	5224.451	3.7
5	1	5	0	4	0	4	0	5245.931	5245.931	-0.1
5	2	4	0	5	1	5	0	5427.895	5427.876	19.0
6	1	6	0	5	0	5	0	5885.734	5885.732	1.8

J'	K_a'	K_c'	v'	J"	K_a"	K_c"	v"	ν_{obs}/MHz	ν_{calc}/MHz	$\Delta\nu$/kHz
7	1	7	0	6	0	6	0	6514.066	6514.074	-8.4
9	0	9	0	8	1	8	0	6654.197	6654.193	3.4
8	1	8	0	7	0	7	0	7140.531	7140.530	1.4
3	2	2	1	2	1	1	1	7226.643	7226.650	-7.7
3	2	1	0	2	1	2	0	7481.388	7481.403	-14.9
4	2	3	1	3	1	2	1	7949.304	7949.293	11.0
4	2	3	0	3	1	2	0	7951.858	7951.852	6.1

Table S37: Assigned rotational transitions for the $^{13}C_7$ isotopologue of the monomer of xanthene.

J'	K_a'	K_c'	J"	K_a"	K_c"	ν_{obs}/MHz	ν_{calc}/MHz	$\Delta\nu$/kHz
4	1	3	4	0	4	2031.172	2031.19328	-21.2
1	1	1	0	0	0	2394.982	2394.98495	-3.0
5	0	5	4	1	4	2973.562	2973.56468	-2.3
2	1	2	1	0	1	3163.820	3163.82927	-9.3
3	1	3	2	0	2	3893.136	3893.13651	-0.9
6	0	6	5	1	5	3935.502	3935.5024	-0.1
4	2	2	4	1	3	4401.547	4401.5359	11.3
4	1	4	3	0	3	4586.938	4586.9495	-11.5
7	0	7	6	1	6	4891.020	4891.02313	-2.8
3	2	2	3	1	3	5002.599	5002.59619	2.6
5	1	5	4	0	4	5251.695	5251.70087	-6.3
8	0	8	7	1	7	5831.344	5831.33249	11.3
6	1	6	5	0	5	5895.895	5895.90813	-13.2

J'	K_a'	K_c'	J"	K_a"	K_c"	ν_{obs}/MHz	ν_{calc}/MHz	$\Delta\nu$/kHz
2	2	0	1	1	1	6500.740	6500.74198	-2.3
7	1	7	6	0	6	6529.422	6529.43719	-14.9
9	0	9	8	1	8	6750.410	6750.40524	5.2
8	1	8	7	0	7	7162.315	7162.29728	17.8
3	2	2	2	1	1	7184.951	7184.94724	4.1
4	2	3	3	1	2	7912.611	7912.60326	7.7

3.2 Frequency lists of the xanthene-H_2O complexes

Table S38: Assigned rotational transitions for the xanthene-H_2O complex, 1w-I.

J'	K_a'	K_c'	v'	J"	K_a"	K_c"	v"	ν_{obs}/MHz	ν_{calc}/MHz	$\Delta\nu$/kHz
3	2	2	0	3	1	3	0	2028.491	2028.493	-2.1
3	2	2	1	3	1	3	1	2028.491	2028.493	-2.1
8	3	5	0	8	2	6	0	2073.021	2073.021	-0.3
8	3	5	1	8	2	6	1	2073.021	2073.021	-0.3
5	3	2	1	5	2	3	1	2147.219	2147.220	-1.0
5	3	2	0	5	2	3	0	2147.219	2147.220	-1.0
5	1	4	0	5	0	5	0	2163.093	2163.079	13.3
5	1	4	1	5	0	5	1	2163.093	2163.079	13.3
4	1	3	0	3	2	2	0	2200.631	2200.630	1.1
4	1	3	1	3	2	2	1	2200.631	2200.630	1.1
7	2	5	0	7	1	6	0	2272.159	2272.149	9.4
7	2	5	1	7	1	6	1	2272.159	2272.149	9.4
2	1	1	0	1	0	1	1	2307.626	2307.619	7.4

J'	K_a'	K_c'	v'	J"	K_a"	K_c"	v"	ν_{obs}/MHz	ν_{calc}/MHz	$\Delta\nu$/kHz
2	1	1	1	1	0	1	0	2307.676	2307.678	-1.9
4	3	1	1	4	2	2	1	2337.382	2337.385	-3.1
4	3	1	0	4	2	2	0	2337.382	2337.385	-3.1
4	2	3	0	4	1	4	0	2350.869	2350.865	3.5
4	2	3	1	4	1	4	1	2350.869	2350.865	3.5
3	1	3	1	2	0	2	1	2438.000	2438.002	-1.8
3	1	3	0	2	0	2	0	2438.000	2438.002	-1.8
3	3	0	1	3	2	1	1	2488.467	2488.466	1.4
3	3	0	0	3	2	1	0	2488.467	2488.466	1.4
8	3	6	1	7	4	3	1	2540.361	2540.367	-5.8
8	3	6	1	7	4	3	1	2540.361	2540.367	-5.8
7	3	4	1	6	4	3	1	2543.156	2543.156	0.3
7	3	4	0	6	4	3	0	2543.156	2543.156	0.3
10	4	6	1	10	3	7	1	2562.064	2562.067	-2.7
10	4	6	0	10	3	7	0	2562.064	2562.067	-2.7
3	3	1	0	3	2	2	0	2630.622	2630.619	3.3
3	3	1	1	3	2	2	1	2630.622	2630.619	3.3
9	4	6	0	8	5	3	0	2641.483	2641.487	-4.3
9	4	6	1	8	5	3	1	2641.483	2641.487	-4.3
9	4	5	1	9	3	6	1	2649.559	2649.564	-5.0
9	4	5	0	9	3	6	0	2649.559	2649.564	-5.0
4	0	4	1	3	1	3	1	2667.766	2667.767	-1.1
4	0	4	0	3	1	3	0	2667.766	2667.767	-1.1
11	4	7	1	11	3	8	1	2672.066	2672.074	-7.8
11	4	7	0	11	3	8	0	2672.066	2672.074	-7.8
4	3	2	0	4	2	3	0	2706.095	2706.095	0.1

J'	K_a'	K_c'	v'	J"	K_a"	K_c"	v"	ν_{obs}/MHz	ν_{calc}/MHz	$\Delta\nu$/kHz
4	3	2	1	4	2	3	1	2706.095	2706.095	0.1
4	3	1	0	4	2	3	1	2734.263	2734.263	0.5
4	3	1	1	4	2	3	0	2734.309	2734.310	-1.4
5	2	4	1	5	1	5	1	2751.364	2751.355	9.6
5	2	4	0	5	1	5	0	2751.364	2751.355	9.6
5	1	4	0	4	2	2	1	2800.693	2800.692	0.6
5	1	4	1	4	2	2	0	2800.748	2800.744	3.5
6	1	5	0	6	0	6	0	2834.525	2834.508	17.5
6	1	5	1	6	0	6	1	2834.525	2834.508	17.5
5	3	3	1	5	2	4	1	2844.438	2844.437	1.4
5	3	3	0	5	2	4	0	2844.438	2844.437	1.4
8	4	4	1	8	3	5	1	2869.310	2869.310	-0.3
8	4	4	0	8	3	5	0	2869.310	2869.310	-0.3
8	2	6	0	8	1	7	0	2919.575	2919.561	13.9
8	2	6	1	8	1	7	1	2919.575	2919.561	13.9
10	3	7	1	10	2	8	1	2938.661	2938.662	-0.9
10	3	7	0	10	2	8	0	2938.661	2938.662	-0.9
5	3	2	0	5	2	4	1	2951.261	2951.262	-0.9
5	3	2	1	5	2	4	0	2951.318	2951.308	9.2
4	1	4	1	3	0	3	1	2988.552	2988.550	1.8
4	1	4	0	3	0	3	0	2988.552	2988.550	1.8
9	3	7	0	8	4	4	0	3026.425	3026.424	2.0
9	3	7	1	8	4	4	1	3026.425	3026.424	2.0
2	2	1	0	1	1	0	0	3057.459	3057.459	0.9
2	2	1	1	1	1	0	1	3057.459	3057.459	0.9
6	3	4	1	6	2	5	1	3059.601	3059.598	3.3

J'	K_a'	K_c'	v'	J"	K_a"	K_c"	v"	ν_{obs}/MHz	ν_{calc}/MHz	$\Delta\nu$/kHz
6	3	4	0	6	2	5	0	3059.601	3059.598	3.3
6	2	4	0	5	3	3	0	3071.804	3071.801	3.9
6	2	4	1	5	3	3	1	3071.804	3071.801	3.9
2	2	0	0	1	1	0	1	3088.278	3088.280	-2.2
2	2	0	1	1	1	0	0	3088.338	3088.336	2.1
7	4	3	1	7	3	4	1	3133.126	3133.129	-2.9
7	4	3	0	7	3	4	0	3133.126	3133.129	-2.9
5	1	4	0	4	2	3	0	3197.618	3197.620	-2.0
5	1	4	1	4	2	3	1	3197.618	3197.620	-2.0
2	2	1	0	1	1	1	1	3205.114	3205.125	-11.2
2	2	1	1	1	1	1	0	3205.173	3205.180	-6.9
6	2	5	1	6	1	6	1	3218.616	3218.607	9.8
6	2	5	0	6	1	6	0	3218.616	3218.607	9.8
2	2	0	1	1	1	1	1	3236.002	3236.002	0.1
2	2	0	0	1	1	1	0	3236.002	3236.002	0.1
12	5	7	1	12	4	8	1	3284.183	3284.177	5.4
12	5	7	0	12	4	8	0	3284.183	3284.177	5.4
10	3	8	0	9	4	5	0	3286.093	3286.094	-1.5
10	3	8	1	9	4	5	1	3286.093	3286.094	-1.5
3	1	2	0	2	0	2	1	3320.007	3320.003	3.7
3	1	2	1	2	0	2	0	3320.065	3320.061	3.6
6	1	5	0	5	2	3	1	3342.979	3342.988	-9.2
6	1	5	1	5	2	3	0	3343.041	3343.039	2.5
7	3	5	0	7	2	6	0	3358.151	3358.153	-2.0
7	3	5	1	7	2	6	1	3358.151	3358.153	-2.0
6	4	2	0	6	3	3	0	3359.897	3359.902	-5.1

J'	K_a'	K_c'	v'	J"	K_a"	K_c"	v"	ν_{obs}/MHz	ν_{calc}/MHz	$\Delta\nu$/kHz
6	4	2	1	6	3	3	1	3359.897	3359.902	-5.1
5	0	5	1	4	1	4	1	3385.399	3385.406	-6.8
5	0	5	0	4	1	4	0	3385.399	3385.406	-6.8
10	4	7	1	9	5	4	1	3397.835	3397.836	-1.7
10	4	7	0	9	5	4	0	3397.835	3397.836	-1.7
5	4	1	1	5	3	2	1	3508.922	3508.932	-10.5
5	4	1	0	5	3	2	0	3508.922	3508.932	-10.5
7	1	6	0	7	0	7	0	3515.462	3515.451	11.1
7	1	6	1	7	0	7	1	3515.462	3515.451	11.1
5	1	5	1	4	0	4	1	3552.569	3552.573	-4.1
5	1	5	0	4	0	4	0	3552.569	3552.573	-4.1
11	5	6	0	11	4	7	0	3560.245	3560.240	5.0
11	5	6	1	11	4	7	1	3560.245	3560.240	5.0
4	4	0	1	4	3	1	1	3585.841	3585.840	0.9
4	4	0	0	4	3	1	0	3585.841	3585.840	0.9
5	4	2	0	5	3	3	0	3611.731	3611.733	-1.9
5	4	2	0	5	3	3	0	3611.731	3611.733	-1.9
4	4	1	1	4	3	2	1	3613.576	3613.574	2.0
4	4	1	0	4	3	2	0	3613.576	3613.574	2.0
11	3	8	1	11	2	9	1	3631.023	3631.032	-8.9
11	3	8	0	11	2	9	0	3631.023	3631.032	-8.9
6	4	3	0	6	3	4	0	3631.397	3631.395	2.5
6	4	3	1	6	3	4	1	3631.397	3631.395	2.5
9	2	7	1	9	1	8	1	3641.487	3641.487	-0.7
9	2	7	0	9	1	8	0	3641.487	3641.487	-0.7
3	2	2	1	2	1	1	1	3691.506	3691.506	0.4

J'	K_a'	K_c'	v'	J"	K_a"	K_c"	v"	ν_{obs}/MHz	ν_{calc}/MHz	$\Delta\nu$/kHz
3	2	2	0	2	1	1	0	3691.506	3691.506	0.4
7	4	4	0	7	3	5	0	3692.293	3692.291	2.1
7	4	4	1	7	3	5	1	3692.293	3692.291	2.1
7	2	6	0	7	1	7	0	3737.115	3737.104	10.6
7	2	6	1	7	1	7	1	3737.115	3737.104	10.6
8	3	6	0	8	2	7	0	3738.216	3738.209	6.6
8	3	6	1	8	2	7	1	3738.216	3738.209	6.6
8	3	5	1	7	4	4	1	3742.985	3742.985	0.3
8	3	5	0	7	4	4	0	3742.985	3742.985	0.3
8	4	5	0	8	3	6	0	3814.367	3814.358	8.2
8	4	5	1	8	3	6	1	3814.367	3814.358	8.2
3	2	1	0	2	1	1	1	3837.768	3837.767	1.5
3	2	1	1	2	1	1	0	3837.827	3837.821	5.5
10	5	5	1	10	4	6	1	3890.315	3890.312	2.4
10	5	5	0	10	4	6	0	3890.315	3890.312	2.4
15	6	9	0	15	5	10	0	3900.883	3900.866	16.3
15	6	9	1	15	5	10	1	3900.883	3900.866	16.3
7	3	4	0	7	2	6	1	3985.721	3985.718	2.4
7	3	4	1	7	2	6	0	3985.772	3985.762	10.2
9	4	6	0	9	3	7	0	4013.282	4013.282	0.1
9	4	6	1	9	3	7	1	4013.282	4013.282	0.1
6	0	6	1	5	1	5	1	4063.925	4063.926	-1.2
6	0	6	0	5	1	5	0	4063.925	4063.926	-1.2
3	2	2	0	2	1	2	1	4134.557	4134.561	-4.4
3	2	2	1	2	1	2	0	4134.614	4134.616	-1.4
6	1	6	0	5	0	5	0	4143.040	4143.043	-3.4

J'	K_a'	K_c'	v'	J"	K_a"	K_c"	v"	ν_{obs}/MHz	ν_{calc}/MHz	$\Delta\nu$/kHz
6	1	6	1	5	0	5	1	4143.040	4143.043	-3.4
6	1	5	1	5	2	4	1	4147.084	4147.079	5.0
6	1	5	0	5	2	4	0	4147.084	4147.079	5.0
8	1	7	0	8	0	8	0	4174.920	4174.911	8.7
8	1	7	1	8	0	8	1	4174.920	4174.911	8.7
9	5	4	1	9	4	5	1	4185.523	4185.526	-3.2
9	5	4	0	9	4	5	0	4185.523	4185.526	-3.2
9	3	7	0	9	2	8	0	4190.101	4190.099	2.6
9	3	7	1	9	2	8	1	4190.101	4190.099	2.6
7	2	5	1	6	3	4	1	4228.800	4228.790	10.3
7	2	5	0	6	3	4	0	4228.800	4228.790	10.3
4	2	3	1	3	1	2	1	4249.203	4249.208	-5.2
4	2	3	0	3	1	2	0	4249.203	4249.208	-5.2
3	2	1	1	2	1	2	1	4280.880	4280.876	3.9
3	2	1	0	2	1	2	0	4280.880	4280.876	3.9
8	2	7	0	8	1	8	0	4290.750	4290.738	12.3
8	2	7	1	8	1	8	1	4290.750	4290.738	12.3
10	4	7	1	10	3	8	1	4297.270	4297.269	1.0
10	4	7	0	10	3	8	0	4297.270	4297.269	1.0
10	2	8	0	10	1	9	0	4369.901	4369.900	1.7
10	2	8	1	10	1	9	1	4369.901	4369.900	1.7
8	5	3	0	8	4	4	0	4398.210	4398.218	-8.0
8	5	3	1	8	4	4	1	4398.210	4398.218	-8.0
4	1	3	0	3	0	3	1	4437.277	4437.272	4.8
4	1	3	1	3	0	3	0	4437.332	4437.329	3.4
8	5	4	0	8	4	5	0	4575.144	4575.144	-0.2

J'	K_a'	K_c'	v'	J"	K_a"	K_c"	v"	ν_{obs}/MHz	ν_{calc}/MHz	$\Delta\nu$/kHz
8	5	4	1	8	4	5	1	4575.144	4575.144	-0.2
9	5	5	0	9	4	6	0	4578.677	4578.677	0.3
9	5	5	1	9	4	6	1	4578.677	4578.677	0.3
7	5	3	0	7	4	4	0	4593.699	4593.702	-2.9
7	5	3	1	7	4	4	1	4593.699	4593.702	-2.9
6	5	2	0	6	4	2	1	4598.945	4598.952	-6.6
6	5	2	1	6	4	2	0	4598.993	4598.999	-5.6
6	5	2	1	6	4	2	0	4598.993	4598.999	-5.6
6	5	1	0	6	4	2	0	4599.469	4599.472	-2.4
6	5	1	1	6	4	2	1	4599.469	4599.472	-2.4
6	5	2	0	6	4	3	0	4618.612	4618.612	0.5
6	5	2	1	6	4	3	1	4618.612	4618.612	0.5
10	5	6	0	10	4	7	0	4624.220	4624.220	0.3
10	5	6	1	10	4	7	1	4624.220	4624.220	0.3
5	5	0	0	5	4	1	0	4636.322	4636.329	-6.7
5	5	0	1	5	4	1	1	4636.322	4636.329	-6.7
5	5	1	0	5	4	2	0	4640.327	4640.332	-4.9
5	5	1	1	5	4	2	1	4640.327	4640.332	-4.9
4	2	2	0	3	1	2	1	4646.084	4646.083	0.8
4	2	2	1	3	1	2	0	4646.139	4646.136	2.7
11	4	8	1	11	3	9	1	4665.668	4665.677	-9.4
11	4	8	0	11	3	9	0	4665.668	4665.677	-9.4
10	3	8	0	10	2	9	0	4698.941	4698.940	0.9
10	3	8	1	10	2	9	1	4698.941	4698.940	0.9
7	0	7	1	6	1	6	1	4719.381	4719.394	-13.0
7	0	7	0	6	1	6	0	4719.381	4719.394	-13.0

J'	K_a'	K_c'	v'	J"	K_a"	K_c"	v"	ν_{obs}/MHz	ν_{calc}/MHz	$\Delta\nu$/kHz
11	5	7	0	11	4	8	0	4732.002	4731.998	4.1
11	5	7	1	11	4	8	1	4732.002	4731.998	4.1
5	2	4	1	4	1	3	1	4742.568	4742.572	-3.8
5	2	4	0	4	1	3	0	4742.568	4742.572	-3.8
7	1	7	1	6	0	6	1	4754.466	4754.467	-0.6
7	1	7	0	6	0	6	0	4754.466	4754.467	-0.6
9	1	8	0	9	0	9	0	4809.594	4809.585	9.5
9	1	8	1	9	0	9	1	4809.594	4809.585	9.5
3	3	1	1	2	2	0	1	4945.020	4945.018	2.3
3	3	1	0	2	2	0	0	4945.020	4945.018	2.3
3	3	0	0	2	2	0	1	4949.130	4949.128	2.1
3	3	0	1	2	2	0	0	4949.174	4949.176	-1.9
3	3	1	0	2	2	1	1	4975.838	4975.843	-4.9
3	3	1	1	2	2	1	0	4975.896	4975.891	4.7
12	6	6	0	12	5	7	0	4977.617	4977.603	14.7
12	6	6	1	12	5	7	1	4977.617	4977.603	14.7
3	3	0	1	2	2	1	1	4980.004	4980.002	1.9
3	3	0	0	2	2	1	0	4980.004	4980.002	1.9
9	3	6	0	8	4	5	0	5013.186	5013.187	-0.8
9	3	6	1	8	4	5	1	5013.186	5013.187	-0.8
7	1	6	0	6	2	5	0	5016.238	5016.239	-0.7
7	1	6	1	6	2	5	1	5016.238	5016.239	-0.7
12	4	9	1	12	3	10	1	5109.647	5109.661	-14.0
12	4	9	0	12	3	10	0	5109.647	5109.661	-14.0
4	2	3	0	3	1	3	1	5131.213	5131.212	1.3
4	2	3	1	3	1	3	0	5131.264	5131.265	-0.6

J'	K_a'	K_c'	v'	J"	K_a"	K_c"	v"	ν_{obs}/MHz	ν_{calc}/MHz	$\Delta\nu$/kHz
4	3	1	1	4	0	4	1	5197.761	5197.758	3.4
4	3	1	0	4	0	4	0	5197.761	5197.758	3.4
6	2	5	1	5	1	4	1	5198.564	5198.571	-6.4
6	2	5	0	5	1	4	0	5198.564	5198.571	-6.4
11	3	9	0	11	2	10	0	5248.256	5248.273	-16.7
11	3	9	1	11	2	10	1	5248.256	5248.273	-16.7
11	6	5	0	11	5	6	0	5248.992	5248.998	-5.9
11	6	5	1	11	5	6	1	5248.992	5248.998	-5.9
8	2	6	0	7	3	5	0	5362.253	5362.254	-1.0
8	2	6	1	7	3	5	1	5362.253	5362.254	-1.0
8	0	8	1	7	1	7	1	5363.038	5363.040	-2.2
8	0	8	0	7	1	7	0	5363.038	5363.040	-2.2
8	1	8	1	7	0	7	1	5377.903	5377.905	-2.3
8	1	8	0	7	0	7	0	5377.903	5377.905	-2.3
10	1	9	0	10	0	10	0	5426.853	5426.839	14.0
10	1	9	1	10	0	10	1	5426.853	5426.839	14.0
10	6	4	0	10	5	5	0	5429.328	5429.330	-2.8
10	6	4	1	10	5	5	1	5429.328	5429.330	-2.8
10	2	9	0	10	1	10	0	5452.831	5452.824	7.1
10	2	9	1	10	1	10	1	5452.831	5452.824	7.1
12	6	7	0	12	5	8	0	5486.840	5486.844	-4.1
12	6	7	1	12	5	8	1	5486.840	5486.844	-4.1
11	6	6	0	11	5	7	0	5499.624	5499.633	-9.2
11	6	6	1	11	5	7	1	5499.624	5499.633	-9.2
13	6	8	1	13	5	9	1	5517.784	5517.778	6.2
13	6	8	0	13	5	9	0	5517.784	5517.778	6.2

J'	K_a'	K_c'	v'	J"	K_a"	K_c"	v"	ν_{obs}/MHz	ν_{calc}/MHz	$\Delta\nu$/kHz
4	2	2	1	3	1	3	1	5528.149	5528.140	9.1
4	2	2	0	3	1	3	0	5528.149	5528.140	9.1
10	6	5	0	10	5	6	0	5536.018	5536.015	2.8
10	6	5	1	10	5	6	1	5536.018	5536.015	2.8
9	6	3	0	9	5	4	0	5540.822	5540.815	7.6
9	6	3	1	9	5	4	1	5540.822	5540.815	7.6
5	2	3	0	4	1	3	1	5546.614	5546.612	2.3
5	2	3	1	4	1	3	0	5546.666	5546.663	3.2
9	6	4	0	9	5	5	0	5579.707	5579.710	-3.0
9	6	4	1	9	5	5	1	5579.707	5579.710	-3.0
8	6	2	0	8	5	3	0	5608.308	5608.310	-2.0
8	6	2	1	8	5	3	1	5608.308	5608.310	-2.0
14	6	9	1	14	5	10	1	5612.790	5612.806	-15.9
14	6	9	0	14	5	10	0	5612.790	5612.806	-15.9
13	4	10	1	13	3	11	1	5614.640	5614.668	-27.4
13	4	10	0	13	3	11	0	5614.640	5614.668	-27.4
8	6	3	0	8	5	4	0	5620.153	5620.154	-1.2
8	6	3	1	8	5	4	1	5620.153	5620.154	-1.2
7	6	1	0	7	5	2	0	5649.471	5649.469	2.2
7	6	1	1	7	5	2	1	5649.471	5649.469	2.2
7	6	2	0	7	5	3	0	5652.329	5652.328	0.8
7	6	2	1	7	5	3	1	5652.329	5652.328	0.8
7	2	6	1	6	1	5	1	5657.059	5657.063	-4.6
7	2	6	0	6	1	5	0	5657.059	5657.063	-4.6
5	1	4	0	4	0	4	1	5661.077	5661.064	12.8
5	1	4	1	4	0	4	0	5661.126	5661.118	7.9

J'	K_a'	K_c'	v'	J"	K_a"	K_c"	v"	ν_{obs}/MHz	ν_{calc}/MHz	$\Delta\nu$/kHz
4	3	2	0	3	2	1	0	5662.554	5662.552	2.0
4	3	2	1	3	2	1	1	5662.554	5662.552	2.0
6	6	0	0	6	5	1	0	5674.733	5674.734	-0.6
6	6	0	1	6	5	1	1	5674.733	5674.734	-0.6
6	6	1	0	6	5	2	0	5675.225	5675.226	-0.9
6	6	1	1	6	5	2	1	5675.225	5675.226	-0.9
4	3	1	1	3	2	1	0	5690.744	5690.767	-23.5
12	2	10	1	12	1	11	1	5731.443	5731.453	-9.2
12	2	10	0	12	1	11	0	5731.443	5731.453	-9.2
8	1	7	1	7	2	6	1	5800.842	5800.847	-4.7
8	1	7	0	7	2	6	0	5800.842	5800.847	-4.7
4	3	2	0	3	2	2	1	5808.810	5808.816	-6.2
4	3	2	1	3	2	2	0	5808.865	5808.864	1.1
12	3	10	0	12	2	11	0	5823.359	5823.359	0.4
12	3	10	1	12	2	11	1	5823.359	5823.359	0.4
4	3	1	1	3	2	2	1	5837.033	5837.032	1.9
4	3	1	0	3	2	2	0	5837.033	5837.032	1.9
9	0	9	1	8	1	8	1	6001.152	6001.141	11.2
9	0	9	0	8	1	8	0	6001.152	6001.141	11.2
9	1	9	1	8	0	8	1	6007.249	6007.241	7.3
9	1	9	0	8	0	8	0	6007.249	6007.241	7.3
11	1	10	0	11	0	11	0	6033.980	6033.981	-1.5
11	1	10	1	11	0	11	1	6033.980	6033.981	-1.5
11	2	10	0	11	1	11	0	6045.535	6045.521	14.1
11	2	10	1	11	1	11	1	6045.535	6045.521	14.1
8	2	7	1	7	1	6	1	6153.191	6153.192	-1.6

J'	K_a'	K_c'	v'	J"	K_a"	K_c"	v"	ν_{obs}/MHz	ν_{calc}/MHz	$\Delta\nu$/kHz
8	2	7	0	7	1	6	0	6153.191	6153.192	-1.6
5	2	4	0	4	1	4	1	6191.309	6191.296	13.1
5	2	4	1	4	1	4	0	6191.363	6191.348	14.8
5	3	3	1	4	2	2	1	6287.986	6287.992	-5.3
5	3	3	0	4	2	2	0	6287.986	6287.992	-5.3
13	7	6	0	13	6	7	0	6297.886	6297.878	7.8
13	7	6	1	13	6	7	1	6297.886	6297.878	7.8
10	3	7	0	9	4	6	0	6302.926	6302.935	-9.0
10	3	7	1	9	4	6	1	6302.926	6302.935	-9.0
15	7	9	0	15	6	10	0	6364.921	6364.920	1.3
15	7	9	1	15	6	10	1	6364.921	6364.920	1.3
13	2	11	0	13	1	12	0	6368.451	6368.464	-13.0
13	2	11	1	13	1	12	1	6368.451	6368.464	-13.0
14	7	8	0	14	6	9	0	6393.392	6393.391	0.5
14	7	8	1	14	6	9	1	6393.392	6393.391	0.5
5	3	2	0	4	2	2	1	6394.812	6394.818	-5.8
5	3	2	1	4	2	2	0	6394.863	6394.863	0.0
13	3	11	0	13	2	12	0	6413.031	6413.031	0.0
13	3	11	1	13	2	12	1	6413.031	6413.031	0.0
9	2	7	1	8	3	6	1	6423.270	6423.266	4.5
9	2	7	0	8	3	6	0	6423.270	6423.266	4.5
12	7	5	0	12	6	6	0	6448.392	6448.413	-20.9
12	7	5	1	12	6	6	1	6448.392	6448.413	-20.9
9	1	8	0	8	2	7	0	6519.987	6519.987	-0.8
9	1	8	1	8	2	7	1	6519.987	6519.987	-0.8
11	7	4	0	11	6	5	0	6547.141	6547.130	11.2

J'	K_a'	K_c'	v'	J"	K_a"	K_c"	v"	ν_{obs}/MHz	ν_{calc}/MHz	$\Delta\nu$/kHz
11	7	4	1	11	6	5	1	6547.141	6547.130	11.2
6	2	4	0	5	1	4	1	6559.041	6559.049	-8.0
6	2	4	1	5	1	4	0	6559.086	6559.099	-13.2
11	7	5	0	11	6	6	0	6569.214	6569.220	-6.2
11	7	5	1	11	6	6	1	6569.214	6569.220	-6.2
6	3	3	1	6	0	6	1	6593.904	6593.890	14.1
6	3	3	0	6	0	6	0	6593.904	6593.890	14.1
10	7	3	0	10	6	4	0	6613.120	6613.138	-17.7
10	7	3	1	10	6	4	1	6613.120	6613.138	-17.7
10	7	4	0	10	6	5	0	6620.045	6620.038	6.9
10	7	4	1	10	6	5	1	6620.045	6620.038	6.9
12	1	11	0	12	0	12	0	6635.698	6635.696	1.6
12	1	11	1	12	0	12	1	6635.698	6635.696	1.6
10	0	10	0	9	1	9	0	6636.808	6636.802	5.8
10	0	10	1	9	1	9	1	6636.808	6636.802	5.8
10	1	10	0	9	0	9	0	6639.251	6639.246	5.2
10	1	10	1	9	0	9	1	6639.251	6639.246	5.2
12	2	11	0	12	1	12	0	6640.668	6640.671	-2.9
12	2	11	1	12	1	12	1	6640.668	6640.671	-2.9
9	7	2	0	9	6	3	0	6658.297	6658.295	1.9
9	7	2	1	9	6	3	1	6658.297	6658.295	1.9
9	7	3	1	9	6	4	1	6660.104	6660.101	3.7
9	7	3	0	9	6	4	0	6660.104	6660.101	3.7
5	3	3	0	4	2	3	1	6684.873	6684.870	3.2
5	3	3	1	4	2	3	0	6684.917	6684.917	0.6
8	7	1	0	8	6	2	0	6689.490	6689.490	-0.1

J'	K_a'	K_c'	v'	J"	K_a"	K_c"	v"	ν_{obs}/MHz	ν_{calc}/MHz	$\Delta\nu$/kHz
8	7	1	1	8	6	2	1	6689.490	6689.490	-0.1
8	7	2	0	8	6	3	0	6689.861	6689.863	-2.6
8	7	2	1	8	6	3	1	6689.861	6689.863	-2.6
9	2	8	0	8	1	7	0	6698.217	6698.217	-0.2
9	2	8	1	8	1	7	1	6698.217	6698.217	-0.2
7	7	0	0	7	6	1	0	6710.841	6710.846	-5.5
7	7	0	1	7	6	1	1	6710.841	6710.846	-5.5
7	7	1	0	7	6	2	0	6710.841	6710.846	-5.5
7	7	1	1	7	6	2	1	6710.841	6710.846	-5.5
4	4	1	1	3	3	0	1	6787.663	6787.660	2.8
4	4	1	0	3	3	0	0	6787.663	6787.660	2.8
4	4	0	0	3	3	0	1	6788.100	6788.096	4.1
4	4	0	1	3	3	0	0	6788.148	6788.140	7.8
5	3	2	1	4	2	3	1	6791.743	6791.742	0.6
5	3	2	0	4	2	3	0	6791.743	6791.742	0.6
4	4	0	1	3	3	1	1	6792.250	6792.253	-3.1
4	4	0	0	3	3	1	0	6792.250	6792.253	-3.1
6	3	4	0	5	2	3	0	6811.262	6811.266	-4.5
6	3	4	1	5	2	3	1	6811.262	6811.266	-4.5
6	1	5	0	5	0	5	1	6952.982	6952.969	12.8
6	1	5	1	5	0	5	0	6953.033	6953.021	12.0
5	2	3	1	4	1	4	1	6995.388	6995.388	-0.2
5	2	3	0	4	1	4	0	6995.388	6995.388	-0.2
14	3	12	0	14	2	13	0	7009.918	7009.944	-26.4
14	3	12	1	14	2	13	1	7009.918	7009.944	-26.4
6	3	3	0	5	2	3	1	7102.366	7102.374	-7.9

J'	K_a'	K_c'	v'	J"	K_a"	K_c"	v"	ν_{obs}/MHz	ν_{calc}/MHz	$\Delta\nu$/kHz
6	3	3	1	5	2	3	0	7102.413	7102.416	-3.4
6	4	2	1	6	1	5	1	7119.290	7119.284	5.8
6	4	2	0	6	1	5	0	7119.290	7119.284	5.8
10	1	9	0	9	2	8	0	7197.768	7197.754	13.3
10	1	9	1	9	2	8	1	7197.768	7197.754	13.3
13	1	12	0	13	0	13	0	7234.538	7234.548	-10.6
13	1	12	1	13	0	13	1	7234.538	7234.548	-10.6
13	2	12	0	13	1	13	0	7236.636	7236.643	-7.1
13	2	12	1	13	1	13	1	7236.636	7236.643	-7.1
7	3	5	0	6	2	4	0	7246.056	7246.059	-2.5
7	3	5	1	6	2	4	1	7246.056	7246.059	-2.5
11	0	11	0	10	1	10	0	7271.450	7271.443	7.0
11	0	11	1	10	1	10	1	7271.450	7271.443	7.0
11	1	11	0	10	0	10	0	7272.407	7272.404	3.6
11	1	11	1	10	0	10	1	7272.407	7272.404	3.6
10	2	9	0	9	1	8	0	7282.487	7282.485	1.8
10	2	9	1	9	1	8	1	7282.487	7282.485	1.8
6	2	5	0	5	1	5	1	7307.078	7307.063	15.3
6	2	5	1	5	1	5	0	7307.126	7307.114	12.3
7	4	3	1	7	1	6	1	7351.041	7351.039	1.6
7	4	3	0	7	1	6	0	7351.041	7351.039	1.6
10	2	8	1	9	3	7	1	7377.551	7377.555	-4.1
10	2	8	0	9	3	7	0	7377.551	7377.555	-4.1
11	3	8	1	10	4	7	1	7555.645	7555.656	-11.1
11	3	8	0	10	4	7	0	7555.645	7555.656	-11.1
13	8	6	1	13	7	7	1	7561.011	7561.001	9.7

J'	K_a'	K_c'	v'	J"	K_a"	K_c"	v"	ν_{obs}/MHz	ν_{calc}/MHz	$\Delta\nu$/kHz
13	8	6	0	13	7	7	0	7561.011	7561.001	9.7
5	4	2	1	4	3	1	1	7562.343	7562.339	3.8
5	4	2	0	4	3	1	0	7562.343	7562.339	3.8
5	4	1	0	4	3	1	1	7566.363	7566.366	-3.7
5	4	1	1	4	3	1	0	7566.402	7566.409	-7.2
5	4	2	0	4	3	2	1	7590.508	7590.509	-1.1
5	4	2	1	4	3	2	0	7590.543	7590.552	-8.5
5	4	1	1	4	3	2	1	7594.579	7594.579	0.5
5	4	1	0	4	3	2	0	7594.579	7594.579	0.5
6	3	4	0	5	2	4	1	7615.312	7615.308	4.1
6	3	4	1	5	2	4	0	7615.355	7615.356	-1.1
8	3	6	0	7	2	5	0	7619.256	7619.252	3.8
8	3	6	1	7	2	5	1	7619.256	7619.252	3.8
11	8	3	0	11	7	4	0	7663.874	7663.867	7.1
11	8	3	1	11	7	4	1	7663.874	7663.867	7.1
11	8	4	1	11	7	5	1	7664.939	7664.933	6.9
11	8	4	0	11	7	5	0	7664.939	7664.933	6.9
7	2	5	0	6	1	5	1	7697.040	7697.043	-2.9
7	2	5	1	6	1	5	0	7697.040	7697.043	-2.9
11	1	10	0	10	2	9	0	7852.585	7852.601	-15.4
11	1	10	1	10	2	9	1	7852.585	7852.601	-15.4
7	3	4	0	6	2	4	1	7873.622	7873.626	-4.1
7	3	4	1	6	2	4	0	7873.650	7873.664	-14.0
11	2	10	0	10	1	9	0	7891.079	7891.086	-6.6
11	2	10	1	10	1	9	1	7891.079	7891.086	-6.6
12	0	12	0	11	1	11	0	7905.684	7905.676	7.9

J'	K_a'	K_c'	v'	J"	K_a"	K_c"	v"	ν_{obs}/MHz	ν_{calc}/MHz	$\Delta\nu$/kHz
12	0	12	1	11	1	11	1	7905.684	7905.676	7.9
12	1	12	0	11	0	11	0	7906.053	7906.048	5.4
12	1	12	1	11	0	11	1	7906.053	7906.048	5.4
6	3	3	0	5	2	4	0	7906.463	7906.461	1.7
6	3	3	1	5	2	4	1	7906.463	7906.461	1.7
9	3	7	0	8	2	6	0	7968.749	7968.755	-5.8
9	3	7	1	8	2	6	1	7968.749	7968.755	-5.8

Table S39: Assigned rotational transitions for $^{13}C_1$ isotopologue of the xanthene-H_2O complex, 1w-I.

J'	K_a'	K_c'	J"	K_a"	K_c"	ν_{obs}/MHz	ν_{calc}/MHz	$\Delta\nu$/kHz
3	2	2	3	1	3	2028.491	2028.493	-1.2
3	1	3	2	0	2	2436.577	2436.578	-0.4
4	0	4	3	1	3	2664.582	2664.581	1.1
4	1	4	3	0	3	2986.584	2986.582	2.1
5	1	4	4	2	3	3191.326	3191.330	-4.6
6	2	5	6	1	6	3216.189	3216.185	3.6
2	2	0	1	1	1	3234.957	3234.962	-5.6
5	0	5	4	1	4	3381.863	3381.869	-6.4
5	1	5	4	0	4	3549.931	3549.932	-1.1
3	2	2	2	1	1	3690.348	3690.351	-3.1
8	3	5	7	4	4	3728.919	3728.904	15.5
6	0	6	5	1	5	4060.014	4060.015	-1.2
6	1	6	5	0	5	4139.680	4139.684	-4.0

J'	K_a'	K_c'	J"	K_a"	K_c"	ν_{obs}/MHz	ν_{calc}/MHz	$\Delta\nu$/kHz
6	1	5	5	2	4	4140.399	4140.406	-6.6
4	2	3	3	1	2	4247.641	4247.647	-6.2
3	2	1	2	1	2	4278.140	4278.164	-24.6
7	0	7	6	1	6	4715.053	4715.047	6.1
5	2	4	4	1	3	4740.678	4740.680	-2.1
7	1	7	6	0	6	4750.420	4750.420	0.1
3	3	0	3	0	3	4873.650	4873.638	12.1
3	3	1	2	2	0	4944.134	4944.131	2.6
3	3	0	2	2	1	4978.945	4978.941	3.6
7	1	6	6	2	5	5009.548	5009.547	0.7
6	2	5	5	1	4	5196.248	5196.252	-4.1
8	0	8	7	1	7	5358.201	5358.203	-2.1
8	1	8	7	0	7	5373.225	5373.220	5.0
7	2	6	6	1	5	5654.046	5654.048	-2.1
8	1	7	7	2	6	5794.232	5794.239	-7.1
4	3	1	3	2	2	5834.716	5834.715	1.1
9	0	9	8	1	8	5995.778	5995.779	-0.6
9	1	9	8	0	8	6001.959	6001.951	7.9
8	2	7	7	1	6	6149.211	6149.220	-9.5
5	3	3	4	2	2	6286.243	6286.245	-1.9
9	2	7	8	3	6	6411.950	6411.957	-6.6
9	1	8	8	2	7	6513.355	6513.351	3.8
10	0	10	9	1	9	6630.895	6630.895	0.0
10	1	10	9	0	9	6633.378	6633.371	6.7
9	2	8	8	1	7	6693.223	6693.226	-2.8
4	4	1	3	3	0	6786.500	6786.497	3.2

J'	K_a'	K_c'	J"	K_a"	K_c"	ν_{obs}/MHz	ν_{calc}/MHz	$\Delta\nu$/kHz
4	4	0	3	3	1	6791.057	6791.054	2.6
7	3	5	6	2	4	7244.200	7244.197	3.1
11	0	11	10	1	10	7264.986	7264.980	6.1
10	2	9	9	1	8	7276.570	7276.572	-2.4
5	4	2	4	3	1	7560.388	7560.382	6.2
5	4	1	4	3	2	7592.376	7592.377	-0.7
6	3	3	5	2	4	7899.854	7899.858	-3.8
9	3	7	8	2	6	7966.266	7966.262	4.0

Table S40: Assigned rotational transitions for $^{13}C_2$ isotopologue of the xanthene-H_2O complex, 1w-I.

J'	K_a'	K_c'	J"	K_a"	K_c"	ν_{obs}/MHz	ν_{calc}/MHz	$\Delta\nu$/kHz
4	0	4	3	1	3	2655.037	2655.042	-4.2
5	3	3	5	2	4	2841.476	2841.469	7.8
4	1	4	3	0	3	2978.499	2978.507	-8.6
5	0	5	4	1	4	3370.584	3370.592	-8.3
5	1	5	4	0	4	3539.846	3539.851	-5.1
6	0	6	5	1	5	4047.026	4047.028	-1.5
6	1	6	5	0	5	4127.467	4127.475	-7.9
4	2	3	3	1	2	4238.121	4238.135	-13.7
7	0	7	6	1	6	4700.289	4700.288	1.0
5	2	4	4	1	3	4729.830	4729.836	-5.9
7	1	7	6	0	6	4736.092	4736.100	-8.2
3	3	1	2	2	0	4934.522	4934.528	-6.4

J'	K_a'	K_c'	J"	K_a"	K_c"	ν_{obs}/MHz	ν_{calc}/MHz	$\Delta\nu$/kHz
3	3	0	2	2	1	4968.991	4968.995	-3.7
7	1	6	6	2	5	4990.434	4990.435	-1.2
6	2	5	5	1	4	5183.978	5183.985	-6.6
8	0	8	7	1	7	5341.604	5341.603	0.8
8	1	8	7	0	7	5356.829	5356.846	-16.8
7	2	6	6	1	5	5639.911	5639.913	-1.7
4	3	2	3	2	1	5649.369	5649.365	3.2
4	3	2	3	2	1	5649.369	5649.365	3.3
8	1	7	7	2	6	5773.988	5773.988	-0.1
4	3	1	3	2	2	5821.321	5821.318	3.1
9	0	9	8	1	8	5977.294	5977.290	4.0
9	1	9	8	0	8	5983.563	5983.571	-8.7
8	2	7	7	1	6	6132.729	6132.728	1.2
5	3	3	4	2	2	6273.047	6273.055	-8.4
9	1	8	8	2	7	6491.891	6491.889	1.4
10	0	10	9	1	9	6610.487	6610.488	-1.5
10	1	10	9	0	9	6613.011	6613.015	-3.6
9	2	8	8	1	7	6674.187	6674.189	-2.4
5	3	2	4	2	3	6769.800	6769.811	-11.5
4	4	1	3	3	0	6773.397	6773.398	-1.3
4	4	0	3	3	1	6777.896	6777.890	6.4
6	3	4	5	2	3	6795.266	6795.269	-3.8
10	1	9	9	2	8	7168.027	7168.027	0.7
7	3	5	6	2	4	7229.290	7229.285	4.8
11	0	11	10	1	10	7242.665	7242.641	24.3
10	2	9	9	1	8	7255.074	7255.081	-7.5

J'	K_a'	K_c'	J"	K_a"	K_c"	ν_{obs}/MHz	ν_{calc}/MHz	$\Delta\nu$/kHz
5	4	2	4	3	1	7544.737	7544.722	15.1
5	4	1	4	3	2	7576.267	7576.265	1.5
11	1	10	10	2	9	7820.907	7820.895	12.2
12	1	12	11	0	11	7874.780	7874.760	19.7
6	3	3	5	2	4	7876.075	7876.075	-0.2

Table S41: Assigned rotational transitions for $^{13}C_3$ isotopologue of the xanthene-H_2O complex, 1w-I.

J'	K_a'	K_c'	J"	K_a"	K_c"	ν_{obs}/MHz	ν_{calc}/MHz	$\Delta\nu$/kHz
4	0	4	3	1	3	2638.838	2638.852	-13.5
4	1	4	3	0	3	2971.628	2971.621	6.7
2	2	0	1	1	1	3227.776	3227.778	-1.6
5	0	5	4	1	4	3353.579	3353.593	-14.2
5	1	5	4	0	4	3529.611	3529.611	0.0
8	3	5	7	4	4	3610.748	3610.733	14.4
6	0	6	5	1	5	4028.988	4028.994	-5.3
6	1	6	5	0	5	4113.597	4113.595	2.0
4	2	3	3	1	2	4236.723	4236.727	-4.1
3	2	1	2	1	2	4257.247	4257.247	-0.9
7	0	7	6	1	6	4680.742	4680.747	-5.0
5	2	4	4	1	3	4727.305	4727.302	3.1
3	3	1	2	2	0	4939.167	4939.164	2.7
3	3	0	2	2	1	4972.508	4972.511	-3.4
6	2	5	5	1	4	5179.636	5179.622	14.9

J'	K_a'	K_c'	J"	K_a"	K_c"	ν_{obs}/MHz	ν_{calc}/MHz	$\Delta\nu$/kHz
8	0	8	7	1	7	5320.154	5320.154	0.2
8	1	8	7	0	7	5336.541	5336.543	-1.3
7	2	6	6	1	5	5631.889	5631.877	12.4
4	3	2	3	2	1	5651.565	5651.563	1.8
4	3	1	3	2	2	5818.053	5818.061	-8.3
9	0	9	8	1	8	5953.670	5953.668	1.6
9	1	9	8	0	8	5960.504	5960.497	7.0
5	3	3	4	2	2	6274.720	6274.722	-1.6
9	1	8	8	2	7	6460.144	6460.162	-17.7
10	0	10	9	1	9	6584.549	6584.547	2.2
10	1	10	9	0	9	6587.324	6587.323	0.4
4	4	1	3	3	0	6780.133	6780.124	8.5
4	4	0	3	3	1	6784.384	6784.389	-4.4
6	3	4	5	2	3	6797.593	6797.587	5.7
11	0	11	10	1	10	7214.304	7214.303	1.6
11	1	11	10	0	10	7215.401	7215.410	-9.6
10	2	9	9	1	8	7230.604	7230.604	0.0
7	3	5	6	2	4	7232.471	7232.457	13.9
5	4	2	4	3	1	7547.646	7547.650	-3.5
5	4	1	4	3	2	7577.605	7577.610	-4.4

Table S42: Assigned rotational transitions for $^{13}C_4$ isotopologue of the xanthene-H_2O complex, 1w-I.

J'	K_a'	K_c'	J"	K_a"	K_c"	ν_{obs}/MHz	ν_{calc}/MHz	$\Delta\nu$/kHz
3	1	3	2	0	2	2423.091	2423.100	-8.3
4	0	4	3	1	3	2637.182	2637.197	-14.9
4	1	4	3	0	3	2968.332	2968.344	-11.6
5	1	4	4	2	3	3139.470	3139.482	-12.2
5	0	5	4	1	4	3351.012	3351.027	-14.5
5	1	5	4	0	4	3525.924	3525.936	-12.5
3	2	2	2	1	1	3677.718	3677.726	-7.5
6	0	6	5	1	5	4025.588	4025.588	-0.5
6	1	5	5	2	4	4084.505	4084.493	12.4
6	1	6	5	0	5	4109.524	4109.532	-8.3
7	2	5	6	3	4	4130.253	4130.246	6.6
4	2	3	3	1	2	4231.288	4231.300	-11.2
7	0	7	6	1	6	4676.582	4676.590	-7.9
7	1	7	6	0	6	4714.313	4714.323	-10.1
7	1	7	6	0	6	4714.313	4714.323	-10.1
3	3	1	2	2	0	4932.366	4932.359	7.7
7	1	6	6	2	5	4952.505	4952.495	9.8
3	3	0	2	2	1	4965.822	4965.817	4.9
6	2	5	5	1	4	5173.083	5173.081	1.9
8	0	8	7	1	7	5315.308	5315.312	-4.7
8	1	8	7	0	7	5331.521	5331.527	-6.5
7	2	6	6	1	5	5625.107	5625.086	21.5
4	3	2	3	2	1	5644.079	5644.073	6.0
4	3	1	3	2	2	5811.108	5811.110	-1.9

J'	K_a'	K_c'	J"	K_a"	K_c"	ν_{obs}/MHz	ν_{calc}/MHz	$\Delta\nu$/kHz
9	0	9	8	1	8	5948.185	5948.184	1.2
9	1	9	8	0	8	5954.931	5954.931	0.7
5	3	3	4	2	2	6266.382	6266.389	-6.6
10	0	10	9	1	9	6578.454	6578.441	12.6
10	1	10	9	0	9	6581.192	6581.181	10.8
5	3	2	4	2	3	6749.589	6749.603	-14.8
4	4	1	3	3	0	6770.765	6770.760	5.5
4	4	0	3	3	1	6775.055	6775.050	5.3
6	3	4	5	2	3	6788.368	6788.359	8.8
11	0	11	10	1	10	7207.598	7207.587	11.1
5	4	2	4	3	1	7537.722	7537.724	-1.5
5	4	1	4	3	2	7567.855	7567.860	-5.4

Table S43: Assigned rotational transitions for $^{13}C_5$ isotopologue of the xanthene-H_2O complex, 1w-I.

J'	K_a'	K_c'	J"	K_a"	K_c"	ν_{obs}/MHz	ν_{calc}/MHz	$\Delta\nu$/kHz
3	1	3	2	0	2	2424.241	2424.251	-9.4
4	0	4	3	1	3	2652.502	2652.507	-5.5
4	1	4	3	0	3	2971.628	2971.611	16.9
5	0	5	4	1	4	3366.076	3366.072	3.1
5	1	5	4	0	4	3532.366	3532.371	-5.5
6	0	6	5	1	5	4040.727	4040.727	0.4
6	1	6	5	0	5	4119.441	4119.436	4.8
4	2	3	3	1	2	4225.568	4225.557	10.5

J'	K_a'	K_c'	J"	K_a"	K_c"	ν_{obs}/MHz	ν_{calc}/MHz	$\Delta\nu$/kHz
3	2	1	2	1	2	4257.247	4257.265	-18.7
7	0	7	6	1	6	4692.443	4692.450	-7.0
5	2	4	4	1	3	4716.050	4716.044	6.2
7	1	7	6	0	6	4727.335	4727.343	-7.5
3	3	1	2	2	0	4917.906	4917.912	-5.7
7	1	6	6	2	5	4987.661	4987.653	7.9
6	2	5	5	1	4	5169.359	5169.363	-3.8
8	0	8	7	1	7	5332.411	5332.412	-1.3
7	2	6	6	1	5	5625.145	5625.155	-10.5
4	3	2	3	2	1	5631.365	5631.368	-2.2
8	1	7	7	2	6	5767.845	5767.841	3.7
4	3	1	3	2	2	5804.895	5804.894	0.3
9	0	9	8	1	8	5966.864	5966.858	5.7
9	1	9	8	0	8	5972.924	5972.928	-4.1
5	3	3	4	2	2	6253.226	6253.227	-0.6
9	1	8	8	2	7	6482.904	6482.908	-4.1
10	1	10	9	0	9	6601.307	6601.308	-1.0
9	2	8	8	1	7	6660.234	6660.230	4.3
4	4	1	3	3	0	6750.486	6750.484	2.4
5	3	2	4	2	3	6754.233	6754.230	2.9
4	4	0	3	3	1	6755.054	6755.050	3.5
6	3	4	5	2	3	6773.473	6773.471	2.0
10	1	9	9	2	8	7156.821	7156.818	2.9
5	4	1	4	3	2	7552.837	7552.835	2.3

Table S44: Assigned rotational transitions for $^{13}C_6$ isotopologue of the xanthene-H_2O complex, 1w-I.

J'	K_a'	K_c'	J"	K_a"	K_c"	ν_{obs}/MHz	ν_{calc}/MHz	$\Delta\nu$/kHz
4	1	3	3	2	2	2199.700	2199.699	1.0
4	0	4	3	1	3	2663.831	2663.833	-1.8
4	3	2	4	2	3	2698.462	2698.446	16.7
6	1	5	6	0	6	2831.026	2831.028	-2.4
5	3	3	5	2	4	2836.908	2836.907	0.9
4	1	4	3	0	3	2982.843	2982.845	-2.6
2	2	1	1	1	0	3050.437	3050.449	-11.8
5	1	4	4	2	3	3194.904	3194.906	-2.2
2	2	0	1	1	1	3228.910	3228.917	-7.0
5	0	5	4	1	4	3380.002	3380.003	-0.9
5	1	5	4	0	4	3546.034	3546.038	-3.9
3	2	2	2	1	1	3683.408	3683.405	2.2
6	0	6	5	1	5	4057.169	4057.170	-1.2
6	1	6	5	0	5	4135.642	4135.649	-7.6
6	1	5	5	2	4	4142.349	4142.351	-2.0
4	2	3	3	1	2	4240.068	4240.077	-8.3
7	0	7	6	1	6	4711.389	4711.392	-3.0
7	0	7	6	1	6	4711.389	4711.392	-2.8
5	2	4	4	1	3	4732.504	4732.508	-4.0
7	1	7	6	0	6	4746.141	4746.136	5.1
3	3	1	2	2	0	4933.615	4933.620	-5.2
3	3	0	2	2	1	4968.660	4968.660	-0.2
7	1	6	6	2	5	5009.401	5009.400	1.2
6	2	5	5	1	4	5187.742	5187.745	-2.2

J'	K_a'	K_c'	J"	K_a"	K_c"	ν_{obs}/MHz	ν_{calc}/MHz	$\Delta\nu$/kHz
8	0	8	7	1	7	5353.880	5353.863	17.6
8	1	8	7	0	7	5368.575	5368.570	5.0
7	2	6	6	1	5	5645.679	5645.688	-8.9
4	3	2	3	2	1	5649.875	5649.873	1.8
8	1	7	7	2	6	5792.024	5792.024	-0.5
4	3	1	3	2	2	5824.619	5824.614	5.8
9	0	9	8	1	8	5990.835	5990.830	4.5
9	1	9	8	0	8	5996.861	5996.858	2.8
8	2	7	7	1	6	6141.381	6141.384	-3.0
5	3	3	4	2	2	6274.009	6274.014	-4.6
10	0	10	9	1	9	6625.387	6625.380	6.9
9	2	8	8	1	7	6685.896	6685.905	-8.2
4	4	1	3	3	0	6771.969	6771.973	-3.4
4	4	0	3	3	1	6776.589	6776.582	6.4
5	3	2	4	2	3	6778.430	6778.424	6.4
6	3	4	5	2	3	6796.080	6796.082	-1.2
7	3	5	6	2	4	7229.851	7229.845	5.4
5	4	1	4	3	2	7577.759	7577.762	-2.2

Table S45: Assigned rotational transitions for $^{13}C_7$ isotopologue of the xanthene-H_2O complex, 1w-I.

J'	K_a'	K_c'	J"	K_a"	K_c"	ν_{obs}/MHz	ν_{calc}/MHz	$\Delta\nu$/kHz
3	1	3	2	0	8	2428.141	2428.141	0.0
4	1	4	3	0	4	2977.883	2977.893	-10.6

J'	K_a'	K_c'	J"	K_a"	K_c"	ν_{obs}/MHz	ν_{calc}/MHz	$\Delta\nu$/kHz
5	0	5	4	1	6	3380.890	3380.884	5.8
5	1	5	4	0	4	3541.726	3541.733	-7.5
6	0	6	5	1	5	4056.614	4056.623	-9.2
6	1	6	5	0	5	4132.060	4132.055	4.7
7	0	7	6	1	5	4709.849	4709.843	6.1
7	1	7	6	0	6	4742.974	4742.978	-4.7
7	1	6	6	2	2	5017.412	5017.418	-6.3
6	2	5	5	1	5	5173.328	5173.331	-3.6
4	3	2	3	2	4	5627.761	5627.764	-3.6
4	3	1	3	2	1	5805.718	5805.711	6.5
9	0	9	8	1	3	5988.120	5988.122	-2.0
9	1	9	8	0	8	5993.780	5993.782	-2.3
5	3	3	4	2	2	6250.291	6250.293	-2.1
4	4	1	3	3	2	6742.225	6742.223	1.4
4	4	0	3	3	0	6746.979	6746.982	-3.3
11	1	11	10	0	1	7256.406	7256.392	14.4
5	4	1	4	3	10	7549.113	7549.110	3.8

3.3 Frequency list of the xanthene-$(H_2O)_2$ complex

Table S46: Assigned rotational transitions for the xanthene-$(H_2O)_2$ complex, 2w-III.

J'	K_a'	K_c'	J"	K_a"	K_c"	ν_{obs}/MHz	ν_{calc}/MHz	$\Delta\nu$/kHz
3	1	2	2	1	1	2157.425	2157.411	14.2
7	2	5	7	2	6	2240.000	2239.997	3.0

J'	K_a'	K_c'	J"	K_a"	K_c"	ν_{obs}/MHz	ν_{calc}/MHz	$\Delta\nu$/kHz
4	1	4	3	1	3	2256.573	2256.574	-0.2
4	0	4	3	0	3	2287.405	2287.408	-2.5
4	1	4	3	0	3	2303.216	2303.189	27.0
4	2	3	3	2	2	2592.335	2592.330	5.8
3	2	2	2	1	1	2597.007	2597.007	-0.3
4	3	2	3	3	1	2720.666	2720.662	3.7
5	0	5	4	1	4	2771.470	2771.473	-2.6
4	1	3	3	1	2	2776.243	2776.234	-1.8
5	1	5	4	1	4	2776.243	2776.253	-1.8
5	0	5	4	0	4	2787.254	2787.254	0.4
4	2	2	3	2	1	2939.937	2939.929	8.0
9	5	5	9	3	6	2971.628	2971.626	1.8
10	4	6	9	6	3	3137.992	3137.987	5.0
5	2	4	4	2	3	3173.024	3173.019	4.9
6	0	6	5	1	5	3288.283	3288.289	-5.2
6	1	6	5	1	5	3289.639	3289.642	-2.8
6	0	6	5	0	5	3293.062	3293.069	-7.2
6	1	6	5	0	5	3294.428	3294.423	4.7
5	1	4	4	1	3	3309.877	3309.877	-0.3
3	3	0	2	2	0	3371.696	3371.697	-1.5
5	3	3	4	3	2	3388.555	3388.548	7.1
3	3	1	2	2	1	3413.795	3413.799	-4.0
5	4	2	4	4	1	3422.303	3422.292	10.5
3	3	0	2	2	1	3428.512	3428.511	1.7
5	3	2	4	3	1	3601.904	3601.887	16.9
5	2	3	4	2	2	3660.216	3660.213	3.0

J'	K_a'	K_c'	J"	K_a"	K_c"	ν_{obs}/MHz	ν_{calc}/MHz	$\Delta\nu$/kHz
6	1	5	5	2	4	3677.718	3677.712	6.6
6	2	5	5	2	4	3723.692	3723.681	11.4
6	1	5	5	1	4	3796.544	3796.546	-1.8
7	0	7	6	1	6	3800.286	3800.283	2.8
7	1	7	6	1	6	3800.641	3800.650	-8.6
7	0	7	6	0	6	3801.633	3801.637	-4.0
4	3	2	3	2	1	3910.841	3910.856	-15.2
4	2	3	3	1	3	3914.307	3914.287	19.5
4	3	1	3	2	1	4003.967	4003.955	11.2
6	3	4	5	3	3	4026.397	4026.395	2.4
6	4	3	5	4	2	4123.840	4123.840	-0.4
4	3	2	3	2	2	4155.869	4155.862	7.1
6	4	2	5	4	1	4213.775	4213.764	11.6
4	3	1	3	2	2	4248.976	4248.961	14.8
7	2	6	6	2	5	4253.046	4253.056	-10.5
7	1	6	6	1	5	4283.275	4283.278	-2.9
6	2	4	5	2	3	4297.779	4297.773	5.7
8	1	8	7	1	7	4310.889	4310.894	-4.8
8	0	8	7	0	7	4311.158	4311.164	-5.9
5	2	3	4	1	3	4508.516	4508.511	5.6
4	4	1	3	3	1	4619.401	4619.401	-0.4
4	4	0	3	3	1	4622.528	4622.527	1.0
7	3	5	6	3	4	4627.512	4627.507	4.4
5	3	2	4	2	2	4665.907	4665.913	-6.1
4	3	1	3	1	2	4688.545	4688.558	-12.7
8	2	7	7	2	6	4770.641	4770.639	1.1

J'	K_a'	K_c'	J"	K_a"	K_c"	ν_{obs}/MHz	ν_{calc}/MHz	$\Delta\nu$/kHz
8	1	7	7	1	6	4781.404	4781.404	0.3
8	2	7	7	1	6	4786.389	4786.387	1.9
7	4	4	6	4	3	4810.361	4810.357	4.3
9	0	9	8	1	8	4820.921	4820.900	2.0
9	1	9	8	1	8	4820.921	4820.925	2.0
9	0	9	8	0	8	4820.988	4820.996	-14.0
9	1	9	8	0	8	4820.988	4821.021	-14.0
7	2	5	6	2	4	4839.146	4839.161	-14.7
7	5	2	6	5	1	4850.056	4850.046	9.2
7	4	3	6	4	2	5038.100	5038.106	-5.9
7	3	4	6	3	3	5163.205	5163.224	-18.2
8	3	6	7	3	5	5193.319	5193.322	-3.2
9	2	8	8	2	7	5282.990	5282.995	-4.4
9	1	8	8	1	7	5286.485	5286.486	-0.8
8	2	6	7	2	5	5317.707	5317.713	-5.5
10	0	10	9	1	9	5330.920	5330.900	5.2
10	1	10	9	1	9	5330.920	5330.906	5.2
10	0	10	9	0	9	5330.920	5330.924	5.2
10	1	10	9	0	9	5330.920	5330.930	5.2
8	4	5	7	4	4	5467.316	5467.329	-13.2
6	2	4	5	1	4	5496.412	5496.407	5.0
8	6	3	7	6	2	5503.835	5503.830	4.7
8	6	2	7	6	1	5511.246	5511.250	-4.3
8	5	4	7	5	3	5537.140	5537.136	3.4
8	5	3	7	5	2	5632.570	5632.588	-18.2
9	2	7	8	2	6	5789.443	5789.442	1.0

J'	K_a'	K_c'	J"	K_a"	K_c"	ν_{obs}/MHz	ν_{calc}/MHz	$\Delta\nu$/kHz
10	2	9	9	2	8	5793.449	5793.446	3.2
10	1	9	9	1	8	5794.522	5794.509	12.7
8	3	5	7	3	4	5823.184	5823.210	-25.5
5	5	1	4	4	0	5833.432	5833.432	0.5
5	5	0	4	4	0	5834.034	5834.030	4.6
5	5	1	4	4	1	5836.568	5836.558	10.6
5	5	0	4	4	1	5837.163	5837.156	7.1
11	0	11	10	1	10	5840.877	5840.877	0.0
11	1	11	10	1	10	5840.877	5840.879	0.0
11	0	11	10	0	10	5840.877	5840.883	0.0
11	1	11	10	0	10	5840.877	5840.885	0.0
6	4	3	5	3	3	6056.323	6056.323	0.3
9	4	6	8	4	5	6085.936	6085.952	-16.2
10	3	8	9	3	7	6254.024	6254.017	7.1
10	2	8	9	2	7	6276.588	6276.587	1.3
11	2	10	10	2	9	6303.341	6303.332	9.0
11	1	10	10	1	9	6303.641	6303.642	-0.7
12	0	12	11	1	11	6350.849	6350.852	-3.2
12	1	12	11	1	11	6350.849	6350.852	-3.2
9	3	6	8	3	5	6376.332	6376.329	3.1
11	2	9	10	2	8	6775.813	6775.801	11.2
10	3	7	9	3	6	6850.215	6850.231	-15.7
13	0	13	12	1	12	6860.824	6860.826	-2.4
13	1	13	12	1	12	6860.824	6860.826	-2.4
7	4	3	6	3	4	7184.274	7184.299	-24.9
12	3	10	11	3	9	7278.294	7278.286	8.4

J'	K_a'	K_c'	J"	K_a"	K_c"	ν_{obs}/MHz	ν_{calc}/MHz	$\Delta\nu$/kHz
12	2	10	11	2	9	7280.942	7280.930	11.3

3.4 Frequency list of the xanthene-$(H_2O)_3$ complex

Table S47: Assigned rotational transitions for the xanthene-$(H_2O)_3$ complex, 3w-I.

J'	K_a'	K_c'	J"	K_a"	K_c"	ν_{obs}/MHz	ν_{calc}/MHz	$\Delta\nu$/kHz
3	1	2	2	0	2	2489.939	2489.946	-6.5
5	1	4	4	2	2	2609.182	2609.163	19.9
5	0	5	4	1	3	2661.717	2661.703	13.4
3	2	1	2	1	1	2968.759	2968.768	-8.4
3	2	2	2	1	2	3083.555	3083.561	-6.5
6	0	6	5	1	4	3113.324	3113.316	8.6
4	1	3	3	0	3	3263.005	3263.019	-13.4
6	1	5	5	2	3	3300.407	3300.410	-2.8
4	2	2	3	1	2	3616.591	3616.601	-10.4
3	3	0	2	2	0	3677.181	3677.175	5.7
3	3	1	2	2	1	3681.666	3681.650	16.7
4	2	3	3	1	3	3824.427	3824.436	-8.6
5	1	4	4	0	4	4071.604	4071.608	-4.1
5	2	3	4	1	3	4279.999	4280.010	-11.0
10	1	10	9	2	8	4311.563	4311.567	-3.7
4	3	1	3	2	1	4341.482	4341.482	0.1
4	3	2	3	2	2	4362.910	4362.911	-1.3
5	2	4	4	1	4	4587.335	4587.331	4.1

J'	K_a'	K_c'	J"	K_a"	K_c"	ν_{obs}/MHz	ν_{calc}/MHz	$\Delta\nu$/kHz
6	1	5	5	0	5	4918.721	4918.717	4.1
6	2	4	5	1	4	4969.550	4969.566	-15.2
5	3	2	4	2	2	4992.555	4992.567	-12.2
4	4	0	3	3	0	5016.381	5016.368	13.3
4	4	1	3	3	1	5016.674	5016.663	10.4
6	2	5	5	1	5	5371.760	5371.763	-2.9
6	3	3	5	2	3	5627.661	5627.673	-12.0
12	3	10	11	4	8	5656.562	5656.570	-8.1
5	4	1	4	3	1	5689.117	5689.104	12.2
5	4	2	4	3	2	5691.130	5691.127	3.2
7	2	5	6	1	5	5692.600	5692.614	-13.7
6	3	4	5	2	4	5754.266	5754.276	-9.9
7	1	6	6	0	6	5800.964	5800.947	16.9
11	1	10	10	2	8	5893.099	5893.087	12.6
7	2	6	6	1	6	6176.665	6176.648	16.6
7	3	4	6	2	4	6250.759	6250.771	-12.0
6	4	2	5	3	2	6358.476	6358.482	-6.1
6	4	3	5	3	3	6366.319	6366.322	-3.0
8	2	6	7	1	6	6454.575	6454.560	14.8
7	3	5	6	2	5	6471.122	6471.115	7.9
7	4	8	6	3	3	7020.941	7020.950	-9.8
6	5	3	5	4	1	7027.312	7027.300	11.2
6	5	1	5	4	2	7027.455	7027.443	12.4
7	4	4	6	3	4	7043.437	7043.447	-9.3
8	3	6	7	2	6	7205.788	7205.797	-9.2
9	3	6	8	2	6	7509.244	7509.239	5.3

J'	K_a'	K_c'	J"	K_a"	K_c"	ν_{obs}/MHz	ν_{calc}/MHz	$\Delta\nu$/kHz
8	4	4	7	3	4	7671.724	7671.737	-12.9
7	5	6	6	4	2	7700.245	7700.235	10.5
7	5	6	6	4	3	7700.933	7700.933	-0.5
8	4	4	7	3	5	7724.525	7724.542	-17.3
9	3	8	8	2	7	7960.202	7960.190	11.3

3.5 Frequency list of the xanthene-$(H_2O)_4$ complex

Table S48: Assigned rotational transitions for the xanthene-$(H_2O)_4$ complex, 4w-II.

J'	K_a'	K_c'	J"	K_a"	K_c"	ν_{obs}/MHz	ν_{calc}/MHz	$\Delta\nu$/kHz
5	0	5	4	1	3	2544.926	2544.923	2.9
4	2	2	3	1	2	3127.570	3127.547	22.7
6	0	6	5	1	5	3434.717	3434.714	2.9
7	0	7	6	1	6	4039.636	4039.627	9.3
4	4	0	3	3	0	4208.104	4208.105	1.9
4	4	1	3	3	0	4208.104	4208.100	1.9
4	4	1	3	3	1	4208.213	4208.212	-2.1
4	4	0	3	3	1	4208.213	4208.217	-2.1
5	3	3	4	2	3	4308.451	4308.451	0.0
5	3	2	4	2	3	4311.563	4311.569	-6.0
5	4	2	4	3	1	4809.824	4809.803	0.6
5	4	1	4	3	1	4809.824	4809.846	0.6
5	4	2	4	3	2	4810.620	4810.589	8.7
5	4	1	4	3	2	4810.620	4810.631	8.7

J'	K_a'	K_c'	J"	K_a"	K_c"	ν_{obs}/MHz	ν_{calc}/MHz	$\Delta\nu$/kHz
6	3	4	5	2	3	4851.023	4851.022	0.7
6	3	3	5	2	3	4860.269	4860.257	11.8
6	3	4	5	2	4	4924.324	4924.336	-11.5
9	0	9	8	1	8	5225.438	5225.436	1.5
5	5	1	4	4	0	5324.449	5324.443	3.2
5	5	1	4	4	1	5324.449	5324.448	3.2
5	5	0	4	4	0	5324.449	5324.444	3.2
5	5	0	4	4	1	5324.449	5324.448	3.2
7	3	5	6	2	4	5409.046	5409.051	-5.4
6	4	3	5	3	2	5410.025	5410.014	10.4
6	4	2	5	3	2	5410.226	5410.225	1.2
6	4	3	5	3	3	5413.137	5413.132	4.8
6	4	2	5	3	3	5413.340	5413.343	-2.3
7	3	4	6	2	4	5431.671	5431.665	6.5
8	1	7	7	0	7	5669.935	5669.932	2.6
10	0	10	9	1	9	5809.483	5809.503	-20.0
10	1	10	9	0	9	5843.194	5843.168	26.1
7	4	4	6	3	3	6006.995	6007.001	-5.8
7	4	4	6	3	4	6016.235	6016.236	-1.3
7	4	3	6	3	4	6016.992	6017.002	-10.3
11	1	11	10	0	10	6410.323	6410.339	-15.7
8	4	5	7	3	5	6620.652	6620.664	-12.2
8	4	4	7	3	5	6622.934	6622.938	-4.0
7	6	2	6	5	1	7042.935	7042.923	11.2
7	6	2	6	5	2	7042.935	7042.925	11.2
8	5	4	7	4	3	7129.441	7129.441	-23.8

J'	K_a'	K_c'	J"	K_a"	K_c"	ν_{obs}/MHz	ν_{calc}/MHz	$\Delta\nu$/kHz
8	5	3	7	4	3	7129.441	7129.491	-23.8
8	5	4	7	4	4	7130.230	7130.206	-2.5
8	5	3	7	4	4	7130.230	7130.257	-2.5
9	4	5	8	3	6	7233.427	7233.411	15.6

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