Supplementary materials for:

How does the composition of a PAH influence its microsolvation? A rotational spectroscopy study of the phenanthrene-water and phenanthridine-water clusters

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S1. Phenanthridine

S1.1 Experimental results: rotational constants

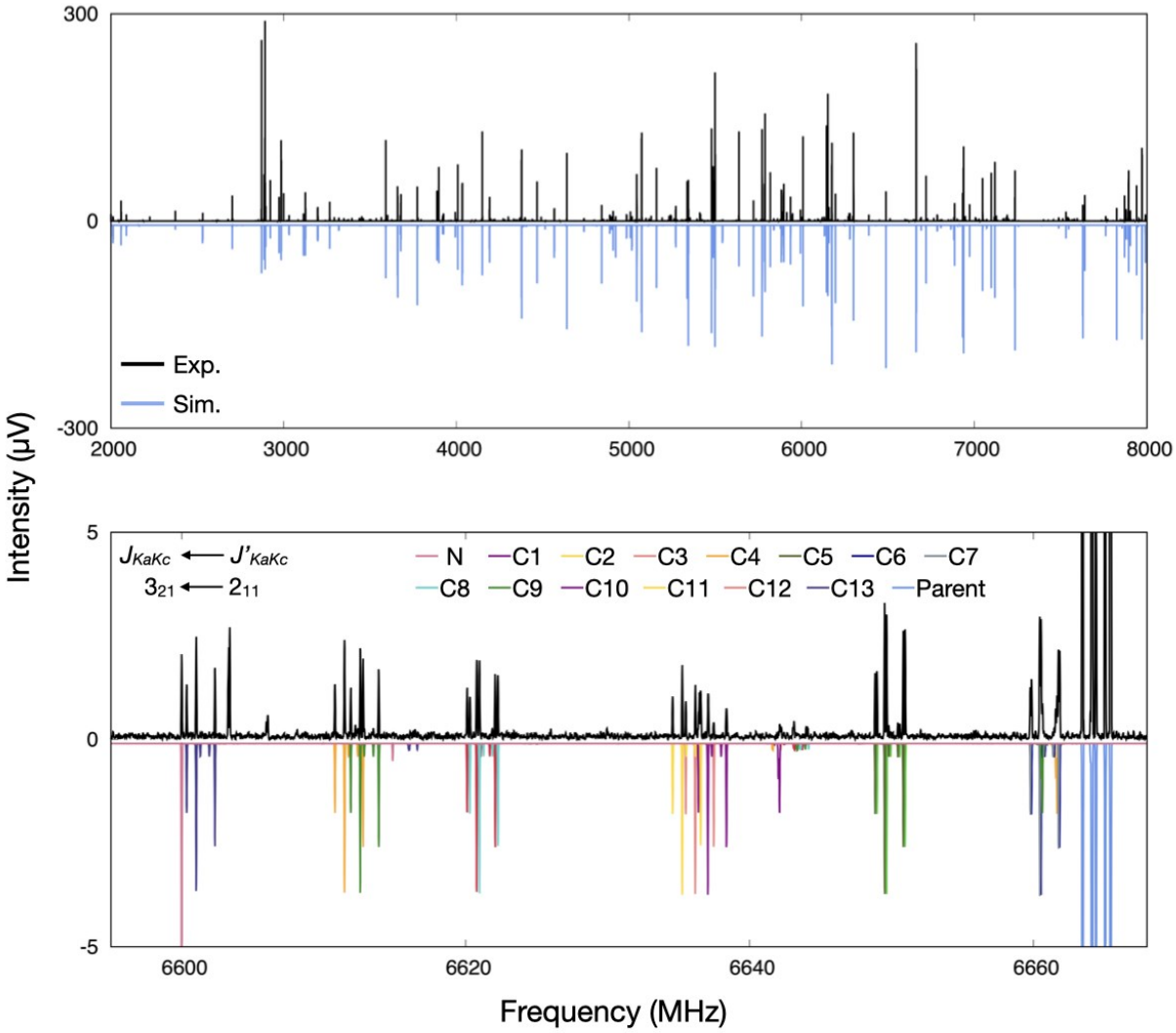


Figure S1 The broadband rotational spectrum of phenanthridine (Pan). The spectrum was recorded in the 2-8 GHz frequency range by heating the sample to 130 °C and using 3.5 bars of the carrier gas neon. The final spectrum was obtained by averaging together 1.4 M free induction decays (FIDs). The top panel shows the spectrum of the monomer in the 2-8 GHz frequency range. The bottom panel corresponds to a zoom of the spectrum showing the assignment of all the ^{13}C and ^{15}N isotopologues of Pan in natural abundance. In both panels, the upper trace (black) corresponds to the experimental spectrum, whereas the lower trace (coloured) represents the simulated spectra generated from the fitted rotational constants. All the spectra, except the one arising from the ^{15}N isotopologue, exhibit the characteristic hyperfine structure generated by the ^{14}N quadrupolar nucleus.

Table S1 Experimental spectroscopic parameters of the monomer of Pan obtained from a global fit. Overall 882 transitions were fitted, of which 600 transitions were measured from this experiment and 282 transitions were measured by McNaughton *et al*. [1] The fit was obtained by using the Watson's Hamiltonian in the A-reduction and the I^r representation implemented in the Pickett's SPFIT/SPCAT program.[2] *A*, *B* and *C* are the rotational constants. $\Delta_J, \Delta_{JK}, \Delta_K, \delta_J$, and δ_K are the centrifugal distortion constants. χ_{aa}, χ_{bb}, and χ_{cc} are the nuclear quadrupole coupling constants. P_a, P_b and P_c are the planar moments of inertia. N is the number of transitions included in the fit. σ is the deviation of the fit.

	Pan global
A (MHz)	1642.457212(25)
*B (*MHz)	557.734698(15)
C (MHz)	416.509513(11)
Δ_J (kHz)	0.003595(17)
Δ_{JK} (kHz)	-0.00176(12)
Δ_K (kHz)	0.05601(16)
δ_J (kHz)	0.0010345(80)
δ_K (kHz)	0.00928(13)
χ_{aa} (MHz)	-0.6131(18)
χ_{bb} (MHz)	-2.5792(21)
χ_{cc} (MHz)	3.1923(21)
P_a (uÅ^2)	905.89916(2)
P_b (uÅ^2)	307.46810(2)
P_c (uÅ^2)	0.22881(2)
N	882
σ (kHz)	7.1

Table S2 Experimental spectroscopic constants for all the ^{13}C and ^{15}N isotopologues of Pan. The fit was obtained by using the Watson's Hamiltonian in the A-reduction and the I^r representation implemented in the Pickett's SPFIT/SPCAT program.[2] *A, B* and *C* are the rotational constants. P_a, P_b and P_c are the planar moments of inertia. N is the number of transitions included in the fit. σ is the deviation of the fit. Centrifugal distortion constants and nuclear quadrupole coupling constants have been kept fixed to the values of the parent species.

	$^{13}C_1$	**$^{13}C_2$**	**$^{13}C_3$**	**$^{13}C_4$**	**$^{13}C_5$**	**$^{13}C_6$**	**$^{13}C_7$**
A (MHz)	1638.82494(48)	1638.41216(51)	1642.04916(54)	1630.21838(49)	1629.07357(48)	1641.55995(68)	1641.56164(77)
*B (*MHz)	556.57858(17)	552.99681(16)	550.19377(17)	552.70008(15)	556.37389(15)	557.44132(21)	557.41992(25)
C (MHz)	415.63129(11)	413.604921(94)	412.264093(92)	412.914597(94)	414.887523(93)	416.28863(16)	416.27667(17)
P_a (uÅ^2)	907.78118(35)	913.66153(20)	918.31811(20)	914.15307(19)	908.11515(19)	906.37541(30)	906.41042(30)
P_b (uÅ^2)	308.14990(35)	308.22675(20)	307.54418(20)	309.77800(19)	309.99573(19)	307.63566(30)	307.63553(30)
P_c (uÅ^2)	0.22898(35)	0.22983(20)	0.22919(20)	0.22893(19)	0.22906(19)	0.22944(30)	0.22924(30)
N	82	95	83	94	91	72	76
σ (kHz)	6.5	6.4	6.2	6.2	6.0	8.2	9.5

	$^{13}C_8$	**$^{13}C_9$**	**$^{13}C_{10}$**	**$^{13}C_{11}$**	**$^{13}C_{12}$**	**$^{13}C_{13}$**	**^{15}N**
A (MHz)	1629.22607(55)	1630.75979(51)	1642.16337(60)	1638.12694(70)	1638.79887(46)	1620.84897(42)	1620.51356(67)
*B (*MHz)	556.30241(18)	552.56739(17)	550.08678(18)	552.96959(15)	556.56265(18)	557.52783(14)	557.42392(20)
C (MHz)	414.85749(10)	412.87539(10)	412.21080(11)	413.571447(80)	415.62068(10)	414.991351(86)	414.91173(11)
P_a (uÅ^2)	908.23212(21)	914.37243(21)	918.49739(23)	913.70662(18)	907.80724(21)	906.23567(17)	906.40474(24)
P_b (uÅ^2)	309.96694(21)	309.67487(21)	307.52339(23)	308.28056(18)	308.15488(21)	311.57044(17)	311.63507(24)
P_c (uÅ^2)	0.22881(21)	0.22915(21)	0.22857(23)	0.22972(18)	0.22891(21)	0.22850(17)	0.22841(24)
N	7.1	6.9	7.6	5.7	6.7	5.9	5.3
σ (kHz)	94	91	90	88	82	94	41

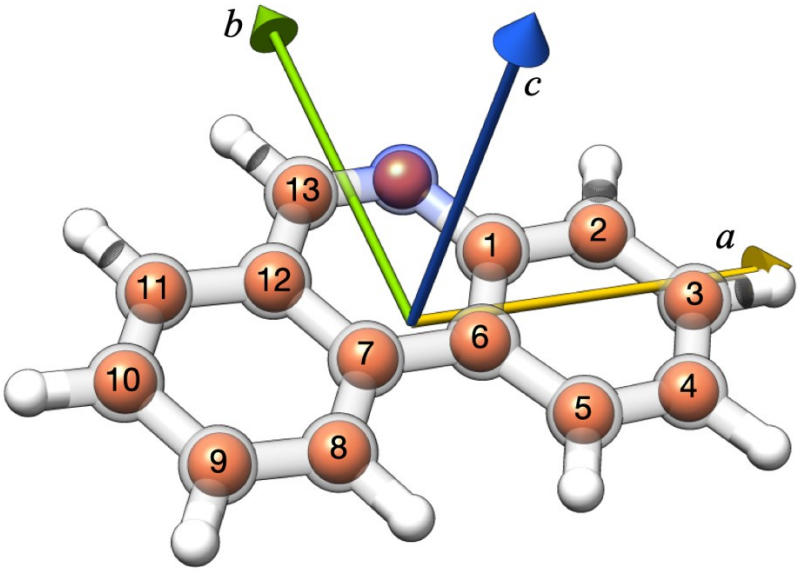


Figure S2 Comparison between the r_e and r_s structures of Pan projected in the principal axis system. The full body of the molecule represents the equilibrium structure (r_e) calculated at the MP2/aug-cc-pVDZ level of theory. The orange spheres represent the carbon and nitrogen positions determined using the Kraitchman's equations (r_s).

Table S3 The r_e, r_s and $r_m^{(1)}$ coordinates (Å) of the carbon and nitrogen atoms of Pan. The theoretical coordinates have been calculated at the MP2/aug-cc-pVDZ level of theory. The numbering of the atoms corresponds to the one reported in Figure S2. Pan is a planar molecule and, therefore, the *c* coordinate of the atoms is not reported.

	r_e	r_s	r_m^1	r_e	r_s	r_m^1
	$\|a\|$	$\|a\|$	$\|a\|$	$\|b\|$	$\|b\|$	$\|b\|$
C1	1.382	1.3726(11)	1.3718(13)	0.839	0.8279(18)	0.8313(14)
C2	2.796	2.7875(5)	2.7853(10)	0.883	0.8776(17)	0.8819(13)
C3	3.541	3.5278(4)	3.5252(9)	0.286	0.2790(54)	0.2866(23)
C4	2.883	2.8706(5)	2.8683(10)	1.535	1.5320(10)	1.5336(8)
C5	1.495	1.4871(10)	1.4862(13)	1.601	1.5946(9)	1.5957(8)
C6	0.711	0.6908(22)	0.6920(22)	0.421	0.4100(37)	0.4136(28)
C7	0.738	0.7157(25)	0.7176(21)	0.420	0.4098(44)	0.4127(28)
C8	1.535	1.5259(10)	1.5251(12)	1.590	1.5856(10)	1.5866(8)
C9	2.922	2.9088(5)	2.9065(10)	1.503	1.4977(10)	1.4993(8)
C10	3.564	3.5532(4)	3.5507(9)	0.245	0.2379(63)	0.2447(23)
C11	2.805	2.7954(5)	2.7933(10)	0.916	0.9082(17)	0.9122(13)
C12	1.392	1.3821(11)	1.3815(13)	0.844	0.8310(18)	0.8342(14)
C13	0.586	0.5788(26)	0.5788(27)	2.035	2.0283(7)	2.0289(6)
N14	0.720	0.7116(21)	0.7104(24)	2.051	2.0509(7)	2.0518(6)

Table S4 The r_e, r_s and r_m^1 bond lengths (Å) of Pan. The theoretical (r_e) bond lengths have been calculated at the MP2/aug-cc-pVDZ level of theory. The numbering of the atoms corresponds to the one reported in Figure S2.

	r_e	r_s	r_m^1
C1–C2	1.42	1.416(2)	1.414(1)
C2–C3	1.39	1.373(5)	1.383(3)
C3–C4	1.41	1.415(5)	1.409(2)
C4–C5	1.39	1.385(1)	1.384(1)
C5–C6	1.42	1.427(3)	1.424(3)
C6–C7	1.45	1.407(3)	1.410(4)
C7–C8	1.42	1.428(11)	1.425(2)
C8–C9	1.39	1.386(9)	1.384(1)
C9–C10	1.41	1.415(6)	1.410(2)
C10–C11	1.39	1.374(6)	1.383(2)
C11–C12	1.41	1.416(3)	1.414(1)
C12–C13	1.44	1.442(3)	1.439(2)
C13–N	1.31	1.291(3)	1.289(5)
N–C1	1.38	1.390(2)	1.388(6)
C1–C6	1.43	1.413(4)	1.414(1)
C12–C7	1.42	1.408(5)	1.413(3)

S2. Phenanthridine-H_2O complexes

S2.1 Experimental results: rotational constants

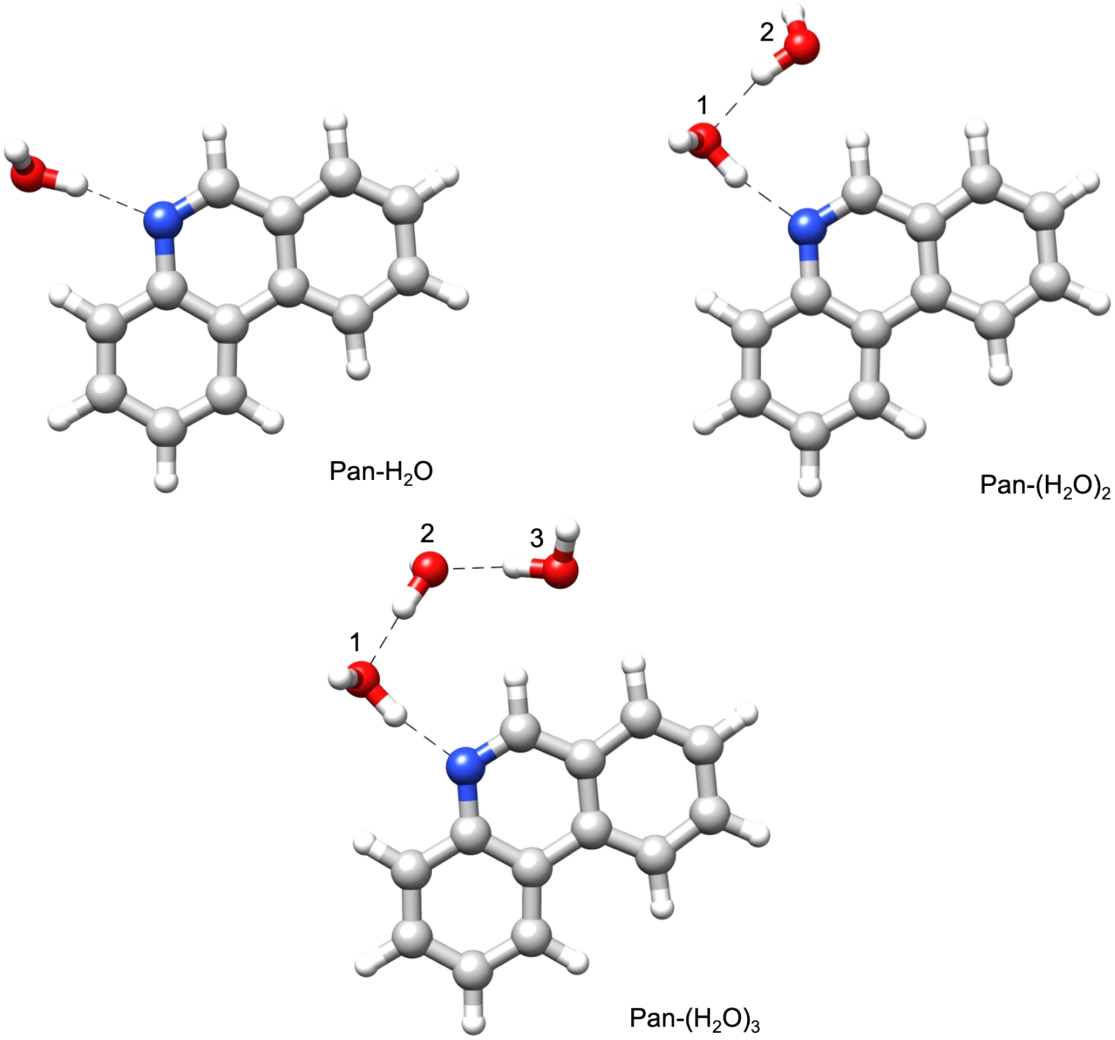


Figure S3 *Ab initio* structures of the observed Pan-$(H_2O)_{n=1\text{-}3}$ complexes, calculated at the MP2/aug-cc-pVDZ level of theory. The numbering scheme corresponds to the labels given to the oxygen atoms upon isotopic substitution.

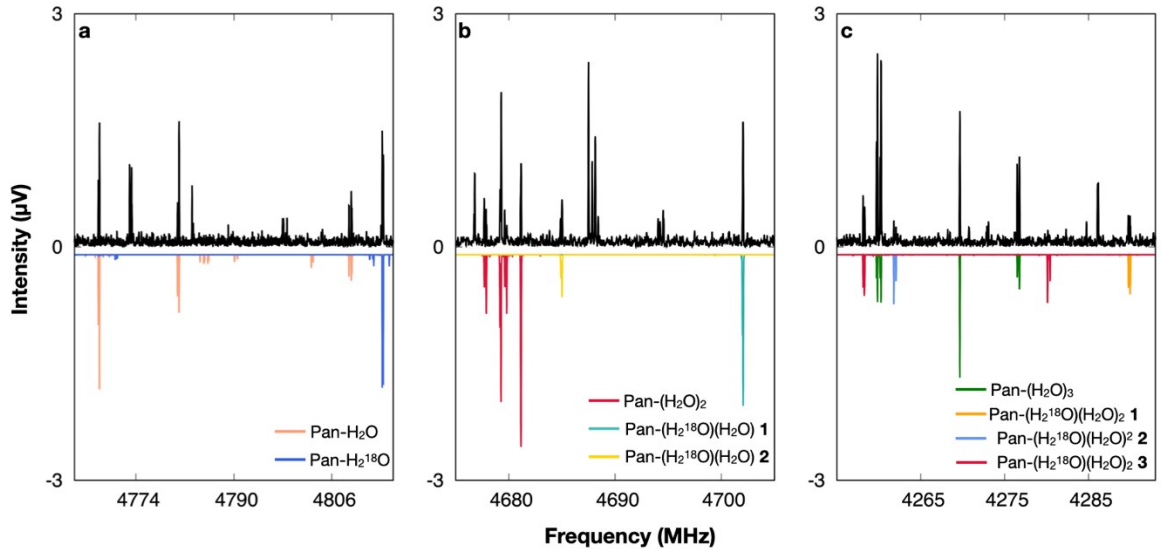


Figure S4 Representative sections of the spectrum arising from the Pan-$(H_2O)_{n=1-3}$ complexes and their ^{18}O singly-substituted isotopologues. The a, b, and c panels show representative transitions arising from Pan-H_2O and its ^{18}O isotopologue, Pan-$(H_2O)_2$ and its two singly-substituted ^{18}O isotopologues, and Pan-$(H_2O)_3$ and its three singly-substituted ^{18}O isotopologues, respectively. In all the panels, the upper trace (black) corresponds to the experimental spectrum, whereas the lower trace corresponds to the simulated spectra generated from the fitted rotational constants. The numbers **1**, **2** and **3** reported in bold correspond to ^{18}O substituted water molecule according to the numbering reported in Figure S3.

Table S5 Experimental spectroscopic parameters of the Pan-H_2O complex and it ^{18}O singly-substituted isotopologue. The fit was obtained by using the Watson's Hamiltonian in the A-reduction and the I^r representation implemented in the Pickett's SPFIT/SPCAT program.[2] *A*, *B* and *C* are the rotational constants. Δ_J, Δ_{JK}, Δ_K, and δ_J are the centrifugal distortion constants. χ_{aa}, χ_{bb}, and χ_{cc} are the nuclear quadrupole coupling constants. P_a, P_b and P_c are the planar moments of inertia. N is the number of transitions included in the fit. σ is the deviation of the fit.

	Pan-(H_2O)	**Pan-($H_2{}^{18}O$)**
A (MHz)	914.41591(24)	889.60643(89)
*B (*MHz)	471.04386(11)	459.92554(25)
C (MHz)	311.110540(89)	303.38357(18)
Δ_J (kHz)	0.01791(53)	0.0210(14)
Δ_{JK} (kHz)	-0.1222(22)	-0.1349(98)
Δ_K (kHz)	0.665(12)	0.594(44)
δ_J (kHz)	0.00759(29)	0.00853(84)
χ_{aa} (MHz)	-2.6107(35)	-2.678(13)
χ_{bb} (MHz)	-0.3110(49)	-0.237(17)
χ_{cc} (MHz)	2.9218(49)	2.915(17)
P_a (uÅ^2)	1072.32376(27)	1098.27191(64)
P_b (uÅ^2)	552.11174(27)	567.53683(64)
P_c (uÅ^2)	0.56785(27)	0.55596(64)
N	441	277
σ (kHz)	6.5	10.0

Table S6 Experimental spectroscopic parameters of the Pan-$(H_2O)_2$ complex and its ^{18}O singly-substituted isotopologues. The (1) and (2) indicate the substituted oxygen atom according to the numbering reported in Figure S3. The fit was obtained by using the Watson's Hamiltonian in the A-reduction and the I^r representation implemented in the Pickett's SPFIT/SPCAT program.[2] *A, B*, and *C* are the rotational constants. Δ_J, Δ_{JK}, Δ_K, δ_J, and δ_K are the centrifugal distortion constants. χ_{aa}, χ_{bb}, and χ_{cc} are the nuclear quadrupole coupling constants. P_a, P_b and P_c are the planar moments of inertia. N is the number of transitions included in the fit. σ is the deviation of the fit.

	Pan-$(H_2O)_2$	**Pan-$(H_2{}^{18}O)$ (H_2O) (1)**	**Pan-(H_2O) $(H_2{}^{18}O)$ (2)**
A (MHz)	517.04406(16)	516.08272(69)	514.8407(12)
B (MHz)	468.95668(11)	455.02784(50)	452.6402(10)
C (MHz)	246.430565(81)	242.32177(14)	241.37218(17)
Δ_J (kHz)	0.01968(82)	0.0197(39)	0.0176(76)
Δ_{JK} (kHz)	0.1830(32)	0.172(11)	0.224(25)
Δ_K (kHz)	-0.1882(45)	-0.176(17)	-0.214(51)
δ_J (kHz)	0.00814(40)	0.0083(19)	0.0067(39)
δ_K (kHz)	0.1141(14)	0.1161(40)	0.137(14)
χ_{aa} (MHz)	-2.761(32)	-2.797(19)	-2.599(56)
χ_{bb} (MHz)	0.059(19)	0.096(25)	-0.113(54)
χ_{cc} (MHz)	2.703(19)	2.701(25)	2.711(54)
P_a (uÅ^2)	1075.51226(39)	1108.4827(11)	1114.3333(18)
P_b (uÅ^2)	975.28450(39)	977.0873(11)	979.4416(18)
P_c (uÅ^2)	2.15445(39)	2.1724(11)	2.1805(18)
N	407	284	275
σ (kHz)	5.8	8.7	10.1

Table S7 Experimental spectroscopic parameters of the Pan-$(H_2O)_3$ complex and it ^{18}O singly-substituted isotopologues. The (1), (2), and (3) indicate the substituted oxygen atom according to the numbering reported in Figure S3. The fit was obtained by using the Watson's Hamiltonian in the A-reduction and the I^r representation implemented in the Pickett's SPFIT/SPCAT program.[2] *A*, *B*, and *C* are the rotational constants. Δ_J, δ_J, and δ_K are the centrifugal distortion constants. χ_{aa}, χ_{bb}, and χ_{cc} are the nuclear quadrupole coupling constants. P_a, P_b and P_c are the planar moments of inertia. N is the number of transitions included in the fit. σ is the deviation of the fit.

	Pan-$(H_2O)_3$	**Pan-$(H_2O)_2(H_2{}^{18}O)$ (1)**	**Pan-$(H_2O)_2(H_2{}^{18}O)$ (2)**	**Pan-$(H_2O)_2(H_2{}^{18}O)$ (3)**
A (MHz)	475.70658(34)	467.4677(14)	473.5451(10)	474.5935(14)
B (MHz)	347.91926(14)	345.01476(54)	338.33188(36)	339.69013(42)
C (MHz)	203.57118(10)	201.08058(20)	200.00152(16)	200.55394(26)
Δ_J (kHz)	0.02792(32)	0.0171(11)	0.0217(12)	0.0164(13)
δ_J (kHz)	0.01050(18)	0.00512(68)	0.00639(69)	0.00462(87)
δ_K (kHz)	0.0351(15)	-	-	-
χ_{aa} (MHz)	0.3453(87)	0.153(63)	0.197(42)	0.457(42)
χ_{bb} (MHz)	-2.898(18)	-2.784(63)	-2.760(45)	-2.992(51)
χ_{cc} (MHz)	2.552(18)	2.596(63)	2.564(45)	2.536(51)
P_a (uÅ^2)	1436.38331(78)	1448.5103(23)	1476.6943	1471.4066(25)
P_b (uÅ^2)	1046.18325(78)	1064.8056(23)	1050.1815(17)	1048.5090(25)
P_c (uÅ^2)	16.19222(78)	16.2937(23)	17.0432(17)	16.3581(25)
N	426	144	145	148
σ (kHz)	6.7	8.8	6.8	9.8

S2.2 Structural determination

The availability of the rotational constants of the parent species and of all the ^{18}O singly-substituted isotopologues for all the observed Pan-$(H_2O)_{n=1-3}$ complexes allowed for the determination of the exact position of the water with respect to the molecule of Pan. In this work, we have determined the substitution structure (r_s),[4] the effective structure (r_0) and the mass dependent structure ($r_m^{(1)}$). [5,6] A comparison of the results obtained with all of the structural determination methods employed in this work is provided below.

Table S8 Comparison of the r_e, r_s, r_0 and $r_m^{(1)}$ principal coordinates for the oxygen atom in the Pan-H_2O complex. All the coordinates are provided in their absolute values. Theoretical coordinates have been calculated at the MP2/aug-cc-pVDZ level of theory. The *c* coordinate of the O atom is not reported because the complex is planar.

	Pan-H_2O			
O	$\|a\|$	δa	$\|b\|$	δb
r_e	3.551	-	2.833	-
r_s	3.5624	0.0004	2.8570	0.0005
r_0^a	3.5624	0.0088	2.8546	0.0035
$r_m^{(1)b}$	3.5777	0.0019	2.8558	0.0026

[a] Fit of 3 parameters to 6 rotational constants, σ_{fit} = 0.111 uÅ^2
[b] Fit of 5 parameters to 6 rotational constants, σ_{fit} = 0.020 uÅ^2

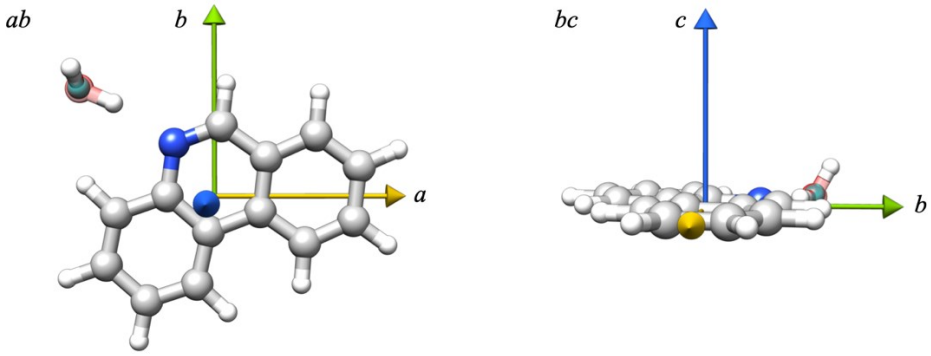


Figure S5 Comparison between the *ab initio* structure (r_e) and the substitution structure (r_s) of the Pan-H_2O complex projected on the *ab* plane (left) and on the *bc* plane (right) . The full body of the molecule represents the *ab initio* structure calculated at the MP2/aug-cc-pVDZ level of theory. The cyan sphere represents the position of the oxygen atom calculated using Kraitchman's equations.[4]

Table S9 Comparison of the r_e, r_s, r_0 and $r_m^{(1)}$ principal coordinates for the O(1) and O(2) oxygen atoms in the Pan-$(H_2O)_2$ complex. All the coordinates are provided in their absolute values. Theoretical coordinates have been calculated at the MP2/aug-cc-pVDZ level of theory.

	O(1)					
	$\|a\|$	δa	$\|b\|$	δb	$\|c\|$	δc
r_e	3.993	-	1.146	-	0.069	-
r_s	4.0379	0.0004	1.0984	0.0017	0.0966	0.0182
r_0 [a]	4.0289	0.0122	0.9549	0.0469	0.1215	0.0103
$r_m^{(1)}$ [b]	4.0421	0.0023	1.1095	0.0078	0.0871	0.0003
	O(2)					
r_e	4.289	-	1.649	-	0.081	-
r_s	4.3288	0.0004	1.7042	0.0012	0.1170	0.0154
r_0 [a]	4.3213	0.0181	1.6174	0.0570	0.1289	0.0166
$r_m^{(1)}$ [b]	4.3326	0.0022	1.7177	0.0053	0.0696	0.0003

[a] Fit of 5 parameters to 9 rotational constants, σ_{fit} = 0.357 uÅ^2
[b] Fit of 7 parameters to 9 rotational constants, σ_{fit} = 0.020 uÅ^2

Table S10 Comparison of the r_e, r_s, r_0 and $r_m^{(1)}$ values of O(1)–O(2) distances (Å) of the Pan-$(H_2O)_2$ complex.

O(1)–O(2)			
r_e	r_s	r_0 [a]	$r_m^{(1)}$ [b]
2.85	2.826(3)	2.60(1)	2.85(1)

[a] Fit of 5 parameters to 9 rotational constants, σ_{fit} = 0.357 uÅ^2
[b] Fit of 7 parameters to 9 rotational constants, σ_{fit} = 0.020 uÅ^2

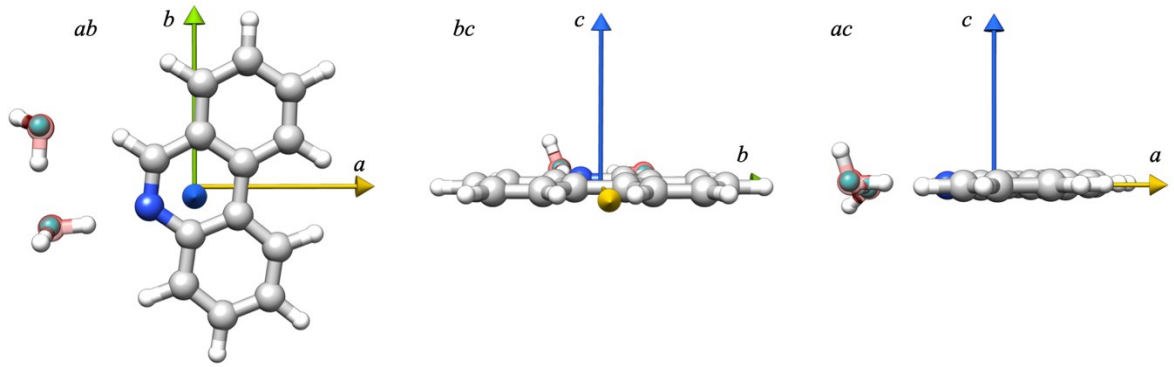


Figure S6 Comparison between the *ab initio* structure (r_e) and the substitution structure (r_s) of the Pan-$(H_2O)_2$ complex projected on the *ab*, *bc* and *ac* planes of symmetry . The full body of the molecule represents the *ab initio* structure calculated at the MP2/aug-cc-pVDZ level of theory. The cyan spheres represent the position of the oxygen atom calculated using Kraitchman's equations.[4]

Table S11 Comparison of the r_e, r_s, r_0 and $r_m^{(1)}$ principal coordinates for the O(1), O(2), and O(3) oxygen atoms in the Pan-$(H_2O)_3$ complex. All the coordinates are provided in their absolute values. Theoretical coordinates have been calculated at the MP2/aug-cc-pVDZ level of theory.

			O(1)			
	$\lvert a \rvert$	δa	$\lvert b \rvert$	δb	$\lvert c \rvert$	δc
r_e	2.435	-	3.053	-	0.197	-
r_s	2.4106	0.0007	3.1083	0.0005	0.2290	0.0073
r_0 [a]	2.4123	0.0045	3.1103	0.0036	0.1461	0.0240
$r_m^{(1)}$ [b]	2.4106	0.0013	3.1167	0.0016	0.2432	0.0070
			O(2)			
r_e	4.497	-	1.396	-	0.568	-
r_s	4.4795	0.0004	1.4893	0.0011	0.6649	0.0025
r_0 [a]	4.4803	0.0026	1.4927	0.0081	0.6451	0.0017
$r_m^{(1)}$ [b]	4.4827	0.0010	1.5047	0.0038	0.6446	0.0074
			O(3)			
r_e	4.086	-	1.242	-	0.235	-
r_s	4.1854	0.0004	1.1293	0.0015	0.2927	0.0056
r_0 [a]	4.1862	0.0029	1.1340	0.0108	0.2461	0.0331
$r_m^{(1)}$ [b]	4.1892	0.0009	1.1409	0.0039	0.2519	0.0136

[a] Fit of 10 parameters to 12 rotational constants, σ_{fit} = 0.382 uÅ^2
[b] Fit of 10 parameters to 12 rotational constants, σ_{fit} = 0.016 uÅ^2

Table S12 Comparison of the r_e, r_s, r_0 and $r_m^{(1)}$ values of O(1)–O(2) and O(2)–O(3) distances (Å) of the Pan-$(H_2O)_3$ complex.

		O(1)–O(2)		
	r_e	r_s	r_0 [a]	$r_m^{(1)}$ [b]
	2.75	2.775(3)	2.742(9)	2.771(5)
		O(2)–O(3)		
	2.75	2.804(3)	2.79(2)	2.809(7)

[a] Fit of 10 parameters to 12 rotational constants, σ_{fit} = 0.382 uÅ^2
[b] Fit of 10 parameters to 12 rotational constants, σ_{fit} = 0.016 uÅ^2

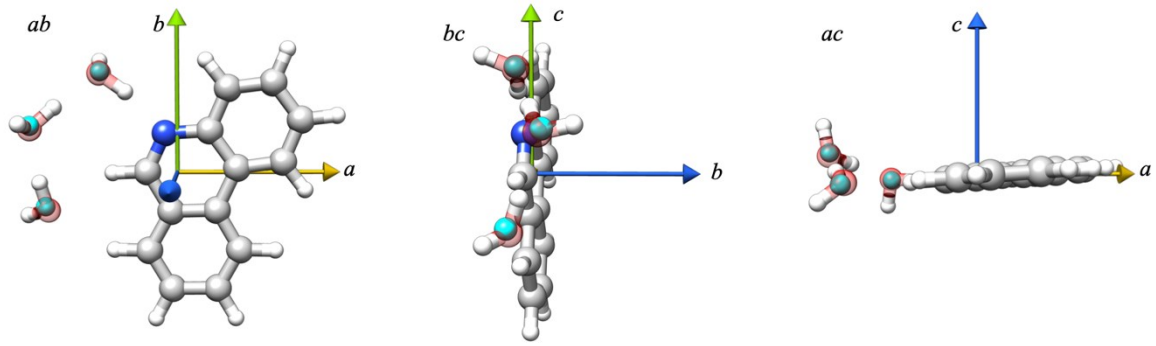


Figure S7 Comparison between the *ab initio* structure (r_e) and the substitution structure (r_s) of the Pan-$(H_2O)_3$ complex projected on the *ab*, *bc* and *ac* planes of symmetry . The full body of the molecule represents the *ab initio* structure calculated at the MP2/aug-cc-pVDZ level of theory. The cyan sphere represents the position of the oxygen atom calculated using Kraitchman's equations.[4]

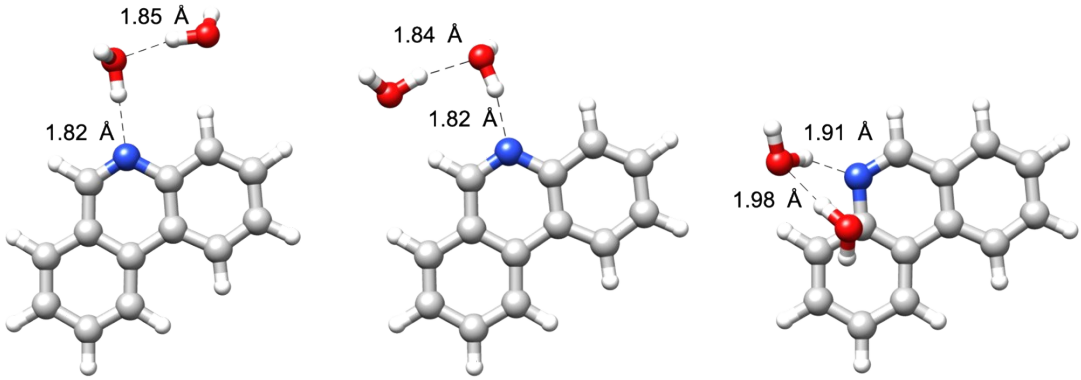
S2.3 Calculated isomers and Cartesian coordinates

The equilibrium theoretical rotational constants (*A*, *B*, *C*) and the principal dipole moment components (μ_a, μ_b, μ_c) are reported in the following tables. The relative energies ($\Delta\Delta E_e$, $\Delta\Delta E(0k)$) for a cluster *k* are defined as: $\Delta\Delta E_k = E_k - \min E_i$ (1) i=0,...n.

Table S13 Theoretical spectroscopic parameters of the isomers of the Pan-$(H_2O)_2$ complex calculated at the MP2/aug-cc-pVDZ and at the B3LYP-D3BJ/def2-TZVP levels of theory.

	pm7-33-3331		hf3c-44-303		pm7-56-139	
	MP2	B3LYP	MP2	B3LYP	MP2	B3LYP
A (MHz)	512.9	522.6	811.8	822.7	776.2	760.9
B (MHz)	470.4	477.1	331.5	337.2	402.2	382.9
C (MHz)	245.8	250.0	236.0	239.8	312.0	288.2
$\lvert\mu_a\rvert$ (D)	3.2	3.5	4.4	4.7	3.0	4.7
$\lvert\mu_b\rvert$ (D)	0.5	0.7	0.4	0.5	0.9	1.2
$\lvert\mu_c\rvert$ (D)	0.4	0.1	0.3	0.1	2.0	2.1
$\Delta\Delta E_e$ (kJ/mol)	0[a]	0[b]	2.4	2.8	10.9	10.4
$\Delta\Delta E$ (0k)	0[c]	0	2.1	2.5	8.1	9.8

[a] MP2-F12/aug-cc-pVTZ-F12//MP2/aug-cc-pVDZ single point energies calculated on the optimised structures at the MP2/aug-cc-pVDZ.
[b] MP2-F12/aug-cc-pVTZ-F12//MP2/aug-cc-pVDZ single point energies combined with harmonic zero-point corrections at the MP2/aug-cc-pVDZ level of theory.
[c] B3LYP-D3BJ/def2-TZVP zero-point corrected energies.



ID:	pm7-33-3331	hf3c-44-303	pm7-56-139
ΔΔEe (kJ/mol)	0.0	2.4	10.9

Figure S8 Theoretical structures calculated at the MP2/aug-cc-pVDZ of the Pan-$(H_2O)_2$ complex. MP2-F12/aug-cc-pVTZ-F12//MP2/aug-cc-pVDZ single point energies calculated on the optimised structures at the MP2/aug-cc-pVDZ are also provided.

Table S14 Calculated spectroscopic parameters at the MP2/aug-cc-pVDZ and at the B3LYP-D3BJ/def2-TZVP levels of theory of the isomers of the Pan-$(H_2O)_3$ complex. At the B3LYP-D3BJ/def2-TZVP isomers hf3c-70-441, hf3c-68-186 and pm7-129-7103 converge into a structure with a low imaginary frequency. Therefore, for these isomers we only provide rotational constants and dipole moment components.

	hf3c-67-452		**hf3c-68-186**		**pm7-78-4104**		**hf3c-70-441**	
	MP2	B3LYP	MP2	B3LYP	MP2	B3LYP	MP2	B3LYP
A (MHz)	472.2	479.2	481.8	478.3	472.5	477.8	472.9	477.7
B (MHz)	349.6	355.8	344.0	351.6	347.1	349.2	345.9	351.0
C (MHz)	202.9	206.2	203.9	204.0	201.0	202.8	200.6	203.3
$\lvert\mu_a\rvert$ (D)	2.3	2.4	3.0	2.9	2.2	2.7	2.5	2.8
$\lvert\mu_b\rvert$ (D)	0.6	0.5	0.1	0.1	0.1	0.0	0.4	0.1
$\lvert\mu_c\rvert$ (D)	0.6	0.8	1.0	1.4	0.3	0.8	1.4	1.4
$\Delta\Delta E_e$(kJ/mol)	**0** [a]	**0**	3.5	-	3.8	3.6	4.0	-
ΔΔE (0k)	**0**[b]	**0**[c]	2.6	-	3.2	3.3	3.5	-

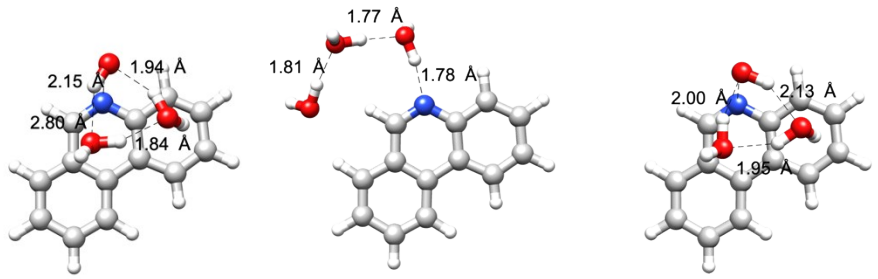
	pm7-123-216		pm7-33-6692		pm7-135-8657		pm7-119-4694	
	MP2	B3LYP	MP2	B3LYP	MP2	B3LYP	MP2	B3LYP
A (MHz)	764.4	770.7	476.5	484.6	731.1	712.2	656.3	626.6
B (MHz)	243.8	248.3	320.3	325.2	253.3	253.6	376.5	382.7
C (MHz)	186.4	190.5	203.7	207.2	199.4	196.8	321.1	311.6
$\lvert\mu_a\rvert$ (D)	4.1	4.5	4.0	4.4	2.3	2.2	3.1	3.3
$\lvert\mu_b\rvert$ (D)	0.5	0.6	2.3	2.2	1.0	0.9	2.8	2.8
$\lvert\mu_c\rvert$ (D)	0.4	0.7	0.7	0.6	0.3	0.0	0.3	0.7
$\Delta\Delta E_e$(kJ/mol)	6.1	7.5	7.1	5.8	7.4	6.6	7.7	7.6
$\Delta\Delta$E (0k)	5.0	7.2	8.7	7.2	8.8	7.5	9.1	8.4
	pm7-108-10038		**pm7-126-12894**		**pm7-120-1962**		**pm7-129-7103**	
	MP2	B3LYP	MP2	B3LYP	MP2	B3LYP	MP2	B3LYP
A (MHz)	647.8	622.1	763.7	743.5	560.6	531.0	759.0	728.4
B (MHz)	379.1	383.2	306.6	271.6	423.0	401.3	309.0	262.2
C (MHz)	320.9	309.2	263.0	215.7	296.6	267.5	266.3	206.0
$\lvert\mu_a\rvert$ (D)	3.1	3.5	3.0	4.3	2.5	4.4	2.9	4.2
$\lvert\mu_b\rvert$ (D)	2.6	2.5	2.2	2.1	3.2	1.9	2.4	2.5
$\lvert\mu_c\rvert$ (D)	0.1	0.4	0.6	0.7	0.2	0.8	0.5	0.2
$\Delta\Delta E_e$(kJ/mol)	8.5	8.4	9.2	5.2	9.2	7.8	10.2	-
$\Delta\Delta$E (0k) (kJ/mol)	10.2	9.2	10.7	6.7	10.3	8.9	11.7	-

[a] MP2-F12/aug-cc-pVTZ-F12//MP2/aug-cc-pVDZ single point energies calculated on the optimised structures at the MP2/aug-cc-pVDZ.

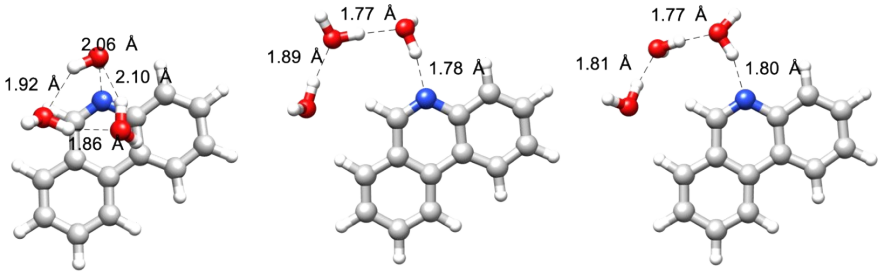
[b] MP2-F12/aug-cc-pVTZ-F12//MP2/aug-cc-pVDZ single point energies combined with harmonic zero-point corrections at the MP2/aug-cc-pVDZ level of theory.

[c] B3LYP-D3BJ/def2-TZVP zero-point corrected energies.

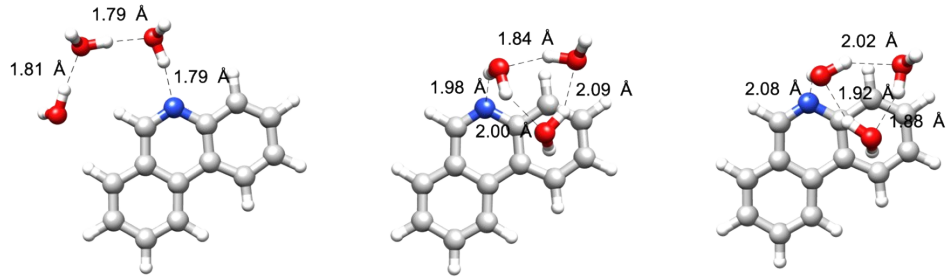
Figure S9 *Ab initio* structures and relative energies (in kJ/mol) calculated at the MP2/aug-cc-pVDZ (bold) level of theory for the isomers of the Pan-$(H_2O)_3$ complex. A comparison of the MP2/aug-cc-pVDZ relative energies with the relative single point energies calculated at the MP2-F12/aug-cc-pVTZ-F12//MP2-aug-cc-pVDZ (non-bold) is also provided to highlight the overestimation of the dispersion interactions by the MP2/aug-cc-pVDZ method, particularly in the Pan-$(H_2O)_3$ complexes in which the water trimer assumes a cyclic motif.



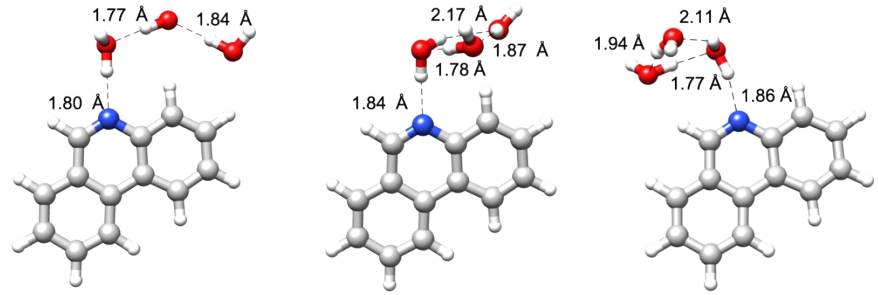
ID:	pm7-119-4694	hf3c-67-452	pm7-108-10038
ΔΔEe (kJ/mol)	**0.0**/7.7	**0.1**/0.0	**0.5**/8.5



ID:	pm7-120-1962	pm7-78-4104	hf3c-68-186
ΔΔEe (kJ/mol)	**2.4**/9.2	**3.6**/3.8	**3.9**/3.5



ID:	hf3c-70-441	pm7-126-12894	pm7-129-7103
ΔΔEe (kJ/mol)	**4.1**/4.0	**4.2**/9.2	**4.4**/10.2



ID:	pm7-123-216	pm7-135-8657	pm7-33-6692
ΔΔEe (kJ/mol)	**6.4**/6.1	**7.4**/7.4	**7.9**/7.1

Table S15 The MP2/aug-cc-pVDZ optimized Cartesian Coordinates of **Pan-H_2O** complex.

	X	Y	Z
N	-1.0556	1.3816	-0.0224
C	1.1977	-0.4126	0.0071
C	-0.1584	-0.9335	0.0053
C	1.3583	1.0080	-0.0105
C	-1.2451	0.0019	-0.0103
C	2.3645	-1.2245	0.0231
C	-0.4636	-2.3226	0.0172
C	0.1821	1.8381	-0.0244
C	2.6572	1.5866	-0.0126
C	-2.5886	-0.4613	-0.0190
C	3.6346	-0.6433	0.0212
C	-1.7894	-2.7612	0.0107
C	3.7858	0.7679	0.0030
C	-2.8585	-1.8297	-0.0082
H	2.2787	-2.3136	0.0368
H	0.3414	-3.0615	0.0297
H	0.3057	2.9290	-0.0381
H	2.7558	2.6770	-0.0271
H	-3.3898	0.2836	-0.0363
H	4.5216	-1.2835	0.0335
H	-2.0020	-3.8344	0.0191
H	4.7863	1.2099	0.0011
H	-3.8933	-2.1833	-0.0161
O	-3.5511	2.8325	-0.0717
H	-2.6536	2.4379	-0.0307
H	-3.6402	3.3092	0.7630

Table S16 The MP2/aug-cc-pVDZ optimized Cartesian Coordinates of the isomer **pm7-33-3331** of the **Pan-$(H_2O)_2$** complex.

	X	Y	Z
N	1.2602	0.5504	-0.0188
C	-1.3587	-0.6438	0.0128
C	-1.2087	0.8014	-0.0003
C	-0.1631	-1.4267	0.0045
C	0.1174	1.3443	-0.0170
C	-2.6100	-1.3176	0.0311
C	-2.3076	1.7047	0.0020
C	1.1146	-0.7631	-0.0109
C	-0.2311	-2.8472	0.0136
C	0.3107	2.7510	-0.0376
C	-2.6633	-2.7134	0.0402
C	-2.0980	3.0852	-0.0151
C	-1.4713	-3.4844	0.0313
C	-0.7831	3.6163	-0.0362
H	-3.5435	-0.7498	0.0381
H	-3.3312	1.3221	0.0155

H	2.0349	-1.3617	-0.0219
H	0.7002	-3.4225	0.0076
H	1.3379	3.1272	-0.0600
H	-3.6345	-3.2166	0.0542
H	-2.9579	3.7615	-0.0138
H	-1.5285	-4.5767	0.0387
H	-0.6280	4.6987	-0.0535
O	3.9935	1.1459	0.0689
H	3.0068	1.0617	0.0452
H	4.1860	1.4772	0.9557
O	4.2893	-1.6489	-0.0813
H	5.0004	-1.9242	-0.6722
H	4.3460	-0.6700	-0.0678

Table S17 The MP2/aug-cc-pVDZ optimized Cartesian Coordinates of the isomer **hf3c-44-303** of the **Pan-$(H_2O)_2$** complex.

	X	Y	Z
N	0.8164	-1.0766	0.0203
C	-1.6971	0.3218	-0.0048
C	-0.4447	1.0577	-0.0224
C	-1.6248	-1.1057	0.0318
C	0.7831	0.3157	-0.0046
C	-2.9812	0.9319	-0.0183
C	-0.3738	2.4776	-0.0542
C	-0.3296	-1.7314	0.0393
C	-2.8116	-1.8887	0.0549
C	2.0326	0.9919	-0.0067
C	-4.1394	0.1514	0.0045
C	0.8616	3.1288	-0.0628
C	-4.0586	-1.2653	0.0418
C	2.0691	2.3863	-0.0364
H	-3.0746	2.0200	-0.0461
H	-1.2899	3.0729	-0.0705
H	-0.2700	-2.8277	0.0624
H	-2.7307	-2.9804	0.0835
H	2.9584	0.4096	0.0261
H	-5.1189	0.6384	-0.0060
H	0.8940	4.2221	-0.0873
H	-4.9736	-1.8642	0.0598
H	3.0333	2.9023	-0.0377
O	3.1526	-2.6350	-0.1498
H	3.1714	-2.9440	-1.0649
H	2.3318	-2.0844	-0.0923
O	5.0172	-0.5677	0.1640
H	5.6607	-0.7551	0.8580
H	4.4723	-1.3806	0.1083

Table S18 The MP2/aug-cc-pVDZ optimized Cartesian Coordinates of the isomer **pm7-56-139** of the **Pan-$(H_2O)_2$** complex.

	X	Y	Z
N	0.7604	-1.2696	-0.9952
C	-1.3121	0.5123	-0.0791
C	0.0664	0.9617	-0.1539
C	-1.5874	-0.8330	-0.4758
C	1.0553	0.0419	-0.6323
C	-2.3930	1.3215	0.3641
C	0.4862	2.2638	0.2350
C	-0.4961	-1.6642	-0.9101
C	-2.9139	-1.3421	-0.4270
C	2.4153	0.4423	-0.7261
C	-3.6919	0.8097	0.4064
C	1.8296	2.6365	0.1495
C	-3.9574	-0.5270	0.0095
C	2.8018	1.7251	-0.3368
H	-2.2182	2.3536	0.6767
H	-0.2426	2.9849	0.6128
H	-0.7063	-2.7058	-1.1869
H	-3.1011	-2.3764	-0.7336
H	3.1446	-0.2874	-1.0883
H	-4.5124	1.4461	0.7502
H	2.1322	3.6404	0.4616
H	-4.9792	-0.9152	0.0492
H	3.8516	2.0246	-0.4008
O	1.8379	-0.9179	2.3402
H	2.2898	-1.5178	1.7183
H	2.0134	-0.0439	1.9663
O	2.9537	-2.6052	0.1965
H	2.9236	-3.5675	0.2706
H	2.2044	-2.3683	-0.3930

Table S19 The MP2/aug-cc-pVDZ optimized Cartesian Coordinates of the isomer **hf3c-67-452** of the **Pan-$(H_2O)_3$** complex.

	X	Y	Z
N	0.3932	-1.1921	-0.1584
C	-1.2149	1.1880	0.0224
C	-1.8381	-0.1248	0.0301
C	0.2099	1.2381	-0.0747
C	-0.9921	-1.2784	-0.0563
C	-1.9278	2.4143	0.1083
C	-3.2434	-0.3258	0.1231
C	0.9484	0.0065	-0.1667
C	0.9013	2.4817	-0.0770
C	-1.5581	-2.5804	-0.0402
C	-1.2427	3.6319	0.1014
C	-3.7825	-1.6140	0.1336
C	0.1740	3.6684	0.0105

C	-2.9391	-2.7514	0.0536
H	-3.0180	2.4174	0.1825
H	-3.9156	0.5332	0.1888
H	2.0395	0.0593	-0.2515
H	1.9941	2.4714	-0.1434
H	-0.8783	-3.4359	-0.0985
H	-1.8060	4.5673	0.1690
H	-4.8663	-1.7447	0.2063
H	0.6939	4.6309	0.0109
H	-3.3693	-3.7568	0.0665
O	4.4965	-1.3956	0.5678
H	4.6695	-1.5981	1.4952
H	3.7858	-2.0247	0.3028
O	4.0855	1.2421	-0.2346
H	4.3006	0.3346	0.0710
H	4.8288	1.4815	-0.8014
O	2.4348	-3.0528	-0.1972
H	2.5124	-3.4089	-1.0917
H	1.6269	-2.4736	-0.2209

Table S20 The MP2/aug-cc-pVDZ optimized Cartesian Coordinates of the isomer **hf3c-68-186** of the **Pan-$(H_2O)_3$** complex.

	X	Y	Z
N	-0.4108	-1.2220	-0.2088
C	1.2377	1.1276	0.0218
C	1.8359	-0.1966	0.0325
C	-0.1829	1.2055	-0.1107
C	0.9708	-1.3334	-0.0832
C	1.9720	2.3391	0.1339
C	3.2353	-0.4234	0.1536
C	-0.9420	-0.0123	-0.2238
C	-0.8499	2.4625	-0.1238
C	1.5167	-2.6441	-0.0776
C	1.3111	3.5698	0.1170
C	3.7528	-1.7203	0.1584
C	-0.1016	3.6339	-0.0109
C	2.8921	-2.8414	0.0422
H	3.0598	2.3205	0.2356
H	3.9203	0.4233	0.2434
H	-2.0302	0.0611	-0.3327
H	-1.9404	2.4748	-0.2195
H	0.8271	-3.4880	-0.1732
H	1.8906	4.4937	0.2045
H	4.8323	-1.8704	0.2520
H	-0.6028	4.6062	-0.0190
H	3.3048	-3.8541	0.0448
O	-4.0429	1.4140	-0.3561
H	-4.7378	1.5945	-1.0008
H	-4.2917	0.5459	0.0278

O	-4.5339	-1.1096	0.7254
H	-3.8993	-1.7854	0.3962
H	-4.4875	-1.1757	1.6870
O	-2.6652	-2.8230	-0.3408
H	-2.5367	-3.7570	-0.1375
H	-1.7644	-2.4093	-0.2983

Table S21 The MP2/aug-cc-pVDZ optimized Cartesian Coordinates of the isomer **pm7-78-4104** of the **Pan-$(H_2O)_3$** complex.

	X	Y	Z
N	-0.4888	-1.1658	-0.0040
C	1.3164	1.0758	0.0205
C	1.8294	-0.2831	-0.0226
C	-0.1028	1.2418	0.0393
C	0.8885	-1.3640	-0.0343
C	2.1314	2.2397	0.0433
C	3.2166	-0.5977	-0.0531
C	-0.9436	0.0739	0.0276
C	-0.6886	2.5379	0.0801
C	1.3461	-2.7072	-0.0823
C	1.5493	3.5091	0.0848
C	3.6483	-1.9250	-0.0972
C	0.1377	3.6612	0.1029
C	2.7115	-2.9897	-0.1130
H	3.2206	2.1537	0.0302
H	3.9594	0.2038	-0.0444
H	-2.0305	0.2140	0.0410
H	-1.7805	2.6173	0.0883
H	0.5969	-3.5046	-0.0997
H	2.1907	4.3953	0.1032
H	4.7200	-2.1432	-0.1212
H	-0.3007	4.6629	0.1360
H	3.0581	-4.0262	-0.1514
O	-3.9756	1.7120	-0.2366
H	-4.2901	0.7963	-0.0880
H	-4.3244	1.9368	-1.1080
O	-4.6508	-0.9738	0.2148
H	-5.4749	-1.4043	-0.0403
H	-3.9722	-1.6879	0.1998
O	-2.6527	-2.8725	0.2491
H	-2.5783	-3.2583	1.1319
H	-1.8118	-2.3533	0.1383

Table S22 The MP2/aug-cc-pVDZ optimized Cartesian Coordinates of the isomer **hf3c-70-441** of the **Pan-$(H_2O)_3$** complex.

	X	Y	Z
N	0.3105	-1.2223	-0.0525
C	-1.1624	1.2484	0.0627
C	-1.8611	-0.0253	0.0290
C	0.2656	1.2149	0.0252
C	-1.0811	-1.2262	-0.0305
C	-1.8056	2.5139	0.1266
C	-3.2787	-0.1434	0.0515
C	0.9343	-0.0583	-0.0289
C	1.0277	2.4162	0.0502
C	-1.7240	-2.4914	-0.0746
C	-1.0509	3.6894	0.1526
C	-3.8932	-1.3967	0.0117
C	0.3678	3.6432	0.1134
C	-3.1157	-2.5810	-0.0532
H	-2.8958	2.5806	0.1570
H	-3.9013	0.7535	0.0978
H	2.0296	-0.0700	-0.0558
H	2.1194	2.3421	0.0134
H	-1.0952	-3.3850	-0.1323
H	-1.5610	4.6560	0.2025
H	-4.9850	-1.4632	0.0287
H	0.9426	4.5737	0.1338
H	-3.6047	-3.5585	-0.0892
O	4.1489	1.0950	-0.3107
H	4.6981	1.3321	-1.0680
H	4.3251	0.1386	-0.1815
O	4.5102	-1.6424	0.1037
H	4.9685	-1.8671	0.9227
H	3.7307	-2.2437	0.0802
O	2.2326	-3.2171	-0.0009
H	2.0499	-3.7946	0.7512
H	1.4655	-2.5853	-0.0234

Table S 23 The MP2/aug-cc-pVDZ optimized Cartesian Coordinates of the isomer **pm7-123-216** of the **Pan-$(H_2O)_3$** complex.

	X	Y	Z
N	0.2341	-1.2537	-0.1102
C	-2.1204	0.3910	0.0289
C	-0.8011	0.9973	-0.0110
C	-2.1938	-1.0370	0.0009
C	0.3425	0.1343	-0.0777
C	-3.3348	1.1272	0.0957
C	-0.5821	2.4022	0.0143
C	-0.9709	-1.7912	-0.0704
C	-3.4533	-1.6964	0.0402
C	1.6515	0.6830	-0.1109

C	-4.5654	0.4676	0.1334
C	0.7144	2.9221	-0.0223
C	-4.6291	-0.9502	0.1061
C	1.8417	2.0640	-0.0842
H	-3.3161	2.2193	0.1185
H	-1.4309	3.0887	0.0643
H	-1.0237	-2.8876	-0.0935
H	-3.4842	-2.7908	0.0184
H	2.5067	0.0041	-0.1530
H	-5.4894	1.0509	0.1850
H	0.8581	4.0066	-0.0014
H	-5.5995	-1.4540	0.1367
H	2.8605	2.4575	-0.1115
O	4.7175	-1.4472	0.5344
H	3.9425	-1.9828	0.2492
H	4.8321	-1.6624	1.4682
O	4.9648	1.2748	-0.1367
H	4.9075	0.3238	0.0888
H	5.8514	1.3741	-0.5037
O	2.5047	-2.8616	-0.2927
H	1.6878	-2.2986	-0.2495
H	2.5547	-3.1564	-1.2111

Table S24 The MP2/aug-cc-pVDZ optimized Cartesian Coordinates of the isomer **pm7-119-4694** of the **Pan-$(H_2O)_3$** complex.

	X	Y	Z
N	-0.5184	-0.9654	-1.6889
C	1.2070	0.7115	-0.0900
C	-0.1999	1.0336	-0.2417
C	1.6889	-0.4492	-0.7683
C	-1.0074	0.1750	-1.0569
C	2.1192	1.4689	0.6917
C	-0.8200	2.1502	0.3852
C	0.7642	-1.2389	-1.5381
C	3.0529	-0.8308	-0.6604
C	-2.3871	0.4600	-1.2386
C	3.4575	1.0812	0.7930
C	-2.1814	2.4097	0.2029
C	3.9298	-0.0730	0.1151
C	-2.9731	1.5652	-0.6194
H	1.7832	2.3617	1.2246
H	-0.2333	2.8173	1.0215
H	1.1343	-2.1468	-2.0324
H	3.4004	-1.7263	-1.1862
H	-2.9688	-0.2171	-1.8711
H	4.1475	1.6734	1.4012
H	-2.6379	3.2725	0.6966
H	4.9802	-0.3657	0.2033
H	-4.0369	1.7758	-0.7602

O	-2.0274	-2.7919	0.1018
H	-1.7722	-2.4509	-0.7727
H	-1.1759	-2.7824	0.5794
O	0.1573	-1.7852	1.6860
H	0.5458	-2.1103	2.5080
H	-0.6147	-1.2452	1.9680
O	-2.3545	-0.6498	1.9461
H	-2.5429	-1.3152	1.2507
H	-2.4790	0.1986	1.4951

Table S 25 The MP2/aug-cc-pVDZ optimized Cartesian Coordinates of the isomer **pm7-108-10038** of the **Pan-$(H_2O)_3$** complex.

	X	Y	Z
N	-0.5197	0.9424	-1.7021
C	1.1857	-0.7285	-0.0754
C	-0.2228	-1.0429	-0.2315
C	1.6804	0.4176	-0.7692
C	-1.0200	-0.1892	-1.0622
C	2.0877	-1.4812	0.7224
C	-0.8538	-2.1502	0.4014
C	0.7649	1.2066	-1.5506
C	3.0479	0.7873	-0.6638
C	-2.4000	-0.4673	-1.2499
C	3.4294	-1.1049	0.8213
C	-2.2161	-2.4026	0.2124
C	3.9152	0.0330	0.1256
C	-2.9971	-1.5615	-0.6226
H	1.7414	-2.3618	1.2688
H	-0.2757	-2.8148	1.0481
H	1.1435	2.1073	-2.0514
H	3.4052	1.6714	-1.2019
H	-2.9730	0.2066	-1.8940
H	4.1116	-1.6933	1.4418
H	-2.6809	-3.2577	0.7118
H	4.9681	0.3166	0.2122
H	-4.0616	-1.7658	-0.7665
O	-2.3277	0.6447	1.9631
H	-1.3765	0.8466	2.0613
H	-2.3422	-0.2439	1.5776
O	-1.9470	2.8217	0.1106
H	-1.7158	2.4191	-0.7448
H	-2.3912	2.0984	0.5970
O	0.1961	1.9152	1.6195
H	-0.4303	2.4542	1.0837
H	0.5595	2.5295	2.2702

Table S26 The MP2/aug-cc-pVDZ optimized Cartesian Coordinates of the isomer **pm7-126-12894** of the **Pan-$(H_2O)_3$** complex.

	X	Y	Z
N	0.3683	-1.1046	-1.5253
C	-1.7050	0.1352	0.0572
C	-0.4780	0.8523	-0.2433
C	-1.8359	-1.1890	-0.4655
C	0.5101	0.1978	-1.0504
C	-2.7714	0.6667	0.8318
C	-0.2002	2.1644	0.2331
C	-0.7514	-1.7418	-1.2359
C	-3.0092	-1.9503	-0.2112
C	1.7216	0.8644	-1.3710
C	-3.9195	-0.0917	1.0725
C	1.0046	2.7996	-0.0858
C	-4.0429	-1.4055	0.5498
C	1.9724	2.1506	-0.8936
H	-2.7040	1.6755	1.2460
H	-0.9286	2.6879	0.8574
H	-0.8416	-2.7710	-1.6073
H	-3.0872	-2.9635	-0.6190
H	2.4562	0.3315	-1.9803
H	-4.7314	0.3325	1.6704
H	1.2013	3.8045	0.2992
H	-4.9470	-1.9885	0.7473
H	2.9201	2.6434	-1.1241
O	2.7175	-2.0530	0.0131
H	2.0786	-1.9892	-0.7191
H	2.2714	-1.5699	0.7370
O	4.4287	0.1240	0.2148
H	3.9887	-0.7266	-0.0118
H	5.3068	-0.1326	0.5243
O	2.0980	0.0421	1.9026
H	1.4428	0.6863	1.5950
H	2.9295	0.3439	1.4870

Table S27 The MP2/aug-cc-pVDZ optimized Cartesian Coordinates of the isomer **pm7-120-1962** of the Pan-$(H_2O)_3$ complex.

	X	Y	Z
N	-0.7270	0.8920	-1.4688
C	0.8509	-1.0986	-0.0952
C	-0.6002	-1.1829	-0.1007
C	1.4451	0.0043	-0.7820
C	-1.3342	-0.1695	-0.8024
C	1.7017	-2.0275	0.5627
C	-1.3295	-2.2012	0.5752
C	0.5909	0.9577	-1.4416
C	2.8565	0.1661	-0.7978

C	-2.7538	-0.2017	-0.8133
C	3.0882	-1.8604	0.5343
C	-2.7266	-2.2121	0.5557
C	3.6708	-0.7587	-0.1455
C	-3.4466	-1.2097	-0.1421
H	1.2800	-2.8826	1.0966
H	-0.7986	-2.9851	1.1211
H	1.0539	1.8153	-1.9444
H	3.2866	1.0295	-1.3149
H	-3.2780	0.5892	-1.3579
H	3.7302	-2.5840	1.0450
H	-3.2671	-3.0012	1.0865
H	4.7577	-0.6363	-0.1534
H	-4.5400	-1.2238	-0.1498
O	-1.5980	3.1986	0.0814
H	-1.5238	2.6263	-0.7051
H	-0.6846	3.5231	0.1830
O	1.2649	3.0083	0.7583
H	0.8182	2.3176	1.2942
H	1.7646	3.5269	1.4017
O	-0.6168	1.3584	2.0001
H	-1.2156	1.8874	1.4296
H	-0.7826	0.4429	1.7331

Table S28 The MP2/aug-cc-pVDZ optimized Cartesian Coordinates of the isomer **pm7-129-7103** of the Pan-$(H_2O)_3$ complex.

	X	Y	Z
N	-0.3158	-1.1901	-1.4834
C	1.6770	0.2480	0.0340
C	0.4066	0.8723	-0.2936
C	1.8902	-1.0875	-0.4290
C	-0.5402	0.1199	-1.0645
C	2.7081	0.8795	0.7807
C	0.0475	2.1851	0.1236
C	0.8422	-1.7413	-1.1707
C	3.1090	-1.7616	-0.1447
C	-1.7932	0.6930	-1.4068
C	3.9016	0.2061	1.0516
C	-1.1961	2.7272	-0.2171
C	4.1069	-1.1195	0.5879
C	-2.1229	1.9820	-0.9885
H	2.5778	1.8997	1.1496
H	0.7433	2.7818	0.7187
H	0.9977	-2.7779	-1.4976
H	3.2501	-2.7853	-0.5067
H	-2.4953	0.0879	-1.9866
H	4.6854	0.7066	1.6274
H	-1.4546	3.7347	0.1218
H	5.0457	-1.6355	0.8086

H	-3.1003	2.4032	-1.2361
O	-2.4447	-2.2331	0.2672
H	-3.2626	-1.7403	0.0672
H	-1.9059	-2.1393	-0.5381
O	-2.0948	0.0404	1.9287
H	-1.4222	0.6255	1.5487
H	-1.9532	-0.8168	1.4729
O	-4.3991	-0.0883	0.3258
H	-5.1946	-0.1813	0.8655
H	-3.6981	0.1697	0.9637

Table S29 The MP2/aug-cc-pVDZ optimized Cartesian Coordinates of the isomer **pm7-33-6692** of the **Pan-$(H_2O)_3$** complex.

	X	Y	Z
N	-0.7519	0.7063	-0.3274
C	1.6695	-0.8094	0.0325
C	1.7020	0.6432	0.0386
C	0.3994	-1.4362	-0.1601
C	0.4681	1.3490	-0.1456
C	2.8135	-1.6355	0.2031
C	2.8924	1.4011	0.2169
C	-0.7702	-0.6147	-0.3326
C	0.2907	-2.8541	-0.1796
C	0.4523	2.7689	-0.1494
C	2.6931	-3.0270	0.1823
C	2.8576	2.7972	0.2111
C	1.4283	-3.6424	-0.0098
C	1.6333	3.4893	0.0271
H	3.7997	-1.1893	0.3523
H	3.8495	0.8934	0.3598
H	-1.7465	-1.0947	-0.4808
H	-0.6937	-3.3089	-0.3301
H	-0.5093	3.2700	-0.2957
H	3.5838	-3.6481	0.3151
H	3.7852	3.3604	0.3496
H	1.3492	-4.7333	-0.0246
H	1.6160	4.5828	0.0227
O	-4.6629	0.2013	1.6617
H	-4.5711	-0.4953	0.9833
H	-4.3509	-0.2024	2.4806
O	-3.4328	1.5390	-0.6420
H	-2.4624	1.4049	-0.5280
H	-3.7764	1.5178	0.2683
O	-4.1046	-1.0917	-0.8042
H	-3.9201	-0.1321	-0.9647
H	-4.7758	-1.3335	-1.4543

Table S30 The MP2/aug-cc-pVDZ optimized Cartesian Coordinates of the isomer **pm7-135-8657** of the **Pan-$(H_2O)_3$** complex.

	X	Y	Z
N	-0.4719	-0.9719	-0.4280
C	2.1101	0.1995	0.0600
C	0.9186	1.0301	0.0310
C	1.9438	-1.2027	-0.1652
C	-0.3447	0.3988	-0.2187
C	3.4220	0.6945	0.2944
C	0.9405	2.4371	0.2365
C	0.6189	-1.7135	-0.3990
C	3.0677	-2.0738	-0.1525
C	-1.5357	1.1712	-0.2663
C	4.5177	-0.1718	0.3038
C	-0.2399	3.1822	0.1916
C	4.3440	-1.5626	0.0796
C	-1.4833	2.5499	-0.0619
H	3.5860	1.7603	0.4702
H	1.8862	2.9489	0.4310
H	0.4871	-2.7906	-0.5659
H	2.9153	-3.1440	-0.3268
H	-2.4884	0.6749	-0.4663
H	5.5199	0.2270	0.4860
H	-0.2007	4.2636	0.3530
H	5.2106	-2.2299	0.0898
H	-2.4043	3.1384	-0.0974
O	-4.7524	0.2107	-0.9090
H	-4.8550	-0.0242	0.0371
H	-5.6142	0.5450	-1.1846
O	-4.2793	-0.8798	1.5917
H	-4.7996	-1.4574	2.1631
H	-3.7755	-1.4895	1.0002
O	-3.0387	-2.1542	-0.4830
H	-3.5660	-1.6035	-1.0852
H	-2.1339	-1.7620	-0.5342

S3. Phenanthrene-H_2O complexes

S3.1 Experimental results: rotational constants

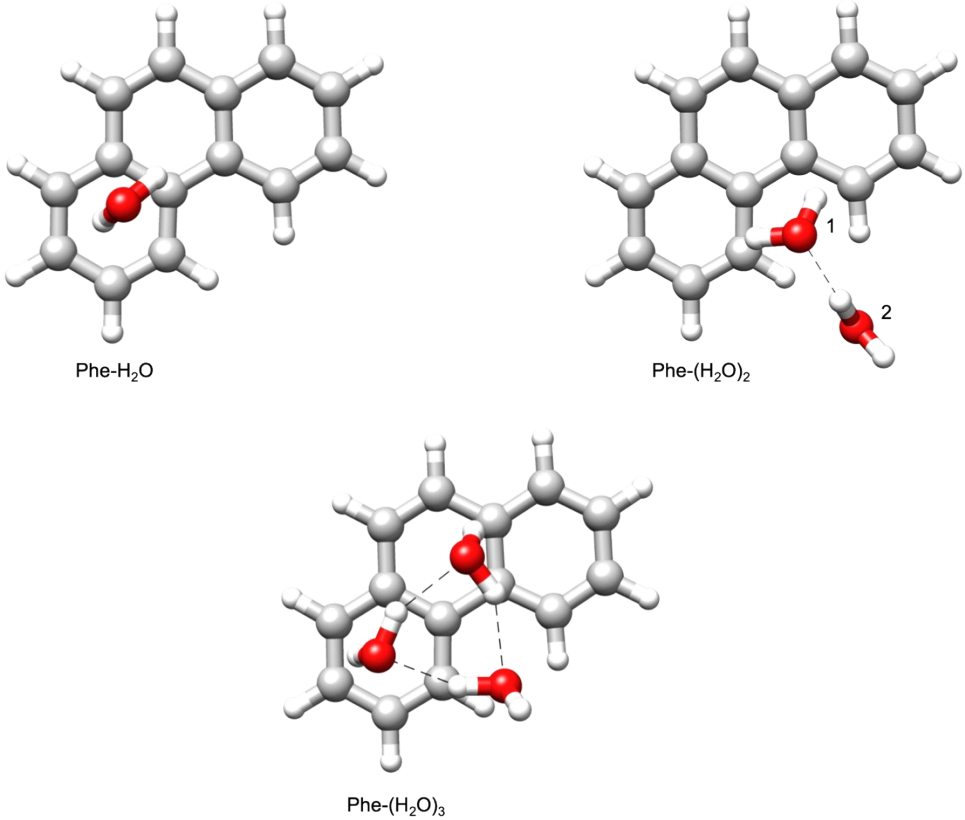


Figure S10 *Ab initio* structures of the Phe-$(H_2O)_{n=1-3}$ complexes calculated at the MP2/aug-cc-pVDZ level of theory. The numbering scheme corresponds to the labels given to the atom upon isotopic substitution.

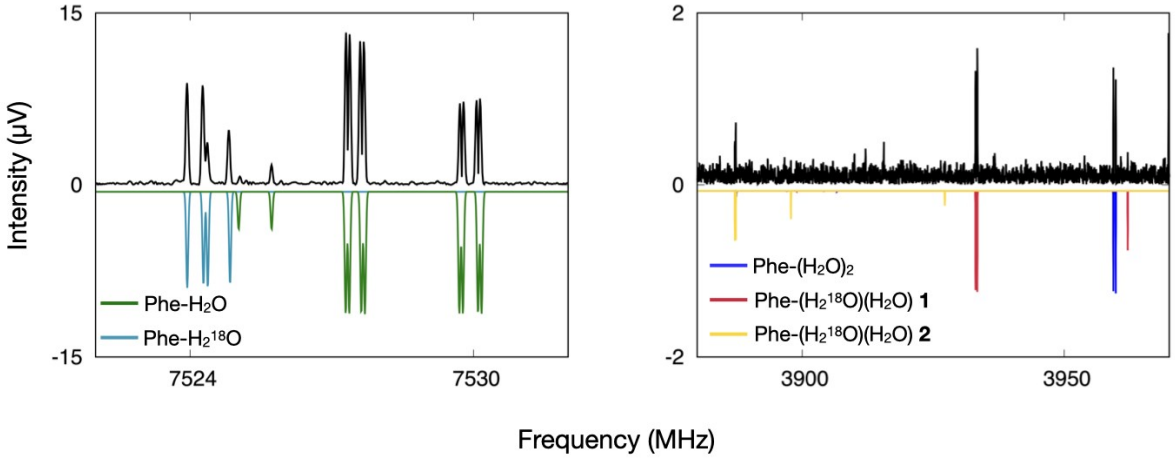


Figure S11 Representative section of the spectrum arising from the Phe-$(H_2O)_{n=1-2}$ complexes and their ^{18}O singly-substituted isotopologues. The left and right panels show representative transitions of the Phe-H_2O and its ^{18}O isotopologue and the Phe-$(H_2O)_2$ and its two ^{18}O singly substituted isotopologues, respectively. In all the panels, the upper trace (black) corresponds to the experimental spectrum, whereas the lower trace corresponds to the simulated spectra generated from the fitted rotational constants. The numbers **1** and **2** reported in bold correspond to ^{18}O substituted water molecule according to the numbering reported in Figure S10.

Table S31 Average of the experimental spectroscopic parameters determined for the four tunneling states of the Phe-H_2O complex and its ^{18}O isotopologue. The experimental frequencies were fitted by using the S-reduction of the Watson's Hamiltonian implemented in the SPFIT/SPCAT program by Pickett.[2] *A, B* and *C* are the rotational constants. Δ_J, Δ_{JK}, Δ_K, d_1, and d_2 are the centrifugal distortion constants. P_a, P_b, *and* P_c are the planar moments of inertia. N is the number of transitions included in the fit. σ is the deviation of the fit.

	PHE···H_2O	PHE···$H_2{}^{18}O$
A (MHz)	1046.790(13)	1013.40(50)
B (MHz)	439.70295(56)	430.7208(15)
C (MHz)	393.331(13)	391.14(50)
Δ_J (kHz)	1.759(34)	1.342(51)
Δ_{JK} (kHz)	-4.112(35)	-3.805(55)
Δ_K (kHz)	0.71475(34)	1.38(10)
d_1 (kHz)	-1.6438(35)	-1.216(51)
d_2 (kHz)	0.1638(15)	0.1177(66)
P_a (uÅ^2)	975.722(21)	983.37(16)
P_b (uÅ^2)	308.147(21)	308.708(16)
P_c (uÅ^2)	173.642(21)	189.99(16)
N	405	279
σ (kHz)	12.5	10.7

Table S32 Experimental spectroscopic parameters of the Phe-$(H_2O)_2$ complex and it ^{18}O singly-substituted isotopologues. The (1) and (2) indicate the substituted oxygen atoms according to the numbering reported in Figure S10. The experimental frequencies were fitted by using the A-reduction of the Watson's Hamiltonian in the I^r representation implemented in the SPFIT/SPCAT program by Pickett.[2] *A, B* and *C* are the rotational constants. Δ_J, Δ_{JK}, Δ_K, and δ_K are the centrifugal distortion constants. P_a, P_b and P_c are the planar moments of inertia. *N* is the number of transitions included in the fit. σ is the deviation of the fit.

	Phe-$(H_2O)_2$	**Phe-$(H_2{}^{18}O)$ (H_2O) (1)**	**Phe-(H_2O) $(H_2{}^{18}O)$ (2)**
A (MHz)	608.34055(28)	595.67255(32)	586.52185(31)
B (MHz)	488.36362(13)	484.32549(18)	488.35976(15)
C (MHz)	310.79554(15)	309.08065(17)	304.99618(19)
Δ_J (kHz)	0.02422(82)	0.02550(84)	0.02315(94)
Δ_{JK} (kHz)	0.2972(66)	0.2841(72)	0.2870(81)
Δ_K (kHz)	-0.1409(93)	-0.1115(93)	-0.136(12)
δ_K (kHz)	0.0749(39)	0.0746(61)	0.0675(61)
P_a (uÅ^2)	915.08669(46)	915.07814(54)	915.09836(59)
P_b (uÅ^2)	710.99522(46)	720.02586(54)	741.90273(59)
P_c (uÅ^2)	119.75494(46)	128.39163(54)	119.75145(59)
N	122	77	79
σ (kHz)	5.4	4.4	4.9

S3.2 Structural determination

Table S33 Comparison of the r_e, r_s, r_0 and $r_m^{(1)}$ principal coordinates for the oxygen atom in the Phe-H_2O complex. All the coordinates are provided in their absolute values. Theoretical coordinates have been calculated at the MP2/aug-cc-pVDZ level of theory. For the O atom, due to its proximity to the *b* principal inertial axis, Kraitchman's equations yielded an imaginary *b* coordinate. For the determination of the r_s structure, this value was fixed to zero.

	Phe-H_2O					
	$\|a\|$	δa	$\|b\|$	δb	$\|c\|$	δc
r_e	1.775	-	0.151	-	2.724	-
r_s	1.942	0.015	-	-	2.881	0.010
$r_m^{(1)}$ [a]	1.886	0.006	0.151	0.002	2.836	0.003

[a] Fit of 3 parameters to 6 rotational constants, σ_{fit} = 0.390 uÅ^2

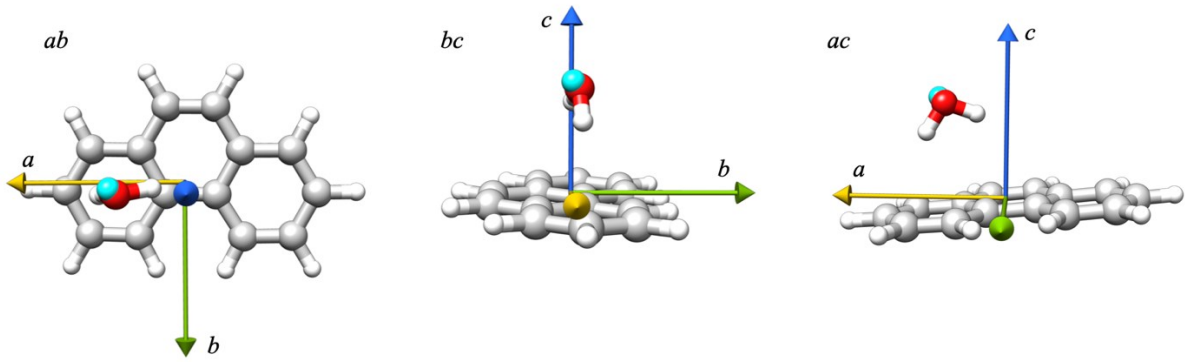


Figure S12 Comparison between the *ab initio* structure (r_e) and the substitution structure (r_s) of the Phe-H_2O complex projected on the *ab* plane (left), *bc* plane (middle) and *ac* plane (right) . The full body of the molecule represents the *ab initio* structure calculated at the MP2/aug-cc-pVDZ level of theory. The cyan sphere represents the position of the oxygen atom calculated using Kraitchman's equations. [4]

Table S34 Comparison of the r_e, r_s, r_0 and $r_m^{(1)}$ principal coordinates and distances for the O(1) and O(2) oxygen atoms in the Phe-$(H_2O)_2$ complex. All the coordinates are provided in their absolute values. Theoretical coordinates have been calculated at the MP2/aug-cc-pVDZ level of theory. For the O(1) and O(2) atoms, due to their proximity to one of the principal inertial axis, Kraitchman's equations yielded imaginary *a* and *c* coordinates, respectively. For the determination of the r_s structure, these values were fixed to zero.

	O(1)					
	$\|a\|$	δa	$\|b\|$	δb	$\|c\|$	δc
r_e	0.017	-	1.894	-	2.079	-
r_s	-	-	2.1169	0.0007	2.1014	0.0007
$r_0{}^a$	0.0096	0.0426	2.1093	0.0043	2.1001	0.0055
$r_m{}^{(1)b}$	0.0713	0.0224	2.1163	0.0016	2.1081	0.0014
	O(2)					
r_e	0.106	-	3.837	-	-0.008	-
r_s	0.0706	0.0214	3.9454	0.0004	-	-
$r_0{}^a$	0.0627	0.1511	3.9410	0.0019	-0.0711	0.0077
$r_m{}^{(1)\,b}$	0.0454	0.0305	3.9502	0.0009	0.0047	0.0017

[a] Fit of 6 parameters to 9 rotational constants, σ_{fit} = 0.045 uÅ^2
[b] Fit of 7 parameters to 9 rotational constants, σ_{fit} = 0.011 uÅ^2

Table S35 Comparison of the r_e, r_s, r_0 and $r_m^{(1)}$ values of O(1)–O(2) distances (Å) of the Phe-$(H_2O)_2$ complex.

	O(1)–O(2)			
	r_e	r_s	$r_0{}^a$	$r_m{}^{(1)b}$
	2.85	2.79(3)	2.84(1)	2.793(3)

[a] Fit of 6 parameters to 9 rotational constants, σ_{fit} = 0.045 uÅ^2
[b] Fit of 7 parameters to 9 rotational constants, σ_{fit} = 0.011 uÅ^2

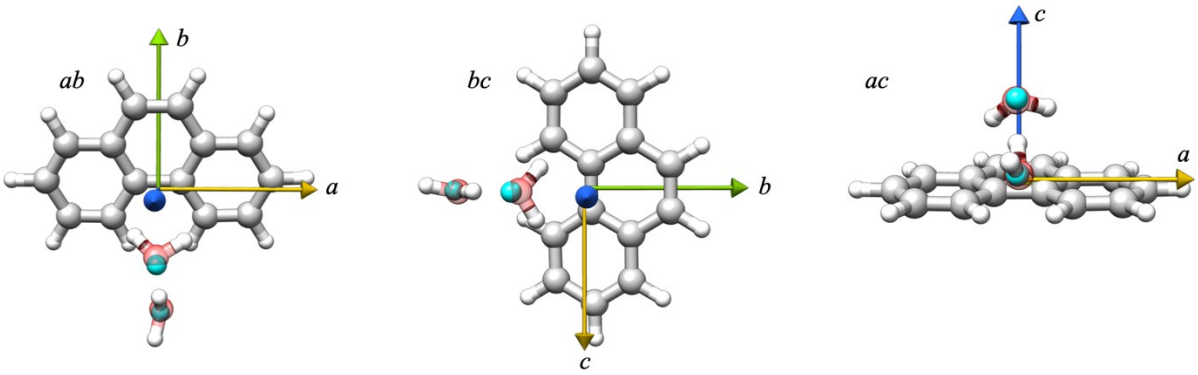


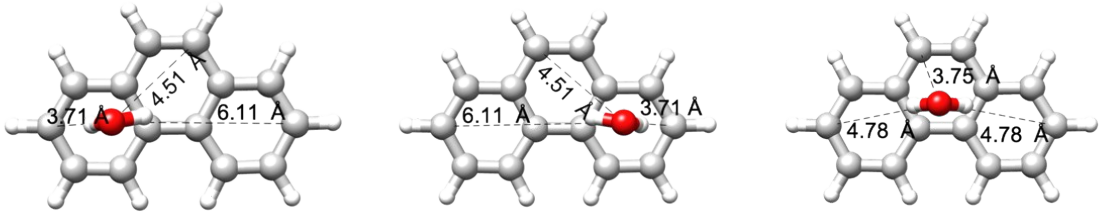
Figure S13 Comparison between the *ab initio* structure (r_e) and the substitution structure (r_s) Phe-$(H_2O)_2$ complex projected on the *ab* plane (left), *bc* plane (middle) and *ac* plane (right) . The full body of the molecule represents the *ab initio* structure calculated at the MP2/aug-cc-pVDZ level of theory. The cyan sphere represents the position of the oxygen atom calculated using Kraitchman's equations.[4]

S3.3 Calculated isomers and Cartesian coordinates

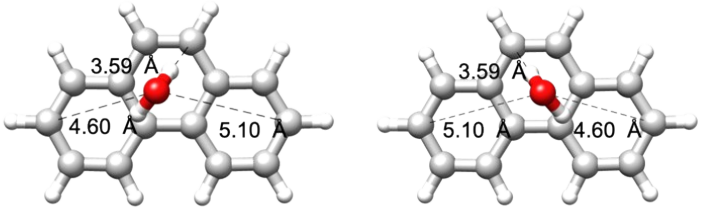
Table S36 Theoretical spectroscopic parameters of the isomers of the Phe-H_2O complex calculated at the MP2/aug-cc-pVDZ and at the B3LYP-D3BJ/def2-TZVP levels of theory.

	Far-left/right		Int-left/right		Sym-middle	
	MP2	**B3LYP**	**MP2**	**B3LYP**	**MP2**	**B3LYP**
A (MHz)	1077.0	1083.4	1054.9	1042.8	1064.2	1061.2
B (MHz)	447.1	445.5	468.8	473.6	466.3	470.0
C (MHz)	389.4	391.8	400.6	404.6	405.0	413.0
$\lvert\mu_a\rvert$ (D)	1.0	1.0	0.1	0.0	0.0	0.0
$\lvert\mu_b\rvert$ (D)	0.1	0.1	0.8	1.0	0.3	0.3
$\lvert\mu_c\rvert$ (D)	2.2	2.2	2.2	2.2	2.3	2.3
$\Delta\Delta E_e$ (kJ/mol)	0.0[a]	0.3	0.1	0.0	0.1	0.1
$\Delta\Delta E$ (0k)[b] (kJ/mol)	0.6[b]	0.3[c]	1.3	0.1	0.0	0.0

[a] MP2-F12/aug-cc-pVTZ-F12//MP2/aug-cc-pVDZ single point energies calculated on the optimised structures at the MP2/aug-cc-pVDZ.
[b] MP2-F12/aug-cc-pVTZ-F12//MP2/aug-cc-pVDZ single point energies combined with harmonic zero-point corrections at the MP2/aug-cc-pVDZ level of theory.
[c] B3LYP-D3BJ/def2-TZVP zero-point corrected energies.



ID:	Far-left	Far-right	Sym-middle
ΔΔEe (kJ/mol)	0.0	0.0	0.1



ID:	Int-left	Far-right
ΔΔEe (kJ/mol)	0.1	0.1

Figure S14 Theoretical structures calculated at the MP2/aug-cc-pVDZ of the Phe-H_2O complex. MP2-F12/aug-cc-pVTZ-F12//MP2-aug-cc-pVDZ single point energies calculated on the optimised structures at the MP2/aug-cc-pVDZ are also provided.

Table S37 The MP2/aug-cc-pVDZ optimized Cartesian Coordinates of the isomer **far-left** of the **Phe-H_2O** complex.

	X	Y	Z
C	-0.1119	0.3208	-0.9953
C	-0.3709	-0.7764	-0.0697
C	0.2736	1.6023	-0.4699
C	-0.2288	-0.5471	1.3419
C	0.4095	1.7873	0.9510
C	0.1655	0.7510	1.8243
C	-0.2462	0.1841	-2.4062
C	-0.7666	-2.0730	-0.5046
C	0.4991	2.6896	-1.3615
C	-0.4839	-1.6080	2.2566
C	-0.0249	1.2653	-3.2620
C	-1.0113	-3.0986	0.4108
C	0.3484	2.5305	-2.7394
C	-0.8691	-2.8685	1.8027
H	0.7026	2.7735	1.3257
H	0.2659	0.9001	2.9045
H	-0.5421	-0.7733	-2.8401
H	-0.8860	-2.2835	-1.5697
H	0.7819	3.6618	-0.9444
H	-0.3712	-1.4162	3.3290
H	-0.1468	1.1347	-4.3410
H	-1.3146	-4.0851	0.0486
H	0.5142	3.3762	-3.4127

H	-1.0625	-3.6753	2.5156
O	-2.9690	2.0455	-1.1553
H	-2.7040	1.3638	-0.5223
H	-2.1465	2.2164	-1.6379

Table S38 MP2/aug-cc-pVDZ optimized Cartesian Coordinates of the isomer **far-right** of the **Phe-H_2O** complex.

	X	Y	Z
C	-0.2191	-0.3765	0.9024
C	-0.3745	-0.3652	-0.5479
C	-0.1052	0.8738	1.6019
C	-0.4043	0.8957	-1.2379
C	-0.1462	2.1139	0.8713
C	-0.2921	2.1250	-0.4979
C	-0.1696	-1.5797	1.6618
C	-0.4766	-1.5576	-1.3193
C	0.0523	0.8769	3.0170
C	-0.5243	0.9189	-2.6568
C	-0.0146	-1.5524	3.0492
C	-0.5887	-1.5118	-2.7105
C	0.0966	-0.3168	3.7357
C	-0.6105	-0.2658	-3.3888
H	-0.0564	3.0529	1.4277
H	-0.3160	3.0718	-1.0473
H	-0.2516	-2.5484	1.1639
H	-0.4525	-2.5332	-0.8292
H	0.1380	1.8384	3.5344
H	-0.5350	1.8872	-3.1680
H	0.0208	-2.4924	3.6075
H	-0.6537	-2.4440	-3.2788
H	0.2183	-0.3010	4.8226
H	-0.6917	-0.2346	-4.4790
O	2.7259	-0.1505	-1.7748
H	2.4187	-0.0099	-0.8685
H	1.8962	-0.2174	-2.2707

Table S39 The MP2/aug-cc-pVDZ optimized Cartesian Coordinates of the isomer **int-left** of the **Phe-H_2O** complex.

	X	Y	Z
C	-0.1443	0.5104	-0.8612
C	-0.5280	-0.8493	-0.4983
C	0.9745	1.1240	-0.1984
C	0.2038	-1.5290	0.5346
C	1.6881	0.4029	0.8233
C	1.3135	-0.8749	1.1795
C	-0.8404	1.2699	-1.8443
C	-1.6156	-1.5318	-1.1115
C	1.3541	2.4532	-0.5383

C	-0.1714	-2.8490	0.9135
C	-0.4523	2.5742	-2.1597
C	-1.9657	-2.8271	-0.7252
C	0.6541	3.1731	-1.5054
C	-1.2416	-3.4936	0.2953
H	2.5309	0.8940	1.3209
H	1.8564	-1.4139	1.9632
H	-1.6973	0.8384	-2.3664
H	-2.1953	-1.0469	-1.9000
H	2.2056	2.9057	-0.0193
H	0.3971	-3.3514	1.7032
H	-1.0081	3.1349	-2.9168
H	-2.8064	-3.3279	-1.2140
H	0.9529	4.1952	-1.7550
H	-1.5217	-4.5074	0.5956
O	-1.4180	1.2625	2.1239
H	-0.6781	0.6378	2.0951
H	-1.4463	1.5933	1.2151

Table S40 The MP2/aug-cc-pVDZ optimized Cartesian Coordinates of the isomer **int-right** of the **Phe-H_2O** complex.

	X	Y	Z
C	-0.4983	-0.5280	0.8493
C	-0.8612	-0.1443	-0.5104
C	0.5346	0.2038	1.5290
C	-0.1984	0.9745	-1.1240
C	1.1795	1.3135	0.8749
C	0.8233	1.6881	-0.4029
C	-1.1115	-1.6156	1.5318
C	-1.8443	-0.8404	-1.2699
C	0.9135	-0.1714	2.8490
C	-0.5383	1.3541	-2.4532
C	-0.7252	-1.9657	2.8271
C	-2.1597	-0.4523	-2.5742
C	0.2953	-1.2416	3.4936
C	-1.5054	0.6541	-3.1731
H	1.9632	1.8564	1.4139
H	1.3209	2.5309	-0.8940
H	-1.9000	-2.1953	1.0469
H	-2.3664	-1.6973	-0.8384
H	1.7032	0.3971	3.3514
H	-0.0193	2.2056	-2.9057
H	-1.2140	-2.8064	3.3279
H	-2.9168	-1.0081	-3.1349
H	0.5956	-1.5217	4.5074
H	-1.7550	0.9529	-4.1952
O	2.1239	-1.4180	-1.2625
H	1.2151	-1.4463	-1.5933

H	2.0951	-0.6781	-0.6378

Table S41 The MP2/aug-cc-pVDZ optimized Cartesian Coordinates of the isomer **sym-middle** of the **Phe-H_2O** complex.

	X	Y	Z
C	-0.2782	-0.4224	0.7295
C	-0.2781	-0.4224	-0.7296
C	-0.3420	0.8328	1.4280
C	-0.3418	0.8328	-1.4281
C	-0.4174	2.0660	0.6882
C	-0.4173	2.0660	-0.6883
C	-0.1978	-1.6175	1.4989
C	-0.1976	-1.6175	-1.4990
C	-0.3218	0.8473	2.8520
C	-0.3215	0.8474	-2.8521
C	-0.1790	-1.5788	2.8947
C	-0.1787	-1.5787	-2.8948
C	-0.2414	-0.3391	3.5801
C	-0.2411	-0.3390	-3.5802
H	-0.4661	3.0082	1.2439
H	-0.4660	3.0082	-1.2439
H	-0.1437	-2.5885	1.0019
H	-0.1436	-2.5885	-1.0021
H	-0.3695	1.8119	3.3683
H	-0.3693	1.8120	-3.3684
H	-0.1137	-2.5128	3.4602
H	-0.1134	-2.5127	-3.4603
H	-0.2236	-0.3139	4.6734
H	-0.2233	-0.3138	-4.6736
O	2.8508	0.3553	0.0005
H	2.2455	0.2958	-0.7528
H	2.2474	0.2990	0.7555

Table S42 Theoretical spectroscopic parameters of the isomer of the Phe-$(H_2O)_2$ complex calculated at the MP2/aug-cc-pVDZ and at the B3LYP-D3BJ/def2-TZVP levels of theory.

	hf3c-0-1176		**dftb-45-4724**		**hf3c-113-2386**	
	MP2	**B3LYP**	**MP2**	**B3LYP**	**MP2**	**B3LYP**
A (MHz)	637.6	622.1	823.8	792.5	803.3	792.2
B (MHz)	485.1	495.9	385.0	373.0	390.5	391.0
C (MHz)	314.8	312.9	320.1	286.5	374.9	380.0
$\lvert\mu_a\rvert$ (D)	0.1	0.3	1.3	0.9	2.5	2.7
$\lvert\mu_b\rvert$ (D)	1.1	0.9	1.0	0.6	0.4	0.2
$\lvert\mu_c\rvert$ (D)	0.5	0.7	0.3	0.7	3.8	3.8
$\Delta\Delta E_e$ (kJ/mol)	0[a]	0	3.2	4.4	4.1	3.5
$\Delta\Delta E$ (0k) (kJ/mol)	0[b]	0[c]	2.5	4.1	4.3	3.0
	hf3c-114-134		**pm7-66-2057**			
	MP2	**B3LYP**	**MP2**	**B3LYP**		
A (MHz)	775.5	759.1	732.8	724.9		
B (MHz)	418.0	432.4	415.6	419.6		
C (MHz)	347.8	350.2	380.2	384.4		
$\lvert\mu_a\rvert$ (D)	0.0	0.2	0.0	0.0		
$\lvert\mu_b\rvert$ (D)	3.9	3.7	2.4	3.2		
$\lvert\mu_c\rvert$ (D)	0.6	0.9	3.7	3.3		
$\Delta\Delta E_e$(kJ/mol)	4.5	7.5	7.2	5.8		
$\Delta\Delta E$ (0k) kJ/mol)	5.1	7.2	8.9	7.2		

[a] MP2-F12/aug-cc-pVTZ-F12//MP2/aug-cc-pVDZ single point energies calculated on the optimised structures at the MP2/aug-cc-pVDZ.
[b] MP2-F12/aug-cc-pVTZ-F12//MP2/aug-cc-pVDZ single point energies combined with harmonic zero-point corrections at the MP2/aug-cc-pVDZ level of theory.
[c] B3LYP-D3BJ/def2-TZVP zero-point corrected energies.

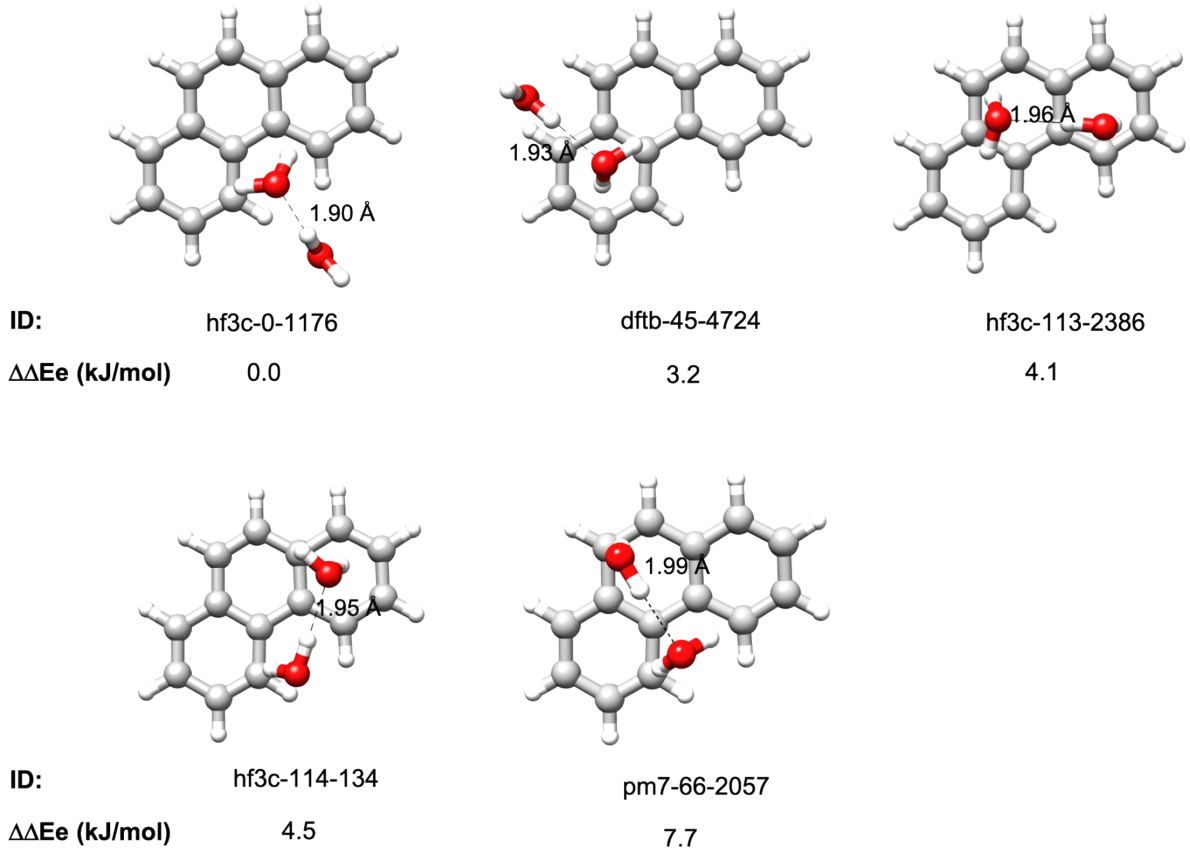


Figure S15 Theoretical structures calculated at the MP2/aug-cc-pVDZ of the Phe-$(H_2O)_2$ complex. MP2-F12/aug-cc-pVTZ-F12//MP2-aug-cc-pVDZ single point energies calculated on the optimised structures at the MP2/aug-cc-pVDZ are also provided.

Table S43 The MP2/aug-cc-pVDZ optimized Cartesian Coordinates of the isomer **hf3c-0-1176** of the **Phe-$(H_2O)_2$** complex.

	X	Y	Z
C	-0.8037	0.3026	0.3529
C	0.4036	0.0190	-0.4172
C	-2.0122	0.6470	-0.3446
C	0.3516	0.0946	-1.8519
C	-2.0226	0.6997	-1.7837
C	-0.8835	0.4335	-2.5102
C	-0.8266	0.2691	1.7774
C	1.6447	-0.3141	0.2011
C	-3.1923	0.9390	0.3969
C	1.5268	-0.1660	-2.6122
C	-1.9968	0.5657	2.4812
C	2.7849	-0.5587	-0.5693
C	-3.1895	0.9013	1.7910
C	2.7299	-0.4875	-1.9844
H	-2.9572	0.9599	-2.2919
H	-0.8989	0.4794	-3.6044

H	0.0758	0.0275	2.3426
H	1.7274	-0.3654	1.2890
H	-4.1059	1.1979	-0.1488
H	1.4706	-0.1061	-3.7044
H	-1.9867	0.5369	3.5746
H	3.7259	-0.8086	-0.0706
H	-4.1021	1.1303	2.3492
H	3.6265	-0.6821	-2.5802
O	1.1977	2.8192	1.1170
H	0.2350	2.7584	1.2142
H	1.3764	2.1941	0.3956
O	2.0277	1.1015	3.2400
H	2.7193	1.4625	3.8079
H	1.8385	1.8123	2.5955

Table S44 The MP2/aug-cc-pVDZ optimized Cartesian Coordinates of the isomer **dftb-45-4724** of the **Phe-$(H_2O)_2$** complex.

	X	Y	Z
C	0.6622	-0.2548	-0.8057
C	0.3510	-0.4630	0.6040
C	-0.0899	-0.9733	-1.7977
C	-0.6891	-1.3889	0.9622
C	-1.1294	-1.8842	-1.3935
C	-1.4199	-2.0866	-0.0627
C	1.6803	0.6376	-1.2472
C	1.0148	0.2414	1.6493
C	0.1985	-0.7746	-3.1780
C	-1.0207	-1.5842	2.3333
C	1.9455	0.8156	-2.6067
C	0.6661	0.0435	2.9887
C	1.2008	0.1060	-3.5826
C	-0.3573	-0.8771	3.3358
H	-1.6947	-2.4101	-2.1702
H	-2.2300	-2.7558	0.2403
H	2.2751	1.1965	-0.5210
H	1.8044	0.9589	1.4151
H	-0.3836	-1.3299	-3.9211
H	-1.8364	-2.2689	2.5811
H	2.7348	1.5062	-2.9174
H	1.1864	0.6040	3.7709
H	1.4124	0.2486	-4.6463
H	-0.6308	-1.0231	4.3847
O	-2.2394	1.3868	1.2795
H	-1.4958	1.1354	1.8517
H	-1.8611	1.3033	0.3917
O	-3.9797	-0.9116	1.5889
H	-3.4343	-0.1076	1.4854
H	-4.8836	-0.5752	1.6289

Table S45 The MP2/aug-cc-pVDZ optimized Cartesian Coordinates of the isomer **hf3c-113-2386** of the **Phe-$(H_2O)_2$** complex.

	X	Y	Z
C	-0.3307	0.5217	0.8189
C	0.4130	-0.7322	0.7849
C	-1.6697	0.5284	1.3425
C	-0.2313	-1.9399	1.2219
C	-2.2713	-0.7015	1.7922
C	-1.5802	-1.8932	1.7245
C	0.2106	1.7499	0.3448
C	1.7527	-0.8185	0.3123
C	-2.4083	1.7451	1.3786
C	0.4708	-3.1767	1.1640
C	-0.5337	2.9314	0.3853
C	2.4251	-2.0428	0.2670
C	-1.8518	2.9340	0.9083
C	1.7810	-3.2334	0.6912
H	-3.2937	-0.6738	2.1838
H	-2.0490	-2.8256	2.0566
H	1.2210	1.7817	-0.0684
H	2.2748	0.0768	-0.0317
H	-3.4275	1.7305	1.7791
H	-0.0398	-4.0882	1.4914
H	-0.0940	3.8595	0.0089
H	3.4522	-2.0811	-0.1066
H	-2.4296	3.8622	0.9382
H	2.3082	-4.1901	0.6419
O	0.2384	-2.1713	-2.4810
H	-0.6102	-1.7779	-2.2081
H	0.7685	-2.1442	-1.6726
O	-2.2185	-0.8683	-1.5575
H	-2.3326	-1.1011	-0.6223
H	-2.0107	0.0766	-1.5221

Table S46 The MP2/aug-cc-pVDZ optimized Cartesian Coordinates of the isomer **hf3c-114-134** of the **Phe-$(H_2O)_2$** complex.

	X	Y	Z
C	0.7824	0.2930	-0.2217
C	0.1778	-0.6046	0.7548
C	0.9649	-0.1650	-1.5721
C	-0.2527	-1.9092	0.3331
C	0.5398	-1.4881	-1.9481
C	-0.0537	-2.3263	-1.0306
C	1.1800	1.6210	0.1013
C	-0.0187	-0.2373	2.1173
C	1.5449	0.7069	-2.5383
C	-0.8687	-2.7850	1.2714
C	1.7408	2.4613	-0.8636
C	-0.6287	-1.1126	3.0191

C	1.9289	2.0045	-2.1941
C	-1.0598	-2.3954	2.5964
H	0.6942	-1.8155	-2.9819
H	-0.3821	-3.3287	-1.3253
H	1.0202	2.0126	1.1073
H	0.3004	0.7442	2.4741
H	1.6775	0.3444	-3.5633
H	-1.1923	-3.7751	0.9331
H	2.0235	3.4821	-0.5921
H	-0.7726	-0.8023	4.0580
H	2.3648	2.6676	-2.9467
H	-1.5385	-3.0756	3.3067
O	-1.5563	2.1211	-1.8862
H	-0.6007	1.9873	-1.9911
H	-1.9465	1.3831	-2.3738
O	-2.0836	1.9988	0.9904
H	-1.8648	1.0774	1.1858
H	-1.9428	2.0658	0.0280

Table S47 The MP2/aug-cc-pVDZ optimized Cartesian Coordinates of the isomer **pm7-66-2057** of the **Phe-$(H_2O)_2$** complex.

	X	Y	Z
C	0.3588	-0.2987	0.2202
C	-0.8770	0.4064	-0.0995
C	1.6115	0.2533	-0.2153
C	-0.8095	1.6346	-0.8416
C	1.6374	1.5033	-0.9303
C	0.4692	2.1698	-1.2325
C	0.3775	-1.5370	0.9246
C	-2.1618	-0.0883	0.2677
C	2.8217	-0.4450	0.0557
C	-2.0106	2.3119	-1.1944
C	1.5777	-2.2080	1.1748
C	-3.3283	0.5909	-0.0944
C	2.8104	-1.6616	0.7367
C	-3.2556	1.7992	-0.8326
H	2.6053	1.9098	-1.2416
H	0.4956	3.1134	-1.7874
H	-0.5541	-1.9813	1.2840
H	-2.2529	-1.0121	0.8445
H	3.7666	-0.0128	-0.2895
H	-1.9403	3.2432	-1.7659
H	1.5624	-3.1589	1.7153
H	-4.3017	0.1866	0.1982
H	3.7465	-2.1922	0.9319
H	-4.1714	2.3252	-1.1165
O	-0.9112	-2.1150	-2.2002
H	-0.2723	-2.2365	-1.4806
H	-1.5566	-1.5040	-1.8120

O	0.6225	-0.1355	-3.7677
H	0.1070	-0.8567	-3.3644
H	0.7750	0.4676	-3.0267

Table S48 Theoretical spectroscopic parameters of the isomers of the Phe-$(H_2O)_3$ complex at the MP2/aug-cc-pVDZ and at the B3LYP-D3BJ/def2-TZVP levels of theory. Rotational constants, dipole moment components and relative energies are also provided for the anti-clockwise directionality of the hydrogen bond network at the B3LYP-D3BJ/def2-TZVP level of theory. The labels **a** and **c** indicate a clockwise and an anti-clockwise directionality of the hydrogen bond network, respectively.

	Isomer1(c)		**Isomer1(a)**	**Isomer2(c)**		**Isomer2(a)**
	MP2	**B3LYP**	**B3LYP**	**MP2**	**B3LYP**	**B3LYP**
A (MHz)	648.1	623.6	621.3	643.8	620.4	622.9
B (MHz)	383.5	392.0	392.2	385.0	393.2	392.7
C (MHz)	336.9	333.0	333.3	336.2	333.1	333.0
$\lvert\mu_a\rvert$ (D)	0.5	0.4	0.4	0.5	0.4	0.4
$\lvert\mu_b\rvert$ (D)	0.9	1.1	1.1	1.0	1.1	1.1
$\lvert\mu_c\rvert$ (D)	1.7	1.5	1.5	1.7	1.5	1.5
$\Delta\Delta E_e$ (kJ/mol)	**0**[a]	1.4	1.4	0.3	1.7	1.7
$\Delta\Delta E$ (0k)[b] (kJ/mol)	**0**[b]	1.2[c]	1.1	0.3	1.1	1.1
	Isomer3(c)		**Isomer3(a)**	**Isomer4(c)**		**Isomer4a)**
	MP2	**B3LYP**	**B3LYP**	**MP2**	**B3LYP**	**B3LYP**
A (MHz)	662.2	648.3	637.3	626.9	616.1	616.3
B (MHz)	363.4	362.7	366.9	366.8	371.3	371.5
C (MHz)	317.5	316.9	319.7	352.4	353.5	353.1
$\lvert\mu_a\rvert$ (D)	0.7	0.7	0.7	0.3	0.4	0.4
$\lvert\mu_b\rvert$ (D)	1.1	1.1	1.1	4.4	4.9	4.8
$\lvert\mu_c\rvert$ (D)	1.6	1.5	1.5	2.7	1.7	1.8
$\Delta\Delta E_e$ (kJ/mol)	1.4	3.0	1.7	1.5	**0**	0
$\Delta\Delta E$ (0k)[b] (kJ/mol)	2.1	2.4	2.5	2.5	**0**	0

[a]MP2-F12/aug-cc-pVTZ-F12//MP2/aug-cc-pVDZ single point energies calculated on the optimised structures at the MP2/aug-cc-pVDZ.
[b] MP2-F12/aug-cc-pVTZ-F12//MP2/aug-cc-pVDZ single point energies combined with harmonic zero-point corrections at the MP2/aug-cc-pVDZ level of theory.
[c] B3LYP-D3BJ/def2-TZVP zero-point corrected energies.

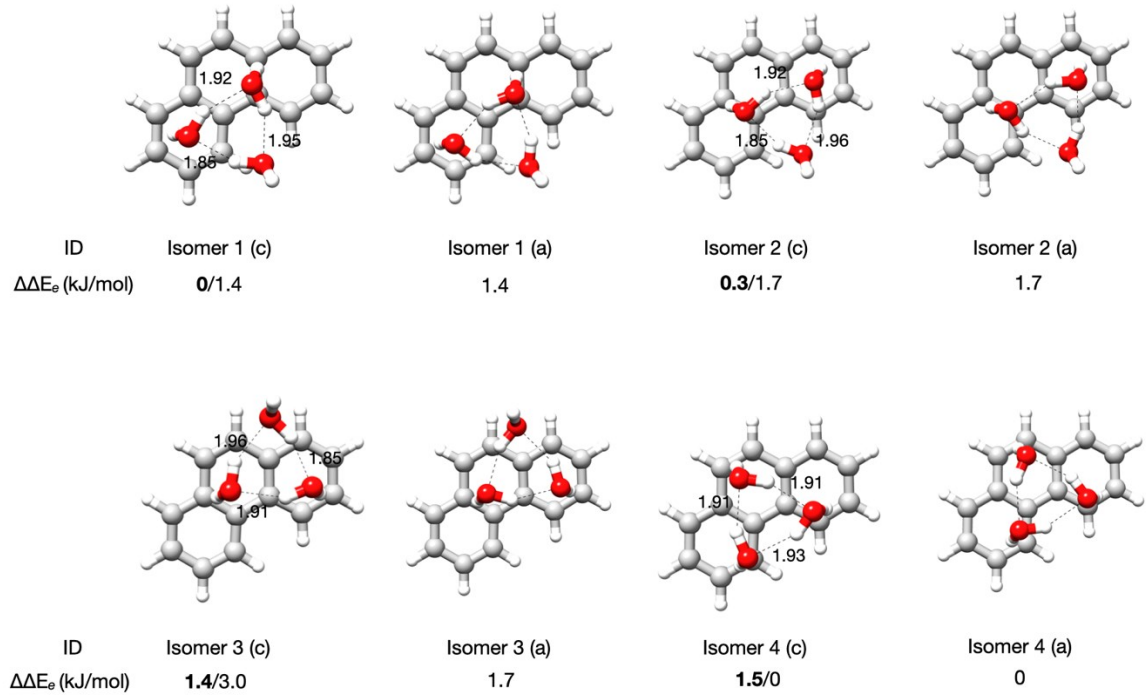


Figure S16 Theoretical structures of the Phe-$(H_2O)_3$ complex. Relative energies at the MP2-F12/aug-cc-pVTZ-F12//MP2-aug-cc-pVDZ (bold) and B3LYP-D3BJ/def2-TZVP (non-bold) are provided. The label c and a indicate a clockwise and an anti-clockwise directionality of the hydrogen bond network, respectively. Hydrogen bond distances (in Å) are also given.

Table S49 The MP2/aug-cc-pVDZ optimized Cartesian Coordinates of the isomer **isomer 1 (c)** of the **Phe-$(H_2O)_3$** complex.

	X	Y	Z
C	0.0911	-1.1531	-0.6383
C	-0.7908	-0.0311	-0.3429
C	1.2460	-0.9352	-1.4682
C	-0.4604	1.2708	-0.8550
C	1.5301	0.3836	-1.9741
C	0.7126	1.4499	-1.6694
C	-0.1266	-2.4585	-0.1158
C	-1.9666	-0.1673	0.4470
C	2.1227	-2.0206	-1.7557
C	-1.2998	2.3810	-0.5508
C	0.7482	-3.5066	-0.4095
C	-2.7786	0.9333	0.7287
C	1.8796	-3.2917	-1.2368
C	-2.4442	2.2201	0.2329
H	2.4182	0.5254	-2.5993
H	0.9424	2.4519	-2.0467
H	-0.9721	-2.6482	0.5471
H	-2.2391	-1.1395	0.8602
H	2.9980	-1.8372	-2.3879
H	-1.0313	3.3678	-0.9428

H	0.5614	-4.4989	0.0110
H	-3.6732	0.8018	1.3437
H	2.5620	-4.1168	-1.4603
H	-3.0802	3.0804	0.4609
O	0.0922	1.6746	2.5150
H	-0.4782	2.0080	1.8054
H	0.9080	1.3889	2.0535
O	2.1666	0.0287	1.5374
H	1.5476	-0.6431	1.8850
H	2.2149	-0.1723	0.5912
O	-0.1421	-1.0810	2.8600
H	-0.0344	-1.3122	3.7920
H	-0.2680	-0.1048	2.86397

Table S 50 The MP2/aug-cc-pVDZ optimized Cartesian Coordinates of the isomer **isomer 2 (c)** of the **Phe-$(H_2O)_3$** complex.

	X	Y	Z
C	2.8651	0.0198	-0.5520
C	1.7404	0.5731	-1.2954
C	3.2383	-1.3528	-0.7691
C	1.0347	-0.2668	-2.2239
C	2.5060	-2.1576	-1.7133
C	1.4402	-1.6346	-2.4120
C	3.5959	0.7730	0.4087
C	1.2975	1.9155	-1.1285
C	4.3175	-1.9154	-0.0285
C	-0.0775	0.2574	-2.9435
C	4.6502	0.1999	1.1225
C	0.2075	2.4107	-1.8476
C	5.0163	-1.1529	0.9065
C	-0.4899	1.5788	-2.7617
H	2.8079	-3.2003	-1.8586
H	0.8831	-2.2549	-3.1221
H	3.3225	1.8087	0.6156
H	1.7956	2.5717	-0.4133
H	4.5864	-2.9626	-0.2032
H	-0.6080	-0.3969	-3.6435
H	5.1915	0.7998	1.8597
H	-0.1159	3.4443	-1.6954
H	5.8403	-1.5967	1.4726
H	-1.3466	1.9695	-3.3184
O	0.8196	-1.4465	1.4738
H	1.5140	-1.7006	0.8478
H	0.0547	-1.2141	0.9066
O	-1.2485	0.0636	0.2766
H	-0.7535	0.7546	0.7583
H	-1.1594	0.3231	-0.6532
O	0.7443	1.2986	1.9539
H	0.5471	1.4748	2.8832

H	0.9710	0.3412	1.9322

Table S51 The MP2/aug-cc-pVDZ optimized Cartesian Coordinates of the isomer **isomer 3 (c)** of the **Phe-$(H_2O)_3$** complex.

	X	Y	Z
C	1.9284	0.0506	3.1770
C	2.2622	-0.3799	4.5295
C	2.9851	0.4501	2.2892
C	3.6384	-0.3574	4.9486
C	4.3501	0.4490	2.7450
C	4.6640	0.0703	4.0311
C	0.5919	0.0731	2.6862
C	1.2833	-0.8309	5.4593
C	2.6761	0.8485	0.9581
C	3.9802	-0.7854	6.2638
C	0.3097	0.4727	1.3759
C	1.6425	-1.2462	6.7432
C	1.3584	0.8618	0.5021
C	2.9998	-1.2244	7.1526
H	5.1350	0.7412	2.0414
H	5.7044	0.0715	4.3728
H	0.2376	-0.2241	3.3317
H	0.2293	-0.8640	5.1746
H	3.4980	1.1276	0.2919
H	5.0329	-0.7660	6.5653
H	0.7266	0.4825	1.0254
H	0.8692	-1.5931	7.4346
H	1.1331	1.1642	-0.5244
H	3.2761	-1.5534	8.1583
O	1.8881	-2.5266	0.8726
H	2.2391	-2.7910	1.7487
H	1.3259	-1.7608	1.0661
O	4.5614	-1.8137	0.5178
H	3.5972	-1.9824	0.4179
H	4.9734	-2.4050	-0.1258
O	3.6758	-3.0279	2.9906
H	4.2667	-2.5792	2.3549
H	3.6619	-2.4354	3.75699

Table S52 The MP2/aug-cc-pVDZ optimized Cartesian Coordinates of the isomer **isomer 4 (c)** of the **Phe-$(H_2O)_3$** complex.

	X	Y	Z
C	1.0509	-0.1137	0.4334
C	0.0911	0.5046	-0.4712
C	1.9127	0.7247	1.2202
C	0.0202	1.9375	-0.5431
C	1.8386	2.1569	1.0881

C	0.9247	2.7423	0.2367
C	1.1625	-1.5249	0.5866
C	-0.8111	-0.2545	-1.2700
C	2.8253	0.1339	2.1392
C	-0.9481	2.5553	-1.3847
C	2.0666	-2.0842	1.4946
C	-1.7563	0.3726	-2.0867
C	2.9017	-1.2510	2.2828
C	-1.8313	1.7882	-2.1430
H	2.5189	2.7756	1.6832
H	0.8677	3.8324	0.1478
H	0.5275	-2.1947	0.0026
H	-0.7838	-1.3462	-1.2458
H	3.4660	0.7884	2.7394
H	-0.9933	3.6487	-1.4208
H	2.1255	-3.1715	1.5980
H	-2.4424	-0.2352	-2.6837
H	3.6005	-1.6932	2.9983
H	-2.5775	2.2736	-2.7781
O	-2.6509	0.1249	1.4363
H	-2.2291	0.9376	1.7878
H	-2.4502	0.1516	0.4894
O	-0.7010	-0.8786	3.2782
H	-1.4031	-0.8394	2.5965
H	0.0540	-1.2664	2.8112
O	-0.9873	1.9030	2.8656
H	-0.2403	2.2163	2.3339
H	-0.6847	1.0339	3.20371

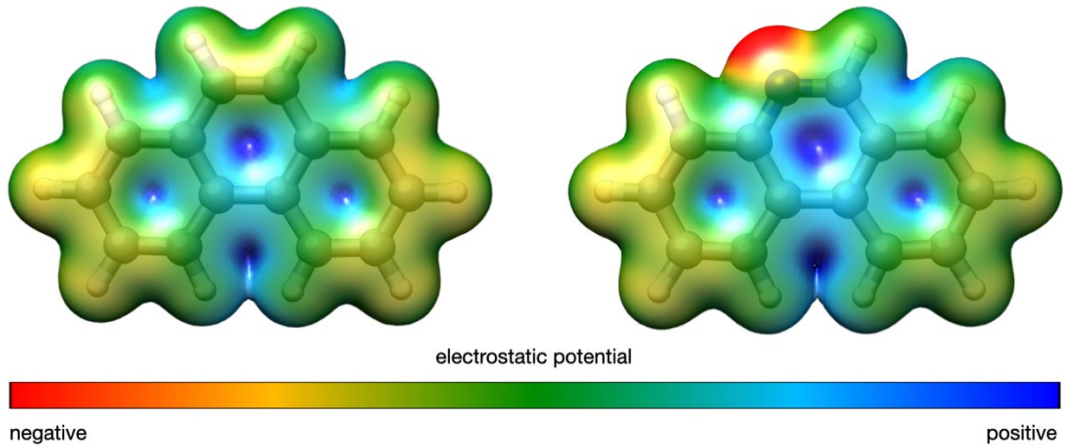


Figure S17 This figure shows the electrostatic potential map for the monomer of Pan (left) and Phe (right). The areas coloured in red are those experiencing a negative electrostatic potential while those coloured in blue are the areas with a positive electrostatic potential. The electrostatic potential of Phe and Pan was calculated using the program Multiwfn.[7]

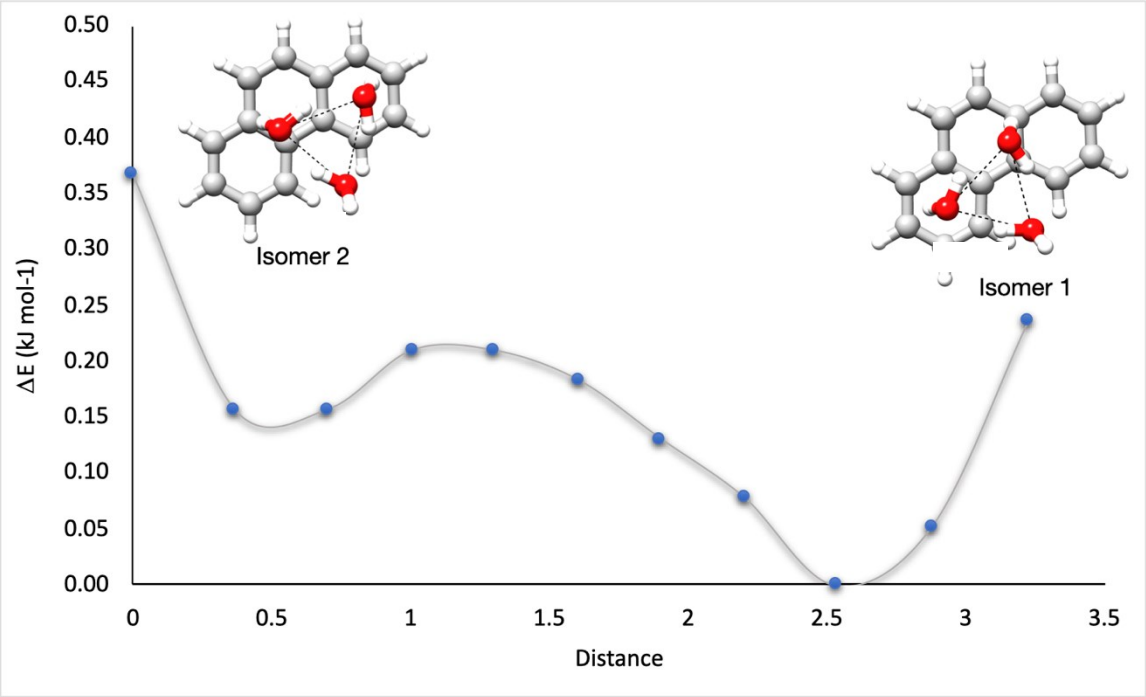


Figure S18 Energy barrier calculated using the NEB method at the B3LYP-D3BJ/def2-TZVP level of theory for the interconversion motion between isomer 1 and 2 of the Phe-$(H_2O)_3$ cluster.

S4. Measured rotational transitions

Table S53 Measured frequencies and residuals (in MHz) for the rotational transitions of the monomer of Pan. The experimental transitions measured by McNaugthon *et al.*[1] are reported in bold.

J'	K_a'	K_c'	F'	←	J''	K_a''	K_c''	F''	ν_{obs}	ν_{obs}-ν_{calc}
4	1	3	3	←	4	0	4	3	2011.0292	-0.0021
4	1	3	5	←	4	0	4	5	2011.3901	-0.0025
4	1	3	4	←	4	0	4	4	2012.7994	-0.0013
7	2	5	8	←	6	3	4	7	2023.9920	0.0060
7	2	5	7	←	6	3	4	6	2024.6527	0.0017
1	1	1	1	←	0	0	0	1	2058.3204	-0.0021
1	1	1	2	←	0	0	0	1	2059.0928	-0.0029
1	1	1	0	←	0	0	0	1	2060.2569	-0.0021
2	1	1	1	←	1	1	0	1	2088.2731	-0.0007
2	1	1	2	←	1	1	0	1	2089.5594	-0.0025
2	1	1	3	←	1	1	0	2	2089.6881	-0.0010
2	1	1	2	←	1	1	0	2	2090.5145	-0.0030
2	1	1	1	←	1	1	0	0	2090.6642	-0.0009
5	4	1	4	←	6	3	4	5	2160.1546	-0.0070
5	4	1	6	←	6	3	4	7	2160.1914	0.0001
5	4	1	5	←	6	3	4	6	2160.3304	0.0067
10	2	9	10	←	9	3	6	9	2160.7520	-0.0010
10	2	9	11	←	9	3	6	10	2161.8867	-0.0023
10	2	9	9	←	9	3	6	8	2162.0095	0.0007
11	2	10	11	←	10	3	7	10	2246.2029	0.0001
11	2	10	12	←	10	3	7	11	2247.5534	-0.0023
11	2	10	10	←	10	3	7	9	2247.6876	0.0024
5	1	4	4	←	4	2	3	3	2372.8972	-0.0041
5	1	4	6	←	4	2	3	5	2373.0513	-0.0020
5	1	4	5	←	4	2	3	4	2373.7692	-0.0044
7	5	3	6	←	8	4	4	7	2446.4798	0.0082
7	5	3	8	←	8	4	4	9	2446.4798	0.0008
7	5	3	7	←	8	4	4	8	2446.4798	-0.0319
7	5	2	6	←	8	4	5	7	2463.5114	0.0060
7	5	2	8	←	8	4	5	9	2463.5114	-0.0048
7	5	2	7	←	8	4	5	8	2463.5759	-0.0001
11	3	9	11	←	10	4	6	10	2520.4952	0.0035
11	3	9	12	←	10	4	6	11	2520.7730	-0.0151
5	1	4	4	←	5	0	5	4	2530.5066	0.0058
5	1	4	6	←	5	0	5	6	2530.8179	0.0044
5	1	4	5	←	5	0	5	6	2531.4152	-0.0075
5	1	4	4	←	5	0	5	5	2531.6315	0.0029
5	1	4	6	←	5	0	5	5	2531.7395	-0.0122
5	1	4	5	←	5	0	5	5	2532.3598	-0.0012
3	1	3	3	←	2	1	2	3	2702.0740	0.0003
3	1	3	2	←	2	1	2	1	2703.0980	0.0438
3	1	3	3	←	2	1	2	2	2703.0980	-0.0015
3	1	3	4	←	2	1	2	3	2703.2240	0.0011
3	1	3	2	←	2	1	2	2	2704.6477	-0.0033
10	3	7	9	←	9	4	6	8	2726.9671	-0.0008

10	3	7	11	←	9	4	6	10	2727.0174	-0.0004
10	3	7	10	←	9	4	6	9	2727.5284	-0.0022
9	2	7	8	←	9	2	8	8	2760.8248	-0.0001
9	2	7	10	←	9	2	8	10	2760.9739	0.0030
9	2	7	9	←	9	2	8	9	2762.2686	-0.0050
3	0	3	3	←	2	0	2	3	2871.3530	-0.0023
3	0	3	3	←	2	0	2	2	2871.6621	-0.0016
3	0	3	4	←	2	0	2	3	2871.8409	-0.0019
3	0	3	2	←	2	0	2	2	2872.3227	-0.0003
5	2	3	4	←	5	1	4	5	2886.2189	-0.0007
5	2	3	6	←	5	1	4	5	2886.3263	-0.0005
5	2	3	5	←	5	1	4	5	2886.8513	0.0003
5	2	3	6	←	5	1	4	6	2886.9320	-0.0040
5	2	3	4	←	5	1	4	4	2886.9320	-0.0202
5	2	3	5	←	5	1	4	6	2887.4620	0.0018
5	2	3	5	←	5	1	4	4	2887.5822	-0.0012
2	1	2	2	←	1	0	1	2	2891.1553	-0.0019
2	1	2	2	←	1	0	1	1	2891.3404	-0.0013
2	1	2	3	←	1	0	1	2	2892.1831	0.0000
2	1	2	1	←	1	0	1	0	2892.4782	-0.0017
2	1	2	1	←	1	0	1	1	2892.9389	0.0002
6	2	4	7	←	6	1	5	6	2895.0761	-0.0003
6	2	4	5	←	6	1	5	5	2895.5640	0.0282
6	2	4	7	←	6	1	5	7	2895.5640	0.0012
6	2	4	6	←	6	1	5	6	2895.7288	0.0026
6	1	5	5	←	6	1	6	5	2904.4452	0.0033
6	1	5	7	←	6	1	6	7	2904.7635	0.0004
6	1	5	6	←	6	1	6	6	2906.6697	0.0062
3	2	2	3	←	2	2	1	2	2922.5782	-0.0021
3	2	2	4	←	2	2	1	3	2922.7760	-0.0008
3	2	2	2	←	2	2	1	1	2922.8846	-0.0006
3	2	2	2	←	2	2	1	1	2922.8846	-0.0006
4	2	2	3	←	4	1	3	4	2972.6549	0.0013
4	2	2	5	←	4	1	3	4	2972.7663	0.0138
4	2	2	4	←	4	1	3	4	2973.1364	-0.0019
3	2	1	2	←	2	2	0	2	2973.2573	-0.0035
4	2	2	5	←	4	1	3	5	2973.4569	0.0028
4	2	2	3	←	4	1	3	3	2973.5336	-0.0006
3	2	1	3	←	2	2	0	2	2973.6766	0.0340
3	2	1	4	←	2	2	0	3	2973.6766	0.0055
3	2	1	2	←	2	2	0	1	2973.7392	-0.0056
4	2	2	4	←	4	1	3	5	2973.8427	0.0027
3	2	1	3	←	2	2	0	3	2973.9522	-0.0021
4	2	2	4	←	4	1	3	3	2974.0257	0.0065
4	0	4	4	←	3	1	3	4	2985.2935	-0.0002
4	0	4	3	←	3	1	3	2	2985.7798	-0.0002
4	0	4	5	←	3	1	3	4	2986.0000	-0.0002
4	0	4	4	←	3	1	3	3	2986.4427	-0.0003
4	0	4	3	←	3	1	3	3	2987.3325	0.0009
7	2	5	6	←	7	1	6	7	3031.1812	-0.0042
7	2	5	6	←	7	1	6	6	3031.5497	-0.0121

7	2	5	8	←	7	1	6	8	3031.6142	-0.0057
7	2	5	7	←	7	1	6	7	3032.0207	-0.0033
7	2	5	7	←	7	1	6	8	3032.3518	-0.0014
7	2	5	7	←	7	1	6	6	3032.3985	-0.0019
3	2	1	2	←	3	1	2	3	3113.9128	0.0019
3	2	1	4	←	3	1	2	3	3114.0109	0.0016
3	2	1	3	←	3	1	2	3	3114.2932	0.0007
3	2	1	4	←	3	1	2	4	3114.7803	0.0030
3	2	1	2	←	3	1	2	2	3114.9560	0.0043
3	2	1	3	←	3	1	2	4	3115.0632	0.0026
3	2	1	3	←	3	1	2	2	3115.3394	0.0060
3	1	2	2	←	2	1	1	2	3124.9918	0.0038
3	1	2	3	←	2	1	1	2	3126.0257	-0.0029
3	1	2	4	←	2	1	1	3	3126.0942	0.0050
3	1	2	2	←	2	1	1	1	3126.2782	0.0021
3	1	2	3	←	2	1	1	3	3126.8583	0.0010
6	1	5	5	←	6	0	6	5	3196.6628	-0.0023
6	1	5	7	←	6	0	6	7	3196.9412	-0.0008
6	1	5	6	←	6	0	6	5	3197.2314	-0.0015
6	1	5	6	←	6	0	6	7	3197.4279	-0.0005
6	1	5	5	←	6	0	6	6	3198.0101	-0.0004
6	1	5	7	←	6	0	6	6	3198.0923	0.0002
6	1	5	6	←	6	0	6	6	3198.5748	-0.0035
12	3	10	12	←	11	4	7	11	3242.2774	-0.0015
12	3	10	13	←	11	4	7	12	3242.7150	0.0088
12	3	10	11	←	11	4	7	10	3242.7150	-0.0287
2	2	0	1	←	2	1	1	2	3266.1937	-0.0010
2	2	0	3	←	2	1	1	2	3266.3634	-0.0035
2	2	0	2	←	2	1	1	2	3266.6784	-0.0002
2	2	0	3	←	2	1	1	3	3267.1931	-0.0023
2	2	0	1	←	2	1	1	1	3267.4791	-0.0037
2	2	0	2	←	2	1	1	1	3267.9707	0.0039
8	2	6	7	←	8	1	7	7	3319.5191	0.0052
8	2	6	9	←	8	1	7	9	3319.5924	-0.0022
8	2	6	8	←	8	1	7	8	3320.2221	0.0005
8	2	6	7	←	7	3	5	6	3440.6565	0.0009
8	2	6	9	←	7	3	5	8	3440.7454	-0.0008
8	2	6	8	←	7	3	5	7	3441.4677	0.0000
4	1	4	4	←	3	1	3	4	3589.5781	-0.0034
4	1	4	4	←	3	1	3	3	3590.7342	0.0034
4	1	4	5	←	3	1	3	4	3590.8263	-0.0008
4	1	4	3	←	3	1	3	3	3592.2961	0.0007
3	1	3	3	←	2	0	2	3	3658.6413	-0.0002
3	1	3	3	←	2	0	2	2	3658.9510	0.0010
3	1	3	4	←	2	0	2	3	3659.7930	0.0021
3	1	3	2	←	2	0	2	1	3660.0188	0.0000
3	1	3	2	←	2	0	2	2	3660.4990	-0.0025
6	1	5	5	←	5	2	4	4	3675.0742	-0.0009
6	1	5	7	←	5	2	4	6	3675.1918	-0.0061
6	1	5	6	←	5	2	4	5	3675.8788	-0.0054
2	2	1	1	←	2	1	2	1	3676.8794	-0.0114

2	2	1	2	←	2	1	2	1	3677.1943	-0.0033
2	2	1	3	←	2	1	2	3	3677.5635	-0.0073
2	2	1	2	←	2	1	2	3	3677.7629	-0.0057
2	2	1	1	←	2	1	2	2	3678.4840	-0.0037
2	2	1	3	←	2	1	2	2	3678.5921	-0.0046
2	2	1	2	←	2	1	2	2	3678.7915	-0.0030
4	0	4	4	←	3	0	3	4	3773.2276	-0.0140
4	0	4	4	←	3	0	3	3	3773.7301	0.0009
4	0	4	5	←	3	0	3	4	3773.9429	-0.0052
4	0	4	5	←	3	0	3	4	3773.9522	0.0040
4	0	4	3	←	3	0	3	2	3773.9522	-0.0063
4	0	4	3	←	3	0	3	3	3774.6143	-0.0035
9	2	7	8	←	9	1	8	8	3776.1235	0.0013
9	2	7	10	←	9	1	8	10	3776.2160	0.0011
9	2	7	9	←	9	1	8	9	3777.0410	0.0000
7	1	6	6	←	7	1	7	6	3806.4596	0.0009
7	1	6	8	←	7	1	7	8	3806.7223	0.0005
7	1	6	7	←	7	1	7	7	3808.5463	0.0032
13	3	11	13	←	12	4	8	12	3811.5610	-0.0019
13	3	11	14	←	12	4	8	13	3812.1452	-0.0037
13	3	11	12	←	12	4	8	11	3812.1948	-0.0018
4	2	3	4	←	3	2	2	3	3886.8297	0.0000
4	2	3	5	←	3	2	2	4	3886.9425	0.0003
3	2	2	2	←	3	1	3	2	3896.7194	-0.0025
3	2	2	4	←	3	1	3	4	3897.1239	-0.0009
3	2	2	3	←	3	1	3	3	3898.2772	0.0018
4	3	2	3	←	3	3	1	3	3920.4213	0.0009
4	3	2	4	←	3	3	1	3	3920.6224	0.0047
4	3	2	5	←	3	3	1	4	3920.7528	0.0024
4	3	2	3	←	3	3	1	2	3920.8221	0.0110
4	3	1	4	←	3	3	0	3	3925.0509	-0.0032
4	3	1	5	←	3	3	0	4	3925.1655	-0.0048
4	3	1	3	←	3	3	0	2	3925.2169	-0.0102
4	3	1	4	←	3	3	0	4	3925.3451	-0.0037
7	1	6	6	←	7	0	7	6	3993.7805	-0.0020
7	1	6	8	←	7	0	7	8	3994.0221	0.0000
7	1	6	7	←	7	0	7	7	3995.6735	-0.0056
4	2	2	3	←	3	2	1	3	4009.5578	-0.0004
4	2	2	5	←	3	2	1	4	4009.9413	0.0009
4	2	2	4	←	3	2	1	3	4010.0443	0.0012
4	2	2	4	←	3	2	1	4	4010.3254	-0.0008
5	0	5	5	←	4	1	4	5	4034.5408	-0.0005
5	0	5	4	←	4	1	4	3	4035.3494	-0.0007
5	0	5	6	←	4	1	4	5	4035.4803	0.0006
5	0	5	5	←	4	1	4	4	4035.7853	-0.0016
5	0	5	4	←	4	1	4	4	4036.9069	-0.0078
4	1	3	3	←	3	1	2	3	4150.3145	-0.0019
4	1	3	4	←	3	1	2	3	4151.1895	-0.0076
4	1	3	5	←	3	1	2	4	4151.2660	0.0024
4	1	3	3	←	3	1	2	2	4151.3540	-0.0031
4	1	3	4	←	3	1	2	4	4151.9627	-0.0024

4	2	3	4	←	4	1	4	3	4192.8112	0.0015
4	2	3	3	←	4	1	4	3	4192.9519	0.0023
4	2	3	4	←	4	1	4	5	4193.1298	0.0011
4	2	3	5	←	4	1	4	5	4193.2433	0.0035
4	2	3	4	←	4	1	4	4	4194.3767	0.0024
4	1	4	4	←	3	0	3	4	4377.5216	-0.0077
4	1	4	4	←	3	0	3	3	4378.0117	-0.0052
4	1	4	5	←	3	0	3	4	4378.7714	-0.0037
4	1	4	3	←	3	0	3	2	4378.9170	-0.0052
4	1	4	3	←	3	0	3	3	4379.5783	-0.0032
10	3	7	10	←	10	2	8	10	4384.2776	0.0005
10	3	7	11	←	10	2	8	11	4384.3602	0.0026
10	3	7	9	←	10	2	8	9	4384.3602	-0.0055
11	3	8	10	←	11	2	9	10	4391.8708	0.0074
11	3	8	12	←	11	2	9	12	4391.8708	-0.0025
11	3	8	11	←	11	2	9	11	4391.9912	0.0000
10	2	8	9	←	10	1	9	9	4406.1496	0.0000
10	2	8	11	←	10	1	9	11	4406.2519	0.0030
10	2	8	10	←	10	1	9	10	4407.2372	0.0029
5	1	5	5	←	4	1	4	5	4467.5961	-0.0021
5	1	5	5	←	4	1	4	4	4468.8435	-0.0005
5	1	5	4	←	4	1	4	3	4468.9207	0.0367
5	1	5	6	←	4	1	4	5	4468.9207	-0.0085
5	1	5	4	←	4	1	4	4	4470.4520	0.0033
9	3	6	9	←	9	2	7	9	4514.6149	-0.0019
9	3	6	10	←	9	2	7	10	4514.8678	-0.0089
9	3	6	8	←	9	2	7	8	4514.9149	0.0088
5	2	4	5	←	5	1	5	4	4566.4109	0.0005
5	2	4	4	←	5	1	5	4	4566.6478	-0.0038
5	2	4	6	←	5	1	5	6	4566.8809	-0.0031
5	2	4	5	←	5	1	5	5	4568.0110	-0.0039
5	2	4	6	←	5	1	5	5	4568.2467	0.0316
5	2	4	4	←	5	1	5	5	4568.2467	-0.0096
12	3	9	11	←	12	2	10	11	4569.5416	-0.0014
12	3	9	13	←	12	2	10	13	4569.5838	0.0141
12	3	9	12	←	12	2	10	12	4569.8929	0.0068
5	0	5	5	←	4	0	4	5	4639.3671	-0.0011
5	0	5	5	←	4	0	4	4	4640.0804	0.0056
5	0	5	6	←	4	0	4	5	4640.3085	0.0019
5	0	5	4	←	4	0	4	4	4641.1927	-0.0098
8	3	5	7	←	8	2	6	8	4739.2915	-0.0026
8	3	5	9	←	8	2	6	8	4739.3342	-0.0029
8	3	5	8	←	8	2	6	8	4739.7032	-0.0071
8	3	5	9	←	8	2	6	9	4740.1181	0.0122
8	3	5	7	←	8	2	6	7	4740.1564	-0.0028
8	3	5	8	←	8	2	6	9	4740.4813	0.0023
8	3	5	8	←	8	2	6	7	4740.5707	-0.0046
8	1	7	7	←	8	1	8	7	4772.9890	0.0037
8	1	7	9	←	8	1	8	9	4773.1984	0.0000
8	1	7	8	←	8	1	8	8	4774.9038	-0.0009
4	2	3	3	←	4	0	4	3	4797.8969	-0.0163

4	2	3	5	←	4	0	4	5	4798.0739	0.0071
4	2	3	4	←	4	0	4	4	4798.6600	-0.0020
5	2	4	5	←	4	2	3	5	4842.3670	-0.0064
5	2	4	5	←	4	2	3	4	4842.4809	-0.0037
5	2	4	6	←	4	2	3	5	4842.5725	-0.0010
5	2	4	4	←	4	2	3	4	4842.7227	-0.0033
8	1	7	7	←	8	0	8	7	4888.4695	-0.0004
8	1	7	9	←	8	0	8	9	4888.6713	0.0003
8	1	7	8	←	8	0	8	8	4890.2851	0.0046
5	4	2	5	←	4	4	1	4	4899.7952	-0.0041
5	4	2	6	←	4	4	1	5	4899.9348	0.0146
5	4	2	4	←	4	4	1	3	4899.9348	-0.0269
5	4	1	5	←	4	4	0	4	4900.0755	-0.0059
5	4	1	6	←	4	4	0	5	4900.2170	0.0156
5	4	1	4	←	4	4	0	3	4900.2170	-0.0257
5	3	3	5	←	4	3	2	4	4908.2987	0.0019
5	3	3	6	←	4	3	2	5	4908.3440	-0.0093
5	3	3	4	←	4	3	2	3	4908.3440	-0.0266
9	2	7	8	←	8	3	6	7	4917.1507	0.0005
9	2	7	10	←	8	3	6	9	4917.2262	-0.0027
9	2	7	9	←	8	3	6	8	4917.9559	-0.0052
5	3	2	4	←	4	3	1	4	4923.4322	-0.0029
5	3	2	4	←	4	3	1	5	4923.6011	-0.0124
5	3	2	6	←	4	3	1	5	4923.6572	0.0127
5	3	2	4	←	4	3	1	3	4923.6572	-0.0022
5	3	2	5	←	4	3	1	5	4923.8059	0.0066
7	1	6	6	←	6	2	5	5	4986.0358	-0.0026
7	1	6	8	←	6	2	5	7	4986.1276	-0.0013
7	1	6	7	←	6	2	5	6	4986.7451	0.0010
5	2	4	4	←	5	0	5	4	5000.1864	0.0008
5	2	4	6	←	5	0	5	6	5000.3335	-0.0002
5	2	4	5	←	5	0	5	5	5001.0816	0.0096
7	3	4	7	←	7	2	5	7	5008.5275	0.0009
7	3	4	8	←	7	2	5	8	5008.9942	-0.0029
7	3	4	6	←	7	2	5	6	5009.0682	0.0038
6	2	5	5	←	6	1	6	5	5017.0883	-0.0077
6	2	5	7	←	6	1	6	7	5017.2860	-0.0064
6	2	5	6	←	6	1	6	6	5018.4175	-0.0032
6	0	6	6	←	5	1	5	6	5043.9897	-0.0002
6	0	6	5	←	5	1	5	4	5045.0511	-0.0105
6	0	6	7	←	5	1	5	6	5045.1329	-0.0070
6	0	6	6	←	5	1	5	5	5045.3125	-0.0083
6	0	6	5	←	5	1	5	5	5046.6701	0.0038
5	1	5	5	←	4	0	4	5	5072.4229	-0.0023
5	2	3	4	←	4	2	2	4	5072.7151	-0.0012
5	1	5	5	←	4	0	4	4	5073.1295	-0.0022
5	2	3	4	←	4	2	2	3	5073.2083	0.0071
5	2	3	6	←	4	2	2	5	5073.2083	-0.0011
5	2	3	5	←	4	2	2	4	5073.3485	0.0008
5	1	5	6	←	4	0	4	5	5073.7587	0.0025
5	1	5	4	←	4	0	4	3	5073.8476	-0.0001

5	1	5	4	←	4	0	4	4	5074.7370	0.0006
5	1	4	4	←	4	1	3	4	5158.9025	0.0000
5	1	4	5	←	4	1	3	4	5159.6367	0.0016
5	1	4	6	←	4	1	3	5	5159.7287	0.0013
5	1	4	4	←	4	1	3	3	5159.7888	0.0056
5	1	4	5	←	4	1	3	5	5160.3337	-0.0028
11	2	9	10	←	11	1	10	10	5196.6922	0.0131
11	2	9	12	←	11	1	10	12	5196.7852	0.0057
11	2	9	11	←	11	1	10	11	5197.8836	0.0140
6	3	3	5	←	6	2	4	6	5270.4063	-0.0099
6	3	3	7	←	6	2	4	6	5270.4433	-0.0044
6	3	3	6	←	6	2	4	6	5270.6320	-0.0034
6	3	3	7	←	6	2	4	7	5271.0891	-0.0082
6	3	3	5	←	6	2	4	5	5271.1627	-0.0116
6	3	3	6	←	6	2	4	7	5271.2882	0.0032
6	3	3	6	←	6	2	4	5	5271.3832	-0.0102
6	2	5	5	←	6	0	6	5	5309.3212	0.0018
6	2	5	7	←	6	0	6	7	5309.4751	0.0035
6	2	5	6	←	6	0	6	6	5310.3439	0.0083
6	1	6	6	←	5	1	5	6	5335.9015	-0.0032
6	1	6	6	←	5	1	5	5	5337.2327	-0.0030
6	1	6	5	←	5	1	5	4	5337.3081	0.0230
6	1	6	7	←	5	1	5	6	5337.3081	-0.0108
2	2	1	1	←	1	1	0	1	5342.9493	0.0168
2	2	1	2	←	1	1	0	1	5343.2269	-0.0122
2	2	1	3	←	1	1	0	2	5344.0066	0.0096
2	2	1	2	←	1	1	0	2	5344.2049	0.0101
2	2	1	1	←	1	1	0	0	5345.3339	0.0101
6	0	6	6	←	5	0	5	6	5477.4408	0.0011
6	0	6	6	←	5	0	5	5	5478.3771	-0.0008
6	0	6	7	←	5	0	5	6	5478.5917	0.0021
6	0	6	5	←	5	0	5	5	5479.7105	-0.0127
5	3	2	4	←	5	2	3	5	5486.3880	-0.0105
5	3	2	6	←	5	2	3	5	5486.4223	-0.0071
5	3	2	5	←	5	2	3	5	5486.5822	-0.0018
5	3	2	6	←	5	2	3	6	5486.9508	-0.0027
5	3	2	4	←	5	2	3	4	5487.0312	0.0013
5	3	2	5	←	5	2	3	6	5487.0959	-0.0123
5	3	2	5	←	5	2	3	4	5487.2175	0.0020
2	2	0	1	←	1	1	1	0	5496.4862	0.0009
2	2	0	1	←	1	1	1	2	5497.6452	-0.0033
2	2	0	3	←	1	1	1	2	5497.8216	0.0009
2	2	0	2	←	1	1	1	2	5498.1325	0.0000
2	2	0	1	←	1	1	1	1	5498.4195	-0.0023
2	2	0	2	←	1	1	1	1	5498.9032	-0.0025
7	2	6	7	←	7	1	7	6	5540.7465	0.0013
7	2	6	6	←	7	1	7	6	5541.1721	0.0059
7	2	6	8	←	7	1	7	8	5541.3360	0.0080
7	2	6	7	←	7	1	7	7	5542.4345	-0.0186
4	3	1	3	←	4	2	2	4	5636.0844	-0.0022
4	3	1	5	←	4	2	2	4	5636.1211	-0.0113

4	3	1	4	←	4	2	2	4	5636.3088	-0.0021
4	3	1	5	←	4	2	2	5	5636.5271	0.0087
4	3	1	3	←	4	2	2	3	5636.5534	-0.0180
4	3	1	4	←	4	2	2	5	5636.6937	-0.0032
4	3	1	4	←	4	2	2	3	5636.7941	-0.0016
3	3	0	2	←	3	2	1	3	5720.9022	-0.0002
3	3	0	4	←	3	2	1	3	5721.0050	-0.0001
3	3	0	4	←	3	2	1	4	5721.2878	-0.0005
3	3	0	3	←	3	2	1	4	5721.5873	0.0041
3	3	0	3	←	3	2	1	2	5721.6795	-0.0019
7	2	6	6	←	7	0	7	6	5728.4816	-0.0085
7	2	6	8	←	7	0	7	8	5728.6326	0.0042
7	2	6	7	←	7	0	7	7	5729.5797	-0.0096
6	1	6	6	←	5	0	5	6	5769.3550	0.0005
6	1	6	6	←	5	0	5	5	5770.2912	-0.0016
6	1	6	7	←	5	0	5	6	5770.7702	0.0016
6	1	6	5	←	5	0	5	4	5770.8203	0.0014
6	1	6	5	←	5	0	5	5	5771.9486	0.0019
3	3	1	2	←	3	2	2	2	5784.2243	-0.0051
3	3	1	4	←	3	2	2	4	5784.3249	-0.0050
3	3	1	3	←	3	2	2	3	5784.6146	-0.0037
6	2	5	6	←	5	2	4	6	5787.4372	-0.0042
6	2	5	6	←	5	2	4	5	5787.6386	-0.0029
6	2	5	7	←	5	2	4	6	5787.7239	-0.0033
6	2	5	5	←	5	2	4	5	5787.9668	-0.0038
4	3	2	3	←	4	2	3	3	5818.0627	-0.0064
4	3	2	5	←	4	2	3	5	5818.1368	-0.0013
4	3	2	3	←	4	2	3	4	5818.1965	-0.0125
4	3	2	5	←	4	2	3	4	5818.2424	-0.0069
4	3	2	4	←	4	2	3	5	5818.2978	0.0026
4	3	2	4	←	4	2	3	4	5818.4043	-0.0020
9	1	8	8	←	9	0	9	8	5838.9164	-0.0076
9	1	8	10	←	9	0	9	10	5839.0872	-0.0049
9	1	8	9	←	9	0	9	9	5840.5934	-0.0048
6	5	2	6	←	5	5	1	5	5877.7851	0.0081
6	5	1	6	←	5	5	0	5	5877.7851	-0.0070
6	5	2	7	←	5	5	1	6	5877.8948	0.0054
6	5	1	7	←	5	5	0	6	5877.8948	-0.0096
6	5	2	5	←	5	5	1	4	5877.9399	0.0198
6	5	1	5	←	5	5	0	4	5877.9399	0.0047
5	3	3	4	←	5	2	4	4	5883.8450	-0.0087
5	3	3	6	←	5	2	4	6	5883.9173	-0.0006
5	3	3	5	←	5	2	4	6	5884.0145	-0.0039
5	3	3	4	←	5	2	4	5	5884.0912	-0.0039
5	3	3	6	←	5	2	4	5	5884.1332	0.0151
5	3	3	5	←	5	2	4	5	5884.2157	-0.0028
6	4	3	6	←	5	4	2	5	5888.9315	0.0072
6	4	3	7	←	5	4	2	6	5888.9808	-0.0021
6	4	3	5	←	5	4	2	4	5888.9808	-0.0188
6	4	2	6	←	5	4	1	5	5890.1957	0.0112
6	4	2	7	←	5	4	1	6	5890.2390	-0.0011

6	4	2	5	←	5	4	1	4	5890.2390	-0.0173
6	3	4	7	←	5	3	3	6	5897.5566	-0.0157
14	4	10	14	←	14	3	11	14	5903.8614	0.0035
14	4	10	15	←	14	3	11	15	5904.0617	0.0069
14	4	10	13	←	14	3	11	13	5904.0617	-0.0073
6	3	3	7	←	5	3	2	6	5937.4820	-0.0066
6	3	3	6	←	5	3	2	5	5937.5155	-0.0061
6	3	4	5	←	6	2	5	5	5993.7108	0.0022
6	3	4	7	←	6	2	5	7	5993.7618	-0.0011
6	3	4	6	←	6	2	5	6	5994.1122	-0.0050
7	0	7	6	←	6	1	6	5	6009.3985	0.0465
7	0	7	8	←	6	1	6	7	6009.3985	-0.0008
7	0	7	7	←	6	1	6	6	6009.4832	-0.0024
12	2	10	11	←	12	1	11	11	6115.8866	0.0084
12	2	10	13	←	12	1	11	13	6115.9870	0.0139
12	2	10	12	←	12	1	11	12	6117.0995	-0.0082
8	2	7	7	←	8	1	8	7	6133.1377	-0.0130
8	2	7	9	←	8	1	8	9	6133.2872	-0.0030
8	2	7	8	←	8	1	8	8	6134.4041	0.0043
6	1	5	5	←	5	1	4	5	6144.0248	-0.0025
6	1	5	6	←	5	1	4	5	6144.5904	-0.0048
6	1	5	7	←	5	1	4	6	6144.7207	0.0025
6	1	5	5	←	5	1	4	4	6144.7207	-0.0392
6	1	5	6	←	5	1	4	6	6145.2056	0.0012
6	2	4	5	←	5	2	3	5	6152.7124	0.0002
6	2	4	7	←	5	2	3	6	6153.3454	0.0005
6	2	4	6	←	5	2	3	5	6153.4713	0.0009
6	2	4	6	←	5	2	3	6	6153.9946	0.0001
7	3	5	6	←	7	2	6	6	6159.0680	0.0005
7	3	5	8	←	7	2	6	8	6159.1194	-0.0079
7	3	5	7	←	7	2	6	7	6159.5377	-0.0036
3	2	2	2	←	2	1	1	2	6176.2602	0.0044
3	2	2	3	←	2	1	1	2	6176.2602	0.0026
3	2	2	3	←	2	1	1	3	6177.0883	0.0023
3	2	2	4	←	2	1	1	3	6177.0883	0.0036
3	2	2	2	←	2	1	1	1	6177.5472	0.0033
7	1	7	7	←	6	1	6	6	6196.6270	0.0053
7	1	7	8	←	6	1	6	7	6196.7108	0.0111
8	1	7	7	←	7	2	6	6	6280.1998	-0.0093
8	1	7	9	←	7	2	6	8	6280.2748	-0.0041
8	1	7	8	←	7	2	6	7	6280.7763	-0.0112
7	0	7	7	←	6	0	6	7	6300.2450	-0.0054
7	0	7	7	←	6	0	6	6	6301.3990	-0.0014
7	0	7	8	←	6	0	6	7	6301.5757	-0.0026
7	0	7	6	←	6	0	6	6	6302.9274	0.0067
8	3	6	7	←	8	2	7	7	6389.6948	0.0095
8	3	6	9	←	8	2	7	9	6389.7545	0.0056
8	3	6	8	←	8	2	7	8	6390.2361	0.0078
10	2	8	9	←	9	3	7	8	6429.3228	0.0074
10	2	8	11	←	9	3	7	10	6429.3949	0.0081
10	2	8	10	←	9	3	7	9	6430.0928	0.0038

7	1	7	7	←	6	0	6	7	6487.3860	-0.0006
7	1	7	7	←	6	0	6	6	6488.5382	0.0016
7	1	7	8	←	6	0	6	7	6488.8740	-0.0047
7	1	7	6	←	6	0	6	6	6490.2325	-0.0121
12	4	8	12	←	12	3	9	12	6524.6409	0.0122
12	4	8	13	←	12	3	9	13	6525.0301	-0.0092
12	4	8	11	←	12	3	9	11	6525.0889	0.0150
3	2	1	2	←	2	1	2	1	6663.4538	-0.0062
3	2	1	4	←	2	1	2	3	6664.1242	-0.0052
3	2	1	3	←	2	1	2	3	6664.4059	-0.0067
3	2	1	2	←	2	1	2	2	6665.0499	-0.0070
3	2	1	3	←	2	1	2	2	6665.4319	-0.0067
9	3	7	8	←	9	2	8	8	6692.7643	-0.0037
9	3	7	10	←	9	2	8	10	6692.8148	-0.0138
9	3	7	9	←	9	2	8	9	6693.3628	-0.0107
7	2	6	7	←	6	2	5	7	6720.3720	0.0036
7	2	6	7	←	6	2	5	6	6720.6540	-0.0002
7	2	6	8	←	6	2	5	7	6720.7458	0.0106
7	2	6	6	←	6	2	5	5	6720.7458	-0.0003
7	2	6	6	←	6	2	5	6	6721.0853	0.0100
9	2	8	8	←	9	1	9	8	6785.1077	-0.0044
9	2	8	10	←	9	1	9	10	6785.2306	-0.0026
9	2	8	9	←	9	1	9	9	6786.3157	-0.0018
10	1	9	9	←	10	0	10	9	6806.2268	0.0035
10	1	9	11	←	10	0	10	11	6806.3616	0.0002
10	1	9	10	←	10	0	10	10	6807.7454	0.0087
9	2	8	8	←	9	0	9	8	6854.2214	0.0001
9	2	8	10	←	9	0	9	10	6854.3320	-0.0042
9	2	8	9	←	9	0	9	9	6855.3574	-0.0082
7	6	2	7	←	6	6	1	6	6855.9227	0.0033
7	6	1	7	←	6	6	0	6	6855.9227	0.0026
7	6	2	8	←	6	6	1	7	6856.0174	-0.0058
7	6	1	8	←	6	6	0	7	6856.0174	-0.0065
7	6	2	6	←	6	6	1	5	6856.0590	0.0121
7	6	1	6	←	6	6	0	5	6856.0590	0.0114
7	5	3	7	←	6	5	2	6	6865.6662	0.0269
7	5	3	8	←	6	5	2	7	6865.7165	0.0142
7	5	3	6	←	6	5	2	5	6865.7165	-0.0003
7	5	2	7	←	6	5	1	6	6865.7165	-0.0058
7	5	2	8	←	6	5	1	7	6865.7944	0.0093
7	5	2	6	←	6	5	1	5	6865.7944	-0.0052
7	4	4	7	←	6	4	3	6	6882.3800	-0.0141
7	4	4	8	←	6	4	3	7	6882.4194	-0.0003
7	4	4	6	←	6	4	3	5	6882.4194	-0.0058
7	3	5	7	←	6	3	4	6	6886.0595	-0.0188
7	3	5	8	←	6	3	4	7	6886.1192	0.0196
7	3	5	6	←	6	3	4	5	6886.1192	0.0142
7	4	3	7	←	6	4	2	6	6886.5236	-0.0185
7	4	3	8	←	6	4	2	7	6886.5764	0.0141
7	4	3	6	←	6	4	2	5	6886.5764	0.0052
11	4	7	11	←	11	3	8	11	6903.0858	-0.0046

11	4	7	12	←	11	3	8	12	6903.5091	-0.0186
11	4	7	12	←	11	3	8	12	6903.5395	0.0117
11	4	7	10	←	11	3	8	10	6903.5871	0.0189
8	0	8	8	←	7	1	7	8	6931.4712	0.0028
8	0	8	7	←	7	1	7	6	6932.8910	-0.0143
8	0	8	9	←	7	1	7	8	6932.9747	0.0387
8	0	8	8	←	7	1	7	7	6932.9747	0.0143
4	2	3	4	←	3	1	2	3	6937.0627	0.0042
4	2	3	3	←	3	1	2	3	6937.2027	0.0043
4	2	3	4	←	3	1	2	4	6937.8311	0.0046
4	2	3	5	←	3	1	2	4	6937.9388	0.0012
4	2	3	3	←	3	1	2	2	6938.2406	0.0014
7	3	4	8	←	6	3	3	7	6972.6156	0.0002
7	3	4	7	←	6	3	3	6	6972.6920	0.0015
8	1	8	8	←	7	1	7	8	7046.8417	-0.0023
8	1	8	8	←	7	1	7	7	7048.3410	0.0049
8	1	8	7	←	7	1	7	6	7048.4075	0.0175
8	1	8	9	←	7	1	7	8	7048.4075	-0.0008
10	3	8	11	←	10	2	9	11	7072.4666	0.0041
10	3	8	10	←	10	2	9	10	7073.0788	0.0152
7	1	6	6	←	6	1	5	6	7098.1129	-0.0120
7	1	6	7	←	6	1	5	6	7098.4918	-0.0095
7	1	6	8	←	6	1	5	7	7098.6521	-0.0062
7	1	6	7	←	6	1	5	7	7098.9715	-0.0160
8	0	8	8	←	7	0	7	8	7118.7704	0.0018
8	0	8	8	←	7	0	7	7	7120.0946	-0.0019
8	0	8	9	←	7	0	7	8	7120.2310	-0.0052
8	0	8	7	←	7	0	7	7	7121.7408	-0.0087
7	2	5	8	←	6	2	4	7	7234.7000	-0.0155
7	2	5	7	←	6	2	4	6	7234.7956	-0.0036
8	1	8	8	←	7	0	7	7	7235.4679	-0.0043
8	1	8	9	←	7	0	7	8	7235.7123	0.0035
8	1	8	7	←	7	0	7	7	7237.2334	-0.0007
10	4	6	10	←	10	3	7	10	7255.6860	-0.0046
10	4	6	11	←	10	3	7	11	7256.1002	0.0004
10	4	6	9	←	10	3	7	9	7256.1421	0.0029
10	2	9	9	←	10	1	10	9	7487.6035	-0.0037
10	2	9	11	←	10	1	10	11	7487.7068	-0.0059
10	2	9	10	←	10	1	10	10	7488.7658	0.0025
11	3	9	10	←	11	2	10	10	7529.2726	-0.0004
11	3	9	12	←	11	2	10	12	7529.3285	-0.0035
11	3	9	11	←	11	2	10	11	7529.9779	-0.0015
9	1	8	8	←	8	2	7	7	7530.7551	0.0419
9	1	8	10	←	8	2	7	9	7530.7551	-0.0077
9	1	8	9	←	8	2	7	8	7531.1366	-0.0117
9	4	5	9	←	9	3	6	9	7546.5705	-0.0049
9	4	5	10	←	9	3	6	10	7546.9010	-0.0092
9	4	5	8	←	9	3	6	8	7546.9559	0.0087
5	2	4	5	←	4	1	3	4	7628.3503	0.0043
5	2	4	4	←	4	1	3	4	7628.5924	0.0050
5	2	4	5	←	4	1	3	5	7629.0463	-0.0012

5	2	4	6	←	4	1	3	5	7629.2501	0.0024
5	2	4	4	←	4	1	3	3	7629.4698	0.0017
8	2	7	8	←	7	2	6	7	7640.2715	-0.0110
8	2	7	9	←	7	2	6	8	7640.3634	-0.0072
8	4	4	8	←	8	3	5	8	7761.1586	-0.0092
8	4	4	9	←	8	3	5	9	7761.3900	-0.0179
8	4	4	7	←	8	3	5	7	7761.4376	0.0031
11	1	10	10	←	11	0	11	10	7763.1153	-0.0073
11	1	10	12	←	11	0	11	12	7763.2291	-0.0067
11	1	10	11	←	11	0	11	11	7764.4679	-0.0086
9	0	9	8	←	8	1	8	7	7824.9458	0.0058
9	0	9	9	←	8	1	8	8	7824.9458	-0.0040
9	0	9	10	←	8	1	8	9	7824.9458	-0.0151
8	6	3	8	←	7	6	2	7	7842.7806	-0.0132
8	6	2	8	←	7	6	1	7	7842.7806	-0.0179
8	6	3	9	←	7	6	2	8	7842.8425	-0.0154
8	6	2	9	←	7	6	1	8	7842.8425	-0.0202
8	6	3	7	←	7	6	2	6	7842.8766	0.0060
8	6	2	7	←	7	6	1	6	7842.8766	0.0013
8	5	4	8	←	7	5	3	7	7857.2172	-0.0146
8	5	4	9	←	7	5	3	8	7857.2693	0.0036
8	5	4	7	←	7	5	3	6	7857.2693	-0.0035
8	5	3	8	←	7	5	2	7	7857.5434	-0.0182
8	5	3	9	←	7	5	2	8	7857.6031	0.0081
8	5	3	7	←	7	5	2	6	7857.6031	0.0010
8	3	6	9	←	7	3	5	8	7870.9914	-0.0006
8	4	5	9	←	7	4	4	8	7880.1363	-0.0079
8	4	4	7	←	7	4	3	6	7891.3649	-0.0003
8	4	4	9	←	7	4	3	8	7891.3649	-0.0010
8	4	4	8	←	7	4	3	7	7891.3649	-0.0090
9	1	9	9	←	8	1	8	8	7893.9976	-0.0004
9	1	9	9	←	8	1	8	8	7894.0154	0.0173
9	1	9	9	←	8	1	8	8	7894.0154	0.0173
7	4	3	7	←	7	3	4	7	7903.8692	-0.0037
7	4	3	8	←	7	3	4	8	7904.0191	0.0085
7	4	3	6	←	7	3	4	6	7904.0191	-0.0137
9	0	9	9	←	8	0	8	8	7940.3300	0.0043
9	0	9	10	←	8	0	8	9	7940.4322	-0.0011
4	2	2	3	←	3	1	3	2	7970.3439	-0.0017
4	2	2	5	←	3	1	3	4	7970.8461	-0.0008
4	2	2	4	←	3	1	3	4	7971.2314	-0.0014
4	2	2	3	←	3	1	3	3	7971.8986	0.0013
4	2	2	3	←	3	1	3	3	7971.8986	0.0013
4	2	2	4	←	3	1	3	3	7972.3847	0.0026
6	4	2	7	←	6	3	3	7	7990.0544	-0.0093
17	**2**	**16**	**16**	←	**17**	**1**	**17**	**16**	**13098.1884**	**0.0000**
17	**2**	**16**	**18**	←	**17**	**1**	**17**	**18**	**13098.2331**	**0.0010**
17	**2**	**16**	**17**	←	**17**	**1**	**17**	**17**	**13098.9752**	**-0.0002**
24	**6**	**19**	**23**	←	**24**	**5**	**20**	**23**	**13357.4890**	**-0.0040**
24	**6**	**19**	**25**	←	**24**	**5**	**20**	**25**	**13357.5057**	**0.0021**
24	**6**	**19**	**24**	←	**24**	**5**	**20**	**24**	**13357.7565**	**-0.0020**

15	1	14	15	←	14	1	13	14	13783.7578	0.0004
15	1	14	16	←	14	1	13	15	13783.8611	0.0009
15	1	14	14	←	14	1	13	13	13783.8611	-0.0014
15	2	14	15	←	14	1	13	14	13860.0937	0.0000
15	2	14	16	←	14	1	13	15	13860.2324	-0.0005
15	2	14	14	←	14	1	13	13	13860.2388	0.0010
14	4	11	14	←	13	4	10	13	13870.3592	0.0005
14	4	11	15	←	13	4	10	14	13870.3754	0.0007
14	4	11	13	←	13	4	10	12	13870.3754	-0.0009
21	1	20	20	←	21	0	21	20	16439.4799	-0.0001
21	1	20	22	←	21	0	21	22	16439.5088	-0.0003
21	1	20	21	←	21	0	21	21	16440.1222	-0.0008
21	2	20	20	←	21	1	21	20	16442.2960	0.0002
21	2	20	22	←	21	1	21	22	16442.3242	-0.0007
21	2	20	21	←	21	1	21	21	16442.9376	0.0001
9	4	6	9	←	8	3	5	8	16625.6881	0.0000
9	4	6	10	←	8	3	5	9	16625.9538	0.0007
9	4	6	8	←	8	3	5	7	16625.9836	-0.0003
21	8	14	21	←	21	7	15	21	16730.1794	-0.0012
21	8	14	22	←	21	7	15	22	16730.2341	0.0026
21	8	14	20	←	21	7	15	20	16730.2341	-0.0002
17	4	14	17	←	16	4	13	16	16747.1192	0.0003
17	4	14	18	←	16	4	13	17	16747.1663	0.0015
17	4	14	16	←	16	4	13	15	16747.1663	-0.0012
20	8	12	20	←	20	7	13	20	16788.3323	-0.0017
20	8	12	21	←	20	7	13	21	16788.3978	0.0017
20	8	12	19	←	20	7	13	19	16788.3978	-0.0021
9	4	5	8	←	8	3	6	7	16979.0026	-0.0006
9	4	5	10	←	8	3	6	9	16979.0164	0.0004
9	4	5	9	←	8	3	6	8	16979.1533	-0.0001
19	1	18	19	←	18	2	17	18	17071.1063	0.0001
19	1	18	18	←	18	2	17	17	17071.1568	0.0008
19	1	18	20	←	18	2	17	19	17071.1568	-0.0003
19	2	18	19	←	18	2	17	18	17080.0250	0.0000
19	2	18	18	←	18	2	17	17	17080.0796	0.0009
19	2	18	20	←	18	2	17	19	17080.0796	-0.0001
10	3	7	9	←	9	2	8	8	17506.4479	-0.0013
10	3	7	11	←	9	2	8	10	17506.5740	0.0011
10	3	7	10	←	9	2	8	9	17507.7401	0.0004
24	1	23	24	←	23	2	22	23	21244.1047	0.0014
24	1	23	23	←	23	2	22	22	21244.1365	-0.0007
24	1	23	25	←	23	2	22	24	21244.1365	-0.0020
24	2	23	24	←	23	2	22	23	21244.6010	0.0009
24	2	23	23	←	23	2	22	22	21244.6345	0.0002
24	2	23	25	←	23	2	22	24	21244.6345	-0.0010
24	1	23	24	←	23	1	22	23	21245.0000	0.0001
24	1	23	23	←	23	1	22	22	21245.0345	0.0002
24	1	23	25	←	23	1	22	24	21245.0345	-0.0010
24	2	23	24	←	23	1	22	23	21245.4965	-0.0002
24	2	23	23	←	23	1	22	22	21245.5306	-0.0005
24	2	23	25	←	23	1	22	24	21245.5306	-0.0018

9	6	4	10	←	8	5	3	9	21486.4867	-0.0002
9	6	4	8	←	8	5	3	7	21486.4867	-0.0004
9	6	4	9	←	8	5	3	8	21486.5027	-0.0006
9	6	3	10	←	8	5	4	9	21486.9440	0.0006
9	6	3	8	←	8	5	4	7	21486.9440	0.0006
9	6	3	9	←	8	5	4	8	21486.9606	0.0000
21	5	16	20	←	20	5	15	19	21853.1743	0.0003
21	5	16	22	←	20	5	15	21	21853.1743	-0.0008
21	5	16	21	←	20	5	15	20	21853.2398	0.0005
14	10	4	13	←	14	9	5	13	21863.1344	0.0031
14	10	5	13	←	14	9	6	13	21863.1344	0.0030
14	10	4	15	←	14	9	5	15	21863.1344	0.0006
14	10	5	15	←	14	9	6	15	21863.1344	0.0005
14	10	4	14	←	14	9	5	14	21863.1695	0.0000
14	10	5	14	←	14	9	6	14	21863.1695	-0.0001
15	5	10	14	←	14	4	11	13	25378.5362	0.0000
15	5	10	16	←	14	4	11	15	25378.5511	0.0012
15	5	10	15	←	14	4	11	14	25378.7604	0.0000
22	12	11	22	←	21	11	10	21	48021.7500	0.0072
22	12	10	22	←	21	11	11	21	48021.7500	0.0069
15	15	0	15	←	14	14	1	14	48119.8200	-0.0063
15	15	1	15	←	14	14	0	14	48119.8200	-0.0063
20	13	7	20	←	19	12	8	19	48392.0500	-0.0325
20	13	8	20	←	19	12	7	19	48392.0500	-0.0325
30	9	21	30	←	29	8	22	29	48480.8600	-0.0136
25	11	15	25	←	24	10	14	24	48570.9800	0.0490
25	11	14	25	←	24	10	15	24	48570.9800	-0.1117
18	14	4	18	←	17	13	5	17	48747.8800	-0.0171
18	14	5	18	←	17	13	4	17	48747.8800	-0.0171
28	10	19	28	←	27	9	18	27	48952.2900	-0.0382
28	10	18	28	←	27	9	19	27	48978.8100	0.0510
23	12	12	23	←	22	11	11	22	48989.9400	-0.0129
23	12	11	23	←	22	11	12	22	48989.9400	-0.0137
16	15	1	16	←	15	14	2	15	49098.3500	0.0144
16	15	2	16	←	15	14	1	15	49098.3500	0.0144
21	13	8	21	←	20	12	9	20	49366.6500	0.0020
21	13	9	21	←	20	12	8	20	49366.6500	0.0020
31	9	22	31	←	30	8	23	30	49513.2400	0.0004
19	14	5	19	←	18	13	6	18	49725.2500	-0.0243
19	14	6	19	←	18	13	5	18	49725.2500	-0.0243
29	10	20	29	←	28	9	19	28	49843.0000	-0.0246
29	10	19	29	←	28	9	20	28	49892.9200	0.0540
24	12	13	24	←	23	11	12	23	49955.6800	-0.0260
24	12	12	24	←	23	11	13	23	49955.6800	-0.0283
17	15	2	17	←	16	14	3	16	50076.7900	0.0558
17	15	3	17	←	16	14	2	16	50076.7900	0.0558
20	14	6	20	←	19	13	7	19	50702.0500	-0.0282
20	14	7	20	←	19	13	6	19	50702.0500	-0.0282
18	15	3	18	←	17	14	4	17	51054.9300	-0.0118
18	15	4	18	←	17	14	3	17	51054.9300	-0.0118
23	13	10	23	←	22	12	11	22	51311.8400	0.0255

23	13	11	23	←	22	12	10	22	51311.8400	0.0255
16	16	0	16	←	15	15	1	15	51404.5600	-0.0244
16	16	1	16	←	15	15	0	15	51404.5600	-0.0244
31	10	22	31	←	30	9	21	30	51547.7200	0.0031
31	10	21	31	←	30	9	22	30	51710.1200	0.0801
26	12	15	26	←	25	11	14	25	51878.3200	-0.0414
26	12	14	26	←	25	11	15	25	51878.3200	-0.0570
19	15	4	19	←	18	14	5	18	52032.9000	0.0303
19	15	5	19	←	18	14	4	18	52032.9000	0.0303
24	13	12	24	←	23	12	11	23	52281.9800	0.0243
24	13	11	24	←	23	12	12	23	52281.9800	0.0243
29	11	19	29	←	28	10	18	28	52332.6600	-0.0452
29	11	18	29	←	28	10	19	28	52336.4100	0.0806
32	10	23	32	←	31	9	22	31	52341.5200	0.0736
17	16	1	17	←	16	15	2	16	52383.1100	0.0114
17	16	2	17	←	16	15	1	16	52383.1100	0.0114
32	10	22	32	←	31	9	23	31	52622.3200	0.0341
22	14	8	22	←	21	13	9	21	52653.3700	-0.0229
22	14	9	22	←	21	13	8	21	52653.3700	-0.0229
27	12	16	27	←	26	11	15	26	52834.4700	0.0453
27	12	15	27	←	26	11	16	26	52834.4700	0.0072
20	15	5	20	←	19	14	6	19	53010.4100	-0.0095
20	15	6	20	←	19	14	5	19	53010.4100	-0.0095
33	10	24	33	←	32	9	23	32	53075.6100	0.0669
25	13	13	25	←	24	12	12	24	53250.1300	0.0003
25	13	12	25	←	24	12	13	24	53250.1300	0.0001
18	16	2	18	←	17	15	3	17	53361.5100	-0.0066
18	16	3	18	←	17	15	2	17	53361.5100	-0.0066
33	10	23	33	←	32	9	24	32	53548.2100	0.0058
23	14	9	23	←	22	13	10	22	53627.5700	-0.0161
23	14	10	23	←	22	13	9	22	53627.5700	-0.0161
21	15	6	21	←	20	14	7	20	53987.4800	-0.0038
21	15	7	21	←	20	14	6	20	53987.4800	-0.0038
26	13	14	26	←	25	12	13	25	54216.0000	-0.0555
26	13	13	26	←	25	12	14	25	54216.0000	-0.0560
19	16	3	19	←	18	15	4	18	54339.8100	0.0404
19	16	4	19	←	18	15	3	18	54339.8100	0.0404
34	10	24	34	←	33	9	25	33	54501.7600	0.0176
24	14	10	24	←	23	13	11	23	54600.5200	-0.0496
24	14	11	24	←	23	13	10	23	54600.5200	-0.0496
17	17	0	17	←	16	16	1	16	54689.3100	-0.0109
17	17	1	17	←	16	16	0	16	54689.3100	-0.0109
22	15	7	22	←	21	14	8	21	54963.9600	0.0143
22	15	8	22	←	21	14	7	21	54963.9600	0.0143
20	16	4	20	←	19	15	5	19	55317.8100	0.0289
20	16	5	20	←	19	15	4	19	55317.8100	0.0289
25	14	11	25	←	24	13	12	24	55572.1600	0.0092
25	14	12	25	←	24	13	11	24	55572.1600	0.0092
18	17	1	18	←	17	16	2	17	55667.8700	0.0312
18	17	2	18	←	17	16	1	17	55667.8700	0.0312
23	15	8	23	←	22	14	9	22	55939.7000	0.0215

23	15	9	23	←	22	14	8	22	55939.7000	0.0215
21	16	5	21	←	20	15	6	20	56295.4600	-0.0075
21	16	6	21	←	20	15	5	20	56295.4600	-0.0075
26	14	12	26	←	25	13	13	25	56542.1400	0.0177
26	14	13	26	←	25	13	12	25	56542.1400	0.0177
19	17	2	19	←	18	16	3	18	56646.2500	-0.0221
19	17	3	19	←	18	16	2	18	56646.2500	-0.0221
24	15	9	24	←	23	14	10	23	56914.5300	-0.0153
24	15	10	24	←	23	14	9	23	56914.5300	-0.0153
22	16	6	22	←	21	15	7	21	57272.7500	0.0124
22	16	7	22	←	21	15	6	21	57272.7500	0.0124
20	17	3	20	←	19	16	4	19	57624.5600	-0.0013
20	17	4	20	←	19	16	3	19	57624.5600	-0.0013
25	15	10	25	←	24	14	11	24	57888.4200	0.0207
25	15	11	25	←	24	14	10	24	57888.4200	0.0207
18	18	0	18	←	17	17	1	17	57974.0100	-0.0243
18	18	1	18	←	17	17	0	17	57974.0100	-0.0243
23	16	7	23	←	22	15	8	22	58249.4700	-0.0224
23	16	8	23	←	22	15	7	22	58249.4700	-0.0224
21	17	4	21	←	20	16	5	20	58602.6800	0.0398
21	17	5	21	←	20	16	4	20	58602.6800	0.0398
26	15	11	26	←	25	14	12	25	58861.0400	-0.0421
26	15	12	26	←	25	14	11	25	58861.0400	-0.0421
19	18	1	19	←	18	17	2	18	58952.5400	-0.0148
19	18	2	19	←	18	17	1	18	58952.5400	-0.0148
24	16	8	24	←	23	15	9	23	59225.6300	0.0048
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22	17	5	22	←	21	16	6	21	59580.4000	-0.0364
22	17	6	22	←	21	16	5	21	59580.4000	-0.0364
20	18	2	20	←	19	17	3	19	59931.0000	-0.0006
20	18	3	20	←	19	17	2	19	59931.0000	-0.0006
25	16	9	25	←	24	15	10	24	60201.0300	0.0089
25	16	10	25	←	24	15	9	24	60201.0300	0.0089
23	17	6	23	←	22	16	7	22	60557.8800	0.0082
23	17	7	23	←	22	16	6	22	60557.8800	0.0082
21	18	3	21	←	20	17	4	20	60909.3300	0.0107
21	18	4	21	←	20	17	3	20	60909.3300	0.0107
19	19	0	19	←	18	18	1	18	61258.7400	0.0166
19	19	1	19	←	18	18	0	18	61258.7400	0.0166
24	17	7	24	←	23	16	8	23	61534.8700	0.0085
24	17	8	24	←	23	16	7	23	61534.8700	0.0085
22	18	4	22	←	21	17	5	21	61887.4900	0.0370
22	18	5	22	←	21	17	4	21	61887.4900	0.0370
20	19	1	20	←	19	18	2	19	62237.2900	0.0442
20	19	2	20	←	19	18	1	19	62237.2900	0.0442
25	17	8	25	←	24	16	9	24	62511.3300	0.0156
25	17	9	25	←	24	16	8	24	62511.3300	0.0156
23	18	5	23	←	22	17	6	22	62865.3600	0.0213
23	18	6	23	←	22	17	5	22	62865.3600	0.0213
21	19	2	21	←	20	18	3	20	63215.7400	0.0383
21	19	3	21	←	20	18	2	20	63215.7400	0.0383

24	18	6	24	←	23	17	7	23	63842.8900	-0.0185
24	18	7	24	←	23	17	6	23	63842.8900	-0.0185
22	19	3	22	←	21	18	4	21	64194.0900	0.0456
22	19	4	22	←	21	18	3	21	64194.0900	0.0456
20	20	0	20	←	19	19	1	19	64543.3900	0.0033
20	20	1	20	←	19	19	0	19	64543.3900	0.0033
23	19	4	23	←	22	18	5	22	65172.2200	-0.0030
23	19	5	23	←	22	18	4	22	65172.2200	-0.0030
21	20	1	21	←	20	19	2	20	65521.9300	0.0197
21	20	2	21	←	20	19	1	20	65521.9300	0.0197
33	15	19	33	←	32	14	18	32	65621.2500	0.0461
33	15	18	33	←	32	14	19	32	65621.2500	0.0456
31	16	15	31	←	30	15	16	30	66030.4000	0.0053
31	16	16	31	←	30	15	15	30	66030.4000	0.0053
22	20	2	22	←	21	19	3	21	66500.4300	0.0557
22	20	3	22	←	21	19	2	21	66500.4300	0.0557
27	21	6	27	←	26	20	7	26	73697.5700	0.0023
27	21	7	27	←	26	20	6	26	73697.5700	0.0023
25	22	3	25	←	24	21	4	24	74048.0500	0.0261
25	22	4	25	←	24	21	3	24	74048.0500	0.0261
30	20	10	30	←	29	19	11	29	74320.1600	-0.0166
30	20	11	30	←	29	19	10	29	74320.1600	-0.0166
23	23	0	23	←	22	22	1	22	74397.2000	-0.0079
23	23	1	23	←	22	22	0	22	74397.2000	-0.0079
28	21	7	28	←	27	20	8	27	74675.1400	-0.0064
28	21	8	28	←	27	20	7	27	74675.1400	-0.0064
26	22	4	26	←	25	21	5	25	75026.2400	-0.0580
26	22	5	26	←	25	21	4	25	75026.2400	-0.0580
31	20	11	31	←	30	19	12	30	75295.8000	0.0114
31	20	12	31	←	30	19	11	30	75295.8000	0.0114
24	23	1	24	←	23	22	2	23	75375.7300	-0.0027
24	23	2	24	←	23	22	1	23	75375.7300	-0.0027
29	21	8	29	←	28	20	9	28	75652.3600	-0.0403
29	21	9	29	←	28	20	8	28	75652.3600	-0.0403
34	19	15	34	←	33	18	16	33	75902.3300	-0.0310
34	19	16	34	←	33	18	15	33	75902.3300	-0.0310
27	22	5	27	←	26	21	6	26	76004.4400	0.0258
27	22	6	27	←	26	21	5	26	76004.4400	0.0258
32	20	12	32	←	31	19	13	31	76270.7200	-0.0360
32	20	13	32	←	31	19	12	31	76270.7200	-0.0360
25	23	2	25	←	24	22	3	24	76354.2100	-0.0026
25	23	3	25	←	24	22	2	24	76354.2100	-0.0026
30	21	9	30	←	29	20	10	29	76629.2600	-0.0127
30	21	10	30	←	29	20	9	29	76629.2600	-0.0127
28	22	6	28	←	27	21	7	27	76982.2500	-0.0805
28	22	7	28	←	27	21	6	27	76982.2500	-0.0805
26	23	3	26	←	25	22	4	25	77332.6400	0.0226
26	23	4	26	←	25	22	3	25	77332.6400	0.0226
24	24	0	24	←	23	23	1	23	77681.7300	-0.0243
24	24	1	24	←	23	23	0	23	77681.7300	-0.0243
30	23	7	30	←	29	22	8	29	81244.7900	-0.0013

30	**23**	**8**	**30**	←	**29**	**22**	**7**	**29**	**81244.7900**	**-0.0013**
28	**24**	**4**	**28**	←	**27**	**23**	**5**	**27**	**81595.5000**	**0.0078**
28	**24**	**5**	**28**	←	**27**	**23**	**4**	**27**	**81595.5000**	**0.0078**
33	**22**	**11**	**33**	←	**32**	**21**	**12**	**32**	**81867.2300**	**-0.0274**
33	**22**	**12**	**33**	←	**32**	**21**	**11**	**32**	**81867.2300**	**-0.0274**
26	**25**	**1**	**26**	←	**25**	**24**	**2**	**25**	**81944.7900**	**-0.0018**
26	**25**	**2**	**26**	←	**25**	**24**	**1**	**25**	**81944.7900**	**-0.0018**
31	**23**	**8**	**31**	←	**30**	**22**	**9**	**30**	**82222.3300**	**0.0503**
31	**23**	**9**	**31**	←	**30**	**22**	**8**	**30**	**82222.3300**	**0.0503**
36	**21**	**15**	**36**	←	**35**	**20**	**16**	**35**	**82478.9200**	**0.0194**
36	**21**	**16**	**36**	←	**35**	**20**	**15**	**35**	**82478.9200**	**0.0194**
29	**24**	**5**	**29**	←	**28**	**23**	**6**	**28**	**82573.6700**	**-0.0073**
29	**24**	**6**	**29**	←	**28**	**23**	**5**	**28**	**82573.6700**	**-0.0073**
27	**25**	**2**	**27**	←	**26**	**24**	**3**	**26**	**82923.2800**	**0.0023**
27	**25**	**3**	**27**	←	**26**	**24**	**2**	**26**	**82923.2800**	**0.0023**
28	**25**	**3**	**28**	←	**27**	**24**	**4**	**27**	**83901.7400**	**0.0397**
28	**25**	**4**	**28**	←	**27**	**24**	**3**	**27**	**83901.7400**	**0.0397**
26	**26**	**0**	**26**	←	**25**	**25**	**1**	**25**	**84250.7200**	**-0.0275**
26	**26**	**1**	**26**	←	**25**	**25**	**0**	**25**	**84250.7200**	**-0.0275**
27	**26**	**1**	**27**	←	**26**	**25**	**2**	**26**	**85229.2400**	**-0.0305**
27	**26**	**2**	**27**	←	**26**	**25**	**1**	**26**	**85229.2400**	**-0.0305**

Table S54 Measured frequencies and residuals (in MHz) for the rotational transitions of the ^{13}C1 isotopologue of the monomer of Pan.

J'	K_a'	K_c'	*F'*	←	*J"*	K_a"	K_c"	*F"*	ν_{obs}	ν_{obs}-ν_{calc}
3	1	3	4	←	2	1	2	3	2697.5516	0.0019
3	0	3	3	←	2	0	2	2	2865.6391	-0.0073
3	0	3	4	←	2	0	2	3	2865.8233	-0.0022
2	1	2	2	←	1	0	1	2	2884.8873	-0.0029
2	1	2	2	←	1	0	1	1	2885.0801	0.0053
2	1	2	3	←	1	0	1	2	2885.9172	0.0010
2	1	2	1	←	1	0	1	1	2886.6735	0.0018
3	2	1	4	←	2	2	0	3	2967.4776	-0.0047
3	2	1	2	←	2	2	0	1	2967.5476	-0.0084
4	0	4	5	←	3	1	3	4	2979.9428	-0.0050
4	0	4	4	←	3	1	3	3	2980.3908	0.0003
3	1	2	4	←	2	1	1	3	3119.5840	0.0006
4	1	4	4	←	3	1	3	3	3583.1941	0.0046
4	1	4	5	←	3	1	3	4	3583.2869	0.0009
3	1	3	3	←	2	0	2	2	3651.0574	0.0003
3	1	3	4	←	2	0	2	3	3651.8947	-0.0030
3	1	3	2	←	2	0	2	1	3652.1215	-0.0043
4	0	4	4	←	3	0	3	3	3765.8068	0.0057
4	0	4	5	←	3	0	3	4	3766.0227	0.0026
4	2	3	4	←	3	2	2	3	3878.7131	0.0040
4	2	2	5	←	3	2	1	4	4001.6102	-0.0003
4	2	2	4	←	3	2	1	3	4001.7136	0.0003
5	0	5	4	←	4	1	4	3	4027.0665	-0.0007
5	0	5	6	←	4	1	4	5	4027.1975	0.0007
5	0	5	5	←	4	1	4	4	4027.5042	0.0002

4	1	3	5	←	3	1	2	4	4142.6288	0.0119
4	1	3	3	←	3	1	2	2	4142.7026	-0.0079
4	1	4	4	←	3	0	3	3	4368.6068	0.0067
4	1	4	5	←	3	0	3	4	4369.3662	0.0080
4	1	4	3	←	3	0	3	2	4369.5131	0.0077
5	0	5	5	←	4	0	4	4	4630.3201	0.0171
5	0	5	6	←	4	0	4	5	4630.5400	0.0052
5	2	4	6	←	4	2	3	5	4832.4602	0.0103
5	1	5	5	←	4	0	4	4	5062.2442	-0.0061
2	2	1	2	←	1	1	0	1	5331.4648	0.0006
2	2	1	3	←	1	1	0	2	5332.2216	-0.0002
6	0	6	6	←	5	0	5	5	5466.8227	0.0007
6	0	6	7	←	5	0	5	6	5467.0385	0.0048
2	2	0	1	←	1	1	1	0	5484.4172	0.0065
2	2	0	3	←	1	1	1	2	5485.7444	-0.0017
2	2	0	2	←	1	1	1	2	5486.0599	0.0019
2	2	0	2	←	1	1	1	1	5486.8327	0.0014
6	1	6	6	←	5	0	5	5	5757.9671	0.0099
6	1	6	7	←	5	0	5	6	5758.4505	0.0177
6	2	5	6	←	5	2	4	5	5775.5398	0.0075
6	2	5	7	←	5	2	4	6	5775.6165	-0.0016
6	3	4	7	←	5	3	3	6	5885.2731	-0.0009
6	3	3	7	←	5	3	2	6	5925.1351	0.0006
7	0	7	8	←	6	1	6	7	5996.8623	-0.0159
7	0	7	7	←	6	1	6	6	5996.9627	-0.0015
6	1	5	6	←	5	1	4	5	6131.7493	-0.0084
6	2	4	7	←	5	2	3	6	6140.5830	-0.0039
6	2	4	6	←	5	2	3	5	6140.7158	0.0034
3	2	2	3	←	2	1	1	2	6162.7291	0.0031
3	2	2	4	←	2	1	1	3	6163.5525	-0.0007
3	2	2	2	←	2	1	1	1	6164.0146	0.0022
7	0	7	8	←	6	0	6	7	6288.2732	-0.0041
7	1	7	7	←	6	0	6	6	6474.6983	-0.0162
3	2	1	2	←	2	1	2	1	6648.9857	-0.0019
3	2	1	4	←	2	1	2	3	6649.6555	-0.0014
3	2	1	2	←	2	1	2	2	6650.5891	0.0045
3	2	1	3	←	2	1	2	2	6650.9619	-0.0042
7	2	6	7	←	6	2	5	6	6706.5855	0.0051
7	2	6	8	←	6	2	5	7	6706.6524	-0.0088
4	2	3	4	←	3	1	2	3	6921.9102	-0.0020
4	2	3	5	←	3	1	2	4	6922.7924	0.0009
4	2	3	3	←	3	1	2	2	6923.0921	-0.0007
7	3	4	8	←	6	3	3	7	6958.1322	0.0017
8	1	8	8	←	7	1	7	7	7033.5036	0.0104
8	1	8	9	←	7	1	7	8	7033.5446	-0.0208
7	1	6	7	←	6	1	5	6	7083.6377	0.0006
7	1	6	8	←	6	1	5	7	7083.7891	-0.0050
8	0	8	9	←	7	0	7	8	7105.2081	0.0015
7	2	5	8	←	6	2	4	7	7219.7062	-0.0006
7	2	5	7	←	6	2	4	6	7219.7936	0.0030
5	2	4	5	←	4	1	3	4	7611.7122	-0.0105

5	2	4	6	←	4	1	3	5	7612.6169	-0.0075
5	2	4	4	←	4	1	3	3	7612.8348	-0.0100
9	0	9	10	←	8	0	8	9	7923.6794	0.0033
4	2	2	3	←	3	1	3	2	7953.2231	0.0065
4	2	2	4	←	3	1	3	3	7955.2532	0.0000
9	1	9	8	←	8	0	8	7	7992.5718	0.0032

Table S55 Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C2$ isotopologue of the monomer of Pan.

J'	K_a'	K_c'	*F'*	←	*J"*	K_a"	K_c"	*F"*	ν_{obs}	ν_{obs}-ν_{calc}
1	1	1	1	←	0	0	0	1	2051.3768	0.0039
1	1	1	2	←	0	0	0	1	2052.1451	-0.0010
3	1	3	3	←	2	1	2	2	2683.1042	-0.0117
3	1	3	4	←	2	1	2	3	2683.2367	-0.0021
3	0	3	4	←	2	0	2	3	2850.1986	-0.0003
2	1	2	2	←	1	0	1	1	2878.5780	-0.0048
2	1	2	3	←	1	0	1	2	2879.4218	-0.0025
3	2	2	4	←	2	2	1	3	2899.8460	-0.0033
3	2	1	4	←	2	2	0	3	2949.4508	-0.0095
3	1	2	3	←	2	1	1	2	3100.5631	-0.0106
3	1	2	4	←	2	1	1	3	3100.6377	0.0042
3	1	2	2	←	2	1	1	1	3100.8180	-0.0028
4	1	4	5	←	3	1	3	4	3564.5035	-0.0024
6	1	5	6	←	5	2	4	5	3616.6234	0.0033
3	1	3	3	←	2	0	2	2	3641.1644	0.0026
3	1	3	4	←	2	0	2	3	3642.0018	-0.0017
3	1	3	2	←	2	0	2	1	3642.2207	-0.0115
4	0	4	4	←	3	0	3	3	3746.1563	-0.0106
4	0	4	5	←	3	0	3	4	3746.3888	0.0049
4	2	3	4	←	3	2	2	3	3856.5121	-0.0049
4	2	3	5	←	3	2	2	4	3856.6372	0.0078
4	2	2	5	←	3	2	1	4	3976.6224	-0.0016
4	2	2	4	←	3	2	1	3	3976.7218	-0.0031
5	0	5	4	←	4	1	4	3	3997.3770	0.0052
5	0	5	6	←	4	1	4	5	3997.5021	0.0000
5	0	5	5	←	4	1	4	4	3997.8114	-0.0041
4	1	3	4	←	3	1	2	3	4117.7061	-0.0049
4	1	3	5	←	3	1	2	4	4117.7783	0.0015
4	1	3	3	←	3	1	2	2	4117.8636	-0.0059
4	1	4	4	←	3	0	3	3	4355.5536	0.0037
4	1	4	5	←	3	0	3	4	4356.3092	-0.0012
4	1	4	3	←	3	0	3	2	4356.4582	-0.0005
5	1	5	6	←	4	1	4	5	4436.4644	-0.0111
5	0	5	5	←	4	0	4	4	4607.2022	0.0036
5	0	5	6	←	4	0	4	5	4607.4350	0.0061
5	2	4	5	←	4	2	3	4	4805.0038	-0.0008
5	2	4	6	←	4	2	3	5	4805.0869	-0.0060
6	0	6	6	←	5	1	5	5	5001.7905	-0.0077
5	2	3	6	←	4	2	2	5	5030.4078	-0.0001

5	2	3	5	←	4	2	2	4	5030.5455	0.0000
5	1	5	6	←	4	0	4	5	5046.4083	0.0062
5	1	4	5	←	4	1	3	4	5118.5971	0.0052
5	1	4	6	←	4	1	3	5	5118.6902	0.0074
2	2	1	2	←	1	1	0	1	5328.2095	0.0100
2	2	1	3	←	1	1	0	2	5328.9591	0.0018
6	0	6	6	←	5	0	5	5	5440.3710	-0.0024
6	0	6	7	←	5	0	5	6	5440.5842	-0.0007
2	2	0	1	←	1	1	1	0	5479.2883	0.0047
2	2	0	3	←	1	1	1	2	5480.6202	0.0021
2	2	0	2	←	1	1	1	2	5480.9369	0.0089
2	2	0	1	←	1	1	1	1	5481.2097	-0.0104
2	2	0	2	←	1	1	1	1	5481.7032	0.0019
6	1	6	6	←	5	0	5	5	5737.4109	0.0037
6	1	6	7	←	5	0	5	6	5737.8987	0.0108
6	2	5	6	←	5	2	4	5	5743.2582	0.0033
6	2	5	7	←	5	2	4	6	5743.3391	0.0000
6	3	4	7	←	5	3	3	6	5850.6046	0.0069
7	0	7	8	←	6	1	6	7	5960.9417	-0.0192
7	0	7	7	←	6	1	6	6	5961.0504	-0.0011
6	1	5	6	←	5	1	4	5	6096.6744	0.0007
6	2	4	7	←	5	2	3	6	6101.1726	0.0033
6	2	4	6	←	5	2	3	5	6101.2948	-0.0005
3	2	2	3	←	2	1	1	2	6155.4178	0.0093
3	2	2	4	←	2	1	1	3	6156.2389	0.0032
3	2	2	2	←	2	1	1	1	6156.6921	-0.0027
7	0	7	7	←	6	0	6	6	6258.0855	0.0002
7	0	7	8	←	6	0	6	7	6258.2586	-0.0053
7	1	7	7	←	6	0	6	6	6449.4465	0.0085
7	1	7	8	←	6	0	6	7	6449.7843	-0.0005
3	2	1	2	←	2	1	2	1	6635.4987	-0.0008
3	2	1	4	←	2	1	2	3	6636.1784	0.0106
3	2	1	3	←	2	1	2	2	6637.4684	-0.0051
7	2	6	7	←	6	2	5	6	6669.6428	-0.0075
7	2	6	8	←	6	2	5	7	6669.7356	0.0042
4	2	3	5	←	3	1	2	4	6912.2275	-0.0041
4	2	3	3	←	3	1	2	2	6912.5106	-0.0222
8	1	8	8	←	7	1	7	7	6998.3880	-0.0003
7	1	6	7	←	6	1	5	6	7044.5802	0.0000
7	1	6	8	←	6	1	5	7	7044.7298	-0.0048
8	0	8	9	←	7	0	7	8	7071.3274	0.0018
7	2	5	8	←	6	2	4	7	7173.7342	-0.0016
7	2	5	7	←	6	2	4	6	7173.8247	0.0034
8	1	8	8	←	7	0	7	7	7189.7426	0.0015
8	1	8	9	←	7	0	7	8	7189.9839	0.0025
8	2	7	8	←	7	2	6	7	7582.9699	0.0028
8	2	7	9	←	7	2	6	8	7583.0600	0.0057
5	2	4	6	←	4	1	3	5	7599.5451	-0.0026
5	2	4	4	←	4	1	3	3	7599.7557	-0.0126
9	0	9	9	←	8	1	8	8	7767.0547	-0.0041
9	0	9	9	←	8	0	8	8	7885.6156	0.0006

9	0	9	0	←	8	0	8	9	7885.7218	-0.0018
8	1	7	8	←	7	1	6	7	7955.7498	0.0172
8	1	7	9	←	7	1	6	8	7955.9152	-0.0008
9	1	9	9	←	8	0	8	8	7956.9209	0.0084
9	1	9	0	←	8	0	8	9	7957.0814	0.0034

Table S56 Measured frequencies and residuals (in MHz) for the rotational transitions of the ^{13}C3 isotopologue of the monomer of Pan.

J'	K_a'	K_c'	F'	←	J''	K_a''	K_c''	F''	ν_{obs}	ν_{obs}-ν_{calc}
1	1	1	1	←	0	0	0	1	2053.6618	-0.0072
1	1	1	2	←	0	0	0	1	2054.4370	-0.0052
3	1	3	3	←	2	1	2	2	2673.0589	-0.0076
3	1	3	4	←	2	1	2	3	2673.1866	-0.0023
3	0	3	3	←	2	0	2	2	2838.8492	0.0050
3	0	3	4	←	2	0	2	3	2839.0205	0.0015
2	1	2	2	←	1	0	1	1	2878.1821	-0.0152
2	1	2	3	←	1	0	1	2	2879.0293	-0.0095
4	0	4	3	←	3	1	3	2	2931.9841	-0.0032
4	0	4	5	←	3	1	3	4	2932.2117	0.0013
4	0	4	4	←	3	1	3	3	2932.6599	-0.0042
3	2	1	4	←	2	2	0	3	2935.7746	-0.0027
3	1	2	3	←	2	1	1	2	3086.1651	-0.0019
3	1	2	4	←	2	1	1	3	3086.2258	0.0000
4	1	4	4	←	3	1	3	3	3551.3283	0.0037
4	1	4	5	←	3	1	3	4	3551.4232	0.0034
3	1	3	3	←	2	0	2	2	3638.6895	-0.0016
3	1	3	4	←	2	0	2	3	3639.5363	0.0022
3	1	3	2	←	2	0	2	1	3639.7649	0.0013
4	0	4	4	←	3	0	3	3	3732.5102	-0.0008
4	0	4	5	←	3	0	3	4	3732.7279	0.0023
4	2	3	4	←	3	2	2	3	3840.2015	0.0082
4	2	3	5	←	3	2	2	4	3840.3004	-0.0048
5	0	5	4	←	4	1	4	3	3972.5039	0.0057
5	0	5	6	←	4	1	4	5	3972.6336	0.0038
5	0	5	5	←	4	1	4	4	3972.9484	-0.0017
4	1	3	4	←	3	1	2	3	4098.9391	-0.0100
4	1	3	5	←	3	1	2	4	4099.0050	-0.0089
4	1	4	4	←	3	0	3	3	4351.1703	-0.0012
4	1	4	5	←	3	0	3	4	4351.9358	0.0008
4	1	4	3	←	3	0	3	2	4352.0876	0.0031
5	0	5	6	←	4	0	4	5	4591.8361	-0.0030
5	2	4	6	←	4	2	3	5	4785.0915	0.0031
6	0	6	7	←	5	1	5	6	4975.2392	-0.0022
6	0	6	6	←	5	1	5	5	4975.4441	0.0094
5	2	3	6	←	4	2	2	5	5005.2884	0.0001
5	2	3	5	←	4	2	2	4	5005.4255	0.0006
5	1	5	5	←	4	0	4	4	5039.1210	-0.0026
5	1	5	6	←	4	0	4	5	5039.7564	-0.0002
5	1	5	4	←	4	0	4	3	5039.8518	0.0009

5	1	4	5	←	4	1	3	4	5095.9480	0.0029
5	1	4	6	←	4	1	3	5	5096.0317	-0.0026
6	1	6	6	←	5	1	5	5	5280.2299	0.0005
6	1	6	7	←	5	1	5	6	5280.3030	-0.0086
2	2	1	2	←	1	1	0	1	5337.7669	-0.0027
2	2	1	3	←	1	1	0	2	5338.5348	0.0074
6	0	6	6	←	5	0	5	5	5422.9508	0.0031
6	0	6	7	←	5	0	5	6	5423.1628	0.0039
2	2	0	3	←	1	1	1	2	5488.4025	-0.0014
2	2	0	1	←	1	1	1	1	5489.0098	0.0025
2	2	0	2	←	1	1	1	1	5489.4833	-0.0019
6	2	5	6	←	5	2	4	5	5719.8436	0.0187
6	2	5	7	←	5	2	4	6	5719.9165	0.0089
6	1	6	6	←	5	0	5	5	5727.7364	-0.0060
6	1	6	7	←	5	0	5	6	5728.2410	0.0119
6	3	3	7	←	5	3	2	6	5861.6007	0.0100
3	2	2	3	←	2	1	1	2	6162.2968	0.0000
3	2	2	4	←	2	1	1	3	6163.1260	0.0018
7	0	7	7	←	6	0	6	6	6238.5446	0.0070
7	0	7	8	←	6	0	6	7	6238.7239	0.0071
7	1	7	7	←	6	0	6	6	6436.0329	-0.0070
3	2	1	4	←	2	1	2	3	6637.0838	-0.0124
4	2	3	4	←	3	1	2	3	6916.3293	0.0062
4	2	3	5	←	3	1	2	4	6917.2145	0.0110
4	2	3	3	←	3	1	2	2	6917.5123	0.0078
7	1	6	7	←	6	1	5	6	7016.3884	-0.0025
7	1	6	8	←	6	1	5	7	7016.5422	-0.0005
8	0	8	8	←	7	0	7	7	7049.1532	0.0012
8	0	8	9	←	7	0	7	8	7049.2913	-0.0023
7	2	5	8	←	6	2	4	7	7137.9163	-0.0001
7	2	5	7	←	6	2	4	6	7138.0038	0.0001
8	1	8	8	←	7	0	7	7	7172.2346	-0.0030
8	1	8	7	←	7	0	7	6	7172.4841	-0.0053
8	1	8	9	←	7	0	7	8	7172.4841	0.0013
8	2	7	8	←	7	2	6	7	7553.5310	-0.0079
8	2	7	9	←	7	2	6	8	7553.6238	-0.0015
9	0	9	9	←	8	1	8	8	7737.7736	0.0028
9	0	9	9	←	8	0	8	8	7860.8387	-0.0177
9	0	9	10	←	8	0	8	9	7860.9528	-0.0133
4	2	2	3	←	3	1	3	2	7920.7906	-0.0033
4	2	2	5	←	3	1	3	4	7921.2918	-0.0002
4	2	2	4	←	3	1	3	3	7922.8141	-0.0009
9	1	9	8	←	8	0	8	7	7935.4872	0.0107

Table S57 Measured frequencies and residuals (in MHz) for the rotational transitions of the ^{13}C4 isotopologue of the monomer of Pan.

J'	K_a'	K_c'	*F'*	←	*J"*	K_a"	K_c"	*F"*	ν_{obs}	ν_{obs}-ν_{calc}
1	1	1	1	←	0	0	0	1	2042.4791	-0.0096
1	1	1	2	←	0	0	0	1	2043.2734	0.0113

3	1	3	4	←	2	1	2	3	2679.5965	-0.0006
3	0	3	4	←	2	0	2	3	2846.6333	-0.0041
2	1	2	2	←	1	0	1	1	2868.3045	-0.0136
2	1	2	3	←	1	0	1	2	2869.1601	0.0005
3	2	2	3	←	2	2	1	2	2896.7017	0.0099
3	2	2	4	←	2	2	1	3	2896.8854	-0.0027
4	0	4	3	←	3	1	3	2	2957.2403	-0.0053
4	0	4	5	←	3	1	3	4	2957.4622	-0.0039
4	0	4	4	←	3	1	3	3	2957.9094	-0.0007
3	1	2	3	←	2	1	1	2	3098.0986	0.0020
3	1	2	4	←	2	1	1	3	3098.1588	0.0019
4	1	4	4	←	3	1	3	3	3559.4194	0.0132
4	1	4	5	←	3	1	3	4	3559.5033	0.0007
3	1	3	3	←	2	0	2	2	3629.3758	-0.0095
3	1	3	4	←	2	0	2	3	3630.2276	0.0012
3	1	3	2	←	2	0	2	1	3630.4601	0.0054
4	0	4	4	←	3	0	3	3	3740.8356	-0.0010
4	0	4	5	←	3	0	3	4	3741.0570	0.0019
4	2	3	4	←	3	2	2	3	3852.4602	0.0127
4	2	3	5	←	3	2	2	4	3852.5622	0.0023
4	2	2	3	←	3	2	1	2	3973.9305	-0.0028
4	2	2	5	←	3	2	1	4	3973.9305	-0.0032
4	2	2	4	←	3	2	1	3	3974.0377	0.0016
5	0	5	4	←	4	1	4	3	3997.9550	-0.0060
5	0	5	6	←	4	1	4	5	3998.0871	-0.0037
5	0	5	5	←	4	1	4	4	3998.4007	0.0010
4	1	3	4	←	3	1	2	3	4114.1806	-0.0075
4	1	3	5	←	3	1	2	4	4114.2542	-0.0002
4	1	3	3	←	3	1	2	2	4114.3445	-0.0033
4	1	4	4	←	3	0	3	3	4342.3245	-0.0081
4	1	4	5	←	3	0	3	4	4343.0906	-0.0008
4	1	4	3	←	3	0	3	2	4343.2404	0.0014
5	1	5	5	←	4	1	4	4	4429.9491	0.0102
5	0	5	5	←	4	0	4	4	4599.8886	-0.0071
5	0	5	6	←	4	0	4	5	4600.1213	-0.0058
5	2	4	5	←	4	2	3	4	4799.7375	0.0133
5	2	4	6	←	4	2	3	5	4799.8138	0.0009
6	0	6	6	←	5	1	5	5	4999.6129	0.0014
5	2	3	6	←	4	2	2	5	5027.4851	-0.0009
5	2	3	5	←	4	2	2	4	5027.6340	0.0098
5	1	5	5	←	4	0	4	4	5031.4312	-0.0036
5	1	5	4	←	4	0	4	3	5032.1521	-0.0001
5	1	4	5	←	4	1	3	4	5113.7864	-0.0010
5	1	4	6	←	4	1	3	5	5113.8795	0.0001
2	2	1	2	←	1	1	0	1	5302.9209	-0.0069
2	2	1	3	←	1	1	0	2	5303.6908	0.0052
6	0	6	6	←	5	0	5	5	5431.1502	-0.0004
6	0	6	7	←	5	0	5	6	5431.3741	0.0118
2	2	0	3	←	1	1	1	2	5455.8923	-0.0030
6	1	6	6	←	5	0	5	5	5722.3941	-0.0087
6	2	5	6	←	5	2	4	5	5736.6424	0.0000

6	2	5	7	←	5	2	4	6	5736.7346	0.0069
6	3	3	7	←	5	3	2	6	5884.4050	0.0025
7	0	7	7	←	6	1	6	6	5955.9222	-0.0061
6	1	5	6	←	5	1	4	5	6090.2481	0.0013
6	1	5	7	←	5	1	4	6	6090.3796	0.0103
6	2	4	5	←	5	2	3	4	6097.8204	0.0012
6	2	4	6	←	5	2	3	5	6097.9469	0.0007
3	2	2	3	←	2	1	1	2	6128.7455	-0.0107
3	2	2	4	←	2	1	1	3	6129.5896	0.0061
3	2	2	2	←	2	1	1	1	6130.0605	0.0178
7	0	7	7	←	6	0	6	6	6247.1782	-0.0022
7	0	7	8	←	6	0	6	7	6247.3504	-0.0082
3	2	1	2	←	2	1	2	1	6610.7801	-0.0025
3	2	1	4	←	2	1	2	3	6611.4505	-0.0012
3	2	1	3	←	2	1	2	2	6612.7631	0.0031
7	2	6	7	←	6	2	5	6	6661.5708	-0.0039
7	2	6	8	←	6	2	5	7	6661.6583	0.0025
4	2	3	4	←	3	1	2	3	6883.1007	-0.0064
4	2	3	5	←	3	1	2	4	6883.9947	0.0081
4	2	3	3	←	3	1	2	2	6884.2996	0.0117
7	1	6	7	←	6	1	5	6	7036.0907	-0.0031
7	1	6	8	←	6	1	5	7	7036.2513	0.0010
8	0	8	8	←	7	0	7	7	7058.8502	0.0115
8	0	8	9	←	7	0	7	8	7058.9865	0.0078
7	2	5	8	←	6	2	4	7	7169.5276	-0.0045
7	2	5	7	←	6	2	4	6	7169.6150	-0.0013
8	1	8	8	←	7	0	7	7	7174.2472	-0.0015
8	1	8	9	←	7	0	7	8	7174.4878	0.0015
5	2	4	5	←	4	1	3	4	7568.6340	-0.0090
5	2	4	6	←	4	1	3	5	7569.5441	-0.0008
5	2	4	4	←	4	1	3	3	7569.7674	0.0020
8	2	7	8	←	7	2	6	7	7573.2853	-0.0085
8	2	7	9	←	7	2	6	8	7573.3770	-0.0046
9	0	9	9	←	8	1	8	8	7756.5547	-0.0022
9	0	9	9	←	8	0	8	8	7871.9650	-0.0020
9	0	9	8	←	8	0	8	7	7872.0612	-0.0050
4	2	2	3	←	3	1	3	2	7905.2816	-0.0059
4	2	2	5	←	3	1	3	4	7905.7861	-0.0023
4	2	2	4	←	3	1	3	3	7907.3212	-0.0009
9	1	9	9	←	8	0	8	8	7941.1251	0.0012
9	1	9	0	←	8	0	8	9	7941.2891	0.0018

Table S58 Measured frequencies and residuals (in MHz) for the rotational transitions of the ^{13}C5 isotopologue of the monomer of Pan.

J‘	K_a‘	K_c‘	*F*‘	←	*J*“	K_a“	K_c“	*F*“	ν_{obs}	ν_{obs}-ν_{calc}
1	1	1	2	←	0	0	0	1	2044.0905	0.0003
3	1	3	4	←	2	1	2	3	2693.7762	-0.0015
3	0	3	3	←	2	0	2	2	2862.0252	0.0110
3	0	3	4	←	2	0	2	3	2862.1941	-0.0011
2	1	2	2	←	1	0	1	2	2872.9015	-0.0061

2	1	2	2	←	1	0	1	1	2873.0853	-0.0068
2	1	2	3	←	1	0	1	2	2873.9327	-0.0008
2	1	2	1	←	1	0	1	1	2874.6841	-0.0049
3	2	2	3	←	2	2	1	2	2913.6376	0.0055
3	2	2	4	←	2	2	1	3	2913.8300	0.0015
3	2	2	2	←	2	2	1	1	2913.9288	-0.0080
4	0	4	5	←	3	1	3	4	2984.3743	-0.0013
4	0	4	4	←	3	1	3	3	2984.8192	0.0056
3	1	2	3	←	2	1	1	2	3117.3417	-0.0049
3	1	2	4	←	2	1	1	3	3117.4084	0.0004
3	1	2	2	←	2	1	1	1	3117.5883	-0.0057
4	1	4	4	←	3	1	3	3	3577.9672	0.0005
4	1	4	5	←	3	1	3	4	3578.0644	0.0007
3	1	3	4	←	2	0	2	3	3638.2538	0.0106
4	2	3	4	←	3	2	2	3	3874.7600	0.0035
4	2	3	5	←	3	2	2	4	3874.8691	0.0000
4	2	2	5	←	3	2	1	4	3999.4575	-0.0015
4	2	2	4	←	3	2	1	3	3999.5687	0.0052
5	0	5	4	←	4	1	4	3	4028.8880	-0.0028
5	0	5	6	←	4	1	4	5	4029.0221	0.0026
5	0	5	5	←	4	1	4	4	4029.3227	0.0016
4	1	3	4	←	3	1	2	3	4139.3528	-0.0082
4	1	3	5	←	3	1	2	4	4139.4272	-0.0008
4	1	3	3	←	3	1	2	2	4139.5215	-0.0013
4	1	4	5	←	3	0	3	4	4354.1358	0.0241
5	0	5	6	←	4	0	4	5	4622.7046	-0.0029
5	2	4	5	←	4	2	3	4	4827.1681	0.0012
5	2	4	6	←	4	2	3	5	4827.2535	-0.0030
6	0	6	5	←	5	1	5	4	5033.2383	0.0023
6	0	6	7	←	5	1	5	6	5033.3077	-0.0055
6	0	6	6	←	5	1	5	5	5033.4925	0.0033
5	1	5	5	←	4	0	4	4	5045.8114	-0.0073
5	2	3	6	←	4	2	2	5	5060.5625	-0.0041
5	2	3	5	←	4	2	2	4	5060.7052	-0.0002
5	1	4	5	←	4	1	3	4	5144.3638	0.0017
5	1	4	6	←	4	1	3	5	5144.4526	-0.0032
5	1	4	4	←	4	1	3	3	5144.5072	-0.0046
2	2	1	1	←	1	1	0	1	5301.1617	0.0022
2	2	1	2	←	1	1	0	1	5301.4659	-0.0003
2	2	1	3	←	1	1	0	2	5302.2347	0.0107
2	2	0	1	←	1	1	1	0	5455.1471	-0.0069
2	2	0	3	←	1	1	1	2	5456.4821	-0.0086
6	0	6	7	←	5	0	5	6	5457.0384	-0.0068
2	2	0	2	←	1	1	1	1	5457.5730	-0.0047
6	1	6	6	←	5	0	5	5	5740.9149	-0.0016
6	1	6	7	←	5	0	5	6	5741.3994	0.0118
6	2	5	6	←	5	2	4	5	5768.9431	0.0053
6	2	5	7	←	5	2	4	6	5769.0276	0.0012
6	3	3	7	←	5	3	2	6	5921.1416	0.0059
7	0	7	8	←	6	1	6	7	5992.0755	-0.0142
7	0	7	7	←	6	1	6	6	5992.1739	0.0021

6	1	5	6	←	5	1	4	5	6125.4773	0.0006
6	1	5	7	←	5	1	4	6	6125.6177	0.0161
3	2	2	3	←	2	1	1	2	6131.2378	-0.0029
3	2	2	4	←	2	1	1	3	6132.0691	0.0012
3	2	2	2	←	2	1	1	1	6132.5293	0.0023
6	2	4	7	←	5	2	3	6	6138.2519	0.0095
7	0	7	8	←	6	0	6	7	6276.4255	-0.0065
7	1	7	7	←	6	0	6	6	6457.5200	-0.0008
3	2	1	2	←	2	1	2	1	6620.1106	0.0043
3	2	1	4	←	2	1	2	3	6620.7790	0.0022
3	2	1	3	←	2	1	2	2	6622.0836	-0.0055
4	2	3	4	←	3	1	2	3	6888.6519	0.0013
4	2	3	5	←	3	1	2	4	6889.5339	0.0049
7	3	4	8	←	6	3	3	7	6954.3608	-0.0042
7	3	4	7	←	6	3	3	6	6954.4459	0.0041
8	1	8	8	←	7	1	7	7	7021.6448	0.0097
8	1	8	9	←	7	1	7	8	7021.7057	-0.0018
8	0	8	8	←	7	0	7	7	7091.6649	-0.0015
8	0	8	9	←	7	0	7	8	7091.7927	-0.0126
8	1	8	8	←	7	0	7	7	7202.8968	-0.0044
8	1	8	9	←	7	0	7	8	7203.1368	0.0026
7	2	5	8	←	6	2	4	7	7216.5826	-0.0014
7	2	5	7	←	6	2	4	6	7216.6635	-0.0028
5	2	4	5	←	4	1	3	4	7576.4488	-0.0075
5	2	4	6	←	4	1	3	5	7577.3576	0.0001
5	2	4	4	←	4	1	3	3	7577.5814	0.0036
8	2	7	8	←	7	2	6	7	7614.3557	-0.0021
8	2	7	9	←	7	2	6	8	7614.4414	-0.0052
9	0	9	9	←	8	1	8	8	7797.5533	0.0050
8	5	4	7	←	7	5	3	6	7834.3006	-0.0033
8	3	6	9	←	7	3	5	8	7847.4653	0.0068
9	0	9	9	←	8	0	8	8	7908.7835	0.0003
9	0	9	10	←	8	0	8	9	7908.8809	-0.0091
9	1	9	9	←	8	0	8	8	7975.0465	0.0012
9	1	9	10	←	8	0	8	9	7975.2105	0.0052

Table S59 Measured frequencies and residuals (in MHz) for the rotational transitions of the ^{13}C6 isotopologue of the monomer of Pan.

J'	K_a'	K_c'	*F'*	←	*J"*	K_a"	K_c"	*F"*	ν_{obs}	ν_{obs}-ν_{calc}
1	1	1	1	←	0	0	0	1	2057.2177	0.0133
3	1	3	4	←	2	1	2	3	2701.7934	0.0009
3	0	3	3	←	2	0	2	2	2870.1462	0.0011
3	0	3	4	←	2	0	2	3	2870.3194	-0.0048
2	1	2	2	←	1	0	1	2	2889.5826	-0.0146
2	1	2	2	←	1	0	1	1	2889.7634	-0.0183
2	1	2	3	←	1	0	1	2	2890.6051	-0.0181
2	1	2	1	←	1	0	1	0	2890.9066	-0.0134
3	2	2	3	←	2	2	1	2	2921.0331	-0.0044

3	2	2	4	←	2	2	1	3	2921.2360	0.0019
4	0	4	5	←	3	1	3	4	2984.4490	-0.0021
4	0	4	4	←	3	1	3	3	2984.8923	-0.0015
3	1	3	3	←	2	0	2	2	3656.9879	0.0057
3	1	3	4	←	2	0	2	3	3657.8294	0.0064
3	1	3	2	←	2	0	2	1	3658.0566	0.0055
4	0	4	5	←	3	0	3	4	3771.9563	0.0064
4	2	3	5	←	3	2	2	4	3884.8915	0.0017
4	3	2	4	←	3	3	1	3	3918.5461	-0.0032
4	3	2	5	←	3	3	1	4	3918.6878	0.0058
4	2	2	5	←	3	2	1	4	4007.8239	-0.0055
4	2	2	4	←	3	2	1	3	4007.9322	0.0000
5	0	5	6	←	4	1	4	5	4033.3734	0.0024
5	0	5	5	←	4	1	4	4	4033.6788	0.0005
4	1	3	4	←	3	1	2	3	4149.0077	-0.0006
4	1	3	5	←	3	1	2	4	4149.0765	0.0016
5	0	5	5	←	4	0	4	4	4637.6250	0.0104
5	0	5	6	←	4	0	4	5	4637.8547	0.0084
5	2	4	6	←	4	2	3	5	4840.0178	0.0019
6	0	6	6	←	5	1	5	5	5042.6649	-0.0067
5	1	5	5	←	4	0	4	4	5070.4190	0.0053
5	1	5	6	←	4	0	4	5	5071.0412	0.0030
5	1	5	4	←	4	0	4	3	5071.1389	0.0092
5	1	4	5	←	4	1	3	4	5156.9012	-0.0115
5	1	4	6	←	4	1	3	5	5157.0094	0.0043
5	1	4	4	←	4	1	3	3	5157.0552	-0.0056
6	0	6	7	←	5	0	5	6	5475.6894	0.0069
2	2	0	1	←	1	1	1	0	5493.4837	-0.0102
2	2	0	3	←	1	1	1	2	5494.8229	-0.0065
2	2	0	2	←	1	1	1	2	5495.1291	-0.0120
2	2	0	1	←	1	1	1	1	5495.4244	-0.0061
2	2	0	2	←	1	1	1	1	5495.9068	-0.0076
6	1	6	6	←	5	0	5	5	5767.2119	0.0043
6	3	4	7	←	5	3	3	6	5894.4617	0.0002
6	3	3	7	←	5	3	2	6	5934.3558	-0.0044
7	0	7	8	←	6	1	6	7	6006.2200	-0.0127
7	0	7	7	←	6	1	6	6	6006.3169	-0.0019
6	2	4	7	←	5	2	3	6	6150.1110	0.0023
6	2	4	6	←	5	2	3	5	6150.2359	0.0017
3	2	2	3	←	2	1	1	2	6172.8943	-0.0088
3	2	2	4	←	2	1	1	3	6173.7160	-0.0142
7	0	7	8	←	6	0	6	7	6298.2477	0.0141
7	1	7	7	←	6	0	6	6	6485.0785	0.0039
7	1	7	6	←	6	0	6	5	6485.4225	-0.0147
3	2	1	2	←	2	1	2	1	6659.8668	0.0089
3	2	1	4	←	2	1	2	3	6660.5334	0.0061
3	2	1	3	←	2	1	2	2	6661.8448	0.0084
7	2	6	7	←	6	2	5	6	6717.1086	0.0071
7	2	6	8	←	6	2	5	7	6717.1901	0.0078
4	2	3	4	←	3	1	2	3	6933.3074	0.0081
4	2	3	5	←	3	1	2	4	6934.1888	0.0103

4	2	3	3	←	3	1	2	2	6934.4923	0.0123
7	3	4	8	←	6	3	3	7	6968.9445	-0.0003
7	1	6	7	←	6	1	5	6	7094.7340	-0.0140
7	1	6	8	←	6	1	5	7	7094.9121	0.0070
8	0	8	7	←	7	0	7	6	7116.4363	-0.0137
7	2	5	6	←	6	2	4	5	7230.9121	-0.0005
7	2	5	7	←	6	2	4	6	7231.0000	0.0068
8	1	8	9	←	7	0	7	8	7231.8523	-0.0030
8	4	4	7	←	7	4	3	6	7887.1949	-0.0107
4	2	2	3	←	3	1	3	2	7966.0630	0.0000
4	2	2	5	←	3	1	3	4	7966.5716	0.0074
4	2	2	4	←	3	1	3	3	7968.1074	0.0080

Table S60 Measured frequencies and residuals (in MHz) for the rotational transitions of the ^{13}C7 isotopologue of the monomer of Pan.

J'	K_a'	K_c'	*F'*	←	*J"*	K_a"	K_c"	*F"*	ν_{obs}	ν_{obs}-ν_{calc}
3	1	3	4	←	2	1	2	3	2701.6983	-0.0093
3	0	3	3	←	2	0	2	2	2870.0529	0.0003
3	0	3	4	←	2	0	2	3	2870.2281	-0.0035
2	1	2	2	←	1	0	1	2	2889.5829	0.0197
2	1	2	2	←	1	0	1	1	2889.7636	0.0159
2	1	2	3	←	1	0	1	2	2890.6051	0.0160
2	1	2	1	←	1	0	1	0	2890.9063	0.0203
3	2	2	3	←	2	2	1	2	2920.9251	-0.0123
3	2	2	4	←	2	2	1	3	2921.1351	0.0011
4	0	4	3	←	3	1	3	2	2984.0794	0.0029
4	0	4	5	←	3	1	3	4	2984.3041	0.0074
4	0	4	4	←	3	1	3	3	2984.7430	0.0035
4	1	4	4	←	3	1	3	3	3588.7236	0.0047
3	1	3	3	←	2	0	2	2	3656.9207	-0.0073
3	1	3	4	←	2	0	2	3	3657.7604	-0.0083
3	1	3	2	←	2	0	2	1	3657.9877	-0.0092
4	2	3	4	←	3	2	2	3	3884.6427	-0.0027
4	3	2	5	←	3	3	1	4	3918.5470	0.0018
4	2	2	5	←	3	2	1	4	4007.6821	0.0020
5	0	5	5	←	4	1	4	4	4033.4979	-0.0011
4	1	3	4	←	3	1	2	3	4148.8587	-0.0016
4	1	3	5	←	3	1	2	4	4148.9370	0.0100
5	0	5	5	←	4	0	4	4	4637.4821	0.0036
5	0	5	6	←	4	0	4	5	4637.7159	0.0056
5	2	4	5	←	4	2	3	4	4839.7609	-0.0034
5	2	4	6	←	4	2	3	5	4839.8500	-0.0033
6	0	6	5	←	5	1	5	4	5042.2075	-0.0064
6	0	6	7	←	5	1	5	6	5042.2912	-0.0010
5	1	5	6	←	4	0	4	5	5070.9376	-0.0074
5	1	5	4	←	4	0	4	3	5071.0413	0.0047
5	1	4	5	←	4	1	3	4	5156.7351	0.0025
5	1	4	6	←	4	1	3	5	5156.8298	0.0048

6	0	6	6	←	5	0	5	5	5475.3166	0.0012
6	0	6	7	←	5	0	5	6	5475.5247	-0.0022
2	2	0	1	←	1	1	1	0	5493.4839	0.0081
2	2	0	3	←	1	1	1	2	5494.8230	0.0118
2	2	0	2	←	1	1	1	2	5495.1291	0.0062
2	2	0	1	←	1	1	1	1	5495.4248	0.0125
2	2	0	2	←	1	1	1	1	5495.9071	0.0108
6	1	6	6	←	5	0	5	5	5767.0845	-0.0053
6	1	6	7	←	5	0	5	6	5767.5789	0.0132
6	2	5	7	←	5	2	4	6	5784.4758	-0.0016
6	3	4	7	←	5	3	3	6	5894.2541	-0.0008
6	3	3	7	←	5	3	2	6	5934.1388	-0.0059
7	0	7	8	←	6	1	6	7	6006.0093	-0.0092
7	0	7	7	←	6	1	6	6	6006.1015	-0.0031
6	1	5	6	←	5	1	4	5	6141.1440	0.0020
6	2	4	7	←	5	2	3	6	6149.8751	0.0023
6	2	4	6	←	5	2	3	5	6150.0032	0.0049
3	2	2	3	←	2	1	1	2	6172.8944	0.0221
3	2	2	4	←	2	1	1	3	6173.7159	0.0164
3	2	2	2	←	2	1	1	1	6174.1742	0.0156
7	0	7	7	←	6	0	6	6	6297.8893	0.0101
7	0	7	8	←	6	0	6	7	6298.0707	0.0136
7	1	7	7	←	6	0	6	6	6484.9264	-0.0019
3	2	1	2	←	2	1	2	1	6659.7771	-0.0122
3	2	1	4	←	2	1	2	3	6660.4478	-0.0108
3	2	1	3	←	2	1	2	2	6661.7577	-0.0101
7	2	6	7	←	6	2	5	6	6716.8858	0.0034
7	2	6	8	←	6	2	5	7	6716.9728	0.0095
4	2	3	4	←	3	1	2	3	6933.2344	-0.0150
4	2	3	5	←	3	1	2	4	6934.1128	-0.0158
4	2	3	3	←	3	1	2	2	6934.4139	-0.0162
7	3	4	8	←	6	3	3	7	6968.6847	-0.0006
7	3	4	7	←	6	3	3	6	6968.7591	-0.0012
7	1	6	7	←	6	1	5	6	7094.5155	-0.0013
7	1	6	8	←	6	1	5	7	7094.6799	0.0060
8	0	8	8	←	7	0	7	7	7116.1175	-0.0004
8	0	8	9	←	7	0	7	8	7116.2563	-0.0013
7	2	5	8	←	6	2	4	7	7230.6460	0.0115
7	2	5	7	←	6	2	4	6	7230.7222	0.0038
8	1	8	8	←	7	0	7	7	7231.4336	-0.0083
8	1	8	9	←	7	0	7	8	7231.6571	-0.0212
4	2	2	3	←	3	1	3	2	7965.9145	-0.0152
4	2	2	5	←	3	1	3	4	7966.4200	-0.0110
4	2	2	4	←	3	1	3	3	7967.9543	-0.0118

Table S61 Measured frequencies and residuals (in MHz) for the rotational transitions of the ^{13}C8 isotopologue of the monomer of Pan.

J'	K_a'	K_c'	*F'*	←	*J"*	K_a"	K_c"	*F"*	ν_{obs}	ν_{obs}-ν_{calc}

1	1	1	1	←	0	0	0	1	2043.4450	0.0055
1	1	1	2	←	0	0	0	1	2044.2124	-0.0002
3	0	3	3	←	2	0	2	2	2861.7453	-0.0030
3	0	3	4	←	2	0	2	3	2861.9186	-0.0107
2	1	2	2	←	1	0	1	2	2872.9700	0.0000
2	1	2	2	←	1	0	1	1	2873.1614	0.0068
2	1	2	3	←	1	0	1	2	2873.9985	0.0025
2	1	2	1	←	1	0	1	1	2874.7587	0.0072
3	2	2	3	←	2	2	1	2	2913.3185	-0.0090
3	2	2	4	←	2	2	1	3	2913.5306	0.0066
4	0	4	3	←	3	1	3	2	2983.5532	-0.0018
4	0	4	5	←	3	1	3	4	2983.7793	0.0050
4	1	4	4	←	3	1	3	3	3577.6674	0.0064
4	1	4	5	←	3	1	3	4	3577.7620	0.0040
3	1	3	3	←	2	0	2	2	3637.4189	-0.0032
3	1	3	4	←	2	0	2	3	3638.2538	-0.0082
3	1	3	2	←	2	0	2	1	3638.4831	-0.0064
4	0	4	5	←	3	0	3	4	3760.1097	0.0027
4	2	3	4	←	3	2	2	3	3874.3614	0.0031
4	2	3	5	←	3	2	2	4	3874.4762	0.0053
4	2	2	5	←	3	2	1	4	3998.9700	-0.0015
4	2	2	4	←	3	2	1	3	3999.0712	-0.0044
5	0	5	4	←	4	1	4	3	4028.2447	0.0013
5	0	5	6	←	4	1	4	5	4028.3729	0.0008
5	0	5	5	←	4	1	4	4	4028.6758	0.0018
4	1	3	4	←	3	1	2	3	4138.8856	-0.0093
4	1	3	5	←	3	1	2	4	4138.9610	-0.0010
4	1	3	3	←	3	1	2	2	4139.0473	-0.0095
4	1	4	4	←	3	0	3	3	4353.3477	0.0129
4	1	4	5	←	3	0	3	4	4354.0763	-0.0143
4	1	4	3	←	3	0	3	2	4354.2311	-0.0057
5	0	5	5	←	4	0	4	4	4622.1104	-0.0121
5	0	5	6	←	4	0	4	5	4622.3536	-0.0022
5	2	4	5	←	4	2	3	4	4826.6953	0.0139
5	2	4	6	←	4	2	3	5	4826.7651	-0.0060
6	0	6	5	←	5	1	5	4	5032.5748	0.0030
6	0	6	7	←	5	1	5	6	5032.6436	-0.0054
6	0	6	6	←	5	1	5	5	5032.8237	-0.0014
5	2	3	6	←	4	2	2	5	5059.9249	-0.0009
5	2	3	5	←	4	2	2	4	5060.0625	-0.0021
5	1	4	5	←	4	1	3	4	5143.8118	0.0069
5	1	4	6	←	4	1	3	5	5143.9000	0.0014
2	2	1	2	←	1	1	0	1	5301.9066	0.0129
2	2	1	3	←	1	1	0	2	5302.6607	0.0092
2	2	0	1	←	1	1	1	0	5455.5280	-0.0022
6	0	6	7	←	5	0	5	6	5456.6568	-0.0025
2	2	0	3	←	1	1	1	2	5456.8664	-0.0004
2	2	0	2	←	1	1	1	2	5457.1768	-0.0036
2	2	0	1	←	1	1	1	1	5457.4551	-0.0117
2	2	0	2	←	1	1	1	1	5457.9388	-0.0148
6	1	6	6	←	5	0	5	5	5740.7670	0.0000

6	1	6	7	←	5	0	5	6	5741.2502	0.0120
6	2	5	6	←	5	2	4	5	5768.3840	0.0109
6	2	5	7	←	5	2	4	6	5768.4700	0.0086
6	3	4	7	←	5	3	3	6	5879.5483	-0.0086
6	3	3	5	←	5	3	2	4	5920.4466	0.0014
7	0	7	8	←	6	1	6	7	5991.4105	-0.0126
7	0	7	7	←	6	1	6	6	5991.5113	0.0060
6	1	5	6	←	5	1	4	5	6124.8505	0.0011
6	1	5	7	←	5	1	4	6	6124.9879	0.0137
3	2	2	3	←	2	1	1	2	6131.6186	0.0104
3	2	2	4	←	2	1	1	3	6132.4323	-0.0030
3	2	2	2	←	2	1	1	1	6132.8862	-0.0081
6	2	4	7	←	5	2	3	6	6137.4635	0.0069
6	2	4	6	←	5	2	3	5	6137.5861	0.0045
7	0	7	7	←	6	0	6	6	6275.8194	-0.0050
7	0	7	8	←	6	0	6	7	6275.9966	-0.0052
7	1	7	7	←	6	0	6	6	6457.2747	0.0003
3	2	1	2	←	2	1	2	1	6620.3044	0.0036
3	2	1	4	←	2	1	2	3	6620.9694	-0.0018
3	2	1	3	←	2	1	2	2	6622.2744	-0.0092
4	2	3	4	←	3	1	2	3	6888.9900	0.0103
4	2	3	5	←	3	1	2	4	6889.8734	0.0152
4	2	3	3	←	3	1	2	2	6890.1577	-0.0024
7	3	4	8	←	6	3	3	7	6953.5149	-0.0028
8	1	8	8	←	7	1	7	7	7021.1056	0.0069
8	1	8	9	←	7	1	7	8	7021.1618	-0.0093
8	0	8	8	←	7	0	7	7	7091.1748	-0.0059
8	0	8	9	←	7	0	7	8	7091.3124	-0.0073
8	1	8	8	←	7	0	7	7	7202.5480	-0.0005
8	1	8	9	←	7	0	7	8	7202.7810	-0.0004
7	2	5	8	←	6	2	4	7	7215.6743	-0.0010
7	2	5	7	←	6	2	4	6	7215.7623	0.0046
5	2	4	5	←	4	1	3	4	7576.7727	0.0067
5	2	4	6	←	4	1	3	5	7577.6644	-0.0027
5	2	4	4	←	4	1	3	3	7577.8777	-0.0096
8	2	7	8	←	7	2	6	7	7613.6529	-0.0073
8	2	7	9	←	7	2	6	8	7613.7439	-0.0052
9	0	9	9	←	8	1	8	8	7796.8735	0.0060
8	4	4	7	←	7	4	3	6	7868.1442	0.0000
9	0	9	9	←	8	0	8	8	7908.2288	-0.0062
9	0	9	10	←	8	0	8	9	7908.3357	-0.0063
9	1	9	9	←	8	0	8	8	7974.6003	0.0120
9	1	9	10	←	8	0	8	9	7974.7585	0.0102

Table S62 Measured frequencies and residuals (in MHz) for the rotational transitions of the ^{13}C9 isotopologue of the monomer of Pan.

J'	K_a'	K_c'	F'	←	J''	K_a''	K_c''	F''	ν_{obs}	ν_{obs}-ν_{calc}
1	1	1	1	←	0	0	0	1	2042.9989	0.0079

1	1	1	2	←	0	0	0	1	2043.7618	-0.0024
1	1	1	0	←	0	0	0	1	2044.9076	-0.0199
3	1	3	3	←	2	1	2	2	2679.1028	-0.0096
3	1	3	4	←	2	1	2	3	2679.2375	0.0019
2	1	2	2	←	1	0	1	1	2868.7482	0.0062
2	1	2	3	←	1	0	1	2	2869.5798	-0.0035
3	2	2	4	←	2	2	1	3	2896.3726	0.0001
3	2	2	2	←	2	2	1	1	2896.4928	0.0118
3	2	1	4	←	2	2	0	3	2946.4890	-0.0021
4	0	4	5	←	3	1	3	4	2956.1910	0.0029
4	0	4	4	←	3	1	3	3	2956.6316	-0.0009
3	1	2	3	←	2	1	1	2	3097.4491	-0.0078
3	1	2	4	←	2	1	1	3	3097.5190	0.0019
4	1	4	4	←	3	1	3	3	3558.9498	0.0024
4	1	4	5	←	3	1	3	4	3559.0464	0.0028
3	1	3	3	←	2	0	2	2	3629.7760	0.0085
3	1	3	4	←	2	0	2	3	3630.6064	-0.0021
3	1	3	2	←	2	0	2	1	3630.8266	-0.0103
4	0	4	4	←	3	0	3	3	3740.3663	0.0023
4	0	4	5	←	3	0	3	4	3740.5810	-0.0012
4	2	3	4	←	3	2	2	3	3851.7784	-0.0001
4	2	3	5	←	3	2	2	4	3851.9016	0.0106
4	2	2	5	←	3	2	1	4	3973.0534	0.0030
4	2	2	4	←	3	2	1	3	3973.1507	-0.0017
5	0	5	4	←	4	1	4	3	3996.6567	0.0006
5	0	5	6	←	4	1	4	5	3996.7841	-0.0018
5	0	5	5	←	4	1	4	4	3997.0909	-0.0045
4	1	3	4	←	3	1	2	3	4113.3626	-0.0060
4	1	3	5	←	3	1	2	4	4113.4365	0.0015
4	1	3	3	←	3	1	2	2	4113.5261	-0.0021
4	1	4	4	←	3	0	3	3	4342.6826	0.0038
4	1	4	5	←	3	0	3	4	4343.4340	-0.0037
4	1	4	3	←	3	0	3	2	4343.5780	-0.0073
5	0	5	5	←	4	0	4	4	4599.3922	-0.0180
5	0	5	6	←	4	0	4	5	4599.6340	-0.0075
5	2	4	5	←	4	2	3	4	4798.9193	0.0015
5	2	4	6	←	4	2	3	5	4799.0117	0.0052
5	2	3	6	←	4	2	2	5	5026.3137	0.0067
5	2	3	5	←	4	2	2	4	5026.4515	0.0065
5	1	5	5	←	4	0	4	4	5031.7171	0.0058
5	1	5	6	←	4	0	4	5	5032.3359	-0.0012
5	1	5	4	←	4	0	4	3	5032.4207	-0.0083
5	1	4	5	←	4	1	3	4	5112.8273	0.0037
5	1	4	6	←	4	1	3	5	5112.9214	0.0059
2	2	1	2	←	1	1	0	1	5304.5252	0.0123
2	2	1	3	←	1	1	0	2	5305.2709	0.0003
6	0	6	6	←	5	0	5	5	5430.6610	0.0071
6	0	6	7	←	5	0	5	6	5430.8754	0.0099
2	2	0	1	←	1	1	1	0	5456.0279	0.0001
2	2	0	3	←	1	1	1	2	5457.3583	-0.0046
2	2	0	2	←	1	1	1	1	5458.4439	-0.0034

6	1	6	6	←	5	0	5	5	5722.5545	0.0039
6	3	3	7	←	5	3	2	6	5883.1791	0.0021
7	0	7	7	←	6	1	6	6	5954.7434	-0.0063
6	1	5	6	←	5	1	4	5	6089.1957	0.0061
6	1	5	7	←	5	1	4	6	6089.3322	0.0203
6	2	4	7	←	5	2	3	6	6096.3762	0.0101
6	2	4	6	←	5	2	3	5	6096.4770	-0.0147
3	2	2	3	←	2	1	1	2	6130.2723	0.0094
3	2	2	4	←	2	1	1	3	6131.0906	0.0005
3	2	2	2	←	2	1	1	1	6131.5488	-0.0003
7	0	7	7	←	6	0	6	6	6246.6472	0.0008
7	0	7	8	←	6	0	6	7	6246.8138	-0.0107
3	2	1	2	←	2	1	2	1	6611.8967	0.0042
3	2	1	4	←	2	1	2	3	6612.5671	0.0056
3	2	1	3	←	2	1	2	2	6613.8653	-0.0040
4	2	3	4	←	3	1	2	3	6884.5966	0.0121
4	2	3	5	←	3	1	2	4	6885.4678	0.0038
4	2	3	3	←	3	1	2	2	6885.7629	-0.0023
7	1	6	7	←	6	1	5	6	7035.0123	0.0034
7	1	6	8	←	6	1	5	7	7035.1681	0.0031
8	0	8	8	←	7	0	7	7	7058.2441	0.0061
8	0	8	9	←	7	0	7	8	7058.3833	0.0053
7	2	5	6	←	6	2	4	5	7167.8516	-0.0084
7	2	5	7	←	6	2	4	6	7167.9368	-0.0044
8	1	8	8	←	7	0	7	7	7174.0115	0.0007
8	1	8	9	←	7	0	7	8	7174.2472	-0.0014
5	2	4	5	←	4	1	3	4	7570.1387	0.0051
5	2	4	6	←	4	1	3	5	7571.0295	-0.0058
5	2	4	4	←	4	1	3	3	7571.2471	-0.0087
8	2	7	8	←	7	2	6	7	7572.1893	-0.0042
8	2	7	9	←	7	2	6	8	7572.2811	-0.0002
9	0	9	10	←	8	1	8	9	7755.5128	-0.0062
9	0	9	9	←	8	0	8	8	7871.2786	-0.0030
9	0	9	10	←	8	0	8	9	7871.3822	-0.0074
4	2	2	3	←	3	1	3	2	7905.8714	-0.0040
4	2	2	5	←	3	1	3	4	7906.3757	-0.0004
4	2	2	4	←	3	1	3	3	7907.8929	-0.0163
9	1	9	9	←	8	0	8	8	7940.6930	0.0053
9	1	9	10	←	8	0	8	9	7940.8505	-0.0008

Table S63 Measured frequencies and residuals (in MHz) for the rotational transitions of the ^{13}C10 isotopologue of the monomer of Pan.

J'	K_a'	K_c'	F'	←	J''	K_a''	K_c''	F''	ν_{obs}	ν_{obs}-ν_{calc}
3	1	3	4	←	2	1	2	3	2672.8002	0.0048
3	0	3	3	←	2	0	2	2	2838.4132	0.0048
3	0	3	4	←	2	0	2	3	2838.5840	0.0009
3	2	2	3	←	2	2	1	2	2886.7426	0.0024
3	1	2	3	←	2	1	1	2	3085.6052	-0.0083

3	1	2	4	←	2	1	1	3	3085.6710	-0.0012
3	1	2	2	←	2	1	1	1	3085.8573	-0.0027
4	1	4	3	←	3	1	3	2	3550.8138	-0.0091
4	1	4	5	←	3	1	3	4	3550.9121	0.0057
3	1	3	3	←	2	0	2	2	3638.5613	0.0003
3	1	3	4	←	2	0	2	3	3639.4052	0.0012
3	1	3	2	←	2	0	2	1	3639.6312	-0.0021
4	0	4	4	←	3	0	3	3	3731.9753	0.0004
4	0	4	3	←	3	0	3	2	3732.1910	-0.0082
4	0	4	5	←	3	0	3	4	3732.1910	0.0017
4	2	3	4	←	3	2	2	3	3839.5589	-0.0021
4	2	3	5	←	3	2	2	4	3839.6737	0.0006
5	0	5	4	←	4	1	4	3	3971.5509	-0.0021
5	0	5	6	←	4	1	4	5	3971.6882	0.0036
5	0	5	5	←	4	1	4	4	3972.0007	-0.0046
4	1	4	4	←	3	0	3	3	4350.9651	0.0014
4	1	4	5	←	3	0	3	4	4351.7299	0.0026
4	1	4	3	←	3	0	3	2	4351.8814	0.0047
5	0	5	5	←	4	0	4	4	4591.0021	0.0080
5	0	5	6	←	4	0	4	5	4591.2206	-0.0020
5	2	4	5	←	4	2	3	4	4784.2328	0.0075
5	2	4	6	←	4	2	3	5	4784.3136	0.0010
5	2	3	6	←	4	2	2	5	5004.3301	0.0019
5	2	3	5	←	4	2	2	4	5004.4707	0.0060
5	1	5	5	←	4	0	4	4	5038.8279	0.0022
5	1	5	6	←	4	0	4	5	5039.4622	0.0033
5	1	5	4	←	4	0	4	3	5039.5491	-0.0039
5	1	4	5	←	4	1	3	4	5095.0735	0.0022
5	1	4	6	←	4	1	3	5	5095.1642	0.0037
2	2	1	2	←	1	1	0	1	5338.0643	0.0053
2	2	1	3	←	1	1	0	2	5338.8250	0.0082
6	0	6	6	←	5	0	5	5	5422.2600	0.0051
6	0	6	5	←	5	0	5	4	5422.4731	0.0012
2	2	0	3	←	1	1	1	2	5488.6272	-0.0008
2	2	0	2	←	1	1	1	1	5489.7081	-0.0011
6	2	5	6	←	5	2	4	5	5718.9142	-0.0003
6	2	5	7	←	5	2	4	6	5719.0056	0.0084
6	1	6	6	←	5	0	5	5	5727.3314	0.0035
6	1	6	6	←	5	0	5	5	5727.3320	0.0042
6	3	3	7	←	5	3	2	6	5860.5347	-0.0019
7	0	7	8	←	6	1	6	7	5932.5976	0.0084
7	0	7	7	←	6	1	6	6	5932.6991	0.0135
6	2	4	7	←	5	2	3	6	6069.1886	-0.0009
6	2	4	6	←	5	2	3	5	6069.3121	-0.0041
6	1	5	6	←	5	1	4	5	6069.8174	0.0006
6	1	5	7	←	5	1	4	6	6069.9519	0.0164
7	1	7	7	←	6	1	6	6	6130.4144	0.0047
7	1	7	8	←	6	1	6	7	6130.4922	0.0054
3	2	2	3	←	2	1	1	2	6162.4835	0.0039
3	2	2	4	←	2	1	1	3	6163.3080	0.0011
3	2	2	2	←	2	1	1	1	6163.7585	-0.0076

7	0	7	7	←	6	0	6	6	6237.7643	0.0057
7	0	7	6	←	6	0	6	5	6237.9456	0.0104
7	1	7	7	←	6	0	6	6	6435.4798	-0.0027
7	1	7	8	←	6	0	6	7	6435.8206	-0.0147
3	2	1	4	←	2	1	2	3	6637.0844	0.0229
3	2	1	3	←	2	1	2	2	6638.3639	0.0009
7	3	5	8	←	6	3	4	7	6800.0018	-0.0009
7	3	4	8	←	6	3	3	7	6880.0815	0.0024
4	2	3	4	←	3	1	2	3	6916.4401	0.0128
4	2	3	5	←	3	1	2	4	6917.3191	0.0114
4	2	3	3	←	3	1	2	2	6917.6222	0.0134
7	1	6	7	←	6	1	5	6	7015.2877	-0.0057
7	1	6	8	←	6	1	5	7	7015.4448	-0.0002
7	2	5	6	←	6	2	4	5	7136.5416	-0.0071
7	2	5	7	←	6	2	4	6	7136.6142	-0.0194
8	1	8	8	←	7	0	7	7	7171.5271	0.0035
8	1	8	7	←	7	0	7	6	7171.7751	-0.0003
8	1	8	9	←	7	0	7	8	7171.7751	0.0062
8	2	7	8	←	7	2	6	7	7552.3801	-0.0103
8	2	7	9	←	7	2	6	8	7552.4721	-0.0045
5	2	4	5	←	4	1	3	4	7602.4065	-0.0189
5	2	4	6	←	4	1	3	5	7603.3080	-0.0203
5	2	4	4	←	4	1	3	3	7603.5261	-0.0232
9	0	9	10	←	8	1	8	9	7736.6216	-0.0054
9	0	9	9	←	8	1	8	8	7736.6216	0.0007
9	1	9	9	←	8	1	8	8	7811.1921	0.0038
9	1	9	10	←	8	1	8	9	7811.2493	-0.0046
9	0	9	9	←	8	0	8	8	7859.8617	-0.0088
9	0	9	10	←	8	0	8	9	7859.9742	-0.0061
4	2	2	3	←	3	1	3	2	7920.4115	-0.0042
4	2	2	5	←	3	1	3	4	7920.9117	-0.0021
4	2	2	4	←	3	1	3	3	7922.4324	-0.0043
8	3	5	8	←	7	3	4	7	7924.6167	0.0021
8	1	7	8	←	7	1	6	7	7924.9829	-0.0004

Table S64 Measured frequencies and residuals (in MHz) for the rotational transitions of the ^{13}C11 isotopologue of the monomer of Pan.

J'	K_a'	K_c'	F'	←	J''	K_a''	K_c''	F''	ν_{obs}	ν_{obs}-ν_{calc}
1	1	1	1	←	0	0	0	1	2051.0500	-0.0041
1	1	1	2	←	0	0	0	1	2051.8290	0.0015
3	1	3	4	←	2	1	2	3	2683.0416	-0.0034
3	0	3	3	←	2	0	2	2	2849.8225	-0.0021
3	0	3	4	←	2	0	2	3	2849.9890	-0.0128
2	1	2	2	←	1	0	1	1	2878.1828	-0.0144
2	1	2	3	←	1	0	1	2	2879.0294	-0.0092
3	1	2	3	←	2	1	1	2	3100.3930	-0.0053
3	1	2	4	←	2	1	1	3	3100.4596	0.0015
3	1	2	2	←	2	1	1	1	3100.6368	-0.0086

4	1	4	5	←	3	1	3	4	3564.2419	-0.0020
3	1	3	3	←	2	0	2	2	3640.7024	-0.0052
3	1	3	4	←	2	0	2	3	3641.5481	-0.0013
3	1	3	2	←	2	0	2	1	3641.7775	-0.0006
4	0	4	4	←	3	0	3	3	3745.8889	-0.0009
4	0	4	5	←	3	0	3	4	3746.1103	0.0035
4	2	3	4	←	3	2	2	3	3856.2736	0.0023
4	2	3	5	←	3	2	2	4	3856.3839	0.0003
4	2	2	5	←	3	2	1	4	3976.4080	-0.0044
4	2	2	3	←	3	2	1	2	3976.4080	-0.0040
4	2	2	4	←	3	2	1	3	3976.5167	0.0032
5	0	5	4	←	4	1	4	3	3997.2499	-0.0021
5	0	5	6	←	4	1	4	5	3997.3773	-0.0050
5	0	5	5	←	4	1	4	4	3997.6964	0.0007
4	1	3	4	←	3	1	2	3	4117.4703	-0.0014
4	1	3	5	←	3	1	2	4	4117.5393	0.0018
4	1	3	3	←	3	1	2	2	4117.6333	0.0030
4	1	4	4	←	3	0	3	3	4355.0327	0.0017
4	1	4	5	←	3	0	3	4	4355.7962	0.0046
4	1	4	3	←	3	0	3	2	4355.9414	0.0016
5	0	5	5	←	4	0	4	4	4606.8402	0.0033
5	0	5	6	←	4	0	4	5	4607.0735	0.0063
5	2	4	5	←	4	2	3	4	4804.6837	-0.0089
5	2	4	6	←	4	2	3	5	4804.7759	-0.0049
6	0	6	5	←	5	1	5	4	5001.3081	0.0070
6	0	6	7	←	5	1	5	6	5001.3857	0.0054
6	0	6	6	←	5	1	5	5	5001.5754	0.0086
5	2	3	6	←	4	2	2	5	5030.1507	-0.0031
5	2	3	5	←	4	2	2	4	5030.2965	0.0051
5	1	5	6	←	4	0	4	5	5045.8115	-0.0164
5	1	5	4	←	4	0	4	3	5045.9178	-0.0028
5	1	4	5	←	4	1	3	4	5118.2837	0.0012
5	1	4	6	←	4	1	3	5	5118.3795	0.0060
2	2	1	2	←	1	1	0	1	5327.3066	-0.0037
2	2	1	3	←	1	1	0	2	5328.0753	0.0072
6	0	6	6	←	5	0	5	5	5439.9262	-0.0033
6	0	6	7	←	5	0	5	6	5440.1408	-0.0002
6	2	5	6	←	5	2	4	5	5742.8641	-0.0093
6	2	5	7	←	5	2	4	6	5742.9600	0.0023
6	3	4	7	←	5	3	3	6	5850.2481	0.0032
6	3	3	7	←	5	3	2	6	5888.6997	-0.0023
7	0	7	8	←	6	1	6	7	5960.5993	-0.0151
7	0	7	7	←	6	1	6	6	5960.7077	0.0025
6	2	4	7	←	5	2	3	6	6100.8695	0.0028
3	2	2	3	←	2	1	1	2	6154.4519	-0.0004
3	2	2	4	←	2	1	1	3	6155.2896	0.0099
3	2	2	2	←	2	1	1	1	6155.7483	0.0094
7	0	7	7	←	6	0	6	6	6257.5597	-0.0065
7	0	7	6	←	6	0	6	5	6257.7405	-0.0014
7	1	7	7	←	6	0	6	6	6448.7873	-0.0011
7	1	7	8	←	6	0	6	7	6449.1334	-0.0018

7	2	6	7	←	6	2	5	6	6669.1924	-0.0039
7	2	6	8	←	6	2	5	7	6669.2792	0.0017
7	1	6	7	←	6	1	5	6	7044.1009	-0.0015
7	1	6	8	←	6	1	5	7	7044.2542	-0.0028
8	0	8	8	←	7	0	7	7	7070.6013	0.0038
8	0	8	9	←	7	0	7	8	7070.7378	-0.0003
7	2	5	6	←	6	2	4	5	7173.3729	-0.0028
7	2	5	7	←	6	2	4	6	7173.4606	0.0023
8	1	8	8	←	7	0	7	7	7189.0622	0.0013
8	1	8	9	←	7	0	7	8	7189.3047	0.0035
8	1	8	7	←	7	0	7	6	7189.3047	-0.0022
8	1	8	7	←	7	0	7	6	7189.3047	-0.0022
8	1	8	9	←	7	0	7	8	7189.3047	0.0035
8	2	7	8	←	7	2	6	7	7582.4293	-0.0079
8	2	7	7	←	7	2	6	6	7582.5335	0.0051
5	2	4	5	←	4	1	3	4	7597.5385	-0.0077
5	2	4	6	←	4	1	3	5	7598.4461	-0.0023
9	0	9	9	←	8	0	8	8	7884.9640	0.0007
9	0	9	9	←	8	0	8	8	7884.9646	0.0013
9	0	9	10	←	8	0	8	9	7885.0662	-0.0056
9	0	9	10	←	8	0	8	9	7885.0662	-0.0056
9	1	9	9	←	8	0	8	8	7956.2034	0.0056
9	1	9	9	←	8	0	8	8	7956.2034	0.0056
9	1	9	8	←	8	0	8	7	7956.3729	0.0119
9	1	9	8	←	8	0	8	7	7956.3729	0.0119
8	3	5	9	←	7	3	4	8	7965.6012	0.0022
8	3	5	8	←	7	3	4	7	7965.7159	0.0055

Table S65 Measured frequencies and residuals (in MHz) for the rotational transitions of the ^{13}C12 isotopologue of the monomer of Pan.

J'	K_a'	K_c'	*F'*	←	*J"*	K_a"	K_c"	*F"*	ν_{obs}	ν_{obs}-ν_{calc}
3	0	3	3	←	2	0	2	2	2865.5635	-0.0064
3	0	3	4	←	2	0	2	3	2865.7445	-0.0046
2	1	2	2	←	1	0	1	2	2884.8342	0.0018
2	1	2	2	←	1	0	1	1	2885.0087	-0.0081
2	1	2	3	←	1	0	1	2	2885.8564	-0.0019
2	1	2	1	←	1	0	1	0	2886.1604	0.0052
2	1	2	1	←	1	0	1	1	2886.6044	-0.0093
4	0	4	4	←	3	1	3	3	2980.2922	-0.0001
3	1	2	3	←	2	1	1	2	3119.4311	-0.0047
3	1	2	4	←	2	1	1	3	3119.5018	0.0055
4	1	4	4	←	3	1	3	3	3583.1090	0.0135
4	1	4	5	←	3	1	3	4	3583.1930	0.0011
3	1	3	3	←	2	0	2	2	3650.9816	0.0013
3	1	3	4	←	2	0	2	3	3651.8229	0.0019
3	1	3	2	←	2	0	2	1	3652.0507	0.0016
4	0	4	5	←	3	0	3	4	3765.9248	0.0033
4	2	2	5	←	3	2	1	4	4001.4949	-0.0025

5	0	5	4	←	4	1	4	3	4026.9400	-0.0040
5	0	5	6	←	4	1	4	5	4027.0664	-0.0071
5	0	5	5	←	4	1	4	4	4027.3801	-0.0006
4	1	3	4	←	3	1	2	3	4142.4273	-0.0081
4	1	3	5	←	3	1	2	4	4142.5107	0.0087
4	1	4	4	←	3	0	3	3	4368.5135	0.0079
4	1	4	5	←	3	0	3	4	4369.2712	0.0075
5	0	5	5	←	4	0	4	4	4630.2002	0.0163
5	0	5	6	←	4	0	4	5	4630.4220	0.0062
5	2	4	5	←	4	2	3	4	4832.2366	0.0065
5	1	5	5	←	4	0	4	4	5062.1308	-0.0073
5	1	5	6	←	4	0	4	5	5062.7494	-0.0131
6	1	6	6	←	5	1	5	5	5325.8919	0.0205
6	1	6	7	←	5	1	5	6	5325.9446	-0.0100
2	2	1	2	←	1	1	0	1	5331.3704	-0.0049
2	2	1	3	←	1	1	0	2	5332.1329	-0.0002
2	2	1	1	←	1	1	0	0	5333.4652	0.0053
6	0	6	6	←	5	0	5	5	5466.6873	0.0042
6	0	6	7	←	5	0	5	6	5466.8974	0.0027
2	2	0	1	←	1	1	1	0	5484.3167	0.0010
2	2	0	3	←	1	1	1	2	5485.6529	0.0016
2	2	0	2	←	1	1	1	2	5485.9655	0.0025
2	2	0	1	←	1	1	1	1	5486.2624	0.0101
2	2	0	2	←	1	1	1	1	5486.7392	0.0029
6	1	6	6	←	5	0	5	5	5757.8339	0.0082
6	2	5	6	←	5	2	4	5	5775.3766	-0.0001
6	2	5	7	←	5	2	4	6	5775.4596	-0.0030
6	3	4	7	←	5	3	3	6	5885.1098	-0.0021
6	3	3	7	←	5	3	2	6	5924.9696	0.0009
6	2	4	7	←	5	2	3	6	6140.4098	-0.0013
3	2	2	3	←	2	1	1	2	6162.6153	-0.0007
3	2	2	4	←	2	1	1	3	6163.4480	0.0048
3	2	2	2	←	2	1	1	1	6163.9021	-0.0001
7	0	7	7	←	6	0	6	6	6287.9347	-0.0057
7	0	7	8	←	6	0	6	7	6288.1196	0.0012
7	1	7	7	←	6	0	6	6	6474.5495	-0.0126
3	2	1	2	←	2	1	2	1	6648.8546	-0.0028
3	2	1	4	←	2	1	2	3	6649.5246	-0.0022
3	2	1	3	←	2	1	2	3	6649.8054	-0.0048
3	2	1	2	←	2	1	2	2	6650.4500	-0.0044
3	2	1	3	←	2	1	2	2	6650.8338	-0.0023
7	2	6	7	←	6	2	5	6	6706.3964	-0.0044
7	2	6	8	←	6	2	5	7	6706.4788	-0.0030
8	0	8	9	←	7	1	7	8	6918.2253	-0.0156
4	2	3	4	←	3	1	2	3	6921.7818	-0.0020
4	2	3	5	←	3	1	2	4	6922.6665	0.0035
4	2	3	3	←	3	1	2	2	6922.9707	0.0062
7	3	4	8	←	6	3	3	7	6957.9390	0.0052
7	3	4	7	←	6	3	3	6	6958.0180	0.0090
8	1	8	8	←	7	1	7	7	7033.3252	0.0131
8	1	8	9	←	7	1	7	8	7033.3870	0.0025

7	1	6	7	←	6	1	5	6	7083.4396	-0.0080
8	0	8	8	←	7	0	7	7	7104.8926	0.0054
8	0	8	9	←	7	0	7	8	7105.0369	0.0100
7	2	5	8	←	6	2	4	7	7219.4972	-0.0038
7	2	5	7	←	6	2	4	6	7219.5880	0.0032
8	1	8	8	←	7	0	7	7	7219.9317	-0.0022
8	1	8	9	←	7	0	7	8	7220.1660	-0.0042
5	2	4	5	←	4	1	3	4	7611.5757	-0.0026
5	2	4	6	←	4	1	3	5	7612.4731	-0.0069
8	3	6	7	←	7	3	5	6	7854.3567	0.0017
4	2	2	3	←	3	1	3	2	7953.0396	-0.0049
4	2	2	5	←	3	1	3	4	7953.5439	-0.0018
4	2	2	4	←	3	1	3	3	7955.0851	0.0041
9	1	9	9	←	8	0	8	8	7992.1995	-0.0124

Table S66 Measured frequencies and residuals (in MHz) for the rotational transitions of the ^{13}C13 isotopologue of the monomer of Pan.

J'	K_a'	K_c'	*F'*	←	*J"*	K_a"	K_c"	*F"*	ν_{obs}	ν_{obs}-ν_{calc}
1	1	1	1	←	0	0	0	1	2035.1882	-0.0079
1	1	1	2	←	0	0	0	1	2035.9738	0.0043
1	1	1	0	←	0	0	0	1	2037.1356	0.0028
3	0	3	2	←	2	0	2	1	2864.8157	-0.0003
2	1	2	2	←	1	0	1	1	2865.1727	-0.0063
2	1	2	3	←	1	0	1	2	2866.0161	-0.0043
2	1	2	1	←	1	0	1	0	2866.3165	-0.0008
2	1	2	1	←	1	0	1	1	2866.7734	-0.0025
4	0	4	3	←	3	1	3	2	2997.2650	0.0005
4	0	4	5	←	3	1	3	4	2997.4824	0.0004
4	0	4	4	←	3	1	3	3	2997.9081	-0.0057
4	1	4	5	←	3	1	3	4	3580.4778	-0.0011
3	1	3	3	←	2	0	2	2	3629.2984	0.0002
3	1	3	4	←	2	0	2	3	3630.1395	0.0026
3	1	3	2	←	2	0	2	1	3630.3670	0.0035
4	2	3	4	←	3	2	2	3	3879.5630	0.0075
4	2	3	5	←	3	2	2	4	3879.6617	-0.0063
4	3	2	4	←	3	3	1	3	3914.5415	-0.0026
4	3	2	5	←	3	3	1	4	3914.6774	0.0015
4	2	2	5	←	3	2	1	4	4006.9089	-0.0002
4	2	2	4	←	3	2	1	3	4007.0170	0.0016
5	0	5	4	←	4	1	4	3	4041.2861	-0.0065
5	0	5	6	←	4	1	4	5	4041.4158	-0.0048
5	0	5	5	←	4	1	4	4	4041.7212	0.0061
4	1	3	4	←	3	1	2	3	4145.8037	0.0009
4	1	3	5	←	3	1	2	4	4145.8797	0.0095
4	1	3	3	←	3	1	2	2	4145.9762	0.0090
4	1	4	4	←	3	0	3	3	4345.0431	-0.0021
4	1	4	5	←	3	0	3	4	4345.7986	0.0004
4	1	4	3	←	3	0	3	2	4345.9444	0.0014
5	0	5	5	←	4	0	4	4	4624.1895	0.0070

5	0	5	6	←	4	0	4	5	4624.4129	-0.0047
5	2	4	5	←	4	2	3	4	4832.7960	0.0019
5	2	4	6	←	4	2	3	5	4832.8963	0.0113
5	1	5	5	←	4	0	4	4	5037.7648	-0.0034
5	1	5	6	←	4	0	4	5	5038.3855	0.0011
5	1	5	4	←	4	0	4	3	5038.4656	-0.0077
6	0	6	5	←	5	1	5	4	5044.0727	-0.0054
6	0	6	7	←	5	1	5	6	5044.1521	-0.0022
6	0	6	6	←	5	1	5	5	5044.3140	-0.0097
5	2	3	6	←	4	2	2	5	5070.7605	0.0020
5	1	4	5	←	4	1	3	4	5151.6519	-0.0005
5	1	4	6	←	4	1	3	5	5151.7489	0.0010
2	2	1	2	←	1	1	0	1	5276.8932	-0.0031
2	2	1	1	←	1	1	0	0	5278.9803	-0.0005
2	2	0	3	←	1	1	1	2	5433.2740	0.0051
2	2	0	2	←	1	1	1	2	5433.5851	-0.0004
2	2	0	1	←	1	1	1	1	5433.8747	0.0075
2	2	0	2	←	1	1	1	1	5434.3618	0.0029
6	0	6	7	←	5	0	5	6	5458.1230	0.0019
6	2	5	6	←	5	2	4	5	5775.1342	-0.0011
6	2	5	7	←	5	2	4	6	5775.2365	-0.0163
6	3	3	7	←	5	3	2	6	5931.1417	0.0127
7	0	7	8	←	6	1	6	7	6001.0013	-0.0134
7	0	7	7	←	6	1	6	6	6001.0983	0.0067
3	2	2	3	←	2	1	1	2	6106.8767	-0.0019
3	2	2	4	←	2	1	1	3	6107.7060	0.0003
3	2	2	2	←	2	1	1	1	6108.1678	0.0032
6	2	4	7	←	5	2	3	6	6150.8723	0.0031
6	2	4	6	←	5	2	3	5	6150.9981	0.0046
7	0	7	7	←	6	0	6	6	6277.0573	0.0000
7	0	7	8	←	6	0	6	7	6277.2302	-0.0037
7	1	7	7	←	6	0	6	6	6452.1287	0.0132
3	2	1	2	←	2	1	2	1	6600.3409	0.0000
3	2	1	4	←	2	1	2	3	6601.0146	0.0017
3	2	1	3	←	2	1	2	2	6602.3331	0.0037
7	2	6	8	←	6	2	5	7	6705.0676	0.0015
4	2	3	4	←	3	1	2	3	6863.9378	-0.0047
4	2	3	5	←	3	1	2	4	6864.8270	0.0073
4	2	3	3	←	3	1	2	2	6865.1272	0.0041
7	4	3	8	←	6	4	2	7	6877.1297	0.0110
8	0	8	9	←	7	1	7	8	6917.5123	0.0198
7	1	6	7	←	6	1	5	6	7081.8949	-0.0044
7	1	6	8	←	6	1	5	7	7082.0535	-0.0081
8	0	8	8	←	7	0	7	7	7092.5671	-0.0013
8	0	8	7	←	7	0	7	6	7092.7033	0.0043
8	1	8	8	←	7	0	7	7	7199.3597	-0.0060
8	1	8	7	←	7	0	7	6	7199.5937	-0.0043
7	2	5	8	←	6	2	4	7	7230.9124	-0.0117
7	2	5	7	←	6	2	4	6	7231.0010	-0.0033
5	2	4	5	←	4	1	3	4	7550.9268	-0.0071
5	2	4	6	←	4	1	3	5	7551.8322	-0.0021

5	2	4	4	←	4	1	3	3	7552.0523	-0.0019
9	0	9	9	←	8	1	8	8	7803.2027	0.0002
9	1	9	10	←	8	1	8	9	7866.5200	0.0008
8	4	5	9	←	7	4	4	8	7869.2973	0.0068
8	4	4	7	←	7	4	3	6	7881.5616	-0.0022
9	0	9	9	←	8	0	8	8	7909.9963	-0.0033
9	0	9	10	←	8	0	8	9	7910.0998	-0.0058
4	2	2	3	←	3	1	3	2	7911.6091	-0.0057
4	2	2	5	←	3	1	3	4	7912.1096	-0.0096
4	2	2	4	←	3	1	3	3	7913.6674	0.0012
9	1	9	9	←	8	0	8	8	7973.2539	0.0037
9	1	9	8	←	8	0	8	7	7973.4078	0.0044

Table S67 Measured frequencies and residuals (in MHz) for the rotational transitions of the ^{15}N isotopologue of the monomer of Pan.

J'	K_a'	K_c'	←	J''	K_a''	K_c''	ν_{obs}	ν_{obs}-ν_{calc}
1	1	1	←	0	0	0	2035.4222	-0.0030
3	0	3	←	2	0	2	2864.2130	-0.0061
2	1	2	←	1	0	1	2865.2430	-0.0057
4	0	4	←	3	1	3	2997.0416	0.0029
4	1	4	←	3	1	3	3579.7523	0.0007
3	1	3	←	2	0	2	3629.1984	0.0020
4	3	1	←	3	3	0	3918.6242	0.0017
4	2	2	←	3	2	1	4006.1936	0.0007
5	0	5	←	4	1	4	4040.7481	0.0017
4	1	3	←	3	1	2	4145.0896	0.0045
4	1	4	←	3	0	3	4344.7273	-0.0013
5	1	5	←	4	1	4	4454.4961	-0.0025
5	0	5	←	4	0	4	4623.4520	-0.0073
5	2	4	←	4	2	3	4831.9502	0.0035
5	1	5	←	4	0	4	5037.2100	-0.0016
6	0	6	←	5	1	5	5043.2464	-0.0059
5	1	4	←	4	1	3	5150.7508	-0.0081
2	2	1	←	1	1	0	5276.4508	-0.0006
2	2	0	←	1	1	1	5432.3611	0.0086
6	1	6	←	5	0	5	5733.0585	-0.0162
6	2	5	←	5	2	4	5774.1322	-0.0010
6	3	4	←	5	3	3	5887.5664	0.0049
6	3	3	←	5	3	2	5930.0295	0.0015
7	0	7	←	6	1	6	5999.9084	0.0095
3	2	2	←	2	1	1	6106.2758	0.0010
6	1	5	←	5	1	4	6131.9056	-0.0044
6	2	4	←	5	2	3	6149.7643	0.0025
7	1	7	←	6	1	6	6175.0193	0.0035
7	1	7	←	6	0	6	6451.0999	0.0140
3	2	1	←	2	1	2	6599.9870	-0.0002
7	2	6	←	6	2	5	6703.7660	-0.0014
4	2	3	←	3	1	2	6863.2077	0.0034
8	1	8	←	7	1	7	7023.0128	0.0059

7	1	6	←	6	1	5	7080.6701	-0.0038
8	1	8	←	7	0	7	7198.1238	0.0000
7	2	5	←	6	2	4	7229.5978	-0.0039
5	2	4	←	4	1	3	7550.0620	-0.0038
9	0	9	←	8	1	8	7801.7271	0.0060
9	1	9	←	8	1	8	7864.9837	-0.0025
9	0	9	←	8	0	8	7908.5443	-0.0044
4	2	2	←	3	1	3	7910.9488	-0.0010

Table S68 Measured frequencies and residuals (in MHz) for the rotational transitions of the Pan-H_2O complex.

J'	K_a'	K_c'	F'	←	J''	K_a''	K_c''	F''	ν_{obs}	ν_{obs}-ν_{calc}
3	1	3	3	←	2	1	2	2	2085.90880	0.00122
3	1	3	2	←	2	1	2	1	2086.10490	0.00156
3	1	3	4	←	2	1	2	3	2086.19700	0.00128
3	1	3	2	←	2	1	2	2	2087.56140	-0.00343
3	0	3	3	←	2	0	2	2	2212.82140	-0.00252
3	0	3	2	←	2	0	2	1	2212.89840	0.00408
3	0	3	4	←	2	0	2	3	2213.02150	-0.00157
3	0	3	2	←	2	0	2	2	2214.40560	0.01015
3	2	2	3	←	2	2	1	2	2345.81130	-0.00051
3	2	2	4	←	2	2	1	3	2346.65100	0.00028
3	2	2	2	←	2	2	1	1	2347.12230	0.00517
3	1	3	3	←	2	0	2	2	2405.40370	0.00065
3	1	3	4	←	2	0	2	3	2405.67010	0.00437
3	2	1	3	←	2	2	0	2	2479.44260	-0.00658
3	2	1	4	←	2	2	0	3	2480.12070	0.00067
3	2	1	2	←	2	2	0	1	2480.55360	0.00010
3	1	2	3	←	2	1	1	2	2560.46090	-0.00217
3	1	2	3	←	2	1	1	3	2560.56233	-0.00111
3	1	2	4	←	2	1	1	3	2560.72410	-0.00205
3	1	2	2	←	2	1	1	1	2560.83780	-0.00038
10	4	6	9	←	10	3	7	9	2576.23375	-0.01557
10	4	6	11	←	10	3	7	11	2576.27532	0.01042
10	4	6	10	←	10	3	7	10	2576.42065	0.00060
9	4	5	8	←	9	3	6	8	2594.76894	0.00884
9	4	5	10	←	9	3	6	10	2594.76894	-0.00114
9	4	5	9	←	9	3	6	9	2594.85820	-0.00127
4	1	4	4	←	3	1	3	4	2748.36760	0.00409
4	1	4	4	←	3	1	3	3	2749.58830	-0.00258
4	1	4	3	←	3	1	3	2	2749.68400	0.00213
4	1	4	5	←	3	1	3	4	2749.75650	0.00252
8	4	4	7	←	8	3	5	7	2785.93954	0.00444
8	4	4	9	←	8	3	5	9	2785.93954	-0.00398
8	4	4	8	←	8	3	5	8	2786.01150	0.00111
4	0	4	4	←	3	0	3	3	2842.81140	0.01338
4	0	4	3	←	3	0	3	2	2842.91456	-0.00127
4	0	4	5	←	3	0	3	4	2842.97500	-0.00278

4	1	4	4	←	3	0	3	3	2942.17490	0.00489
2	2	1	1	←	1	1	0	1	3052.96990	0.00215
2	2	1	3	←	1	1	0	2	3054.30030	-0.00982
2	2	1	2	←	1	1	0	2	3055.15840	0.00923
2	2	1	1	←	1	1	0	0	3055.15840	-0.00049
4	2	3	4	←	3	2	2	3	3099.94810	-0.00143
4	2	3	5	←	3	2	2	4	3100.34380	0.00649
4	2	3	3	←	3	2	2	2	3100.44460	0.00776
4	2	3	3	←	3	2	2	3	3100.44460	0.00727
4	2	3	3	←	3	2	2	4	3100.44460	0.00712
4	3	2	4	←	3	3	1	3	3187.13118	0.00343
4	3	2	5	←	3	3	1	4	3187.85959	0.00272
4	3	2	3	←	3	3	1	2	3188.15366	0.00474
12	5	7	11	←	12	4	8	11	3195.58286	0.00459
12	5	7	13	←	12	4	8	13	3195.58286	0.00009
12	5	7	12	←	12	4	8	12	3195.63431	-0.00225
10	3	7	9	←	10	2	8	9	3205.76554	0.00704
10	3	7	11	←	10	2	8	11	3205.80530	0.00118
10	3	7	10	←	10	2	8	10	3206.25485	-0.00354
4	3	1	3	←	3	3	0	3	3216.86950	-0.00293
4	3	1	4	←	3	3	0	3	3217.42090	-0.01515
4	3	1	5	←	3	3	0	4	3218.12200	-0.00222
4	3	1	3	←	3	3	0	2	3218.40910	0.00212
2	2	0	1	←	1	1	1	0	3249.41270	-0.00189
2	2	0	1	←	1	1	1	1	3249.64820	-0.00077
2	2	0	3	←	1	1	1	2	3250.09070	0.00017
2	2	0	2	←	1	1	1	2	3251.05390	-0.00133
2	2	0	2	←	1	1	1	1	3251.14810	-0.00114
5	0	5	6	←	4	1	4	5	3351.35940	-0.00311
4	1	3	4	←	3	1	2	3	3358.99800	-0.01389
4	1	3	5	←	3	1	2	4	3359.19507	0.00355
4	1	3	3	←	3	1	2	2	3359.19507	-0.02727
4	1	3	3	←	3	1	2	3	3359.44880	0.00604
4	2	2	3	←	3	2	1	3	3385.05450	-0.00114
4	2	2	4	←	3	2	1	3	3385.13730	0.00078
4	2	2	5	←	3	2	1	4	3385.36440	-0.00119
4	2	2	3	←	3	2	1	2	3385.44410	-0.00748
5	1	5	5	←	4	1	4	4	3397.13660	0.00329
5	1	5	4	←	4	1	4	3	3397.19209	-0.00417
5	1	5	6	←	4	1	4	5	3397.24830	0.00092
11	5	6	10	←	11	4	7	10	3422.77387	-0.01059
11	5	6	12	←	11	4	7	12	3422.77387	-0.01212
11	5	6	11	←	11	4	7	11	3422.77387	-0.02893
5	0	5	5	←	4	0	4	4	3450.64442	0.00075
5	0	5	4	←	4	0	4	3	3450.77402	0.03645
5	0	5	6	←	4	0	4	5	3450.77402	-0.00735
5	1	5	5	←	4	0	4	4	3496.50510	-0.00020
5	1	5	6	←	4	0	4	5	3496.66234	-0.00390
4	4	1	3	←	4	3	2	3	3611.67192	0.00464
4	4	1	5	←	4	3	2	5	3611.88470	-0.01000
5	4	2	4	←	5	3	3	4	3612.38903	0.00482

5	4	2	6	←	5	3	3	6	3612.51285	0.00465
4	4	1	4	←	4	3	2	4	3612.77230	-0.00566
5	4	2	5	←	5	3	3	5	3613.09960	-0.01701
3	2	2	3	←	2	1	1	2	3676.49290	-0.00198
3	2	2	4	←	2	1	1	3	3676.59340	-0.00172
3	2	2	2	←	2	1	1	1	3676.64725	-0.00281
5	2	4	5	←	4	2	3	4	3830.88514	0.01047
5	2	4	6	←	4	2	3	5	3831.10882	-0.00146
5	2	4	4	←	4	2	3	3	3831.15581	0.01837
5	3	3	5	←	4	3	2	4	3989.68420	-0.00043
5	3	3	6	←	4	3	2	5	3990.05220	-0.01189
5	3	3	4	←	4	3	2	3	3990.16220	-0.00019
5	4	2	6	←	4	4	1	5	3990.66430	-0.01330
5	4	2	4	←	4	4	1	3	3990.86950	-0.00983
5	4	1	5	←	4	4	0	4	3994.92310	-0.00874
5	4	1	6	←	4	4	0	5	3995.57770	-0.00231
5	4	1	4	←	4	4	0	3	3995.77460	-0.00595
6	0	6	6	←	5	1	5	5	4013.38547	0.00962
6	0	6	5	←	5	1	5	4	4013.44148	0.02804
6	0	6	7	←	5	1	5	6	4013.44148	-0.01144
6	1	6	6	←	5	1	5	5	4033.04563	-0.00181
6	1	6	5	←	5	1	5	4	4033.10243	0.00592
6	1	6	7	←	5	1	5	6	4033.13297	-0.00138
6	0	6	6	←	5	0	5	5	4059.23912	0.00164
6	0	6	5	←	5	0	5	4	4059.33666	0.03363
6	0	6	7	←	5	0	5	6	4059.33666	-0.00113
6	1	6	6	←	5	0	5	5	4078.90840	-0.00067
6	1	6	5	←	5	0	5	4	4078.98626	0.00015
9	5	4	8	←	9	4	5	8	4085.86111	0.00406
9	5	4	10	←	9	4	5	10	4085.86111	-0.00663
9	5	4	9	←	9	4	5	9	4085.96438	0.00111
5	3	2	5	←	4	3	1	4	4087.51700	0.00123
5	3	2	6	←	4	3	1	5	4087.81882	0.00181
5	3	2	4	←	4	3	1	3	4087.90478	0.00249
5	1	4	5	←	4	1	3	4	4098.89620	0.00300
5	1	4	6	←	4	1	3	5	4099.06510	-0.00358
4	2	3	4	←	3	1	2	3	4215.98380	0.00246
4	2	3	5	←	3	1	2	4	4216.21910	0.01282
5	2	3	5	←	4	2	2	4	4286.08270	-0.00279
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3	2	1	4	←	2	1	2	3	4325.64340	0.00174
3	2	1	3	←	2	1	2	3	4325.94010	0.00459
3	2	1	2	←	2	1	2	2	4326.48140	0.00261
3	2	1	3	←	2	1	2	2	4326.87530	0.00056
7	2	5	8	←	6	3	4	7	4346.26452	-0.00826
7	2	5	6	←	6	3	4	5	4346.26452	-0.00888
6	2	5	6	←	5	2	4	5	4536.10150	-0.00168
6	2	5	7	←	5	2	4	6	4536.27520	0.00126
6	2	5	5	←	5	2	4	4	4536.27520	-0.00576
9	5	5	10	←	9	4	6	10	4587.50616	-0.00242

9	5	5	9	←	9	4	6	9	4587.79276	0.00555
5	5	1	4	←	5	4	2	4	4635.91040	0.00452
3	2	1	2	←	2	0	2	1	4644.47080	-0.00234
3	2	1	4	←	2	0	2	3	4645.11230	0.00062
3	2	1	3	←	2	0	2	3	4645.39110	-0.01443
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10	5	6	10	←	10	4	7	10	4657.58987	0.00608
7	1	7	7	←	6	1	6	6	4661.92542	0.02262
7	1	7	6	←	6	1	6	5	4661.92542	-0.01668
7	1	7	8	←	6	1	6	7	4661.96990	-0.00148
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7	1	7	7	←	6	0	6	6	4681.57861	0.00422
7	1	7	6	←	6	0	6	5	4681.61957	-0.00562
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6	1	5	6	←	5	1	4	5	4767.88860	0.00140
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6	3	4	6	←	5	3	3	5	4780.80160	-0.00238
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6	4	3	6	←	5	4	2	5	4808.79240	-0.00099
6	4	3	7	←	5	4	2	6	4809.16430	-0.00286
6	4	3	5	←	5	4	2	4	4809.24750	-0.00448
6	4	2	6	←	5	4	1	5	4829.94980	-0.00257
6	4	2	7	←	5	4	1	6	4830.30320	-0.00499
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3	3	1	2	←	2	2	0	2	4946.13100	0.00461
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3	3	1	3	←	2	2	0	3	4948.60287	-0.00487
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6	3	3	6	←	5	3	2	5	5004.88580	0.00219
6	3	3	7	←	5	3	2	6	5004.99980	-0.01041
6	3	3	5	←	5	3	2	4	5005.04801	0.01135
7	1	6	6	←	6	2	5	5	5023.73870	0.00682
7	1	6	8	←	6	2	5	7	5023.73870	-0.00159
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8	1	8	8	←	7	1	7	7	5287.04112	0.00499
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8	1	8	9	←	7	1	7	8	5287.09680	0.00548
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7	1	6	7	←	6	1	5	6	5380.83050	0.00076
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11	2	9	10	←	11	1	10	10	5386.66352	0.00492
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7	3	5	7	←	6	3	4	6	5551.99100	-0.00336
7	3	5	8	←	6	3	4	7	5552.15010	-0.01084
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7	4	4	8	←	6	4	3	7	5630.66123	0.00366
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7	4	3	7	←	6	4	2	6	5695.82150	-0.00678
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10	0	10	10	←	9	0	9	9	6533.78520	-0.01304
10	0	10	9	←	9	0	9	8	6533.83508	0.01514
10	0	10	11	←	9	0	9	10	6533.83508	-0.00094
10	1	10	10	←	9	0	9	9	6534.24399	-0.01369
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9	1	8	9	←	8	1	7	8	6568.69370	-0.00281
9	1	8	8	←	8	1	7	7	6568.80860	-0.00218
9	1	8	10	←	8	1	7	9	6568.80860	-0.00366
8	4	4	8	←	7	4	3	7	6605.95013	0.00381
8	4	4	9	←	7	4	3	8	6606.04712	0.00560
8	4	4	7	←	7	4	3	6	6606.04712	-0.00781
9	2	8	9	←	8	1	7	8	6612.09669	0.00052
9	2	8	8	←	8	1	7	7	6612.22876	0.00229
9	2	8	10	←	8	1	7	9	6612.22876	0.00242
8	2	6	8	←	7	2	5	7	6681.21970	0.00774
8	2	6	9	←	7	2	5	8	6681.34870	0.00696
8	2	6	7	←	7	2	5	6	6681.34870	-0.00457
6	3	4	6	←	5	2	3	5	6754.59171	0.00349
6	3	4	7	←	5	2	3	6	6754.74937	-0.00450
6	3	4	5	←	5	2	3	4	6754.79775	0.01787
4	4	1	5	←	3	3	0	4	6794.51550	-0.00668
4	4	1	3	←	3	3	0	2	6794.58320	-0.00825
4	4	1	4	←	3	3	0	3	6794.65970	-0.00338
4	4	0	5	←	3	3	1	4	6800.37881	0.00049
4	4	0	3	←	3	3	1	2	6800.43417	-0.00846
4	4	0	4	←	3	3	1	3	6800.53230	-0.00143
5	3	2	4	←	4	2	3	3	6847.54060	-0.00505
5	3	2	6	←	4	2	3	5	6847.67050	-0.00494
5	3	2	5	←	4	2	3	4	6848.20560	-0.00495
8	3	5	9	←	7	3	4	8	6877.14296	0.00718
8	3	5	7	←	7	3	4	6	6877.14296	0.00213
4	3	1	3	←	3	1	2	2	6975.89954	0.00745
4	3	1	5	←	3	1	2	4	6976.06496	0.00025

4	3	1	4	←	3	1	2	3	6976.68380	0.00767
9	3	7	9	←	8	3	6	8	7013.05070	-0.00933
9	3	7	10	←	8	3	6	9	7013.16790	-0.00832
9	3	7	8	←	8	3	6	7	7013.16790	-0.01393
10	1	9	10	←	9	2	8	9	7131.15705	-0.00448
10	1	9	9	←	9	2	8	8	7131.22811	-0.00743
10	1	9	11	←	9	2	8	10	7131.22811	-0.01245
10	2	9	10	←	9	2	8	9	7150.14160	-0.00350
10	2	9	9	←	9	2	8	8	7150.22584	-0.00009
10	2	9	11	←	9	2	8	10	7150.22584	-0.00448
11	0	11	11	←	10	1	10	10	7155.18382	-0.00868
11	0	11	10	←	10	1	10	9	7155.23330	0.02305
11	0	11	12	←	10	1	10	11	7155.23330	0.00936
11	1	11	11	←	10	1	10	10	7155.35074	-0.01216
11	1	11	10	←	10	1	10	9	7155.40079	0.02006
11	1	11	12	←	10	1	10	11	7155.40079	0.00638
11	0	11	11	←	10	0	10	10	7155.64148	-0.01046
11	0	11	10	←	10	0	10	9	7155.69074	0.02084
11	0	11	12	←	10	0	10	11	7155.69074	0.00717
11	1	11	11	←	10	0	10	10	7155.81533	-0.00701
11	1	11	10	←	10	0	10	9	7155.85733	0.01697
11	1	11	12	←	10	0	10	11	7155.85733	0.00330
7	3	5	7	←	6	2	4	6	7157.96200	-0.00982
7	3	5	8	←	6	2	4	7	7158.19400	-0.01159
7	3	5	6	←	6	2	4	5	7158.23227	-0.00325
5	2	3	4	←	4	1	4	3	7160.91540	0.00115
5	2	3	6	←	4	1	4	5	7161.25660	-0.00420
10	1	9	10	←	9	1	8	9	7174.56160	0.00040
10	1	9	9	←	9	1	8	8	7174.64820	-0.00303
10	2	9	10	←	9	1	8	9	7193.53770	-0.00707
10	2	9	9	←	9	1	8	8	7193.65568	0.01406
10	2	9	11	←	9	1	8	10	7193.65568	0.01128
9	6	4	9	←	8	6	3	8	7222.61340	-0.01093
9	6	4	10	←	8	6	3	9	7222.86840	-0.00330
9	6	3	9	←	8	6	2	8	7224.96320	0.00047
9	6	3	10	←	8	6	2	9	7225.21587	0.00721
9	4	6	9	←	8	4	5	8	7251.15170	0.00530
9	4	6	10	←	8	4	5	9	7251.27710	0.00884
9	4	6	8	←	8	4	5	7	7251.27710	-0.00270
5	2	3	4	←	4	0	4	3	7260.34518	0.00003
5	2	3	6	←	4	0	4	5	7260.68152	0.00185
5	2	3	5	←	4	0	4	4	7261.97101	0.00073
9	5	5	9	←	8	5	4	8	7267.06750	-0.00401
9	5	5	10	←	8	5	4	9	7267.22340	-0.01362
9	5	5	8	←	8	5	4	7	7267.26775	0.00974
9	5	4	9	←	8	5	3	8	7308.31030	-0.00648
9	5	4	8	←	8	5	3	9	7308.45300	-0.00514
9	5	4	8	←	8	5	3	7	7308.47569	-0.00609
9	2	7	9	←	8	2	6	8	7331.67310	-0.00051
9	2	7	10	←	8	2	6	9	7331.81990	0.00160
9	2	7	8	←	8	2	6	7	7331.81990	-0.00900

10	2	8	9	←	9	3	7	8	7422.74888	-0.00271
10	2	8	11	←	9	3	7	10	7422.74888	-0.00569
8	3	6	8	←	7	2	5	7	7502.79430	0.00157
8	3	6	9	←	7	2	5	8	7503.04280	-0.00828
8	3	6	7	←	7	2	5	6	7503.09108	0.01229
9	4	5	9	←	8	4	4	8	7561.66223	-0.00755
9	4	5	10	←	8	4	4	9	7561.70805	0.00175
9	4	5	8	←	8	4	4	7	7561.70805	-0.00209
5	4	2	4	←	4	3	1	3	7567.07737	0.01356
5	4	2	6	←	4	3	1	5	7567.07737	0.00181
5	4	1	4	←	4	3	2	3	7608.05932	-0.01496
5	4	1	6	←	4	3	2	5	7608.12222	0.02076
5	4	1	5	←	4	3	2	4	7608.34780	0.00999
10	3	8	10	←	9	3	7	9	7700.97700	0.00229
10	3	8	11	←	9	3	7	10	7701.07795	-0.00184
10	3	8	9	←	9	3	7	8	7701.07795	-0.00520
5	3	2	4	←	4	1	3	3	7704.57348	0.00144
5	3	2	6	←	4	1	3	5	7704.68863	-0.00157
5	3	2	5	←	4	1	3	4	7705.18181	0.00181
9	3	6	9	←	8	3	5	8	7752.82133	0.00064
9	3	6	10	←	8	3	5	9	7752.88001	0.00028
9	3	6	8	←	8	3	5	7	7752.88001	-0.00513
11	3	8	10	←	10	4	7	9	7758.11801	0.00604
11	3	8	12	←	10	4	7	11	7758.11801	-0.00109
11	1	10	11	←	10	2	9	10	7768.95642	-0.00237
11	1	10	10	←	10	2	9	9	7769.02353	-0.00132
11	1	10	12	←	10	2	9	11	7769.02353	-0.00620
11	2	10	11	←	10	2	9	10	7776.96975	0.00283
11	2	10	10	←	10	2	9	9	7777.03786	0.00211
11	2	10	12	←	10	2	9	11	7777.03786	-0.00254
12	1	12	12	←	11	1	11	11	7777.57601	-0.00322
12	1	12	11	←	11	1	11	10	7777.61221	0.01789
12	1	12	13	←	11	1	11	12	7777.61221	0.00612
12	0	12	12	←	11	0	11	11	7777.68591	-0.00134
12	0	12	11	←	11	0	11	10	7777.71709	0.01470
12	0	12	13	←	11	0	11	12	7777.71709	0.00294
11	1	10	11	←	10	1	9	10	7787.94048	-0.00188
11	1	10	10	←	10	1	9	9	7788.01451	-0.00074
11	1	10	12	←	10	1	9	11	7788.01451	-0.00499
11	2	10	11	←	10	1	9	10	7795.95801	0.00751
11	2	10	10	←	10	1	9	9	7796.02355	-0.00260
11	2	10	12	←	10	1	9	11	7796.02355	-0.00662
9	3	7	9	←	8	2	6	8	7834.64030	-0.00049
9	3	7	10	←	8	2	6	9	7834.89573	0.01017
9	3	7	8	←	8	2	6	7	7834.89573	-0.01162
10	2	8	10	←	9	2	7	9	7925.67290	-0.00693
10	2	8	11	←	9	2	7	10	7925.82865	0.00681
10	2	8	9	←	9	2	7	8	7925.82865	-0.00139

Table S69 Measured frequencies and residuals (in MHz) for the rotational transitions of the ^{18}O isotopologue of the Pan-H_2O complex.

J'	K_a'	K_c'	F'	←	J''	K_a''	K_c''	F''	ν_{obs}	ν_{obs}-ν_{calc}
3	1	3	3	←	2	1	2	3	2033.80395	0.00196
3	1	3	3	←	2	1	2	2	2034.73280	-0.00611
3	1	3	2	←	2	1	2	1	2034.95610	0.01501
3	1	3	4	←	2	1	2	3	2035.03316	0.00168
3	1	3	2	←	2	1	2	2	2036.41386	0.01480
3	0	3	3	←	2	0	2	2	2158.21675	0.01002
3	0	3	2	←	2	0	2	1	2158.25389	-0.01345
3	0	3	4	←	2	0	2	3	2158.39643	-0.00493
3	2	2	3	←	2	2	1	2	2289.27118	0.01209
3	2	2	4	←	2	2	1	3	2290.11059	-0.00906
3	2	2	2	←	2	2	1	1	2290.58713	-0.01099
3	1	3	4	←	2	0	2	3	2343.71644	-0.00461
3	2	1	3	←	2	2	0	2	2421.00402	0.02656
3	2	1	4	←	2	2	0	3	2421.68447	0.00918
3	1	2	3	←	2	1	1	2	2499.14919	0.00432
3	1	2	4	←	2	1	1	3	2499.41166	-0.00130
3	1	2	2	←	2	1	1	1	2499.51816	-0.00364
4	1	4	4	←	3	1	3	3	2681.85794	-0.00226
4	1	4	3	←	3	1	3	2	2681.94907	-0.00305
4	1	4	5	←	3	1	3	4	2682.02609	0.00188
4	0	4	3	←	3	0	3	2	2772.13285	-0.00577
4	0	4	5	←	3	0	3	4	2772.19957	-0.00341
4	1	4	5	←	3	0	3	4	2867.34070	-0.00321
4	2	3	4	←	3	2	2	3	3024.92424	-0.00722
4	2	3	5	←	3	2	2	4	3025.32551	-0.00195
4	2	3	3	←	3	2	2	2	3025.44425	0.01516
2	2	0	3	←	1	1	1	2	3164.07186	0.00342
2	2	0	2	←	1	1	1	1	3165.11976	-0.00282
4	1	3	4	←	3	1	2	3	3277.88514	0.00796
4	1	3	5	←	3	1	2	4	3278.05217	-0.00496
4	1	3	3	←	3	1	2	2	3278.09040	0.00508
4	2	2	5	←	3	2	1	4	3305.74953	0.00285
4	2	2	3	←	3	2	1	2	3305.83945	0.00422
5	1	5	5	←	4	1	4	4	3313.15423	-0.01142
5	1	5	4	←	4	1	4	3	3313.22291	-0.00520
5	1	5	6	←	4	1	4	5	3313.27084	-0.00861
5	0	5	5	←	4	0	4	4	3364.61487	0.00396
5	1	5	4	←	4	0	4	3	3408.37499	-0.00465
5	2	4	5	←	4	2	3	4	3737.70063	-0.00426
5	2	4	6	←	4	2	3	5	3737.95373	0.00995
5	2	4	4	←	4	2	3	3	3737.95373	-0.01743
5	3	3	5	←	4	3	2	4	3894.09787	-0.01522
5	3	3	4	←	4	3	2	5	3894.50956	0.00742
5	3	3	4	←	4	3	2	3	3894.61634	0.01185
6	0	6	6	←	5	1	5	5	3914.51142	0.00297
6	0	6	7	←	5	1	5	6	3914.57505	-0.01087

6	1	6	6	←	5	1	5	5	3933.13682	0.00270
6	1	6	5	←	5	1	5	4	3933.18457	0.00224
6	0	6	6	←	5	0	5	5	3958.17101	0.00813
6	0	6	5	←	5	0	5	4	3958.21253	-0.01321
6	0	6	7	←	5	0	5	6	3958.26036	-0.00069
6	1	6	6	←	5	0	5	5	3976.79665	0.00811
6	1	6	5	←	5	0	5	4	3976.85633	-0.00533
6	1	6	7	←	5	0	5	6	3976.89323	-0.00226
5	3	2	5	←	4	3	1	4	3991.26582	-0.01459
5	3	2	6	←	4	3	1	5	3991.58502	-0.01018
5	3	2	4	←	4	3	1	3	3991.67857	-0.00486
5	1	4	5	←	4	1	3	4	3998.63348	0.00269
5	1	4	6	←	4	1	3	5	3998.80194	-0.00205
5	1	4	4	←	4	1	3	3	3998.80194	-0.01734
4	2	3	5	←	3	1	2	4	4104.88329	-0.01295
4	2	3	3	←	3	1	2	2	4104.92653	-0.00413
5	2	3	5	←	4	2	2	4	4184.69830	-0.00529
5	2	3	6	←	4	2	2	5	4184.82513	-0.00308
5	2	3	4	←	4	2	2	3	4184.85899	0.00327
3	2	1	3	←	2	1	2	2	4216.68938	-0.00303
6	2	5	6	←	5	2	4	5	4425.18018	-0.00385
6	2	5	7	←	5	2	4	6	4425.35903	0.00328
6	2	5	5	←	5	2	4	4	4425.35903	-0.00349
7	1	7	7	←	6	1	6	6	4546.25908	-0.00104
7	1	7	8	←	6	1	6	7	4546.34011	0.01213
7	0	7	7	←	6	0	6	6	4557.31445	-0.00331
7	0	7	8	←	6	0	6	7	4557.38662	-0.00436
5	2	4	6	←	4	1	3	5	4564.77636	-0.00654
5	2	4	4	←	4	1	3	3	4564.82465	0.00816
7	1	7	7	←	6	0	6	6	4564.89455	0.00877
6	1	5	6	←	5	1	4	5	4649.71161	0.00229
6	1	5	7	←	5	1	4	6	4649.87092	-0.01675
6	1	5	5	←	5	1	4	4	4649.91061	0.01192
6	3	4	6	←	5	3	3	5	4665.92479	-0.00410
6	3	4	7	←	5	3	3	6	4666.17827	0.00952
6	3	4	5	←	5	3	3	4	4666.21799	0.00849
3	3	1	4	←	2	2	0	3	4814.20660	-0.00265
3	3	0	4	←	2	2	1	3	4854.94752	-0.00002
3	3	0	2	←	2	2	1	1	4855.02046	0.00207
3	3	0	3	←	2	2	1	2	4855.25903	0.00873
6	3	3	6	←	5	3	2	5	4887.89990	-0.01533
6	3	3	7	←	5	3	2	6	4888.04663	-0.00501
6	3	3	5	←	5	3	2	4	4888.09497	0.01556
6	2	5	7	←	5	1	4	6	4991.31784	-0.01681
6	2	5	5	←	5	1	4	4	4991.36742	0.00768
6	2	4	6	←	5	2	3	5	5025.64810	0.01283
6	2	4	7	←	5	2	3	6	5025.75558	0.01894
6	2	4	5	←	5	2	3	4	5025.75558	0.00479
7	2	6	7	←	6	2	5	6	5087.98369	0.00185
7	2	6	8	←	6	2	5	7	5088.12033	0.00160
7	2	6	6	←	6	2	5	5	5088.12033	0.00175

8	0	8	8	←	7	1	7	7	5152.83595	0.00629
8	1	8	8	←	7	1	7	7	5155.78553	-0.01473
8	1	8	7	←	7	1	7	6	5155.81814	-0.01308
8	1	8	9	←	7	1	7	8	5155.85039	-0.00439
8	0	8	8	←	7	0	7	7	5160.39673	-0.00095
8	0	8	9	←	7	0	7	8	5160.46584	0.01148
8	1	8	8	←	7	0	7	7	5163.36906	0.00080
8	1	8	9	←	7	0	7	8	5163.42922	0.00299
7	1	6	7	←	6	1	5	6	5246.41355	-0.00675
7	1	6	8	←	6	1	5	7	5246.57556	-0.01153
7	1	6	6	←	6	1	5	5	5246.57556	-0.01774
7	3	5	7	←	6	3	4	6	5417.95898	-0.00420
7	3	5	8	←	6	3	4	7	5418.12033	-0.01281
7	3	5	6	←	6	3	4	5	5418.14521	-0.00672
7	2	6	8	←	6	1	5	7	5429.56445	-0.00127
7	2	6	6	←	6	1	5	5	5429.58803	0.00839
7	5	3	7	←	6	5	2	6	5470.91316	-0.00525
7	5	3	8	←	6	5	2	7	5471.30161	0.00284
7	5	3	6	←	6	5	2	5	5471.36586	-0.00755
7	5	2	7	←	6	5	1	6	5474.53550	0.01061
7	5	2	8	←	6	5	1	7	5474.90272	0.00035
7	5	2	6	←	6	5	1	5	5474.96248	-0.01414
4	2	2	3	←	3	1	3	2	5485.74032	-0.00477
4	2	2	5	←	3	1	3	4	5486.19220	0.00616
7	4	4	7	←	6	4	3	6	5496.10978	0.00716
7	4	4	8	←	6	4	3	7	5496.32757	-0.01673
7	4	4	6	←	6	4	3	5	5496.40088	0.01562
4	3	2	5	←	3	2	1	4	5504.13356	-0.01270
4	3	2	3	←	3	2	1	2	5504.13356	-0.00919
7	4	3	7	←	6	4	2	6	5561.59118	0.00498
7	4	3	8	←	6	4	2	7	5561.78540	-0.00475
8	1	7	8	←	7	2	6	7	5640.53497	0.01427
8	1	7	7	←	7	2	6	6	5640.59317	-0.00800
8	1	7	9	←	7	2	6	8	5640.59317	-0.01437
4	3	1	3	←	3	2	2	2	5706.43711	0.00676
4	3	1	5	←	3	2	2	4	5706.55639	0.00950
4	3	1	4	←	3	2	2	3	5707.01882	0.01949
8	2	7	8	←	7	2	6	7	5729.80426	-0.01900
8	2	7	7	←	7	2	6	6	5729.91877	-0.01633
8	2	7	9	←	7	2	6	8	5729.91877	-0.01920
9	1	9	9	←	8	1	8	8	5763.66650	0.00574
9	1	9	10	←	8	1	8	9	5763.70419	-0.00113
9	0	9	9	←	8	0	8	8	5765.49769	0.00267
9	0	9	8	←	8	0	8	7	5765.53305	0.01189
9	0	9	10	←	8	0	8	9	5765.53305	-0.00734
7	2	5	7	←	6	2	4	6	5808.21673	-0.01555
7	2	5	8	←	6	2	4	7	5808.33499	-0.00667
7	2	5	6	←	6	2	4	5	5808.33499	-0.01787
7	3	4	8	←	6	3	3	7	5810.03098	0.00016
7	3	4	6	←	6	3	3	5	5810.03098	-0.00914
8	1	7	8	←	7	1	6	7	5823.46405	0.01812

8	1	7	9	←	7	1	6	8	5823.59770	0.01152
8	1	7	7	←	7	1	6	6	5823.59770	0.01019
8	2	7	8	←	7	1	6	7	5912.76332	0.01483
8	2	7	9	←	7	1	6	8	5912.92659	0.00999
8	2	7	7	←	7	1	6	6	5912.92659	0.00516
5	3	3	6	←	4	2	2	5	6092.89836	-0.00485
5	3	3	4	←	4	2	2	3	6092.89836	-0.01365
8	3	6	8	←	7	3	5	7	6144.15467	0.00617
8	3	6	9	←	7	3	5	8	6144.29359	0.00978
8	3	6	7	←	7	3	5	6	6144.29359	0.00012
8	5	3	8	←	7	5	2	7	6293.41899	-0.01269
8	4	5	8	←	7	4	4	7	6293.47854	-0.00869
8	4	5	9	←	7	4	4	8	6293.64266	-0.01029
8	5	3	9	←	7	5	2	8	6293.67932	0.00638
8	4	5	7	←	7	4	4	6	6293.67932	0.00540
9	1	8	9	←	8	2	7	8	6315.47904	-0.01834
9	1	8	8	←	8	2	7	7	6315.59019	0.01328
9	1	8	10	←	8	2	7	9	6315.59019	0.00777
9	2	8	9	←	8	2	7	8	6356.28136	0.01352
9	2	8	8	←	8	2	7	7	6356.38043	0.01875
9	2	8	10	←	8	2	7	9	6356.38043	0.01468
10	1	10	10	←	9	1	9	9	6370.79884	-0.00410
10	1	10	11	←	9	1	9	10	6370.84615	0.00625
10	0	10	10	←	9	0	9	9	6371.50896	-0.00425
10	0	10	9	←	9	0	9	8	6371.55606	0.02172
10	0	10	11	←	9	0	9	10	6371.55606	0.00559
9	1	8	9	←	8	1	7	8	6404.81587	0.01594
9	1	8	8	←	8	1	7	7	6404.92364	0.01280
9	1	8	10	←	8	1	7	9	6404.92364	0.01080
8	4	4	9	←	7	4	3	8	6451.73747	-0.00330
8	4	4	7	←	7	4	3	6	6451.73747	-0.01744
8	2	6	8	←	7	2	5	7	6517.18734	0.01166
8	2	6	9	←	7	2	5	8	6517.32073	0.01707
8	2	6	7	←	7	2	5	6	6517.32073	0.00637
6	3	4	7	←	5	2	3	6	6574.24960	0.00584
6	3	4	5	←	5	2	3	4	6574.24960	-0.01620
4	4	1	5	←	3	3	0	4	6611.37714	-0.00728
4	4	1	3	←	3	3	0	2	6611.44683	-0.00815
4	4	1	4	←	3	3	0	3	6611.52904	-0.00088
4	4	0	5	←	3	3	1	4	6617.22133	0.00268
4	4	0	3	←	3	3	1	2	6617.28809	0.00370
4	4	0	4	←	3	3	1	3	6617.39116	0.01290
5	3	2	4	←	4	2	3	3	6672.68068	-0.00400
5	3	2	6	←	4	2	3	5	6672.81180	-0.00282
5	3	2	5	←	4	2	3	4	6673.34834	0.00005
8	3	5	9	←	7	3	4	8	6715.06445	-0.01409
8	3	5	7	←	7	3	4	6	6715.06445	-0.01925
9	3	7	9	←	8	3	6	8	6841.80826	0.02365
9	3	7	10	←	8	3	6	9	6841.92245	0.02124
9	3	7	8	←	8	3	6	7	6841.92245	0.01583
10	1	9	10	←	9	2	8	9	6955.15302	0.00685

10	1	9	9	←	9	2	8	8	6955.23766	0.01814
10	1	9	11	←	9	2	8	10	6955.23766	0.01296
7	3	5	8	←	6	2	4	7	6966.63511	-0.00515
7	3	5	6	←	6	2	4	5	6966.68675	0.01982
10	2	9	10	←	9	2	8	9	6972.86859	-0.01443
10	2	9	9	←	9	2	8	8	6972.95201	-0.01045
10	2	9	11	←	9	2	8	10	6972.95201	-0.01507
11	1	11	11	←	10	1	10	10	6977.68215	0.01994
11	1	11	10	←	10	1	10	9	6977.68215	0.00256
11	1	11	12	←	10	1	10	11	6977.68215	-0.01116
11	0	11	11	←	10	0	10	10	6977.95315	0.02208
11	0	11	10	←	10	0	10	9	6977.95315	0.00459
11	0	11	12	←	10	0	10	11	6977.95315	-0.00912
10	1	9	10	←	9	1	8	9	6995.90906	-0.00757
10	1	9	9	←	9	1	8	8	6995.98935	-0.01495
10	1	9	11	←	9	1	8	10	6995.98935	-0.01869
10	2	9	10	←	9	1	8	9	7013.66502	0.01153
10	2	9	9	←	9	1	8	8	7013.76686	0.01963
10	2	9	11	←	9	1	8	10	7013.76686	0.01644
9	4	6	9	←	8	4	5	8	7077.23444	0.02250
9	4	6	10	←	8	4	5	9	7077.32155	-0.01570
9	5	5	9	←	8	5	4	8	7094.19350	0.00759
9	5	5	10	←	8	5	4	9	7094.36243	0.00506
9	5	5	8	←	8	5	4	7	7094.36243	-0.01655
9	5	4	9	←	8	5	3	8	7135.82095	0.00373
9	5	4	10	←	8	5	3	9	7135.98748	0.01787
9	5	4	8	←	8	5	3	7	7135.98748	-0.00177
9	2	7	9	←	8	2	6	8	7149.21758	0.01673
9	2	7	10	←	8	2	6	9	7149.35066	0.00852
9	2	7	8	←	8	2	6	7	7149.35066	-0.00128
5	4	2	4	←	4	3	1	3	7365.04272	-0.00643
5	4	2	6	←	4	3	1	5	7365.04272	-0.01954
5	4	2	5	←	4	3	1	4	7365.24220	-0.00242
9	4	5	10	←	8	4	4	9	7386.18254	0.02054
9	4	5	8	←	8	4	4	7	7386.18254	0.01622
5	4	1	6	←	4	3	2	5	7405.92613	0.00348
5	4	1	5	←	4	3	2	4	7406.16944	0.00459
5	3	2	4	←	4	1	3	3	7499.52481	-0.00521
5	3	2	6	←	4	1	3	5	7499.65598	0.00224
10	3	8	10	←	9	3	7	9	7511.87787	0.00453
10	3	8	11	←	9	3	7	10	7511.98234	0.00432
10	3	8	9	←	9	3	7	8	7511.98234	0.00119
9	3	6	9	←	8	3	5	8	7567.75548	-0.01644
9	3	6	10	←	8	3	5	9	7567.81993	-0.01344
9	3	6	8	←	8	3	5	7	7567.81993	-0.01867
11	1	10	10	←	10	2	9	9	7576.59241	-0.01272
11	1	10	12	←	10	2	9	11	7576.59241	-0.01776
11	2	10	11	←	10	2	9	10	7583.96611	-0.01633
11	2	10	10	←	10	2	9	9	7584.07187	0.02189
11	2	10	12	←	10	2	9	11	7584.07187	0.01706
12	1	12	12	←	11	1	11	11	7584.43703	0.01678

12	1	12	11	←	11	1	11	10	7584.43703	0.00207
12	1	12	13	←	11	1	11	12	7584.43703	-0.00972
12	0	12	12	←	11	0	11	11	7584.53541	0.01520
12	0	12	11	←	11	0	11	10	7584.53541	0.00045
12	0	12	13	←	11	0	11	12	7584.53541	-0.01134
11	1	10	11	←	10	1	9	10	7594.26273	-0.01416
11	1	10	10	←	10	1	9	9	7594.33759	-0.01046
11	1	10	12	←	10	1	9	11	7594.33759	-0.01495
11	2	10	11	←	10	1	9	10	7601.70342	-0.01587
11	2	10	10	←	10	1	9	9	7601.78527	-0.00764
11	2	10	12	←	10	1	9	11	7601.78527	-0.01192
9	3	7	9	←	8	2	6	8	7626.94227	-0.00645
9	3	7	10	←	8	2	6	9	7627.18522	0.00527
9	3	7	8	←	8	2	6	7	7627.18522	-0.01458
10	2	8	10	←	9	2	7	9	7726.99443	-0.01086
10	2	8	11	←	9	2	7	10	7727.12687	-0.01634
10	4	7	10	←	9	4	6	9	7838.78304	0.00310
10	4	7	11	←	9	4	6	10	7838.89440	0.01014
10	4	7	9	←	9	4	6	8	7838.89440	0.00288
10	6	5	10	←	9	6	4	9	7866.06426	0.00176
10	6	5	11	←	9	6	4	10	7866.25545	0.01178
10	6	5	9	←	9	6	4	8	7866.25545	-0.00990
10	6	4	10	←	9	6	3	9	7874.58263	0.00115
10	6	4	11	←	9	6	3	10	7874.76714	0.00852
10	6	4	9	←	9	6	3	8	7874.76714	-0.01278
10	5	6	10	←	9	5	5	9	7909.39643	0.01686
10	5	6	11	←	9	5	5	10	7909.49139	-0.01244

Table S70 Measured frequencies and residuals (in MHz) for the rotational transitions of the Pan-$(H_2O)_2$ complex.

J'	K_a'	K_c'	F'	←	J''	K_a''	K_c''	F''	ν_{obs}	ν_{obs}-ν_{calc}
3	2	2	3	←	2	2	1	2	2145.47260	0.00739
3	2	2	4	←	2	2	1	3	2146.35180	-0.00070
3	2	2	2	←	2	2	1	1	2146.84610	0.00027
4	1	4	4	←	3	1	3	3	2216.53870	-0.00484
4	1	4	3	←	3	1	3	2	2216.64030	0.00199
4	1	4	5	←	3	1	3	4	2216.70480	0.00095
4	0	4	4	←	3	0	3	3	2217.13880	-0.00127
4	0	4	3	←	3	0	3	2	2217.22030	-0.00806
4	0	4	5	←	3	0	3	4	2217.29340	-0.00216
2	2	0	3	←	1	0	1	2	2249.24400	-0.00430
2	2	0	2	←	1	0	1	1	2251.02940	0.00906
3	1	2	3	←	2	1	1	2	2256.30807	0.00587
3	1	2	4	←	2	1	1	3	2256.46799	-0.00086
3	1	2	2	←	2	1	1	1	2256.52147	-0.00109
3	2	1	3	←	2	2	0	2	2564.34880	-0.00068
3	2	1	4	←	2	2	0	3	2565.06215	0.00203
3	2	1	2	←	2	2	0	1	2565.48935	-0.01363
7	2	5	6	←	7	2	6	6	2690.07405	0.00470
7	2	5	8	←	7	2	6	8	2690.15053	0.00419

7	3	5	6	←	7	1	6	6	2690.28862	-0.00065
7	3	5	8	←	7	1	6	8	2690.37524	0.00887
7	2	5	7	←	7	2	6	7	2690.68687	0.00662
4	2	3	4	←	3	2	2	3	2694.54072	0.00273
4	2	3	5	←	3	2	2	4	2694.91200	-0.00177
4	2	3	3	←	3	2	2	2	2695.01480	0.00462
5	1	5	5	←	4	1	4	4	2709.66346	0.00255
5	0	5	4	←	4	0	4	3	2709.77146	0.00281
5	1	5	6	←	4	1	4	5	2709.77146	0.00052
5	0	5	6	←	4	0	4	5	2709.81223	-0.00407
4	1	3	4	←	3	1	2	3	2724.21450	-0.00060
4	1	3	3	←	3	1	2	2	2724.43028	-0.03384
4	1	3	5	←	3	1	2	4	2724.43028	0.00333
4	3	2	4	←	3	3	1	3	3060.79240	0.00204
4	3	2	5	←	3	3	1	4	3061.56780	-0.00300
4	3	2	3	←	3	3	1	2	3061.87740	-0.00277
8	2	6	7	←	8	2	7	7	3181.85275	-0.00140
8	2	6	9	←	8	2	7	9	3181.90181	-0.01489
7	1	6	6	←	7	1	7	6	3186.50964	0.00638
7	2	6	6	←	7	0	7	6	3186.50964	0.00358
7	1	6	8	←	7	1	7	8	3186.59436	-0.00120
7	2	6	8	←	7	0	7	8	3186.59436	-0.00400
7	1	6	7	←	7	1	7	7	3187.24623	0.01009
7	2	6	7	←	7	0	7	7	3187.24623	0.00729
5	2	4	5	←	4	2	3	4	3199.22730	-0.00103
5	2	4	6	←	4	2	3	5	3199.46110	-0.00123
5	2	4	4	←	4	2	3	3	3199.49514	0.00533
6	0	6	6	←	5	0	5	5	3202.55010	0.00643
6	1	6	6	←	5	1	5	5	3202.55010	0.00957
6	0	6	5	←	5	0	5	4	3202.61909	0.03050
6	0	6	7	←	5	0	5	6	3202.61909	-0.00538
6	1	6	5	←	5	1	5	4	3202.61909	0.03362
6	1	6	7	←	5	1	5	6	3202.61909	-0.00225
5	1	4	5	←	4	1	3	4	3203.24620	0.00160
5	1	4	6	←	4	1	3	5	3203.45110	-0.00787
4	2	2	4	←	3	2	1	3	3252.74710	-0.00272
4	2	2	5	←	3	2	1	4	3252.90120	-0.00390
4	2	2	3	←	3	2	1	2	3252.96860	0.00223
3	3	0	2	←	2	1	1	1	3310.02294	-0.00059
3	3	0	2	←	2	1	1	2	3310.06080	0.00684
3	3	0	4	←	2	1	1	3	3310.41690	0.00180
3	3	0	3	←	2	1	1	2	3311.52399	0.00397
4	3	1	4	←	3	3	0	3	3443.21644	-0.00076
4	3	1	5	←	3	3	0	4	3443.92796	0.00183
4	3	1	3	←	3	3	0	2	3444.20520	-0.00421
3	2	1	4	←	2	0	2	3	3564.87980	-0.00480
3	2	1	3	←	2	0	2	2	3566.05610	-0.00539
5	3	3	5	←	4	3	2	4	3657.04440	0.00123
5	3	3	6	←	4	3	2	5	3657.40790	-0.00177
5	3	3	4	←	4	3	2	3	3657.50340	-0.00154
9	2	7	8	←	9	2	8	8	3673.24105	0.00985

9	3	7	8	←	9	1	8	8	3673.24105	0.00826
9	2	7	10	←	9	2	8	10	3673.27877	-0.00410
9	3	7	10	←	9	1	8	10	3673.27877	-0.00569
9	2	7	9	←	9	2	8	9	3673.75449	0.00914
9	3	7	9	←	9	1	8	9	3673.75449	0.00755
6	2	5	6	←	5	2	4	5	3693.47227	0.00022
6	2	5	5	←	5	2	4	4	3693.65007	-0.00426
6	2	5	7	←	5	2	4	6	3693.65007	0.00382
6	1	5	6	←	5	1	4	5	3693.87324	0.00102
6	1	5	7	←	5	1	4	6	3694.04838	0.00369
6	1	5	5	←	5	1	4	4	3694.04838	-0.00403
7	0	7	7	←	6	0	6	6	3695.41289	0.00964
7	1	7	7	←	6	1	6	6	3695.41289	0.00984
7	0	7	8	←	6	0	6	7	3695.46441	-0.00071
7	1	7	8	←	6	1	6	7	3695.46441	-0.00051
5	2	3	5	←	4	2	2	4	3736.30990	-0.00078
5	2	3	6	←	4	2	2	5	3736.42090	-0.00263
5	2	3	4	←	4	2	2	3	3736.45707	0.00645
3	3	1	2	←	2	1	2	1	3844.67919	0.00215
3	3	1	4	←	2	1	2	3	3845.57287	0.00405
3	3	1	3	←	2	1	2	2	3847.60359	-0.00168
5	4	2	5	←	4	4	1	4	3953.89770	0.00006
5	4	2	6	←	4	4	1	5	3954.60920	0.00430
5	4	2	4	←	4	4	1	3	3954.82570	0.00618
6	3	4	6	←	5	3	3	5	4180.04440	0.01050
6	3	4	5	←	5	3	3	4	4180.26729	-0.03494
6	3	4	7	←	5	3	3	6	4180.26729	0.00438
7	1	6	7	←	6	1	5	6	4186.38622	-0.00566
7	1	6	6	←	6	1	5	5	4186.50324	-0.02564
7	1	6	8	←	6	1	5	7	4186.50324	-0.02527
7	2	6	6	←	6	2	5	5	4186.50324	0.00812
7	2	6	8	←	6	2	5	7	4186.50324	0.00851
8	0	8	8	←	7	0	7	7	4188.26614	0.00211
8	1	8	8	←	7	1	7	7	4188.26614	0.00213
8	0	8	9	←	7	0	7	8	4188.31991	0.00699
8	1	8	9	←	7	1	7	8	4188.31991	0.00700
6	2	4	6	←	5	2	3	5	4195.24850	0.00822
6	2	4	7	←	5	2	3	6	4195.42830	0.00832
6	2	4	5	←	5	2	3	4	4195.45174	0.00270
5	3	2	5	←	4	3	1	4	4224.98180	0.00175
5	3	2	6	←	4	3	1	5	4225.17060	0.00066
5	3	2	4	←	4	3	1	3	4225.22870	0.00006
5	4	1	5	←	4	4	0	4	4284.04289	0.00774
5	4	1	6	←	4	4	0	5	4284.77668	0.00838
5	4	1	4	←	4	4	0	3	4284.98689	0.00333
4	4	0	3	←	3	2	1	2	4426.04160	-0.00197
4	4	0	5	←	3	2	1	4	4426.28100	0.00194
4	4	0	4	←	3	2	1	3	4427.27740	0.00029
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4	3	1	5	←	3	1	2	4	4497.87580	0.00343
4	3	1	4	←	3	1	2	3	4498.43530	0.00028

6	4	3	6	←	5	4	2	5	4604.35770	0.00365
6	4	3	7	←	5	4	2	6	4604.71560	0.00692
6	4	3	5	←	5	4	2	4	4604.79000	0.00022
7	3	5	7	←	6	3	4	6	4677.68790	-0.00384
7	3	5	8	←	6	3	4	7	4677.85540	-0.01431
7	3	5	6	←	6	3	4	5	4677.90516	0.01495
8	1	7	8	←	7	1	6	7	4679.16431	0.00184
8	2	7	8	←	7	2	6	7	4679.16431	0.00444
8	1	7	7	←	7	1	6	6	4679.27353	0.00395
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8	2	7	7	←	7	2	6	6	4679.27353	0.00653
7	2	5	7	←	6	2	4	6	4679.61200	-0.01385
7	2	5	8	←	6	2	4	7	4679.79189	-0.00598
7	2	5	6	←	6	2	4	5	4679.83131	0.01396
7	2	5	6	←	6	2	4	6	4680.06665	-0.00200
9	0	9	9	←	8	0	8	8	4681.11565	-0.00838
9	1	9	9	←	8	1	8	8	4681.11565	-0.00838
9	0	9	8	←	8	0	8	7	4681.17334	0.02810
9	0	9	10	←	8	0	8	9	4681.17334	0.00971
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6	3	3	5	←	5	3	2	4	4760.66079	-0.02121
6	3	3	7	←	5	3	2	6	4760.66079	-0.00718
6	5	2	6	←	5	5	1	5	4826.01130	0.00337
6	5	2	7	←	5	5	1	6	4826.66010	-0.00419
6	5	2	5	←	5	5	1	4	4826.81610	-0.00859
4	4	1	3	←	3	2	2	2	4939.78190	0.00310
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4	2	2	5	←	3	0	3	4	5090.30568	0.00091
4	2	2	4	←	3	0	3	3	5091.54066	0.00475
7	4	4	7	←	6	4	3	6	5156.52727	0.01121
7	4	4	6	←	6	4	3	5	5156.74651	-0.02003
7	4	4	8	←	6	4	3	7	5156.74651	0.01699
6	4	2	6	←	5	4	1	5	5164.18200	0.00067
6	4	2	7	←	5	4	1	6	5164.42540	-0.00186
6	4	2	5	←	5	4	1	4	5164.48817	0.00210
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8	3	6	7	←	7	3	5	6	5170.85295	-0.00104
8	3	6	9	←	7	3	5	8	5170.85295	0.01048
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8	2	6	7	←	7	2	5	6	5171.05120	-0.00060
9	1	8	9	←	8	1	7	8	5171.98704	0.00664
9	2	8	9	←	8	2	7	8	5171.98704	0.00683
9	1	8	8	←	8	1	7	7	5172.07391	0.00756
9	1	8	10	←	8	1	7	9	5172.07391	0.00304

9	2	8	10	←	8	2	7	9	5172.07391	0.00323
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7	3	4	7	←	6	3	3	6	5198.58588	-0.00084
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7	3	4	6	←	6	3	3	5	5198.73514	0.00926
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7	5	3	7	←	6	5	2	6	5533.30770	-0.00563
7	5	3	8	←	6	5	2	7	5533.65750	-0.00666
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8	4	5	9	←	7	4	4	8	5662.25090	-0.01280
8	4	5	7	←	7	4	4	6	5662.29234	0.00718
9	3	7	9	←	8	3	6	8	5663.28953	-0.00473
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9	3	7	8	←	8	3	6	7	5663.41764	-0.00781
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7	6	2	8	←	6	6	1	7	5679.95560	-0.00397
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5	3	2	5	←	4	1	3	4	5999.18840	-0.01157
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8	4	4	8	←	7	4	3	7	6218.57927	0.00396
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8	4	4	7	←	7	4	3	6	6218.63368	-0.00671
8	6	3	8	←	7	6	2	7	6441.91430	-0.00882
8	6	3	9	←	7	6	2	8	6442.27500	-0.00083
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8	7	1	8	←	7	7	0	7	6644.07325	0.00111
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9	5	5	9	←	8	5	4	8	6645.78808	0.00154
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9	4	5	9	←	8	4	4	8	6664.91426	0.00058
9	4	5	10	←	8	4	4	9	6665.01091	-0.01817
9	4	5	8	←	8	4	4	7	6665.06464	0.02030
8	5	3	8	←	7	5	2	7	6789.26613	-0.00197
8	5	3	7	←	7	5	2	6	6789.32475	-0.01262
8	5	3	9	←	7	5	2	8	6789.32475	0.00013
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8	6	2	9	←	7	6	1	8	6921.46082	0.00686
8	6	2	7	←	7	6	1	6	6921.51551	0.00056
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9	6	4	8	←	8	6	3	7	7082.41227	0.01362
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6	6	1	7	←	5	4	2	6	7221.18329	0.00433
6	6	1	6	←	5	4	2	5	7222.06259	-0.00180
9	5	4	10	←	8	5	3	9	7255.59921	-0.00110
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9	7	3	9	←	8	7	2	8	7329.53218	-0.00277
9	7	3	10	←	8	7	2	9	7329.89255	0.00104
9	7	3	8	←	8	7	2	7	7329.94241	-0.00280
9	8	2	9	←	8	8	1	8	7342.64068	0.00349
9	8	2	10	←	8	8	1	9	7343.18149	-0.00233
9	8	2	8	←	8	8	1	7	7343.27237	0.00461
7	6	1	6	←	6	4	2	5	7539.88662	0.00328
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7	6	1	7	←	6	4	2	6	7540.44964	0.00126
6	4	3	5	←	5	2	4	4	7604.88407	-0.00403
6	4	3	7	←	5	2	4	6	7605.05649	0.00101
6	4	3	6	←	5	2	4	5	7605.91151	-0.00886
10	6	5	10	←	9	6	4	9	7626.87012	0.00350
10	6	5	11	←	9	6	4	10	7627.00681	0.00312
10	6	5	9	←	9	6	4	8	7627.00681	-0.01430
12	3	9	12	←	11	3	8	11	7632.93397	0.00343
12	4	9	12	←	11	4	8	11	7632.93397	0.00412
12	3	9	11	←	11	3	8	10	7633.03085	-0.00081
12	3	9	13	←	11	3	8	12	7633.03085	0.00345
12	4	9	13	←	11	4	8	12	7633.03085	0.00414
12	4	9	11	←	11	4	8	10	7633.03085	-0.00012

11	5	7	11	←	10	5	6	10	7633.81601	0.00513
11	5	7	10	←	10	5	6	9	7633.93448	-0.00381
11	5	7	12	←	10	5	6	11	7633.93448	0.00623
11	4	7	11	←	10	4	6	10	7634.15214	0.00350
13	2	11	13	←	12	2	10	12	7634.27597	0.00123
13	3	11	13	←	12	3	10	12	7634.27597	0.00124
11	4	7	12	←	10	4	6	11	7634.27597	0.01056
11	4	7	10	←	10	4	6	9	7634.27597	0.00058
13	2	11	14	←	12	2	10	13	7634.34534	0.00104
13	2	11	12	←	12	2	10	11	7634.34534	0.00174
13	3	11	12	←	12	3	10	11	7634.34534	0.00174
13	3	11	14	←	12	3	10	13	7634.34534	0.00104
14	1	13	13	←	13	1	12	12	7636.23495	0.00268
14	1	13	15	←	13	1	12	14	7636.23495	-0.00190
14	2	13	15	←	13	2	12	14	7636.23495	-0.00190
14	2	13	13	←	13	2	12	12	7636.23495	0.00268
15	0	15	16	←	14	0	14	15	7638.26794	-0.00767
15	0	15	15	←	14	0	14	14	7638.26794	0.00781
15	0	15	14	←	14	0	14	13	7638.26794	-0.00020
15	1	15	15	←	14	1	14	14	7638.26794	0.00781
15	1	15	14	←	14	1	14	13	7638.26794	-0.00020
15	1	15	16	←	14	1	14	15	7638.26794	-0.00767
10	5	5	10	←	9	5	4	9	7672.58094	0.00084
10	5	5	9	←	9	5	4	8	7672.65923	-0.00606
10	5	5	11	←	9	5	4	10	7672.65923	0.00426
9	7	2	9	←	8	7	1	8	7734.53116	0.00176
9	7	2	10	←	8	7	1	9	7734.95829	0.00293
9	7	2	8	←	8	7	1	7	7735.00897	-0.00648
7	5	2	6	←	6	3	3	5	7770.89935	-0.00613
7	5	2	8	←	6	3	3	7	7770.93342	0.00726
7	5	2	7	←	6	3	3	6	7771.09705	0.00343

Table S71 Measured frequencies and residuals (in MHz) for the rotational transitions of the ^{18}O(1) singly-substituted isotopologues of the Pan-$(H_2O)_2$ complex.

J'	K_a'	K_c'	F'	←	J''	K_a''	K_c''	F''	ν_{obs}	ν_{obs}-ν_{calc}
4	1	4	4	←	3	1	3	3	2179.33423	-0.00825
4	1	4	3	←	3	1	3	2	2179.43669	0.00028
4	1	4	5	←	3	1	3	4	2179.49556	-0.00689
4	0	4	4	←	3	0	3	3	2180.56447	-0.00012
4	0	4	3	←	3	0	3	2	2180.65680	0.00847
4	0	4	5	←	3	0	3	4	2180.71963	0.00261
4	2	3	4	←	3	2	2	3	2642.18898	-0.01322
4	2	3	5	←	3	2	2	4	2642.59189	0.00297
4	2	3	3	←	3	2	2	2	2642.70211	0.01398
5	1	5	5	←	4	1	4	4	2664.48464	0.00055
5	1	5	4	←	4	1	4	3	2664.54449	-0.00083
5	1	5	6	←	4	1	4	5	2664.60395	0.01069
5	0	5	5	←	4	0	4	4	2664.60395	-0.00116

5	0	5	4	←	4	0	4	3	2664.66665	0.00108
5	0	5	6	←	4	0	4	5	2664.71251	-0.00119
4	1	3	5	←	3	1	2	4	2687.71025	-0.00289
5	2	4	5	←	4	2	3	4	3144.45006	0.00177
5	2	4	6	←	4	2	3	5	3144.68219	-0.00117
5	2	4	4	←	4	2	3	3	3144.71468	0.00421
6	1	6	6	←	5	1	5	5	3149.18678	0.01978
6	1	6	5	←	5	1	5	4	3149.18678	-0.02425
6	0	6	6	←	5	0	5	5	3149.18678	0.00901
6	1	6	7	←	5	1	5	6	3149.25187	0.00475
6	0	6	7	←	5	0	5	6	3149.25187	-0.00598
5	1	4	5	←	4	1	3	4	3152.55256	0.00771
5	1	4	6	←	4	1	3	5	3152.74745	-0.00238
5	1	4	4	←	4	1	3	3	3152.77865	0.00964
4	2	2	4	←	3	2	1	3	3188.68653	0.00267
4	2	2	5	←	3	2	1	4	3188.87921	-0.00496
4	2	2	3	←	3	2	1	2	3188.94712	-0.00951
5	3	3	5	←	4	3	2	4	3577.35201	-0.01754
5	3	3	6	←	4	3	2	5	3577.76255	0.00964
5	3	3	4	←	4	3	2	3	3577.86304	0.01119
6	2	5	6	←	5	2	4	5	3631.88911	0.00106
6	2	5	7	←	5	2	4	6	3632.06196	0.00134
6	2	5	5	←	5	2	4	4	3632.06196	-0.00604
6	1	5	6	←	5	1	4	5	3632.93945	0.00152
6	1	5	7	←	5	1	4	6	3633.10796	0.00086
6	1	5	5	←	5	1	4	4	3633.10796	-0.00581
7	1	7	7	←	6	1	6	6	3633.81735	0.00819
7	1	7	6	←	6	1	6	5	3633.81735	-0.02505
7	0	7	7	←	6	0	6	6	3633.81735	0.00729
7	0	7	6	←	6	0	6	5	3633.81735	-0.02594
7	1	7	8	←	6	1	6	7	3633.87216	0.00163
7	0	7	8	←	6	0	6	7	3633.87216	0.00074
5	4	2	6	←	4	4	1	5	3829.00704	-0.00578
5	4	1	6	←	4	4	0	5	4103.47004	0.00654
5	4	1	4	←	4	4	0	3	4103.68566	-0.00022
6	3	4	6	←	5	3	3	5	4105.32793	-0.00692
6	3	4	7	←	5	3	3	6	4105.56337	-0.00576
6	3	4	5	←	5	3	3	4	4105.60875	-0.00016
7	2	6	7	←	6	2	5	6	4116.71784	-0.00056
7	1	6	7	←	6	1	5	6	4116.81892	-0.01475
7	2	6	8	←	6	2	5	7	4116.85667	0.00307
7	2	6	6	←	6	2	5	5	4116.85667	0.00318
7	1	6	6	←	6	1	5	5	4116.96548	-0.00290
7	1	6	8	←	6	1	5	7	4116.96548	-0.00305
8	1	8	8	←	7	1	7	7	4118.44595	-0.00359
8	0	8	8	←	7	0	7	7	4118.44595	-0.00366
8	1	8	9	←	7	1	7	8	4118.49928	0.00123
8	0	8	9	←	7	0	7	8	4118.49928	0.00116
5	3	2	5	←	4	3	1	4	4120.41936	-0.02112
5	3	2	6	←	4	3	1	5	4120.68102	-0.00096
5	3	2	4	←	4	3	1	3	4120.74943	-0.00235

6	2	4	6	←	5	2	3	5	4135.14366	0.01455
6	2	4	7	←	5	2	3	6	4135.28323	-0.00759
6	2	4	5	←	5	2	3	4	4135.32327	0.00788
4	3	1	3	←	3	1	2	2	4397.96299	-0.00097
4	3	1	5	←	3	1	2	4	4398.14489	0.00167
4	3	1	4	←	3	1	2	3	4398.73933	-0.01861
6	4	3	7	←	5	4	2	6	4491.32970	0.00839
6	4	3	5	←	5	4	2	4	4491.42123	0.01484
7	3	5	7	←	6	3	4	6	4599.44947	0.00720
7	3	5	8	←	6	3	4	7	4599.62175	0.00267
7	3	5	6	←	6	3	4	5	4599.62175	-0.01723
8	2	7	8	←	7	2	6	7	4601.28935	0.00922
8	1	7	8	←	7	1	6	7	4601.28935	-0.00219
8	2	7	7	←	7	2	6	6	4601.39402	0.00831
8	2	7	9	←	7	2	6	8	4601.39402	0.00497
8	1	7	7	←	7	1	6	6	4601.39402	-0.00307
8	1	7	9	←	7	1	6	8	4601.39402	-0.00641
9	1	9	9	←	8	1	8	8	4603.08346	-0.00671
9	0	9	9	←	8	0	8	8	4603.08346	-0.00672
9	1	9	10	←	8	1	8	9	4603.14099	0.01152
9	0	9	10	←	8	0	8	9	4603.14099	0.01151
7	2	5	7	←	6	2	4	6	4604.44182	0.00667
7	2	5	8	←	6	2	4	7	4604.60055	0.00013
7	2	5	6	←	6	2	4	5	4604.60055	-0.01779
6	3	3	7	←	5	3	2	6	4702.04842	-0.00258
6	3	3	5	←	5	3	2	4	4702.04842	-0.01852
6	4	2	7	←	5	4	1	6	5007.27550	-0.01096
6	4	2	5	←	5	4	1	4	5007.35995	0.00416
7	4	4	7	←	6	4	3	6	5057.55544	-0.00399
7	4	4	8	←	6	4	3	7	5057.78708	0.00291
7	4	4	6	←	6	4	3	5	5057.82784	0.00525
8	3	6	8	←	7	3	5	7	5085.00661	-0.00109
8	3	6	9	←	7	3	5	8	5085.15838	0.00496
8	3	6	7	←	7	3	5	6	5085.15838	-0.00598
8	2	6	8	←	7	2	5	7	5085.67149	-0.00325
8	2	6	9	←	7	2	5	8	5085.81776	-0.00126
8	2	6	7	←	7	2	5	6	5085.81776	-0.01199
9	2	8	9	←	8	2	7	8	5085.87047	0.01630
9	1	8	9	←	8	1	7	8	5085.87047	0.01525
9	2	8	8	←	8	2	7	7	5085.94668	0.00773
9	2	8	10	←	8	2	7	9	5085.94668	0.00300
9	1	8	8	←	8	1	7	7	5085.94668	0.00668
9	1	8	10	←	8	1	7	9	5085.94668	0.00195
10	1	10	10	←	9	1	9	9	5087.72796	-0.00263
10	1	10	9	←	9	1	9	8	5087.72796	-0.01973
10	0	10	10	←	9	0	9	9	5087.72796	-0.00263
10	0	10	9	←	9	0	9	8	5087.72796	-0.01973
10	1	10	11	←	9	1	9	10	5087.77886	0.01579
10	0	10	11	←	9	0	9	10	5087.77886	0.01578
7	3	4	7	←	6	3	3	6	5136.14574	0.02222
7	3	4	8	←	6	3	3	7	5136.22503	0.00665

7	3	4	6	←	6	3	3	5	5136.22503	-0.00901
5	4	1	4	←	4	2	2	3	5367.32558	-0.01309
5	4	1	6	←	4	2	2	5	5367.43067	-0.00896
5	4	1	5	←	4	2	2	4	5367.95951	0.01737
7	5	3	8	←	6	5	2	7	5380.09854	0.02110
7	5	3	6	←	6	5	2	5	5380.17158	0.02099
7	6	2	8	←	6	6	1	7	5469.76329	-0.00418
7	6	2	6	←	6	6	1	5	5469.87215	-0.02224
8	4	5	8	←	7	4	4	7	5566.09611	0.00130
8	4	5	9	←	7	4	4	8	5566.24829	-0.01203
8	4	5	7	←	7	4	4	6	5566.29319	0.01168
9	3	7	9	←	8	3	6	8	5569.35273	0.00204
9	2	7	9	←	8	2	6	8	5569.44168	0.01335
9	3	7	10	←	8	3	6	9	5569.49295	0.01923
9	3	7	8	←	8	3	6	7	5569.49295	0.01328
9	2	7	10	←	8	2	6	9	5569.54356	-0.00764
9	2	7	8	←	8	2	6	7	5569.54356	-0.01358
10	2	9	10	←	9	2	8	9	5570.45561	0.00423
10	1	9	10	←	9	1	8	9	5570.45561	0.00414
10	2	9	9	←	9	2	8	8	5570.52135	0.00041
10	2	9	11	←	9	2	8	10	5570.52135	-0.00483
10	1	9	9	←	9	1	8	8	5570.52135	0.00032
10	1	9	11	←	9	1	8	10	5570.52135	-0.00492
11	1	11	11	←	10	1	10	10	5572.37025	-0.00021
11	1	11	10	←	10	1	10	9	5572.37025	-0.01449
11	0	11	11	←	10	0	10	10	5572.37025	-0.00021
11	0	11	10	←	10	0	10	9	5572.37025	-0.01449
11	1	11	12	←	10	1	10	11	5572.40853	0.01076
11	0	11	12	←	10	0	10	11	5572.40853	0.01076
8	3	5	8	←	7	3	4	7	5583.15806	-0.00533
8	3	5	9	←	7	3	4	8	5583.31378	0.01399
8	3	5	7	←	7	3	4	6	5583.31378	-0.00291
7	6	1	7	←	6	6	0	6	5593.15091	0.02250
7	6	1	8	←	6	6	0	7	5593.80612	-0.00503
7	6	1	6	←	6	6	0	5	5593.93915	-0.00775
7	4	3	7	←	6	4	2	6	5693.46532	-0.00781
7	4	3	8	←	6	4	2	7	5693.54414	-0.00657
7	4	3	6	←	6	4	2	5	5693.54414	-0.02335
7	5	2	8	←	6	5	1	7	5842.13237	0.01450
7	5	2	6	←	6	5	1	5	5842.19856	0.01098
8	5	4	8	←	7	5	3	7	5995.62147	-0.02118
8	5	4	9	←	7	5	3	8	5995.85841	-0.00558
8	5	4	7	←	7	5	3	6	5995.89788	-0.00143
10	3	8	10	←	9	3	7	9	6053.69809	0.00229
10	2	8	10	←	9	2	7	9	6053.69809	-0.00593
10	3	8	11	←	9	3	7	10	6053.80351	0.00272
10	3	8	9	←	9	3	7	8	6053.80351	-0.00023
10	2	8	11	←	9	2	7	10	6053.80351	-0.00549
10	2	8	9	←	9	2	7	8	6053.80351	-0.00843
9	4	6	9	←	8	4	5	8	6054.30691	0.00280
9	4	6	10	←	8	4	5	9	6054.44263	-0.00097

9	4	6	8	←	8	4	5	7	6054.44263	-0.01449
11	2	10	11	←	10	2	9	10	6055.05472	-0.00795
11	1	10	11	←	10	1	9	10	6055.05472	-0.00796
11	2	10	10	←	10	2	9	9	6055.11225	-0.00849
11	2	10	12	←	10	2	9	11	6055.11225	-0.01381
11	1	10	10	←	10	1	9	9	6055.11225	-0.00850
11	1	10	12	←	10	1	9	11	6055.11225	-0.01381
12	1	12	12	←	11	1	11	11	6056.99306	-0.01653
12	0	12	12	←	11	0	11	11	6056.99306	-0.01653
12	1	12	11	←	11	1	11	10	6057.02818	0.00649
12	1	12	13	←	11	1	11	12	6057.02818	-0.00468
12	0	12	11	←	11	0	11	10	6057.02818	0.00649
12	0	12	13	←	11	0	11	12	6057.02818	-0.00468
9	3	6	10	←	8	3	5	9	6057.19478	-0.00163
9	3	6	8	←	8	3	5	7	6057.19478	-0.01457
5	4	2	4	←	4	2	3	3	6131.03111	0.00479
5	4	2	6	←	4	2	3	5	6131.26667	0.01409
8	4	4	8	←	7	4	3	7	6157.67146	-0.01558
8	4	4	9	←	7	4	3	8	6157.72482	-0.00037
8	4	4	7	←	7	4	3	6	6157.72482	-0.00793
8	6	3	9	←	7	6	2	8	6242.87205	-0.00495
8	6	3	7	←	7	6	2	6	6242.94829	0.00744
9	5	5	9	←	8	5	4	8	6529.31155	0.00594
9	5	5	10	←	8	5	4	9	6529.46177	0.00221
9	5	5	8	←	8	5	4	7	6529.46177	-0.01762
11	3	9	11	←	10	3	8	10	6538.13936	0.00328
11	2	9	11	←	10	2	8	10	6538.13936	0.00247
11	3	9	12	←	10	3	8	11	6538.22751	0.00101
11	3	9	10	←	10	3	8	9	6538.22751	-0.00007
11	2	9	12	←	10	2	8	11	6538.22751	0.00020
11	2	9	10	←	10	2	8	9	6538.22751	-0.00088
10	4	7	10	←	9	4	6	9	6538.43682	0.00023
10	4	7	11	←	9	4	6	10	6538.55691	-0.00187
10	4	7	9	←	9	4	6	8	6538.55691	-0.01093
10	3	7	10	←	9	3	6	9	6538.80456	-0.00656
10	3	7	11	←	9	3	6	10	6538.93562	0.00288
10	3	7	9	←	9	3	6	8	6538.93562	-0.00608
12	2	11	11	←	11	2	10	10	6539.73629	0.00513
12	2	11	13	←	11	2	10	12	6539.73629	-0.00004
12	1	11	11	←	11	1	10	10	6539.73629	0.00513
12	1	11	13	←	11	1	10	12	6539.73629	-0.00004
13	1	13	13	←	12	1	12	12	6541.66474	0.01690
13	1	13	12	←	12	1	12	11	6541.66474	0.00651
13	1	13	14	←	12	1	12	13	6541.66474	-0.00317
13	0	13	13	←	12	0	12	12	6541.66474	0.01690
13	0	13	12	←	12	0	12	11	6541.66474	0.00651
13	0	13	14	←	12	0	12	13	6541.66474	-0.00317
9	4	5	9	←	8	4	4	8	6575.64570	0.00266
9	4	5	10	←	8	4	4	9	6575.72303	-0.01459
8	5	3	8	←	7	5	2	7	6645.42423	-0.00048
8	5	3	9	←	7	5	2	8	6645.53979	-0.00657

8	5	3	7	←	7	5	2	6	6645.57968	0.01234
11	4	8	11	←	10	4	7	10	7022.30162	-0.00405
11	4	8	12	←	10	4	7	11	7022.40865	-0.00481
11	4	8	10	←	10	4	7	9	7022.40865	-0.01089
11	3	8	12	←	10	3	7	11	7022.46435	0.00569
11	3	8	10	←	10	3	7	9	7022.46435	-0.00041
12	3	10	12	←	11	3	9	11	7022.64443	0.00334
12	2	10	12	←	11	2	9	11	7022.64443	0.00326
12	3	10	11	←	11	3	9	10	7022.71955	0.00000
12	3	10	13	←	11	3	9	12	7022.71955	-0.00009
12	2	10	11	←	11	2	9	10	7022.71955	-0.00007
12	2	10	13	←	11	2	9	12	7022.71955	-0.00016
13	2	12	12	←	12	2	11	11	7024.34067	-0.00736
13	2	12	14	←	12	2	11	13	7024.34067	-0.01228
13	1	12	12	←	12	1	11	11	7024.34067	-0.00736
13	1	12	14	←	12	1	11	13	7024.34067	-0.01228
10	5	6	11	←	9	5	5	10	7024.53544	0.00090
10	5	6	9	←	9	5	5	8	7024.53544	-0.01232
14	1	14	14	←	13	1	13	13	7026.29157	0.00645
14	1	14	13	←	13	1	13	12	7026.29157	-0.00256
14	1	14	15	←	13	1	13	14	7026.29157	-0.01103
14	0	14	14	←	13	0	13	13	7026.29157	0.00645
14	0	14	13	←	13	0	13	12	7026.29157	-0.00256
14	0	14	15	←	13	0	13	14	7026.29157	-0.01103
10	4	6	10	←	9	4	5	9	7033.48036	0.00390
10	4	6	11	←	9	4	5	10	7033.59236	-0.00017
10	4	6	9	←	9	4	5	8	7033.59236	-0.01203
6	5	2	5	←	5	3	3	4	7179.19171	-0.00143
6	5	2	7	←	5	3	3	6	7179.32733	0.00372
9	5	4	10	←	8	5	3	9	7187.85227	-0.00008
9	5	4	8	←	8	5	3	7	7187.85227	-0.00438
10	6	5	10	←	9	6	4	9	7484.89543	0.00230
10	6	5	11	←	9	6	4	10	7485.05206	0.01114
10	6	5	9	←	9	6	4	8	7485.05206	-0.00716
12	4	9	13	←	11	4	8	12	7506.49946	0.01208
12	4	9	11	←	11	4	8	10	7506.49946	0.00806
12	3	9	13	←	11	3	8	12	7506.49946	0.00707
12	3	9	11	←	11	3	8	10	7506.49946	0.00304
13	3	11	12	←	12	3	10	11	7507.26362	0.01017
13	3	11	14	←	12	3	10	13	7507.26362	0.00935
13	2	11	12	←	12	2	10	11	7507.26362	0.01016
13	2	11	14	←	12	2	10	13	7507.26362	0.00934
14	2	13	14	←	13	2	12	13	7508.92332	-0.00889
14	1	13	14	←	13	1	12	13	7508.92332	-0.00889
11	5	7	11	←	10	5	6	10	7508.92332	-0.01096
14	2	13	13	←	13	2	12	12	7508.98188	0.01303
14	2	13	15	←	13	2	12	14	7508.98188	0.00840
14	1	13	13	←	13	1	12	12	7508.98188	0.01303
14	1	13	15	←	13	1	12	14	7508.98188	0.00840
11	5	7	12	←	10	5	6	11	7509.05315	0.00414
11	5	7	10	←	10	5	6	9	7509.05315	-0.00544

11	4	7	11	←	10	4	6	10	7510.38088	0.01444
11	4	7	12	←	10	4	6	11	7510.48768	0.00836
11	4	7	10	←	10	4	6	9	7510.48768	-0.00104
15	1	15	15	←	14	1	14	14	7510.93787	0.01653
15	1	15	14	←	14	1	14	13	7510.93787	0.00864
15	1	15	16	←	14	1	14	15	7510.93787	0.00117
15	0	15	15	←	14	0	14	14	7510.93787	0.01653
15	0	15	14	←	14	0	14	13	7510.93787	0.00864
15	0	15	16	←	14	0	14	15	7510.93787	0.00117
7	6	1	6	←	6	4	2	5	7553.09680	0.01215
7	6	1	8	←	6	4	2	7	7553.16612	0.00064
7	5	2	6	←	6	3	3	5	7554.15359	-0.01497
7	5	2	8	←	6	3	3	7	7554.20212	0.00236
10	5	5	10	←	9	5	4	9	7589.23373	0.00499
10	5	5	11	←	9	5	4	10	7589.27928	0.00299
10	5	5	9	←	9	5	4	8	7589.27928	-0.00375

Table S72 Measured frequencies and residuals (in MHz) for the rotational transitions of the ^{18}O(2) singly-substituted isotopologues of the Pan-$(H_2O)_2$ complex.

J'	K_a'	K_c'	*F'*	←	*J"*	K_a"	K_c"	*F"*	ν_{obs}	ν_{obs}-ν_{calc}
4	1	4	4	←	3	1	3	3	2170.77307	0.00473
4	1	4	3	←	3	1	3	2	2170.87328	0.00944
4	1	4	5	←	3	1	3	4	2170.92902	-0.00053
4	0	4	4	←	3	0	3	3	2172.06685	0.00173
4	0	4	3	←	3	0	3	2	2172.15827	0.00625
4	0	4	5	←	3	0	3	4	2172.22363	0.00366
3	1	2	3	←	2	1	1	2	2211.92157	0.01611
3	1	2	4	←	2	1	1	3	2212.14164	0.00896
4	2	3	5	←	3	2	2	4	2631.41232	-0.00192
4	2	3	3	←	3	2	2	2	2631.50195	-0.00924
5	1	5	5	←	4	1	4	4	2654.04192	0.00224
5	1	5	4	←	4	1	4	3	2654.09996	-0.00221
5	1	5	6	←	4	1	4	5	2654.13989	-0.01007
5	0	5	5	←	4	0	4	4	2654.18185	0.01080
5	0	5	4	←	4	0	4	3	2654.23625	0.00335
5	0	5	6	←	4	0	4	5	2654.28178	0.00094
4	1	3	5	←	3	1	2	4	2678.07949	-0.01080
4	1	3	3	←	3	1	2	2	2678.11815	-0.00968
5	2	4	5	←	4	2	3	4	3131.93925	0.00453
5	2	4	6	←	4	2	3	5	3132.17028	-0.00106
5	2	4	4	←	4	2	3	3	3132.21036	0.01112
6	1	6	6	←	5	1	5	5	3136.81228	-0.01419
6	1	6	7	←	5	1	5	6	3136.91588	0.00847
6	0	6	6	←	5	0	5	5	3136.81228	-0.02616
6	0	6	7	←	5	0	5	6	3136.91588	-0.00346
5	1	4	5	←	4	1	3	4	3140.50773	-0.00571
5	1	4	6	←	4	1	3	5	3140.72646	0.00177
5	1	4	4	←	4	1	3	3	3140.76170	0.01580
4	2	2	4	←	3	2	1	3	3174.77256	-0.00362

4	2	2	5	←	3	2	1	4	3174.98975	0.00392
4	2	2	3	←	3	2	1	2	3175.08246	0.01570
5	3	3	6	←	4	3	2	5	3561.69481	-0.00139
5	3	3	4	←	4	3	2	3	3561.78510	-0.00667
6	2	5	6	←	5	2	4	5	3617.63966	-0.00108
6	2	5	7	←	5	2	4	6	3617.82035	0.00483
6	2	5	5	←	5	2	4	4	3617.82035	-0.00318
6	1	5	6	←	5	1	4	5	3618.77528	-0.00407
6	1	5	7	←	5	1	4	6	3618.95425	0.00302
6	1	5	5	←	5	1	4	4	3618.95425	-0.00438
7	1	7	7	←	6	1	6	6	3619.57876	0.00983
7	1	7	6	←	6	1	6	5	3619.57876	-0.02402
7	1	7	8	←	6	1	6	7	3619.63406	0.00316
7	0	7	7	←	6	0	6	6	3619.57876	0.00881
7	0	7	6	←	6	0	6	5	3619.57876	-0.02503
7	0	7	8	←	6	0	6	7	3619.63406	0.00215
5	2	3	6	←	4	2	2	5	3679.48348	0.00703
6	3	4	6	←	5	3	3	5	4088.61043	0.00573
6	3	4	7	←	5	3	3	6	4088.84310	0.00412
6	3	4	5	←	5	3	3	4	4088.88872	0.00948
5	3	2	6	←	4	3	1	5	4100.50731	-0.00906
5	3	2	4	←	4	3	1	3	4100.58807	0.00106
7	2	6	7	←	6	2	5	6	4100.58807	-0.00837
7	2	6	8	←	6	2	5	7	4100.73034	-0.00300
7	2	6	6	←	6	2	5	5	4100.73034	-0.00328
7	1	6	7	←	6	1	5	6	4100.73034	0.00603
7	1	6	6	←	6	1	5	5	4100.85764	-0.00353
7	1	6	8	←	6	1	5	7	4100.85764	-0.00330
8	1	8	8	←	7	1	7	7	4102.32319	0.01402
8	1	8	7	←	7	1	7	6	4102.32319	-0.01241
8	1	8	9	←	7	1	7	8	4102.37668	0.01854
8	0	8	8	←	7	0	7	7	4102.32319	0.01394
8	0	8	7	←	7	0	7	6	4102.32319	-0.01249
8	0	8	9	←	7	0	7	8	4102.37668	0.01845
6	2	4	7	←	5	2	3	6	4120.25209	0.00285
6	2	4	5	←	5	2	3	4	4120.25209	-0.02461
7	3	5	7	←	6	3	4	6	4581.34159	0.00012
7	3	5	8	←	6	3	4	7	4581.52311	0.00220
7	3	5	6	←	6	3	4	5	4581.56138	0.01985
8	2	7	8	←	7	2	6	7	4583.27476	0.01723
8	2	7	7	←	7	2	6	6	4583.37090	0.00623
8	2	7	9	←	7	2	6	8	4583.37090	0.00312
8	1	7	8	←	7	1	6	7	4583.27476	0.00428
8	1	7	7	←	7	1	6	6	4583.37090	-0.00669
8	1	7	9	←	7	1	6	8	4583.37090	-0.00980
9	0	9	9	←	8	0	8	8	4585.03823	-0.01130
9	0	9	10	←	8	0	8	9	4585.09128	0.00208
9	1	9	9	←	8	1	8	8	4585.03823	-0.01129
9	1	9	10	←	8	1	8	9	4585.09128	0.00209
7	2	5	7	←	6	2	4	6	4586.74936	0.00226
7	2	5	8	←	6	2	4	7	4586.92844	0.01173

7	2	5	6	←	6	2	4	5	4586.92844	-0.00720
6	3	3	7	←	5	3	2	6	4684.99760	0.00545
6	3	3	5	←	5	3	2	4	4684.99760	-0.01720
7	4	4	7	←	6	4	3	6	5036.13062	0.00285
7	4	4	8	←	6	4	3	7	5036.34390	-0.00563
8	3	6	8	←	7	3	5	7	5065.11779	-0.00255
8	3	6	9	←	7	3	5	8	5065.26594	-0.00244
8	3	6	7	←	7	3	5	6	5065.26594	-0.01388
8	2	6	8	←	7	2	5	7	5065.84872	-0.01076
8	2	6	9	←	7	2	5	8	5066.01132	0.00503
8	2	6	7	←	7	2	5	6	5066.01132	-0.00622
9	2	8	9	←	8	2	7	8	5065.92466	-0.00396
9	2	8	8	←	8	2	7	7	5066.01132	-0.00328
9	2	8	10	←	8	2	7	9	5066.01132	-0.00786
9	1	8	9	←	8	1	7	8	5065.92466	-0.00519
9	1	8	8	←	8	1	7	7	5066.01132	-0.00449
9	1	8	10	←	8	1	7	9	5066.01132	-0.00908
10	1	10	10	←	9	1	9	9	5067.77845	-0.01103
10	1	10	9	←	9	1	9	8	5067.82708	0.02022
10	1	10	11	←	9	1	9	10	5067.82708	0.00481
10	0	10	10	←	9	0	9	9	5067.77845	-0.01103
10	0	10	9	←	9	0	9	8	5067.82708	0.02022
10	0	10	11	←	9	0	9	10	5067.82708	0.00481
7	3	4	7	←	6	3	3	6	5118.67536	0.00897
7	3	4	8	←	6	3	3	7	5118.76859	-0.01086
7	3	4	6	←	6	3	3	5	5118.81387	0.01509
5	4	1	4	←	4	2	2	3	5347.58034	0.01342
5	4	1	6	←	4	2	2	5	5347.65513	-0.00739
8	4	5	8	←	7	4	4	7	5543.96482	-0.00958
8	4	5	9	←	7	4	4	8	5544.13104	-0.01134
8	4	5	7	←	7	4	4	6	5544.17730	0.01306
9	3	7	9	←	8	3	6	8	5547.57066	0.00353
9	3	7	10	←	8	3	6	9	5547.69641	0.00443
9	3	7	8	←	8	3	6	7	5547.69641	-0.00185
9	2	7	9	←	8	2	6	8	5547.64822	-0.00692
9	2	7	10	←	8	2	6	9	5547.77983	-0.00002
9	2	7	8	←	8	2	6	7	5547.77983	-0.00629
10	2	9	10	←	9	2	8	9	5548.62612	0.00276
10	2	9	9	←	9	2	8	8	5548.69709	0.00323
10	2	9	11	←	9	2	8	10	5548.69709	-0.00191
10	1	9	10	←	9	1	8	9	5548.62612	0.00265
10	1	9	9	←	9	1	8	8	5548.69709	0.00312
10	1	9	11	←	9	1	8	10	5548.69709	-0.00202
11	1	11	11	←	10	1	10	10	5550.51544	-0.01322
11	1	11	12	←	10	1	10	11	5550.56151	0.00531
11	0	11	11	←	10	0	10	10	5550.51544	-0.01322
11	0	11	12	←	10	0	10	11	5550.56151	0.00531
8	3	5	8	←	7	3	4	7	5562.39127	-0.01077
8	3	5	9	←	7	3	4	8	5562.53708	-0.00823
8	3	5	7	←	7	3	4	6	5562.57406	0.01054
7	4	3	8	←	6	4	2	7	5670.29443	-0.01630

7	4	3	6	←	6	4	2	5	5670.33850	0.00700
7	5	2	8	←	6	5	1	7	5806.23040	0.01533
7	5	2	6	←	6	5	1	5	5806.26871	-0.01028
8	5	4	8	←	7	5	3	7	5968.86074	0.01404
8	5	4	9	←	7	5	3	8	5969.05296	-0.00798
8	5	4	7	←	7	5	3	6	5969.10131	0.00565
10	3	8	10	←	9	3	7	9	6029.99654	-0.00495
10	3	8	11	←	9	3	7	10	6030.10526	-0.00266
10	3	8	9	←	9	3	7	8	6030.10526	-0.00584
10	2	8	10	←	9	2	7	9	6029.99654	-0.01448
10	2	8	11	←	9	2	7	10	6030.10526	-0.01218
10	2	8	9	←	9	2	7	8	6030.10526	-0.01535
9	4	6	9	←	8	4	5	8	6030.64222	-0.00905
9	4	6	10	←	8	4	5	9	6030.80006	0.00652
9	4	6	8	←	8	4	5	7	6030.80006	-0.00754
11	2	10	11	←	10	2	9	10	6031.32752	-0.00505
11	2	10	10	←	10	2	9	9	6031.38537	-0.00604
11	2	10	12	←	10	2	9	11	6031.38537	-0.01128
11	1	10	11	←	10	1	9	10	6031.32752	-0.00506
11	1	10	10	←	10	1	9	9	6031.38537	-0.00605
11	1	10	12	←	10	1	9	11	6031.38537	-0.01129
12	1	12	12	←	11	1	11	11	6033.28365	0.01686
12	1	12	11	←	11	1	11	10	6033.28365	0.00457
12	1	12	13	←	11	1	11	12	6033.28365	-0.00662
12	0	12	12	←	11	0	11	11	6033.28365	0.01686
12	0	12	11	←	11	0	11	10	6033.28365	0.00457
12	0	12	13	←	11	0	11	12	6033.28365	-0.00662
9	3	6	9	←	8	3	5	8	6033.68884	-0.01250
9	3	6	10	←	8	3	5	9	6033.84301	0.00336
9	3	6	8	←	8	3	5	7	6033.84301	-0.01020
5	4	2	4	←	4	2	3	3	6110.93527	0.00940
5	4	2	6	←	4	2	3	5	6111.13890	-0.00943
8	4	4	9	←	7	4	3	8	6137.79164	0.00110
8	4	4	7	←	7	4	3	6	6137.79164	-0.01047
9	5	5	9	←	8	5	4	8	6502.79751	-0.00148
9	5	5	10	←	8	5	4	9	6502.95391	-0.00058
9	5	5	8	←	8	5	4	7	6502.95391	-0.02091
11	3	9	11	←	10	3	8	10	6512.54739	0.01491
11	3	9	12	←	10	3	8	11	6512.63085	0.00677
11	3	9	10	←	10	3	8	9	6512.63085	0.00553
11	2	9	11	←	10	2	8	10	6512.54739	0.01394
11	2	9	12	←	10	2	8	11	6512.63085	0.00581
11	2	9	10	←	10	2	8	9	6512.63085	0.00457
10	4	7	11	←	9	4	6	10	6513.04716	-0.00297
10	4	7	9	←	9	4	6	8	6513.04716	-0.01240
10	3	7	10	←	9	3	6	9	6513.35850	0.00881
10	3	7	11	←	9	3	6	10	6513.48251	0.00890
10	3	7	9	←	9	3	6	8	6513.48251	-0.00045
12	2	11	12	←	11	2	10	11	6514.06153	0.01162
12	2	11	11	←	11	2	10	10	6514.10864	0.00889
12	2	11	13	←	11	2	10	12	6514.10864	0.00377

12	1	11	12	←	11	1	10	11	6514.06153	0.01162
12	1	11	11	←	11	1	10	10	6514.10864	0.00888
12	1	11	13	←	11	1	10	12	6514.10864	0.00377
13	1	13	13	←	12	1	12	12	6516.02313	0.01937
13	1	13	12	←	12	1	12	11	6516.02313	0.00883
13	1	13	14	←	12	1	12	13	6516.02313	-0.00088
13	0	13	13	←	12	0	12	12	6516.02313	0.01937
13	0	13	12	←	12	0	12	11	6516.02313	0.00883
13	0	13	14	←	12	0	12	13	6516.02313	-0.00088
8	5	3	8	←	7	5	2	7	6614.12248	0.00711
8	5	3	9	←	7	5	2	8	6614.22557	-0.01255
8	5	3	7	←	7	5	2	6	6614.26768	0.00715
9	6	4	10	←	8	6	3	9	6881.53299	-0.00485
9	6	4	8	←	8	6	3	7	6881.56665	-0.00276
11	3	8	11	←	10	3	7	10	6994.91688	-0.00829
11	3	8	12	←	10	3	7	11	6995.01526	-0.01942
11	3	8	10	←	10	3	7	9	6995.01526	-0.02577
12	3	10	12	←	11	3	9	11	6995.12133	-0.00914
12	3	10	11	←	11	3	9	10	6995.22683	0.01679
12	3	10	13	←	11	3	9	12	6995.22683	0.01682
12	2	10	12	←	11	2	9	11	6995.12133	-0.00923
12	2	10	11	←	11	2	9	10	6995.22683	0.01670
12	2	10	13	←	11	2	9	12	6995.22683	0.01673
13	2	12	12	←	12	2	11	11	6996.80231	-0.01220
13	2	12	14	←	12	2	11	13	6996.80231	-0.01708
13	1	12	12	←	12	1	11	11	6996.80231	-0.01220
13	1	12	14	←	12	1	11	13	6996.80231	-0.01708
10	5	6	10	←	9	5	5	9	6996.89871	-0.01970
10	5	6	11	←	9	5	5	10	6997.04186	-0.00759
10	5	6	9	←	9	5	5	8	6997.04186	-0.02135
14	1	14	14	←	13	1	13	13	6998.74629	0.00690
14	1	14	13	←	13	1	13	12	6998.74629	-0.00225
14	1	14	15	←	13	1	13	14	6998.74629	-0.01074
14	0	14	14	←	13	0	13	13	6998.74629	0.00690
14	0	14	13	←	13	0	13	12	6998.74629	-0.00225
14	0	14	15	←	13	0	13	14	6998.74629	-0.01074
10	4	6	10	←	9	4	5	9	7006.91031	-0.01489
10	4	6	11	←	9	4	5	10	7007.04688	0.00089
10	4	6	9	←	9	4	5	8	7007.04688	-0.01170
9	5	4	9	←	8	5	3	8	7163.72037	0.03352
9	5	4	10	←	8	5	3	9	7163.72037	-0.00503
9	5	4	8	←	8	5	3	7	7163.72037	-0.01298
10	6	5	11	←	9	6	4	10	7453.54650	0.01112
10	6	5	9	←	9	6	4	8	7453.54650	-0.00743
12	4	9	12	←	11	4	8	11	7477.05325	0.01781
12	4	9	13	←	11	4	8	12	7477.15065	0.01837
12	4	9	11	←	11	4	8	10	7477.15065	0.01415
12	3	9	12	←	11	3	8	11	7477.05325	0.01186
12	3	9	13	←	11	3	8	12	7477.15065	0.01243
12	3	9	11	←	11	3	8	10	7477.15065	0.00821
13	3	11	13	←	12	3	10	12	7477.77932	0.01005

13	3	11	12	←	12	3	10	11	7477.85250	0.01434
13	3	11	14	←	12	3	10	13	7477.85250	0.01361
13	2	11	13	←	12	2	10	12	7477.77932	0.01004
13	2	11	12	←	12	2	10	11	7477.85250	0.01434
13	2	11	14	←	12	2	10	13	7477.85250	0.01360
14	2	13	13	←	13	2	12	12	7479.55288	0.01981
14	2	13	15	←	13	2	12	14	7479.55288	0.01521
14	1	13	13	←	13	1	12	12	7479.55288	0.01981
14	1	13	15	←	13	1	12	14	7479.55288	0.01521
10	5	5	11	←	9	5	4	10	7564.79315	0.00904
10	5	5	9	←	9	5	4	8	7564.79315	0.00018
13	4	10	13	←	12	4	9	12	7959.39519	0.01477
13	4	10	14	←	12	4	9	13	7959.45641	-0.00995
13	4	10	12	←	12	4	9	11	7959.45641	-0.01267
13	3	10	13	←	12	3	9	12	7959.39519	0.01414
13	3	10	14	←	12	3	9	13	7959.45641	-0.01058
13	3	10	12	←	12	3	9	11	7959.45641	-0.01331
14	3	12	14	←	13	3	11	13	7960.41617	-0.01713
14	3	12	13	←	13	3	11	12	7960.47442	-0.01908
14	3	12	15	←	13	3	11	14	7960.47442	-0.02030
14	2	12	14	←	13	2	11	13	7960.41617	-0.01714
14	2	12	13	←	13	2	11	12	7960.47442	-0.01909
14	2	12	15	←	13	2	11	14	7960.47442	-0.02030
12	5	8	12	←	11	5	7	11	7960.94928	0.00230
12	5	8	13	←	11	5	7	12	7961.04429	-0.00896
12	5	8	11	←	11	5	7	10	7961.04429	-0.01634
12	4	8	12	←	11	4	7	11	7961.15979	-0.01449
12	4	8	13	←	11	4	7	12	7961.29308	0.01275
12	5	8	11	←	11	5	7	11	7961.29385	0.02105
15	2	14	14	←	14	2	13	13	7962.24446	-0.00931
15	2	14	16	←	14	2	13	15	7962.24446	-0.01363
15	1	14	14	←	14	1	13	13	7962.24446	-0.00931
15	1	14	16	←	14	1	13	15	7962.24446	-0.01363
11	6	6	11	←	10	6	5	10	7962.64371	0.02072
11	6	6	12	←	10	6	5	11	7962.74352	0.00081
11	6	6	10	←	10	6	5	9	7962.74352	-0.01180
16	1	16	16	←	15	1	15	15	7964.21728	0.01099
16	1	16	15	←	15	1	15	14	7964.21728	0.00392
16	1	16	17	←	15	1	15	16	7964.21728	-0.00275
16	0	16	16	←	15	0	15	15	7964.21728	0.01099
16	0	16	15	←	15	0	15	14	7964.21728	0.00392
16	0	16	17	←	15	0	15	16	7964.21728	-0.00275

Table S73 Measured frequencies and residuals (in MHz) for the rotational transitions of the Pan-$(H_2O)_3$ complex.

J'	K_a'	K_c'	F'	←	J''	K_a''	K_c''	F''	ν_{obs}	ν_{obs}-ν_{calc}
4	2	3	4	←	3	2	2	3	2146.55762	-0.00222
4	2	3	5	←	3	2	2	4	2146.66719	0.00033
4	2	3	3	←	3	2	2	2	2146.66719	-0.02695
5	1	5	6	←	4	1	4	5	2232.81708	-0.00002

5	0	5	5	←	4	0	4	4	2235.87767	-0.00472
5	0	5	4	←	4	0	4	3	2236.01822	0.02899
5	0	5	6	←	4	0	4	5	2236.01822	-0.00150
4	1	3	4	←	3	1	2	3	2275.08677	-0.00114
4	1	3	5	←	3	1	2	4	2275.54071	0.00165
4	1	3	3	←	3	1	2	2	2275.72130	0.00245
4	3	2	3	←	3	3	1	2	2301.75292	-0.00261
4	3	2	5	←	3	3	1	4	2301.82038	0.00161
4	3	2	4	←	3	3	1	3	2302.07357	0.00985
4	3	1	3	←	3	3	0	2	2424.86985	-0.00658
4	3	1	5	←	3	3	0	4	2425.01454	0.00191
4	3	1	4	←	3	3	0	3	2425.59225	-0.00859
5	2	4	5	←	4	2	3	4	2601.47335	0.00045
5	2	4	6	←	4	2	3	5	2601.64732	-0.00401
5	2	4	4	←	4	2	3	3	2601.68568	0.00349
6	0	6	6	←	5	0	5	5	2641.61924	-0.00277
6	0	6	5	←	5	0	5	4	2641.68356	-0.00610
6	0	6	7	←	5	0	5	6	2641.72036	0.00373
5	1	4	5	←	4	1	3	4	2669.08528	0.00167
5	1	4	6	←	4	1	3	5	2669.48238	-0.00463
5	1	4	4	←	4	1	3	3	2669.57923	-0.00253
5	3	3	6	←	4	3	2	5	2846.28081	0.00015
5	3	3	4	←	4	3	2	3	2846.28081	-0.00702
5	3	3	5	←	4	3	2	4	2846.31788	0.00894
5	4	2	4	←	4	4	1	3	2913.14476	0.01203
5	4	2	6	←	4	4	1	5	2913.19660	0.00282
5	4	2	5	←	4	4	1	4	2913.50294	0.01286
5	4	1	4	←	4	4	0	3	2965.40851	0.01624
5	4	1	6	←	4	4	0	5	2965.47451	-0.00982
5	4	1	5	←	4	4	0	4	2965.94281	-0.00069
6	2	5	6	←	5	2	4	5	3029.45779	-0.00056
6	2	5	7	←	5	2	4	6	3029.63380	-0.00714
6	2	5	5	←	5	2	4	4	3029.67260	0.01096
7	1	7	7	←	6	1	6	6	3048.24239	-0.00206
7	1	7	6	←	6	1	6	5	3048.27930	-0.01274
7	1	7	8	←	6	1	6	7	3048.31914	0.00458
7	0	7	7	←	6	0	6	6	3048.39510	-0.00111
7	0	7	8	←	6	0	6	7	3048.47021	0.00323
6	1	5	6	←	5	1	4	5	3053.80470	-0.00266
6	1	5	7	←	5	1	4	6	3054.08194	0.00685
6	1	5	5	←	5	1	4	4	3054.08194	-0.03244
5	2	3	5	←	4	2	2	4	3070.57314	-0.00216
5	2	3	6	←	4	2	2	5	3070.77842	0.00087
5	2	3	4	←	4	2	2	3	3070.87216	-0.00331
5	3	2	6	←	4	3	1	5	3129.30043	-0.00144
5	3	2	5	←	4	3	1	4	3129.64121	0.00806
6	3	4	6	←	5	3	3	5	3348.84173	0.00339
6	3	4	7	←	5	3	3	6	3348.93194	-0.00057
6	3	4	5	←	5	3	3	4	3348.96187	0.00395
7	2	6	7	←	6	2	5	6	3443.55921	-0.00228
7	2	6	8	←	6	2	5	7	3443.72334	0.00249

7	2	6	6	←	6	2	5	5	3443.72334	-0.00852
7	1	6	7	←	6	1	5	6	3450.59009	-0.00074
7	1	6	8	←	6	1	5	7	3450.77402	0.00037
7	1	6	6	←	6	1	5	5	3450.77402	-0.01520
8	1	8	8	←	7	1	7	7	3455.41622	0.01691
8	0	8	8	←	7	0	7	7	3455.41622	-0.01354
8	1	8	7	←	7	1	7	6	3455.41622	-0.01974
8	0	8	7	←	7	0	7	6	3455.48704	0.02049
8	0	8	9	←	7	0	7	8	3455.48704	0.00188
6	4	3	5	←	5	4	2	4	3499.40619	0.01014
6	4	3	7	←	5	4	2	6	3499.40619	-0.00231
6	4	3	6	←	5	4	2	5	3499.53904	-0.00168
6	5	2	5	←	5	5	1	4	3503.73114	0.00988
6	5	2	7	←	5	5	1	6	3503.76771	-0.00489
6	5	2	6	←	5	5	1	5	3504.07151	0.00390
6	5	1	5	←	5	5	0	4	3521.70951	0.00006
6	5	1	7	←	5	5	0	6	3521.76133	-0.00853
6	5	1	6	←	5	5	0	5	3522.11089	-0.00957
6	2	4	6	←	5	2	3	5	3523.04391	0.00127
6	2	4	7	←	5	2	3	6	3523.41436	0.00179
6	2	4	5	←	5	2	3	4	3523.51017	0.00514
6	4	2	5	←	5	4	1	4	3672.28793	0.00079
6	4	2	7	←	5	4	1	6	3672.33644	-0.00381
6	4	2	6	←	5	4	1	5	3672.75184	-0.00205
4	3	1	5	←	3	1	2	4	3718.83497	0.01166
4	3	1	3	←	3	1	2	2	3718.90359	0.03415
4	3	1	4	←	3	1	2	3	3718.90359	0.01136
6	3	3	7	←	5	3	2	6	3783.90521	0.00422
6	3	3	5	←	5	3	2	4	3783.90521	-0.02549
6	3	3	6	←	5	3	2	5	3783.95516	0.00634
7	3	5	7	←	6	3	4	6	3810.17161	0.00030
7	3	5	8	←	6	3	4	7	3810.32267	-0.00134
7	3	5	6	←	6	3	4	5	3810.35671	0.00632
8	2	7	8	←	7	2	6	7	3852.41003	-0.00103
8	2	7	9	←	7	2	6	8	3852.54506	0.00256
8	2	7	7	←	7	2	6	6	3852.54506	-0.00268
8	1	7	8	←	7	1	6	7	3854.20044	0.00054
8	1	7	9	←	7	1	6	8	3854.34068	0.00357
8	1	7	7	←	7	1	6	6	3854.34068	-0.00232
9	1	9	9	←	8	1	8	8	3862.52845	0.00677
9	0	9	9	←	8	0	8	8	3862.52845	0.00087
9	1	9	10	←	8	1	8	9	3862.57245	0.00615
9	0	9	10	←	8	0	8	9	3862.57245	0.00023
7	2	5	7	←	6	2	4	6	3902.04623	-0.00024
7	2	5	8	←	6	2	4	7	3902.39807	0.00497
7	2	5	6	←	6	2	4	5	3902.45496	-0.00021
7	4	4	8	←	6	4	3	7	4052.27875	0.00336
7	4	4	7	←	6	4	3	6	4052.27875	-0.00342
7	4	4	6	←	6	4	3	5	4052.27875	-0.00593
7	5	3	6	←	6	5	2	5	4115.10519	-0.01276
7	5	3	8	←	6	5	2	7	4115.14404	0.00527

7	5	3	7	←	6	5	2	6	4115.32705	0.00114
8	3	6	8	←	7	3	5	7	4241.50836	-0.00013
8	3	6	9	←	7	3	5	8	4241.66593	-0.00754
8	3	6	7	←	7	3	5	6	4241.70559	0.01089
9	2	8	9	←	8	2	7	8	4259.73730	-0.00118
9	2	8	10	←	8	2	7	9	4259.84802	0.00144
9	2	8	8	←	8	2	7	7	4259.84802	0.00012
9	1	8	9	←	8	1	7	8	4260.15908	0.00059
9	1	8	10	←	8	1	7	9	4260.27015	0.00233
9	1	8	8	←	8	1	7	7	4260.27015	0.00086
10	1	10	10	←	9	1	9	9	4269.63781	-0.00394
10	0	10	10	←	9	0	9	9	4269.63781	-0.00506
10	1	10	9	←	9	1	9	8	4269.66828	0.00297
10	0	10	9	←	9	0	9	8	4269.66828	0.00185
10	1	10	11	←	9	1	9	10	4269.66828	-0.01024
10	0	10	11	←	9	0	9	10	4269.66828	-0.01136
8	2	6	8	←	7	2	5	7	4276.52564	0.00924
8	2	6	9	←	7	2	5	8	4276.77931	0.01599
8	2	6	7	←	7	2	5	6	4276.77931	-0.01772
7	3	4	7	←	6	3	3	6	4337.40768	0.00176
7	3	4	8	←	6	3	3	7	4337.59266	0.00323
7	3	4	6	←	6	3	3	5	4337.64081	-0.00296
7	4	3	6	←	6	4	2	5	4400.07722	0.01591
7	4	3	8	←	6	4	2	7	4400.07722	0.00211
7	4	3	7	←	6	4	2	6	4400.32383	-0.00126
8	4	5	8	←	7	4	4	7	4560.12456	0.00149
8	4	5	9	←	7	4	4	8	4560.19505	-0.01040
8	4	5	7	←	7	4	4	6	4560.19505	-0.02852
9	3	7	9	←	8	3	6	8	4656.77722	0.00024
9	3	7	10	←	8	3	6	9	4656.93749	0.00795
9	3	7	8	←	8	3	6	7	4656.93749	-0.00713
10	2	9	10	←	9	2	8	9	4666.74036	-0.00004
10	2	9	9	←	9	2	8	8	4666.83366	0.00428
10	2	9	11	←	9	2	8	10	4666.83366	0.00349
10	1	9	10	←	9	1	8	9	4666.83366	0.00010
10	1	9	9	←	9	1	8	8	4666.92516	0.00234
10	1	9	11	←	9	1	8	10	4666.92516	0.00157
9	2	7	9	←	8	2	6	8	4667.67415	0.00203
9	2	7	10	←	8	2	6	9	4667.84508	-0.00531
9	2	7	8	←	8	2	6	7	4667.84508	-0.02375
11	1	11	11	←	10	1	10	10	4676.79421	0.03076
11	0	11	11	←	10	0	10	10	4676.79421	0.03055
11	1	11	10	←	10	1	10	9	4676.79421	0.01124
11	0	11	10	←	10	0	10	9	4676.79421	0.01104
11	1	11	12	←	10	1	10	11	4676.79421	-0.00008
11	0	11	12	←	10	0	10	11	4676.79421	-0.00028
8	6	3	7	←	7	6	2	6	4707.25126	-0.01694
8	6	3	9	←	7	6	2	8	4707.29279	0.00265
8	5	4	7	←	7	5	3	6	4709.53045	0.00370
8	5	4	9	←	7	5	3	8	4709.53045	0.00064
8	5	4	8	←	7	5	3	7	4709.61729	-0.00070

8	6	2	9	←	7	6	1	8	4737.80832	-0.00310
8	6	2	8	←	7	6	1	7	4738.07706	-0.00141
8	3	5	8	←	7	3	4	7	4772.98903	-0.00293
8	3	5	9	←	7	3	4	8	4773.31243	-0.00107
8	3	5	7	←	7	3	4	6	4773.36554	-0.00585
8	5	3	7	←	7	5	2	6	4932.17684	-0.00446
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9	4	6	8	←	8	4	5	7	5024.56157	-0.02523
8	4	4	9	←	7	4	3	8	5061.80400	-0.01275
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9	7	3	10	←	8	7	2	9	5288.02609	0.00150
9	7	3	9	←	8	7	2	8	5288.20802	-0.01523
9	7	2	8	←	8	7	1	7	5298.16096	0.02467
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18	2	17	19	←	17	2	16	18	7923.17173	0.01112
18	1	17	19	←	17	1	16	18	7923.17173	0.01112
19	1	19	19	←	18	1	18	18	7933.71257	0.00075
19	0	19	19	←	18	0	18	18	7933.71257	0.00075
19	1	19	18	←	18	1	18	17	7933.71257	-0.00587
19	0	19	18	←	18	0	18	17	7933.71257	-0.00587
19	1	19	20	←	18	1	18	19	7933.71257	-0.01026
19	0	19	20	←	18	0	18	19	7933.71257	-0.01026
13	8	5	12	←	12	8	4	11	7952.29260	0.00184
13	8	5	14	←	12	8	4	13	7952.29260	-0.01231

Table S74 Measured frequencies and residuals (in MHz) for the rotational transitions of the ^{18}O(1) singly-substituted isotopologues of the Pan-$(H_2O)_3$ complex.

J'	K_a'	K_c'	F'	←	J''	K_a''	K_c''	F''	ν_{obs}	ν_{obs}-ν_{calc}
5	1	5	5	←	4	1	4	4	2205.5497	0.0000
5	1	5	6	←	4	1	4	5	2205.6595	-0.0103
4	1	3	5	←	3	1	2	4	2247.8178	0.0072
4	1	3	3	←	3	1	2	2	2247.9800	-0.0039
5	2	4	5	←	4	2	3	4	2571.7540	0.0003
5	2	4	6	←	4	2	3	5	2571.9607	0.0190
5	2	4	4	←	4	2	3	3	2571.9607	-0.0123
6	1	6	6	←	5	1	5	5	2608.6441	-0.0134
6	1	6	5	←	5	1	5	4	2608.7477	0.0277
6	1	6	7	←	5	1	5	6	2608.7477	-0.0010
6	0	6	6	←	5	0	5	5	2609.2736	-0.0053
6	0	6	5	←	5	0	5	4	2609.3561	0.0112
6	0	6	7	←	5	0	5	6	2609.3561	-0.0169
5	1	4	6	←	4	1	3	5	2634.9601	0.0049
5	3	3	6	←	4	3	2	5	2818.7545	-0.0064
5	3	3	4	←	4	3	2	3	2818.7545	-0.0208
5	3	3	5	←	4	3	2	4	2818.7545	-0.0034
7	1	7	7	←	6	1	6	6	3010.9959	0.0068
7	1	7	8	←	6	1	6	7	3011.0614	0.0023
7	0	7	7	←	6	0	6	6	3011.1174	0.0013
7	0	7	8	←	6	0	6	7	3011.1961	0.0095
6	1	5	6	←	5	1	4	5	3015.2051	0.0058
6	1	5	7	←	5	1	4	6	3015.4815	0.0227
5	3	2	6	←	4	3	1	5	3106.8942	0.0051
5	3	2	5	←	4	3	1	4	3107.1807	0.0055
6	3	4	6	←	5	3	3	5	3313.3704	0.0054
6	3	4	7	←	5	3	3	6	3313.4811	0.0055
6	3	4	5	←	5	3	3	4	3313.4811	-0.0220
7	2	6	8	←	6	2	5	7	3401.9649	0.0028
7	2	6	6	←	6	2	5	5	3401.9649	-0.0074
7	3	5	7	←	6	3	4	6	3766.7652	-0.0060

7	3	5	8	←	6	3	4	7	3766.9399	0.0085
7	3	5	6	←	6	3	4	5	3766.9399	-0.0181
8	2	7	8	←	7	2	6	7	3805.4237	0.0037
8	2	7	9	←	7	2	6	8	3805.5594	0.0084
8	2	7	7	←	7	2	6	6	3805.5594	0.0040
8	1	7	8	←	7	1	6	7	3806.9331	0.0086
8	1	7	9	←	7	1	6	8	3807.0669	0.0068
8	1	7	7	←	7	1	6	6	3807.0669	0.0018
9	1	9	9	←	8	1	8	8	3815.3152	0.0175
9	1	9	8	←	8	1	8	7	3815.3152	-0.0109
9	1	9	10	←	8	1	8	9	3815.3152	-0.0270
9	0	9	9	←	8	0	8	8	3815.3152	0.0129
9	0	9	8	←	8	0	8	7	3815.3152	-0.0156
9	0	9	10	←	8	0	8	9	3815.3152	-0.0317
7	2	5	7	←	6	2	4	6	3850.5554	0.0042
7	2	5	8	←	6	2	4	7	3850.8902	0.0051
7	2	5	6	←	6	2	4	5	3850.9419	-0.0016
9	2	8	9	←	8	2	7	8	4207.7069	0.0048
9	2	8	10	←	8	2	7	9	4207.8124	0.0028
9	2	8	8	←	8	2	7	7	4207.8124	0.0021
9	1	8	9	←	8	1	7	8	4208.0478	0.0030
9	1	8	10	←	8	1	7	9	4208.1545	0.0012
9	1	8	8	←	8	1	7	7	4208.1545	0.0003
10	1	10	10	←	9	1	9	9	4217.4633	0.0260
10	1	10	9	←	9	1	9	8	4217.4633	0.0028
10	1	10	11	←	9	1	9	10	4217.4633	-0.0106
10	0	10	10	←	9	0	9	9	4217.4633	0.0252
10	0	10	9	←	9	0	9	8	4217.4633	0.0020
10	0	10	11	←	9	0	9	10	4217.4633	-0.0115
8	2	6	8	←	7	2	5	7	4221.7640	0.0061
8	2	6	9	←	7	2	5	8	4222.0028	0.0076
8	2	6	7	←	7	2	5	6	4222.0028	-0.0238
7	3	4	7	←	6	3	3	6	4289.7642	-0.0074
7	3	4	8	←	6	3	3	7	4289.9686	-0.0013
7	3	4	6	←	6	3	3	5	4290.0226	-0.0021
8	3	5	8	←	7	3	4	7	4711.1066	0.0063
8	3	5	9	←	7	3	4	8	4711.4064	-0.0137
8	3	5	7	←	7	3	4	6	4711.4742	-0.0022
10	2	8	10	←	9	2	7	9	5006.2451	-0.0086
10	2	8	11	←	9	2	7	10	5006.3679	-0.0231
11	2	10	11	←	10	2	9	10	5011.7089	-0.0105
11	1	10	11	←	10	1	9	10	5011.7089	-0.0257
11	2	10	10	←	10	2	9	9	5011.8080	0.0156
11	2	10	12	←	10	2	9	11	5011.8080	0.0133
11	1	10	10	←	10	1	9	9	5011.8080	0.0003
11	1	10	12	←	10	1	9	11	5011.8080	-0.0019
12	1	12	13	←	11	1	11	12	5021.7384	-0.0079
12	0	12	13	←	11	0	11	12	5021.7384	-0.0080
11	3	9	11	←	10	3	8	10	5405.6511	-0.0212
11	3	9	12	←	10	3	8	11	5405.7988	0.0136
11	3	9	10	←	10	3	8	9	5405.7988	0.0075

11	2	9	11	←	10	2	8	10	5406.2818	0.0037
11	2	9	12	←	10	2	8	11	5406.4084	0.0162
11	2	9	10	←	10	2	8	9	5406.4084	0.0100
13	0	13	14	←	12	0	12	13	5423.8848	0.0004
13	1	13	14	←	12	1	12	13	5423.8848	0.0004
12	3	10	12	←	11	3	9	11	5807.2908	0.0026
12	3	10	13	←	11	3	9	12	5807.3935	0.0083
12	3	10	11	←	11	3	9	10	5807.3935	0.0046
12	2	10	13	←	11	2	9	12	5807.5298	0.0039
12	2	10	11	←	11	2	9	10	5807.5298	0.0002
13	2	12	12	←	12	2	11	11	5815.8580	-0.0057
13	1	12	12	←	12	1	11	11	5815.8580	-0.0063
13	2	12	14	←	12	2	11	13	5815.8580	-0.0087
13	1	12	14	←	12	1	11	13	5815.8580	-0.0093
14	0	14	14	←	13	0	13	13	5825.9995	-0.0029
14	1	14	14	←	13	1	13	13	5825.9995	-0.0029
14	0	14	13	←	13	0	13	12	5825.9995	-0.0148
14	1	14	13	←	13	1	13	12	5825.9995	-0.0148
14	1	14	15	←	13	1	13	14	5825.9995	-0.0226
14	0	14	15	←	13	0	13	14	5825.9995	-0.0226
14	2	13	13	←	13	2	12	12	6217.9333	-0.0016
14	2	13	15	←	13	2	12	14	6217.9333	-0.0047
14	1	13	13	←	13	1	12	12	6217.9333	-0.0017
14	1	13	15	←	13	1	12	14	6217.9333	-0.0048
15	0	15	15	←	14	0	14	14	6228.1483	0.0067
15	0	15	14	←	14	0	14	13	6228.1483	-0.0036
15	0	15	16	←	14	0	14	15	6228.1483	-0.0105
15	1	15	15	←	14	1	14	14	6228.1483	0.0067
15	1	15	14	←	14	1	14	13	6228.1483	-0.0036
15	1	15	16	←	14	1	14	15	6228.1483	-0.0105
13	4	10	13	←	12	4	9	12	6605.0895	0.0085
13	4	10	14	←	12	4	9	13	6605.1942	0.0036
13	4	10	12	←	12	4	9	11	6605.1942	-0.0030
15	2	14	14	←	14	2	13	13	6620.0250	0.0050
15	2	14	16	←	14	2	13	15	6620.0250	0.0019
15	1	14	14	←	14	1	13	13	6620.0250	0.0050
15	1	14	16	←	14	1	13	15	6620.0250	0.0019
16	0	16	16	←	15	0	15	15	6630.3009	0.0221
16	0	16	15	←	15	0	15	14	6630.3009	0.0129
16	0	16	17	←	15	0	15	16	6630.3009	0.0068
16	1	16	16	←	15	1	15	15	6630.3009	0.0221
16	1	16	15	←	15	1	15	14	6630.3009	0.0129
16	1	16	17	←	15	1	15	16	6630.3009	0.0068
15	2	13	15	←	14	2	12	14	7012.6058	-0.0132
15	2	13	16	←	14	2	12	15	7012.6824	-0.0017
15	2	13	14	←	14	2	12	13	7012.6824	-0.0021
16	2	15	15	←	15	2	14	14	7022.1388	0.0249
16	2	15	17	←	15	2	14	16	7022.1388	0.0219
16	1	15	15	←	15	1	14	14	7022.1388	0.0249
16	1	15	17	←	15	1	14	16	7022.1388	0.0219
17	0	17	17	←	16	0	16	16	7032.4084	-0.0054

17	0	17	16	←	16	0	16	15	7032.4084	-0.0135
17	0	17	18	←	16	0	16	17	7032.4084	-0.0190
17	1	17	17	←	16	1	16	16	7032.4084	-0.0054
17	1	17	16	←	16	1	16	15	7032.4084	-0.0135
17	1	17	18	←	16	1	16	17	7032.4084	-0.0190
19	1	19	19	←	18	1	18	18	7836.6839	0.0079
19	1	19	18	←	18	1	18	17	7836.6839	0.0014
19	1	19	20	←	18	1	18	19	7836.6839	-0.0030
19	0	19	19	←	18	0	18	18	7836.6839	0.0079
19	0	19	18	←	18	0	18	17	7836.6839	0.0014
19	0	19	20	←	18	0	18	19	7836.6839	-0.0030

Table S75 Measured frequencies and residuals (in MHz) for the rotational transitions of the ^{18}O(2) singly-substituted isotopologues of the Pan-$(H_2O)_3$ complex.

J'	K_a'	K_c'	F'	←	J''	K_a''	K_c''	F''	ν_{obs}	ν_{obs}-ν_{calc}
4	2	3	4	←	3	2	2	3	2099.7971	0.0022
4	2	3	5	←	3	2	2	4	2099.9099	0.0019
4	2	3	3	←	3	2	2	2	2099.9099	-0.0268
5	1	5	5	←	4	1	4	4	2192.9582	-0.0031
5	1	5	4	←	4	1	4	3	2193.0639	0.0188
5	1	5	6	←	4	1	4	5	2193.0639	-0.0166
5	0	5	5	←	4	0	4	4	2197.0159	0.0041
5	0	5	4	←	4	0	4	3	2197.1437	0.0218
5	0	5	6	←	4	0	4	5	2197.1437	-0.0080
4	1	3	5	←	3	1	2	4	2234.2065	-0.0061
6	1	6	6	←	5	1	5	5	2594.2881	-0.0083
6	1	6	5	←	5	1	5	4	2594.3768	0.0166
6	1	6	7	←	5	1	5	6	2594.3768	-0.0110
6	0	6	6	←	5	0	5	5	2595.2775	-0.0059
6	0	6	5	←	5	0	5	4	2595.3686	0.0160
6	0	6	7	←	5	0	5	6	2595.3686	-0.0107
5	1	4	5	←	4	1	3	4	2626.5931	0.0016
5	1	4	6	←	4	1	3	5	2626.9863	-0.0039
5	3	3	6	←	4	3	2	5	2777.2580	0.0082
5	3	3	4	←	4	3	2	3	2777.2580	-0.0014
5	3	3	5	←	4	3	2	4	2777.2580	-0.0078
7	1	7	7	←	6	1	6	6	2994.5770	-0.0044
7	1	7	6	←	6	1	6	5	2994.6527	0.0231
7	1	7	8	←	6	1	6	7	2994.6527	0.0006
7	0	7	7	←	6	0	6	6	2994.7994	-0.0056
7	0	7	6	←	6	0	6	5	2994.8865	0.0324
7	0	7	8	←	6	0	6	7	2994.8865	0.0100
5	2	3	5	←	4	2	2	4	3002.2846	0.0138
5	2	3	6	←	4	2	2	5	3002.4418	0.0046
5	2	3	4	←	4	2	2	3	3002.5314	0.0061
6	3	4	6	←	5	3	3	5	3275.0252	-0.0039
6	3	4	7	←	5	3	3	6	3275.1135	-0.0057
7	2	6	8	←	6	2	5	7	3381.9225	-0.0011
7	2	6	6	←	6	2	5	5	3381.9225	-0.0119

7	1	6	7	←	6	1	5	6	3391.2181	-0.0068
7	1	6	8	←	6	1	5	7	3391.3975	-0.0149
8	1	8	7	←	7	1	7	6	3394.6598	0.0085
8	1	8	9	←	7	1	7	8	3394.6598	-0.0100
8	0	8	8	←	7	0	7	7	3394.6598	-0.0026
6	2	4	6	←	5	2	3	5	3462.0418	0.0011
6	2	4	7	←	5	2	3	6	3462.3779	0.0019
6	2	4	5	←	5	2	3	4	3462.4605	-0.0015
6	3	3	7	←	5	3	2	6	3682.3074	0.0041
6	3	3	5	←	5	3	2	4	3682.3074	-0.0189
6	3	3	6	←	5	3	2	5	3682.3737	-0.0017
7	3	5	7	←	6	3	4	6	3733.8831	-0.0054
7	3	5	8	←	6	3	4	7	3734.0263	-0.0075
8	1	7	8	←	7	1	6	7	3786.7170	-0.0118
8	1	7	9	←	7	1	6	8	3786.8705	0.0021
8	1	7	7	←	7	1	6	6	3786.8705	-0.0041
7	2	5	7	←	6	2	4	6	3842.5902	0.0029
7	2	5	8	←	6	2	4	7	3842.9304	-0.0008
7	2	5	6	←	6	2	4	5	3842.9979	0.0044
7	4	4	8	←	6	4	3	7	3953.1745	0.0051
7	4	4	6	←	6	4	3	5	3953.1745	-0.0037
7	4	4	7	←	6	4	3	6	3953.1745	-0.0015
9	2	8	9	←	8	2	7	8	4184.5285	0.0125
9	2	8	10	←	8	2	7	9	4184.6273	0.0024
9	2	8	8	←	8	2	7	7	4184.6273	0.0009
9	1	8	9	←	8	1	7	8	4185.1771	0.0037
9	1	8	10	←	8	1	7	9	4185.2964	0.0124
9	1	8	8	←	8	1	7	7	4185.2964	0.0107
10	1	10	10	←	9	1	9	9	4194.5962	0.0228
10	1	10	9	←	9	1	9	8	4194.5962	-0.0010
10	1	10	11	←	9	1	9	10	4194.5962	-0.0142
10	0	10	10	←	9	0	9	9	4194.5962	0.0207
10	0	10	9	←	9	0	9	8	4194.5962	-0.0030
10	0	10	11	←	9	0	9	10	4194.5962	-0.0162
8	2	6	9	←	7	2	5	8	4208.2963	0.0188
8	2	6	7	←	7	2	5	6	4208.2963	-0.0164
7	4	3	6	←	6	4	2	5	4261.7976	0.0113
7	4	3	8	←	6	4	2	7	4261.7976	-0.0050
7	4	3	7	←	6	4	2	6	4262.0576	0.0017
10	2	9	9	←	9	2	8	8	4584.4986	-0.0034
10	2	9	11	←	9	2	8	10	4584.4986	-0.0041
10	1	9	10	←	9	1	8	9	4584.5644	-0.0047
10	1	9	9	←	9	1	8	8	4584.6682	0.0087
10	1	9	11	←	9	1	8	10	4584.6682	0.0080
11	1	11	11	←	10	1	10	10	4594.5800	0.0293
11	1	11	10	←	10	1	10	9	4594.5800	0.0096
11	1	11	12	←	10	1	10	11	4594.5800	-0.0017
11	0	11	11	←	10	0	10	10	4594.5800	0.0289
11	0	11	10	←	10	0	10	9	4594.5800	0.0092
11	0	11	12	←	10	0	10	11	4594.5800	-0.0021
8	3	5	8	←	7	3	4	7	4694.2460	0.0016

8	3	5	9	←	7	3	4	8	4694.5336	0.0028
8	3	5	7	←	7	3	4	6	4694.5738	-0.0102
8	4	4	9	←	7	4	3	8	4925.4165	0.0041
8	4	4	7	←	7	4	3	6	4925.4165	-0.0076
10	2	8	10	←	9	2	7	9	4980.4758	0.0083
10	2	8	11	←	9	2	7	10	4980.6175	0.0072
10	2	8	9	←	9	2	7	8	4980.6175	-0.0040
11	2	10	10	←	10	2	9	9	4984.3237	0.0110
11	2	10	12	←	10	2	9	11	4984.3237	0.0092
11	1	10	10	←	10	1	9	9	4984.3237	-0.0248
11	1	10	12	←	10	1	9	11	4984.3237	-0.0267
12	1	12	11	←	11	1	11	10	4994.5583	0.0129
12	1	12	13	←	11	1	11	12	4994.5583	0.0031
12	0	12	11	←	11	0	11	10	4994.5583	0.0128
12	0	12	13	←	11	0	11	12	4994.5583	0.0030
11	2	9	12	←	10	2	8	11	5377.3581	0.0016
11	2	9	10	←	10	2	8	9	5377.3581	-0.0052
12	2	11	12	←	11	2	10	11	5384.0809	-0.0039
12	1	11	12	←	11	1	10	11	5384.0809	-0.0118
12	2	11	11	←	11	2	10	10	5384.1441	-0.0033
12	2	11	13	←	11	2	10	12	5384.1441	-0.0058
12	1	11	11	←	11	1	10	10	5384.1441	-0.0112
12	1	11	13	←	11	1	10	12	5384.1441	-0.0137
13	1	13	13	←	12	1	12	12	5394.5225	0.0160
13	1	13	12	←	12	1	12	11	5394.5225	0.0018
13	1	13	14	←	12	1	12	13	5394.5225	-0.0066
13	0	13	13	←	12	0	12	12	5394.5225	0.0160
13	0	13	12	←	12	0	12	11	5394.5225	0.0018
13	0	13	14	←	12	0	12	13	5394.5225	-0.0067
9	4	5	9	←	8	4	4	8	5487.6501	-0.0086
9	4	5	10	←	8	4	4	9	5487.7890	0.0077
9	4	5	8	←	8	4	4	7	5487.8228	0.0118
10	5	6	10	←	9	5	5	9	5649.5906	-0.0121
10	5	6	11	←	9	5	5	10	5649.6763	0.0115
10	5	6	9	←	9	5	5	8	5649.6763	-0.0003
12	2	10	12	←	11	2	9	11	5775.7861	0.0046
12	2	10	13	←	11	2	9	12	5775.8873	0.0064
12	2	10	11	←	11	2	9	10	5775.8873	0.0022
13	2	12	12	←	12	2	11	11	5784.0210	0.0067
13	2	12	14	←	12	2	11	13	5784.0210	0.0039
13	1	12	12	←	12	1	11	11	5784.0210	0.0050
13	1	12	14	←	12	1	11	13	5784.0210	0.0022
14	0	14	14	←	13	0	13	13	5794.4929	0.0100
14	0	14	13	←	13	0	13	12	5794.4929	-0.0022
14	0	14	15	←	13	0	13	14	5794.4929	-0.0097
14	1	14	14	←	13	1	13	13	5794.4929	0.0100
14	1	14	13	←	13	1	13	12	5794.4929	-0.0022
14	1	14	15	←	13	1	13	14	5794.4929	-0.0097
16	1	16	16	←	15	1	15	15	6594.4399	0.0103
16	1	16	15	←	15	1	15	14	6594.4399	0.0009
16	1	16	17	←	15	1	15	16	6594.4399	-0.0050

16	0	16	16	←	15	0	15	15	6594.4399	0.0103
16	0	16	15	←	15	0	15	14	6594.4399	0.0009
16	0	16	17	←	15	0	15	16	6594.4399	-0.0050
17	1	17	17	←	16	1	16	16	6994.4030	0.0041
17	1	17	16	←	16	1	16	15	6994.4030	-0.0041
17	1	17	18	←	16	1	16	17	6994.4030	-0.0095
17	0	17	17	←	16	0	16	16	6994.4030	0.0041
17	0	17	16	←	16	0	16	15	6994.4030	-0.0041
17	0	17	18	←	16	0	16	17	6994.4030	-0.0095

Table S76 Measured frequencies and residuals (in MHz) for the rotational transitions of the ^{18}O(3) singly-substituted isotopologues of the Pan-$(H_2O)_3$ complex.

J'	K_a'	K_c'	F'	←	J''	K_a''	K_c''	F''	ν_{obs}	ν_{obs}-ν_{calc}
4	2	3	4	←	3	2	2	3	2106.8697	-0.0003
4	2	3	5	←	3	2	2	4	2106.9491	-0.0079
4	2	3	3	←	3	2	2	2	2107.0031	0.0239
4	1	3	4	←	3	1	2	3	2240.7448	0.0137
4	1	3	5	←	3	1	2	4	2241.1788	0.0116
5	2	4	5	←	4	2	3	4	2557.9508	-0.0001
5	2	4	6	←	4	2	3	5	2558.1092	-0.0111
6	1	6	6	←	5	1	5	5	2601.6709	-0.0069
6	1	6	7	←	5	1	5	6	2601.7726	0.0027
6	0	6	5	←	5	0	5	4	2602.7125	-0.0005
6	0	6	7	←	5	0	5	6	2602.7125	-0.0263
5	3	3	6	←	4	3	2	5	2787.2807	0.0085
5	3	3	4	←	4	3	2	3	2787.2807	0.0072
5	3	3	5	←	4	3	2	4	2787.3310	0.0058
6	2	5	6	←	5	2	4	5	2982.2939	0.0059
6	2	5	7	←	5	2	4	6	2982.4601	-0.0054
6	2	5	5	←	5	2	4	4	2982.4601	-0.0297
6	1	5	6	←	5	1	4	5	3012.0423	-0.0016
6	1	5	7	←	5	1	4	6	3012.3351	0.0083
5	2	3	5	←	4	2	2	4	3012.8256	0.0010
5	2	3	6	←	4	2	2	5	3012.9997	0.0069
5	2	3	4	←	4	2	2	3	3013.0850	-0.0006
7	2	6	7	←	6	2	5	6	3391.7913	-0.0100
7	2	6	8	←	6	2	5	7	3391.9725	0.0110
7	2	6	6	←	6	2	5	5	3391.9725	-0.0006
8	1	8	8	←	7	1	7	7	3404.2270	0.0278
8	1	8	7	←	7	1	7	6	3404.2270	-0.0100
8	1	8	9	←	7	1	7	8	3404.2270	-0.0282
8	0	8	8	←	7	0	7	7	3404.2270	-0.0187
6	2	4	6	←	5	2	3	5	3472.6769	0.0086
6	2	4	7	←	5	2	3	6	3473.0256	0.0045
6	2	4	5	←	5	2	3	4	3473.1243	0.0111
6	4	2	7	←	5	4	1	6	3567.8348	-0.0021
6	4	2	6	←	5	4	1	5	3568.2625	-0.0015
6	3	3	7	←	5	3	2	6	3696.7397	-0.0061
6	3	3	6	←	5	3	2	5	3696.8456	0.0091
8	2	7	8	←	7	2	6	7	3795.2191	0.0005
8	2	7	9	←	7	2	6	8	3795.3474	-0.0044
8	2	7	7	←	7	2	6	6	3795.3474	-0.0106

8	1	7	8	←	7	1	6	7	3797.7346	-0.0112
8	1	7	9	←	7	1	6	8	3797.8809	-0.0064
8	1	7	7	←	7	1	6	6	3797.8809	-0.0135
9	1	9	9	←	8	1	8	8	3805.3189	0.0305
9	1	9	8	←	8	1	8	7	3805.3189	0.0006
9	1	9	10	←	8	1	8	9	3805.3189	-0.0146
9	0	9	9	←	8	0	8	8	3805.3189	0.0209
9	0	9	8	←	8	0	8	7	3805.3189	-0.0090
9	0	9	10	←	8	0	8	9	3805.3189	-0.0243
7	2	5	8	←	6	2	4	7	3853.8366	0.0029
7	2	5	6	←	6	2	4	5	3853.8921	-0.0077
7	4	4	8	←	6	4	3	7	3967.5859	0.0000
7	4	4	6	←	6	4	3	5	3967.5859	-0.0059
7	4	4	7	←	6	4	3	6	3967.5859	-0.0291
8	3	6	8	←	7	3	5	7	4175.2528	0.0090
8	3	6	9	←	7	3	5	8	4175.3844	-0.0205
9	2	8	9	←	8	2	7	8	4196.6910	-0.0026
9	2	8	10	←	8	2	7	9	4196.8111	0.0074
9	2	8	8	←	8	2	7	7	4196.8111	0.0054
9	1	8	9	←	8	1	7	8	4197.3327	0.0037
9	1	8	10	←	8	1	7	9	4197.4465	0.0055
9	1	8	8	←	8	1	7	7	4197.4465	0.0032
10	1	10	9	←	9	1	9	8	4206.4057	0.0095
10	1	10	11	←	9	1	9	10	4206.4057	-0.0034
10	0	10	9	←	9	0	9	8	4206.4057	0.0076
10	0	10	11	←	9	0	9	10	4206.4057	-0.0053
8	2	6	8	←	7	2	5	7	4220.0391	-0.0007
8	2	6	9	←	7	2	5	8	4220.3196	0.0153
8	2	6	7	←	7	2	5	6	4220.3196	-0.0219
7	3	4	7	←	6	3	3	6	4258.1273	0.0019
7	3	4	8	←	6	3	3	7	4258.3052	0.0362
7	3	4	6	←	6	3	3	5	4258.3052	-0.0133
10	2	9	10	←	9	2	8	9	4597.6957	0.0022
10	2	9	9	←	9	2	8	8	4597.7926	0.0079
10	2	9	11	←	9	2	8	10	4597.7926	0.0076
10	1	9	10	←	9	1	8	9	4597.8547	0.0105
10	1	9	9	←	9	1	8	8	4597.9522	0.0163
10	1	9	11	←	9	1	8	10	4597.9522	0.0161
8	5	4	7	←	7	5	3	6	4601.7764	-0.0056
8	5	4	9	←	7	5	3	8	4601.7764	-0.0116
8	5	4	8	←	7	5	3	7	4601.9097	0.0122
9	2	7	9	←	8	2	6	8	4601.9097	-0.0116
9	2	7	10	←	8	2	6	9	4602.0962	-0.0138
9	2	7	8	←	8	2	6	7	4602.0962	-0.0342
11	1	11	10	←	10	1	10	9	4607.5054	0.0285
11	1	11	12	←	10	1	10	11	4607.5054	0.0174
11	0	11	10	←	10	0	10	9	4607.5054	0.0281
11	0	11	12	←	10	0	10	11	4607.5054	0.0170
8	3	5	8	←	7	3	4	7	4708.4320	-0.0089
8	3	5	9	←	7	3	4	8	4708.7457	0.0016
8	3	5	7	←	7	3	4	6	4708.8046	0.0035

8	4	4	9	←	7	4	3	8	4944.8905	0.0082
8	4	4	7	←	7	4	3	6	4944.8905	-0.0035
8	4	4	8	←	7	4	3	7	4944.9528	-0.0030
10	2	8	10	←	9	2	7	9	4995.1161	0.0048
10	2	8	11	←	9	2	7	10	4995.2711	0.0145
10	2	8	9	←	9	2	7	8	4995.2711	0.0025
11	1	10	10	←	10	1	9	9	4998.7415	0.0040
11	1	10	12	←	10	1	9	11	4998.7415	0.0025
11	3	9	11	←	10	3	8	10	5391.8351	-0.0089
11	3	9	12	←	10	3	8	11	5391.9648	0.0045
11	3	9	10	←	10	3	8	9	5391.9648	-0.0026
12	2	11	11	←	11	2	10	10	5399.6412	-0.0063
12	2	11	13	←	11	2	10	12	5399.6412	-0.0086
12	1	11	11	←	11	1	10	10	5399.6412	-0.0139
12	1	11	13	←	11	1	10	12	5399.6412	-0.0161
13	1	13	13	←	12	1	12	12	5409.6221	-0.0069
13	1	13	12	←	12	1	12	11	5409.6221	-0.0213
13	0	13	13	←	12	0	12	12	5409.6221	-0.0069
13	0	13	12	←	12	0	12	11	5409.6221	-0.0213
12	3	10	12	←	11	3	9	11	5792.4234	-0.0044
12	3	10	13	←	11	3	9	12	5792.5348	0.0069
12	3	10	11	←	11	3	9	10	5792.5348	0.0024
13	2	12	12	←	12	2	11	11	5800.6264	0.0018
13	2	12	14	←	12	2	11	13	5800.6264	-0.0007
13	1	12	12	←	12	1	11	11	5800.6264	0.0002
13	1	12	14	←	12	1	11	13	5800.6264	-0.0023
14	1	14	13	←	13	1	13	12	5810.7436	0.0165
14	1	14	15	←	13	1	13	14	5810.7436	0.0091
14	0	14	13	←	13	0	13	12	5810.7436	0.0165
14	0	14	15	←	13	0	13	14	5810.7436	0.0091
10	4	6	10	←	9	4	5	9	5947.0325	-0.0215
10	4	6	11	←	9	4	5	10	5947.3083	-0.0158
14	2	13	13	←	13	2	12	12	6201.6088	-0.0178
14	2	13	15	←	13	2	12	14	6201.6088	-0.0206
14	1	13	13	←	13	1	12	12	6201.6088	-0.0182
14	1	13	15	←	13	1	12	14	6201.6088	-0.0209
13	4	10	13	←	12	4	9	12	6588.7839	0.0153
13	4	10	14	←	12	4	9	13	6588.8825	0.0003
13	4	10	12	←	12	4	9	11	6588.8825	-0.0073
14	3	12	15	←	13	3	11	14	6593.7397	0.0222
14	3	12	13	←	13	3	11	12	6593.7397	0.0206
14	2	12	15	←	13	2	11	14	6593.7397	0.0043
14	2	12	13	←	13	2	11	12	6593.7397	0.0027
15	2	14	15	←	14	2	13	14	6602.6362	0.0310
15	2	14	14	←	14	2	13	13	6602.6362	-0.0097
15	2	14	16	←	14	2	13	15	6602.6362	-0.0124
15	1	14	15	←	14	1	13	14	6602.6362	0.0309
15	1	14	14	←	14	1	13	13	6602.6362	-0.0097
15	1	14	16	←	14	1	13	15	6602.6362	-0.0125
12	4	8	12	←	11	4	7	11	6645.5282	0.0112
12	4	8	13	←	11	4	7	12	6645.7591	0.0174

12	4	8	11	←	11	4	7	10	6645.7591	-0.0054
17	1	17	17	←	16	1	16	16	7013.9619	0.0006
17	1	17	16	←	16	1	16	15	7013.9619	-0.0078
17	1	17	18	←	16	1	16	17	7013.9619	-0.0131
17	0	17	17	←	16	0	16	16	7013.9619	0.0006
17	0	17	16	←	16	0	16	15	7013.9619	-0.0078
17	0	17	18	←	16	0	16	17	7013.9619	-0.0131

Table S77 Measured frequencies and residuals (in MHz) for the rotational transitions of the Phe-H_2O complex.

J'	K_a'	K_c'		←	J''	K_a''	K_c''		ν_{obs}	ν_{obs}-ν_{calc}
2	1	1	3	←	1	0	1	3	2367.42070	0.03067
2	1	1	1	←	1	0	1	1	2367.55000	0.02057
2	1	1	0	←	1	0	1	0	2370.52080	0.02521
3	1	3	2	←	2	1	2	3	2401.54960	0.01333
3	1	3	0	←	2	1	2	1	2403.19770	0.00242
3	1	3	1	←	2	1	2	0	2423.66990	0.02467
3	1	3	3	←	2	1	2	2	2425.43720	0.01968
3	0	3	0	←	2	0	2	1	2470.04970	0.00568
3	0	3	1	←	2	0	2	0	2486.05890	0.00032
3	0	3	3	←	2	0	2	2	2487.31300	-0.00573
3	1	2	2	←	2	1	1	3	2554.81280	0.02104
3	1	2	0	←	2	1	1	1	2556.04920	0.01474
3	1	2	1	←	2	1	1	0	2568.23110	-0.00225
6	3	4	1	←	6	2	4	1	3036.36355	0.00124
6	3	4	3	←	6	2	4	3	3039.04012	0.00247
5	3	3	0	←	5	2	3	0	3099.52536	0.01473
5	3	3	2	←	5	2	3	2	3101.45038	0.01635
5	3	3	1	←	5	2	3	1	3102.34973	0.00247
4	3	2	0	←	4	2	2	0	3139.51130	-0.00997
4	3	2	2	←	4	2	2	2	3141.24838	-0.01175
4	3	2	1	←	4	2	2	1	3142.26716	0.00875
5	0	5	0	←	4	1	3	0	3174.70561	-0.00995
5	0	5	2	←	4	1	3	2	3174.83326	-0.01972
5	0	5	1	←	4	1	3	1	3177.77056	0.00147
4	3	1	0	←	4	2	3	0	3183.58629	-0.01754
4	3	1	1	←	4	2	3	1	3185.51120	0.01131
5	3	2	0	←	5	2	4	0	3201.41373	-0.00231
5	3	2	1	←	5	2	4	1	3202.75973	-0.00211
5	3	2	2	←	5	2	4	2	3202.96038	-0.00850
5	3	2	3	←	5	2	4	3	3204.55153	-0.00761
4	1	4	2	←	3	1	3	3	3204.69270	0.01004
4	1	4	0	←	3	1	3	1	3206.03840	0.00475
4	1	4	1	←	3	1	3	0	3223.46890	0.01533
4	1	4	3	←	3	1	3	2	3224.99490	0.00795
3	1	2	1	←	2	0	2	1	3271.86940	0.02587
4	0	4	2	←	3	0	3	3	3284.24310	0.01577
4	0	4	0	←	3	0	3	1	3285.18460	0.01343
4	0	4	1	←	3	0	3	0	3296.84090	0.00193
4	0	4	3	←	3	0	3	2	3297.76660	0.01168
4	2	3	0	←	3	2	2	1	3310.87400	0.00354

4	2	3	1	←	3	2	2	0	3323.48200	0.01719
4	2	3	3	←	3	2	2	2	3324.35850	0.01802
4	2	2	0	←	3	2	1	1	3339.91140	-0.00377
4	2	2	1	←	3	2	1	0	3351.36100	0.02050
4	2	2	3	←	3	2	1	2	3352.00890	0.02497
8	2	6	2	←	8	1	8	2	3353.04837	0.00564
8	2	6	0	←	8	1	8	0	3355.39772	0.02076
8	3	5	1	←	8	2	7	1	3371.02078	0.02078
8	3	5	2	←	8	2	7	2	3371.08343	0.00929
8	3	5	3	←	8	2	7	3	3371.88519	0.03169
4	1	3	2	←	3	1	2	3	3409.79070	0.00543
4	1	3	0	←	3	1	2	1	3410.40190	0.00597
4	1	3	3	←	3	1	2	2	3414.58710	-0.00827
4	1	3	1	←	3	1	2	0	3414.64880	-0.00492
6	1	5	1	←	5	2	3	1	3454.69358	-0.00742
6	1	5	2	←	5	2	3	2	3459.72078	-0.01086
6	1	5	0	←	5	2	3	0	3460.96292	-0.01037
9	3	6	1	←	9	2	8	1	3494.68896	0.00122
2	2	0	1	←	1	1	0	1	3542.38090	0.01716
2	2	0	0	←	1	1	0	0	3542.46470	-0.01820
2	2	0	3	←	1	1	0	3	3543.42210	0.01268
2	2	0	2	←	1	1	0	2	3543.52450	-0.02270
2	2	1	1	←	1	1	1	1	3588.60373	0.01279
2	2	1	3	←	1	1	1	3	3589.47309	0.01627
2	2	1	0	←	1	1	1	0	3589.65839	-0.00839
2	2	1	2	←	1	1	1	2	3590.71177	-0.01366
6	0	6	0	←	5	1	4	0	3800.86603	0.00561
6	0	6	2	←	5	1	4	2	3801.33807	0.00265
6	0	6	1	←	5	1	4	1	3806.60074	-0.00067
6	0	6	3	←	5	1	4	3	3808.07712	-0.00343
8	2	6	0	←	7	3	4	0	3833.25963	-0.00593
5	1	5	2	←	4	1	4	3	4005.53510	0.00360
5	1	5	0	←	4	1	4	1	4006.55780	0.00453
5	1	5	1	←	4	1	4	0	4020.78230	0.00449
5	1	5	3	←	4	1	4	2	4022.08150	0.00888
5	0	5	2	←	4	0	4	3	4089.54770	0.00784
5	0	5	0	←	4	0	4	1	4090.08020	0.00817
5	0	5	1	←	4	0	4	0	4097.99240	0.01302
5	0	5	3	←	4	0	4	2	4098.67580	0.02571
5	2	4	2	←	4	2	3	3	4139.32410	0.01146
5	2	4	0	←	4	2	3	1	4139.90110	0.01306
5	2	4	1	←	4	2	3	0	4145.74470	-0.01086
5	2	4	3	←	4	2	3	2	4146.01990	-0.00262
5	3	3	2	←	4	3	2	3	4152.62600	0.00383
5	2	2	2	←	4	2	1	3	4152.62630	0.00413
5	3	3	0	←	4	3	2	1	4153.56250	-0.00457
5	2	2	0	←	4	2	1	1	4153.56270	-0.00437
5	3	2	2	←	4	3	1	3	4154.84770	0.00385
5	3	2	0	←	4	3	1	1	4155.81280	0.00862
5	2	2	1	←	4	2	1	0	4162.72510	0.01784
5	3	3	1	←	4	3	2	0	4162.72520	0.01794

5	2	2	3	←	4	2	1	2	4163.21030	0.01391
5	3	3	3	←	4	3	2	2	4163.21030	0.01391
5	3	2	1	←	4	3	1	0	4164.92590	0.01232
5	3	2	3	←	4	3	1	2	4165.40120	0.01730
5	2	3	2	←	4	2	2	3	4195.65390	-0.01168
5	2	3	0	←	4	2	2	1	4196.30360	-0.01124
5	2	3	3	←	4	2	2	2	4199.72320	0.01552
5	2	3	1	←	4	2	2	0	4199.89130	0.01003
4	1	3	1	←	3	0	3	1	4205.40780	0.02634
4	1	3	0	←	3	0	3	0	4212.22220	0.02676
5	1	4	3	←	4	1	3	2	4256.89400	0.00898
5	1	4	1	←	4	1	3	0	4257.67090	0.00190
5	1	4	0	←	4	1	3	1	4261.23610	-0.00869
9	4	6	0	←	9	3	6	0	4333.75776	-0.03049
9	4	6	1	←	9	3	6	1	4333.88217	0.00928
3	2	1	1	←	2	1	1	1	4334.03190	0.00999
3	2	1	0	←	2	1	1	0	4334.39120	-0.00959
3	2	1	3	←	2	1	1	3	4335.06400	0.00462
3	2	1	2	←	2	1	1	2	4335.48300	-0.01733
9	4	6	2	←	9	3	6	2	4336.97438	-0.03285
9	4	6	3	←	9	3	6	3	4337.07494	0.00272
7	1	6	2	←	6	2	4	2	4338.23307	0.01709
7	1	6	0	←	6	2	4	0	4339.46235	-0.00049
9	1	9	1	←	8	2	7	1	4351.61038	0.01536
7	0	7	0	←	6	1	5	0	4369.40412	0.00376
7	0	7	2	←	6	1	5	2	4370.41101	0.00588
7	0	7	1	←	6	1	5	1	4377.42435	-0.00824
8	4	5	0	←	8	3	5	0	4378.81666	0.00175
8	4	5	1	←	8	3	5	1	4379.64281	0.00562
8	4	5	2	←	8	3	5	2	4381.68677	-0.00128
8	4	5	3	←	8	3	5	3	4382.61949	0.00123
7	4	4	0	←	7	3	4	0	4406.83231	0.01077
7	4	4	1	←	7	3	4	1	4408.29625	-0.01290
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7	4	4	2	←	7	3	4	2	4409.46355	0.00594
7	4	4	3	←	7	3	4	3	4411.16255	-0.01569
6	4	3	0	←	6	3	3	0	4423.24146	0.01050
6	4	3	1	←	6	3	3	1	4425.33712	-0.00511
6	4	3	2	←	6	3	3	2	4425.71787	0.01236
8	4	4	0	←	8	3	6	0	4427.66759	0.03822
6	4	3	3	←	6	3	3	3	4428.16205	-0.01071
8	4	4	1	←	8	3	6	1	4428.63493	0.00373
7	4	3	0	←	7	3	5	0	4429.24942	0.04070
9	4	5	0	←	9	3	7	0	4430.02935	0.01572
8	4	4	2	←	8	3	6	2	4430.14353	0.03639
7	4	3	1	←	7	3	5	1	4430.70633	-0.00416
5	4	2	0	←	5	3	2	0	4432.16603	-0.02158
6	4	2	0	←	6	3	4	0	4432.24092	0.01088
10	4	6	0	←	10	3	8	2	4433.39279	-0.00758
7	4	3	3	←	7	3	5	3	4433.46600	0.05282
6	4	2	1	←	6	3	4	1	4434.30217	-0.01038

5	4	2	2	←	5	3	2	2	4434.52417	-0.02348
5	4	2	1	←	5	3	2	1	4434.91936	0.00912
5	4	1	0	←	5	3	3	0	4435.17584	-0.01809
6	4	2	3	←	6	3	4	3	4437.05679	-0.01658
4	4	0	0	←	4	3	2	0	4437.31572	-0.07206
5	4	1	2	←	5	3	3	2	4437.50911	-0.02281
5	4	2	3	←	5	3	2	3	4437.75962	0.00992
8	4	4	2	←	8	3	6	0	4437.75962	0.07056
5	4	1	1	←	5	3	3	1	4437.90559	0.01126
4	4	0	2	←	4	3	2	2	4439.58989	-0.06626
4	4	1	1	←	4	3	1	1	4439.99178	0.03392
4	4	0	1	←	4	3	2	1	4440.72480	0.02370
5	4	1	3	←	5	3	3	3	4440.72480	0.01533
4	4	0	3	←	4	3	2	3	4443.61001	0.03980
3	2	2	1	←	2	1	2	1	4467.10160	0.00151
3	2	2	3	←	2	1	2	3	4467.65680	0.00511
3	2	2	0	←	2	1	2	0	4470.06470	0.00178
3	2	2	2	←	2	1	2	2	4471.14660	0.00029
9	2	7	1	←	8	3	5	1	4801.66530	-0.01822
9	2	7	0	←	8	3	5	0	4802.82535	0.02246
6	1	6	2	←	5	1	5	3	4803.62890	-0.01237
6	1	6	0	←	5	1	5	1	4804.33320	-0.00912
6	1	6	1	←	5	1	5	0	4815.51390	-0.00551
6	1	6	3	←	5	1	5	2	4816.60490	-0.00041
10	2	9	1	←	9	3	7	1	4824.76952	-0.02129
10	2	9	0	←	9	3	7	0	4825.75343	0.03015
8	0	8	0	←	7	1	6	0	4881.07986	0.00255
8	0	8	2	←	7	1	6	2	4882.81001	0.00832
6	0	6	2	←	5	0	5	3	4884.14090	-0.00444
6	0	6	0	←	5	0	5	1	4884.33260	-0.00352
6	0	6	1	←	5	0	5	0	4889.56860	0.01375
6	0	6	3	←	5	0	5	2	4890.13570	0.02311
8	0	8	1	←	7	1	6	1	4890.46644	-0.01990
8	0	8	3	←	7	1	6	3	4893.78913	-0.01644
6	2	5	3	←	5	2	4	2	4965.51110	-0.01257
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6	2	5	0	←	5	2	4	1	4966.33932	0.00829
6	4	3	2	←	5	4	2	3	4984.82249	0.02211
6	4	2	2	←	5	4	1	3	4984.94002	0.02453
6	4	3	0	←	5	4	2	1	4985.58253	0.01928
6	4	2	0	←	5	4	1	1	4985.69582	0.01617
6	2	3	2	←	5	2	2	3	4990.99980	0.01038
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6	2	3	0	←	5	2	2	1	4991.35370	0.00977
6	3	4	0	←	5	3	3	1	4991.35380	0.00987
6	4	3	1	←	5	4	2	0	4992.06445	0.00084
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6	4	2	3	←	5	4	1	2	4992.40095	0.00363
6	2	3	3	←	5	2	2	2	4992.85180	-0.00406
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6	2	3	1	←	5	2	2	0	4993.05720	-0.00386
6	3	4	1	←	5	3	3	0	4993.05720	-0.00386
6	3	3	2	←	5	3	2	3	4996.86460	0.02002
6	3	3	0	←	5	3	2	1	4997.25860	0.01607
6	3	3	3	←	5	3	2	2	4998.64250	-0.01484
6	3	3	1	←	5	3	2	0	4998.89330	-0.01571
6	2	4	3	←	5	2	3	2	5055.26320	0.01095
6	2	4	1	←	5	2	3	0	5056.21780	0.00842
6	2	4	2	←	5	2	3	3	5059.96820	-0.02780
6	2	4	0	←	5	2	3	1	5060.14460	-0.02393
6	1	5	3	←	5	1	4	2	5095.25360	0.02191
6	1	5	1	←	5	1	4	0	5096.60290	0.01653
6	1	5	0	←	5	1	4	1	5106.70840	-0.02273
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5	1	4	3	←	4	0	4	3	5171.60190	0.03000
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8	1	7	1	←	7	2	5	1	5177.99822	-0.00624
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5	1	4	0	←	4	0	4	0	5181.45840	0.00332
9	0	9	0	←	8	1	7	0	5341.04714	0.00674
9	0	9	1	←	8	1	7	1	5350.71543	0.01348
4	2	3	1	←	3	1	3	1	5369.87050	-0.01200
4	2	3	3	←	3	1	3	3	5370.06200	-0.00728
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7	1	7	2	←	6	1	6	3	5598.78650	-0.01776
7	1	7	0	←	6	1	6	1	5599.19740	-0.01764
7	1	7	1	←	6	1	6	0	5607.70510	-0.01123
7	1	7	3	←	6	1	6	2	5608.63630	-0.00555
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3	3	0	1	←	2	2	0	1	5662.63280	0.02375
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3	3	0	3	←	2	2	0	3	5664.29550	0.02008
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3	3	1	1	←	2	2	1	1	5665.39000	0.02023
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7	0	7	3	←	6	0	6	2	5673.72490	0.00867
9	5	4	2	←	9	4	6	2	5690.46099	0.00106
8	5	4	3	←	8	4	4	3	5697.62619	-0.03419
8	5	3	2	←	8	4	5	2	5697.85311	0.03671
7	5	3	0	←	7	4	3	0	5699.46273	0.02100
7	5	2	0	←	7	4	4	0	5700.00217	0.02349

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6	5	1	3	←	6	4	3	3	5710.24234	0.00288
10	2	8	0	←	9	3	6	0	5780.33685	-0.00316
7	2	6	3	←	6	2	5	2	5782.75380	-0.01211
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7	3	4	1	←	6	3	3	0	5837.50490	-0.02090
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7	2	5	1	←	6	2	4	0	5918.82030	0.00361
7	2	5	0	←	6	2	4	1	5928.67970	-0.02346
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9	1	8	3	←	8	2	6	3	5970.69175	0.00797
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9	1	8	2	←	8	2	6	2	5971.71889	-0.04387
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11	0	11	1	←	10	1	9	1	6151.01591	-0.00818
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6	1	5	3	←	5	0	5	3	6178.05630	0.01469
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6	1	5	2	←	5	0	5	2	6189.29620	-0.00154
6	1	5	0	←	5	0	5	0	6189.67140	-0.01317
5	2	4	3	←	4	1	4	3	6296.85360	-0.01478

5	2	4	1	←	4	1	4	1	6297.06150	-0.01576
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8	0	8	0	←	7	0	7	1	6448.57130	-0.00380
8	0	8	2	←	7	0	7	3	6448.81130	0.00729
8	0	8	1	←	7	0	7	0	6451.39720	-0.01069
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4	3	1	1	←	3	2	1	1	6486.70180	0.00339
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4	3	2	2	←	3	2	2	2	6503.45940	-0.00323
8	2	7	3	←	7	2	6	2	6597.57470	-0.01339
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8	4	4	1	←	7	4	3	0	6656.29536	-0.02868
8	2	5	1	←	7	2	4	0	6656.91000	0.00845
8	4	5	0	←	7	4	4	1	6661.81089	0.02191
8	4	5	2	←	7	4	4	3	6662.02465	0.02027
8	4	4	0	←	7	4	3	1	6662.86016	0.01858
8	4	4	2	←	7	4	3	3	6663.06623	0.02140
8	7	1	2	←	7	7	0	1	6663.41212	-0.00836
8	3	6	0	←	7	3	5	1	6665.89190	-0.03080
8	3	6	2	←	7	3	5	3	6666.31221	-0.03866
8	3	5	3	←	7	3	4	2	6681.10060	-0.01151
8	3	5	1	←	7	3	4	0	6682.43820	-0.01520
8	3	5	0	←	7	3	4	1	6691.30030	0.01708
8	3	5	2	←	7	3	4	3	6691.51390	0.01933
6	2	4	1	←	5	1	4	1	6701.96930	0.00208
6	2	4	0	←	5	1	4	0	6702.04930	-0.00461
6	2	4	2	←	5	1	4	2	6702.80400	-0.03400
6	2	4	3	←	5	1	4	3	6702.80400	0.01770
10	1	9	1	←	9	2	7	1	6705.67053	0.03586
10	1	9	3	←	9	2	7	3	6705.82165	0.05716
10	1	9	0	←	9	2	7	0	6706.13209	-0.00459
10	1	9	2	←	9	2	7	2	6706.39744	-0.01022
8	1	7	3	←	7	1	6	2	6755.57820	-0.00889
8	1	7	1	←	7	1	6	0	6757.35600	-0.00231
8	1	7	3	←	7	1	6	0	6760.03557	-0.01782
8	1	7	0	←	7	1	6	1	6773.99440	0.01217
8	1	7	2	←	7	1	6	3	6775.08915	0.02677

8	2	6	3	←	7	2	5	2	6782.89490	-0.00347
8	2	6	1	←	7	2	5	0	6784.82640	-0.00563
8	2	6	0	←	7	2	5	1	6797.99650	0.00839
8	2	6	2	←	7	2	5	3	6798.25480	0.00504
9	1	9	0	←	8	1	8	1	7180.54490	0.01156
9	1	9	1	←	8	1	8	0	7185.16960	0.00978
9	1	9	3	←	8	1	8	2	7185.93260	0.00438
9	0	9	0	←	8	0	8	1	7224.56440	0.02811
9	0	9	1	←	8	0	8	0	7226.98220	-0.00075
9	0	9	3	←	8	0	8	2	7227.67380	-0.01091
7	1	6	3	←	6	0	6	3	7227.80960	-0.00419
7	1	6	1	←	6	0	6	1	7230.44690	-0.00474
7	1	6	2	←	6	0	6	2	7239.72310	0.00454
7	1	6	0	←	6	0	6	0	7240.64690	-0.00943
6	2	5	3	←	5	1	5	3	7248.12870	-0.02160
6	2	5	1	←	5	1	5	1	7248.75150	-0.01750
6	2	5	0	←	5	1	5	0	7256.83670	-0.01833
6	2	5	2	←	5	1	5	2	7257.62130	-0.01769
5	3	2	1	←	4	2	2	1	7301.39910	0.00038
5	3	2	0	←	4	2	2	0	7302.60529	0.01787
5	3	2	3	←	4	2	2	3	7303.01960	-0.00339
5	3	2	2	←	4	2	2	2	7304.43751	0.01801
5	3	3	1	←	4	2	3	1	7340.94810	0.00292
5	3	3	3	←	4	2	3	3	7342.32350	0.00496
5	3	3	0	←	4	2	3	0	7342.95060	0.00644
5	3	3	2	←	4	2	3	2	7344.66570	0.00743
9	2	8	3	←	8	2	7	2	7409.73470	-0.00610
9	2	8	1	←	8	2	7	0	7410.92660	0.01103
9	2	8	0	←	8	2	7	1	7423.42750	-0.02396
9	2	8	2	←	8	2	7	3	7424.44970	-0.01376
9	4	6	3	←	8	4	5	2	7489.04445	0.05729
9	3	7	1	←	8	3	6	0	7489.85207	0.04856
9	4	6	1	←	8	4	5	0	7490.33628	0.03645
9	4	6	0	←	8	4	5	1	7499.99829	-0.02539
9	4	6	2	←	8	4	5	3	7500.38495	-0.03751
9	4	5	0	←	8	4	4	1	7502.49781	-0.02803
9	4	5	2	←	8	4	4	3	7502.84638	-0.04960
7	2	5	0	←	6	1	5	0	7523.93770	-0.00155
7	2	5	1	←	6	1	5	1	7524.26820	-0.01602
7	2	5	2	←	6	1	5	2	7524.36270	-0.01117
7	2	5	3	←	6	1	5	3	7524.81780	-0.02810
9	3	6	3	←	8	3	5	2	7533.63996	0.03696
9	3	6	1	←	8	3	5	0	7535.26100	0.01915
9	3	6	0	←	8	3	5	1	7545.87765	0.00503
9	3	6	2	←	8	3	5	3	7546.02426	-0.00924
9	1	8	3	←	8	1	7	2	7574.22515	-0.03983
9	1	8	1	←	8	1	7	0	7575.84680	-0.03535
9	1	8	0	←	8	1	7	1	7592.35027	0.04618
9	1	8	2	←	8	1	7	3	7593.49951	0.05048
9	2	7	3	←	8	2	6	2	7648.88380	0.01259
9	2	7	1	←	8	2	6	0	7650.85890	-0.01246

4	4	0	1	←	3	3	0	1	7763.59010	0.02445
4	4	1	1	←	3	3	1	1	7763.69290	0.02476
4	4	0	0	←	3	3	0	0	7764.07200	-0.02176
4	4	1	0	←	3	3	1	0	7764.17640	-0.02147
4	4	0	3	←	3	3	0	3	7765.93740	0.02404
4	4	1	3	←	3	3	1	3	7766.03900	0.02405
4	4	0	2	←	3	3	0	2	7766.50200	-0.02937
4	4	1	2	←	3	3	1	2	7766.60480	-0.03001

Table S78 Measured frequencies and residuals (in MHz) for the rotational transitions of the ^{18}O singly-substituted isotopologue of the Phe-H_2O complex.

J'	K_a'	K_c'		←	J''	K_a''	K_c''		ν_{obs}	$\nu_{obs}-\nu_{calc}$
2	1	1	3	←	1	0	1	3	2308.2052	0.0298
2	1	1	1	←	1	0	1	1	2308.2052	-0.0099
2	1	1	0	←	1	0	1	0	2310.0962	0.0236
2	1	1	2	←	1	0	1	2	2310.3914	0.0311
3	1	3	0	←	2	1	2	1	2383.1900	-0.0105
3	1	3	1	←	2	1	2	0	2393.6156	0.0237
3	1	3	3	←	2	1	2	2	2394.4631	0.0286
3	0	3	2	←	2	0	2	3	2440.9848	-0.0092
3	0	3	0	←	2	0	2	1	2441.7148	-0.0025
3	0	3	1	←	2	0	2	0	2449.3408	0.0044
4	0	4	0	←	3	1	2	0	2502.4752	-0.0094
4	0	4	1	←	3	1	2	1	2502.8398	-0.0010
3	1	2	2	←	2	1	1	3	2514.7980	0.0083
3	1	2	0	←	2	1	1	1	2515.5102	0.0167
3	1	2	1	←	2	1	1	0	2520.7827	-0.0032
5	1	4	3	←	4	2	2	3	2538.3668	-0.0082
5	1	4	1	←	4	2	2	1	2540.6362	0.0035
6	2	5	2	←	6	0	6	3	2568.2291	-0.0692
6	1	6	0	←	5	2	4	0	2606.1255	-0.0019
6	1	6	3	←	5	2	4	3	2608.2912	0.1156
7	3	5	0	←	7	2	5	0	2846.7983	-0.0035
7	3	5	1	←	7	2	5	1	2847.5850	0.0050
7	3	5	2	←	7	2	5	2	2849.5414	0.0121
7	3	5	3	←	7	2	5	3	2850.4099	0.0111
6	3	4	0	←	6	2	4	0	2926.0446	0.0209
6	3	4	1	←	6	2	4	1	2927.2430	-0.0028
5	3	3	0	←	5	2	3	0	2979.3450	0.0152
5	3	3	1	←	5	2	3	1	2980.7680	-0.0008
5	3	3	2	←	5	2	3	2	2981.4217	0.0193
5	3	3	3	←	5	2	3	3	2983.0786	0.0107
4	3	1	0	←	4	2	3	0	3046.2530	-0.0145
4	3	1	1	←	4	2	3	1	3047.4672	0.0107
4	3	1	3	←	4	2	3	3	3049.4231	0.0123
5	3	2	0	←	5	2	4	0	3060.2840	0.0010
5	3	2	1	←	5	2	4	1	3061.1518	-0.0061
5	3	2	3	←	5	2	4	3	3063.0132	0.0018
6	3	3	0	←	6	2	5	0	3085.6463	0.0133

6	3	3	1	←	6	2	5	1	3086.2763	0.0000
6	3	3	2	←	6	2	5	2	3087.2339	0.0303
6	3	3	3	←	6	2	5	3	3087.9771	0.0020
9	3	7	2	←	8	4	5	2	3144.3990	0.0194
4	1	4	2	←	3	1	3	3	3177.0548	-0.0071
4	1	4	0	←	3	1	3	1	3177.7435	-0.0077
4	1	4	1	←	3	1	3	0	3186.2575	0.0081
4	1	4	3	←	3	1	3	2	3186.9457	0.0039
3	1	2	3	←	2	0	2	3	3191.2531	0.0047
3	1	2	1	←	2	0	2	1	3191.5950	0.0003
3	1	2	0	←	2	0	2	0	3194.6489	0.0234
3	1	2	2	←	2	0	2	2	3194.8346	0.0272
5	0	5	1	←	4	1	3	1	3195.7950	0.0053
4	0	4	2	←	3	0	3	3	3247.2970	0.0060
4	0	4	0	←	3	0	3	1	3247.7772	0.0034
4	0	4	1	←	3	0	3	0	3252.7199	0.0018
4	0	4	3	←	3	0	3	2	3252.9969	0.0008
7	1	7	2	←	6	2	5	2	3256.7616	-0.0386
7	1	7	0	←	6	2	5	0	3257.0196	-0.0049
7	1	7	1	←	6	2	5	1	3260.1565	-0.0015
7	1	7	3	←	6	2	5	3	3260.4520	-0.0300
4	2	3	2	←	3	2	2	3	3267.7018	-0.0124
4	2	3	0	←	3	2	2	1	3268.3522	0.0040
4	2	3	1	←	3	2	2	0	3273.8942	0.0055
4	2	3	3	←	3	2	2	2	3274.1084	0.0043
4	2	2	0	←	3	2	1	1	3291.3099	-0.0019
4	2	2	1	←	3	2	1	0	3296.3436	0.0054
4	1	3	2	←	3	1	2	3	3353.9765	0.0029
4	1	3	0	←	3	1	2	1	3354.3676	0.0093
4	1	3	3	←	3	1	2	2	3354.4981	-0.0089
4	1	3	1	←	3	1	2	0	3354.8897	-0.0102
6	1	5	1	←	5	2	3	1	3429.2528	0.0103
6	1	5	0	←	5	2	3	0	3432.7288	-0.0086
2	2	0	1	←	1	1	0	1	3440.3978	0.0239
2	2	0	0	←	1	1	0	0	3440.3978	-0.0389
2	2	0	3	←	1	1	0	3	3441.4574	0.0235
2	2	0	2	←	1	1	0	2	3441.4928	-0.0166
2	2	1	1	←	1	1	1	1	3481.0362	0.0052
2	2	1	0	←	1	1	1	0	3481.7091	-0.0013
2	2	1	3	←	1	1	1	3	3481.9550	0.0055
2	2	1	2	←	1	1	1	2	3482.7496	-0.0032
6	0	6	2	←	5	1	4	2	3840.1846	-0.0040
6	0	6	1	←	5	1	4	1	3843.0662	0.0015
5	1	5	2	←	4	1	4	3	3969.8806	0.0011
5	1	5	0	←	4	1	4	1	3970.3878	0.0022
5	1	5	1	←	4	1	4	0	3976.9229	-0.0035
5	1	5	3	←	4	1	4	2	3977.4601	-0.0138
5	0	5	2	←	4	0	4	3	4045.2622	0.0042
5	0	5	0	←	4	0	4	1	4045.5138	0.0084
5	0	5	1	←	4	0	4	0	4048.2090	0.0041
5	0	5	3	←	4	0	4	2	4048.3446	-0.0008

5	2	4	2	←	4	2	3	3	4084.9127	0.0097
5	2	4	0	←	4	2	3	1	4085.2468	0.0130
5	2	4	3	←	4	2	3	2	4086.5826	-0.0115
5	2	4	1	←	4	2	3	0	4086.7450	-0.0120
4	1	3	3	←	3	0	3	3	4099.4941	0.0081
4	1	3	1	←	3	0	3	1	4100.1949	0.0058
5	3	2	3	←	4	3	1	2	4101.6529	0.0656
5	3	2	1	←	4	3	1	0	4101.6529	0.0055
4	1	3	2	←	3	0	3	2	4104.2457	0.0178
4	1	3	0	←	3	0	3	0	4104.2457	0.0103
5	2	3	2	←	4	2	2	3	4129.5137	-0.0010
5	2	3	0	←	4	2	2	1	4130.0008	-0.0031
5	2	3	3	←	4	2	2	2	4130.1639	0.0022
5	2	3	1	←	4	2	2	0	4130.6022	-0.0019
5	1	4	3	←	4	1	3	2	4185.6267	0.0002
5	1	4	1	←	4	1	3	0	4186.4587	0.0000
5	1	4	2	←	4	1	3	3	4190.2548	-0.0050
5	1	4	0	←	4	1	3	1	4190.3490	0.0006
3	2	1	1	←	2	1	1	1	4224.4590	0.0073
3	2	1	0	←	2	1	1	0	4224.6284	-0.0037
3	2	1	3	←	2	1	1	3	4225.5023	0.0020
3	2	1	2	←	2	1	1	2	4225.7045	-0.0030
7	4	4	1	←	7	3	4	1	4226.3362	-0.0066
7	4	4	3	←	7	3	4	3	4229.2063	-0.0014
7	4	3	0	←	7	3	5	2	4231.7059	0.0022
7	1	6	1	←	6	2	4	1	4300.2443	-0.0056
7	1	6	0	←	6	2	4	0	4302.5450	0.0132
3	2	2	1	←	2	1	2	1	4341.9284	-0.0073
3	2	2	3	←	2	1	2	3	4342.5928	-0.0061
3	2	2	0	←	2	1	2	0	4343.7966	0.0094
3	2	2	2	←	2	1	2	2	4344.7862	0.0078
6	1	6	2	←	5	1	5	3	4760.4366	-0.0027
6	1	6	0	←	5	1	5	1	4760.7698	0.0024
6	1	6	1	←	5	1	5	0	4765.4857	-0.0101
6	1	6	3	←	5	1	5	2	4765.8966	-0.0243
6	0	6	0	←	5	0	5	1	4834.3406	-0.0055
6	0	6	1	←	5	0	5	0	4835.5394	0.0039
6	0	6	3	←	5	0	5	2	4835.6274	-0.0063
6	2	5	3	←	5	2	4	2	4897.3983	-0.0137
6	2	5	1	←	5	2	4	0	4897.8927	-0.0116
6	2	5	2	←	5	2	4	3	4899.9331	-0.0065
6	2	5	0	←	5	2	4	1	4900.0042	0.0067
6	4	3	2	←	5	4	2	3	4915.4885	0.0151
6	4	2	2	←	5	4	1	3	4915.5597	0.0100
6	4	3	0	←	5	4	2	1	4915.9945	0.0049
6	4	2	0	←	5	4	1	1	4916.0740	0.0072
6	3	4	1	←	5	3	3	0	4919.6118	-0.0101
6	3	4	2	←	5	3	3	3	4919.9110	0.0023
6	3	4	0	←	5	3	3	1	4920.2117	-0.0002
6	3	3	3	←	5	3	2	2	4923.3871	-0.0198
6	3	3	1	←	5	3	2	0	4923.8821	-0.0156

6	3	3	2	←	5	3	2	3	4924.1613	0.0293
6	3	3	0	←	5	3	2	1	4924.4856	0.0130
6	2	4	0	←	5	2	3	3	4966.3399	-0.0022
6	2	4	3	←	5	2	3	2	4970.7978	0.0000
6	2	4	1	←	5	2	3	0	4971.7090	0.0032
6	2	4	2	←	5	2	3	3	4974.6078	-0.0018
6	2	4	0	←	5	2	3	1	4974.9445	-0.0127
4	2	2	1	←	3	1	2	1	5000.1896	0.0053
4	2	2	0	←	3	1	2	0	5000.2683	-0.0018
4	2	2	3	←	3	1	2	3	5001.2292	0.0042
4	2	2	2	←	3	1	2	2	5001.3080	-0.0021
6	1	5	3	←	5	1	4	2	5013.7281	0.0093
6	1	5	1	←	5	1	4	0	5014.8781	0.0097
6	1	5	0	←	5	1	4	1	5022.0919	-0.0168
6	1	5	2	←	5	1	4	3	5022.2194	-0.0150
5	1	4	3	←	4	0	4	3	5036.8705	0.0122
5	1	4	1	←	4	0	4	1	5037.9849	0.0087
5	1	4	2	←	4	0	4	2	5042.4469	-0.0079
5	1	4	0	←	4	0	4	0	5042.7516	-0.0119
4	2	3	1	←	3	1	3	1	5224.0715	-0.0123
4	2	3	3	←	3	1	3	3	5224.4361	-0.0117
4	2	3	0	←	3	1	3	0	5227.0949	0.0115
4	2	3	2	←	3	1	3	2	5227.9859	0.0134
3	3	0	1	←	2	2	0	1	5492.4792	0.0118
3	3	0	0	←	2	2	0	0	5492.7762	-0.0101
3	3	0	3	←	2	2	0	3	5494.1906	0.0160
3	3	0	2	←	2	2	0	2	5494.5389	-0.0158
3	3	1	1	←	2	2	1	1	5494.6938	0.0123
3	3	1	0	←	2	2	1	0	5495.0268	-0.0101
3	3	1	3	←	2	2	1	3	5496.3903	0.0157
3	3	1	2	←	2	2	1	2	5496.7793	-0.0174
7	1	7	2	←	6	1	6	3	5548.5650	0.0005
7	1	7	0	←	6	1	6	1	5548.7317	0.0000
7	1	7	1	←	6	1	6	0	5551.9284	-0.0066
7	1	7	3	←	6	1	6	2	5552.2493	-0.0203
7	0	7	0	←	6	0	6	1	5615.2216	-0.0034
7	0	7	2	←	6	0	6	3	5615.3237	-0.0034
7	0	7	1	←	6	0	6	0	5615.6371	-0.0021
7	0	7	3	←	6	0	6	2	5615.7554	-0.0159
7	2	6	3	←	6	2	5	2	5706.4506	0.0169
7	2	6	1	←	6	2	5	0	5707.1859	0.0124
7	2	6	0	←	6	2	5	1	5712.0673	-0.0129
7	2	6	2	←	6	2	5	3	5712.2171	-0.0165
7	3	4	3	←	6	3	3	2	5748.8921	-0.0162
7	3	4	1	←	6	3	3	0	5749.7423	-0.0098
7	3	4	2	←	6	3	3	3	5753.2243	0.0144
7	3	4	0	←	6	3	3	1	5753.4210	-0.0022
5	2	3	0	←	4	1	3	0	5775.8202	-0.0098
5	2	3	1	←	4	1	3	1	5775.9756	0.0013
5	2	3	2	←	4	1	3	2	5776.7585	-0.0077
5	2	3	3	←	4	1	3	3	5776.9627	-0.0021

7	2	5	3	←	6	2	4	2	5817.4069	-0.0045
7	2	5	1	←	6	2	4	0	5818.6733	0.0083
7	2	5	2	←	6	2	4	3	5823.9972	-0.0886
7	2	5	0	←	6	2	4	1	5824.4085	-0.0111
7	1	6	3	←	6	1	5	2	5837.9248	0.0081
7	1	6	1	←	6	1	5	0	5839.2282	0.0099
7	1	6	0	←	6	1	5	1	5848.2351	-0.0113
7	1	6	2	←	6	1	5	3	5848.4702	-0.0054
6	1	5	3	←	5	0	5	3	6007.8449	0.0167
6	1	5	1	←	5	0	5	1	6009.4359	0.0088
6	1	5	2	←	5	0	5	2	6013.8341	-0.0007
6	1	5	0	←	5	0	5	0	6014.5676	-0.0118
5	2	4	1	←	4	1	4	1	6127.5892	-0.0019
5	2	4	3	←	4	1	4	3	6127.5892	-0.0356
5	2	4	0	←	4	1	4	0	6131.5727	0.0063
5	2	4	2	←	4	1	4	2	6132.2995	0.0106
4	3	1	1	←	3	2	1	1	6306.1251	0.0014
4	3	1	0	←	3	2	1	0	6306.8320	0.0030
4	3	1	3	←	3	2	1	3	6307.7648	0.0008
4	3	1	2	←	3	2	1	2	6308.5945	0.0013
4	3	2	1	←	3	2	2	1	6317.0141	0.0027
4	3	2	0	←	3	2	2	0	6317.8704	0.0000
4	3	2	3	←	3	2	2	3	6318.5898	0.0042
4	3	2	2	←	3	2	2	2	6319.5926	0.0012
8	1	8	2	←	7	1	7	3	6334.2832	0.0275
8	1	8	1	←	7	1	7	0	6336.3103	-0.0040
8	1	8	3	←	7	1	7	2	6336.5751	-0.0160
8	0	8	0	←	7	0	7	1	6390.2729	0.0030
8	0	8	1	←	7	0	7	0	6390.4123	-0.0102
8	0	8	2	←	7	0	7	3	6390.4806	0.0043
8	0	8	3	←	7	0	7	2	6390.6066	-0.0172
8	2	7	3	←	7	2	6	2	6513.4821	0.0222
8	2	7	1	←	7	2	6	0	6514.3611	0.0122
8	2	7	0	←	7	2	6	1	6521.0194	-0.0187
8	2	7	2	←	7	2	6	3	6521.3034	-0.0224
6	2	4	0	←	5	1	4	0	6560.5806	-0.0026
6	2	4	1	←	5	1	4	1	6561.0790	0.0018
6	2	4	2	←	5	1	4	2	6561.3217	0.0071
6	2	4	3	←	5	1	4	3	6561.9340	-0.0036
8	1	7	3	←	7	1	6	2	6656.9024	-0.0496
8	1	7	1	←	7	1	6	0	6658.2222	-0.0123
8	1	7	0	←	7	1	6	1	6667.4250	0.0119
8	1	7	2	←	7	1	6	3	6667.6691	0.0238
8	2	6	3	←	7	2	5	2	6667.7865	-0.0233
8	2	6	1	←	7	2	5	0	6669.2254	-0.0102
8	2	6	0	←	7	2	5	1	6675.6484	0.0093
7	1	6	3	←	6	0	6	3	7016.1290	0.0112
7	1	6	1	←	6	0	6	1	7018.2599	-0.0024
7	1	6	2	←	6	0	6	2	7022.0214	0.0157
7	1	6	0	←	6	0	6	0	7023.3236	-0.0038
6	2	5	3	←	5	1	5	3	7052.2339	0.0070

6	2	5	1	←	5	1	5	1	7052.5419	-0.0023
6	2	5	0	←	5	1	5	0	7057.1938	-0.0092
6	2	5	2	←	5	1	5	2	7057.6831	-0.0019
5	3	2	1	←	4	2	2	1	7112.1311	-0.0070
5	3	2	0	←	4	2	2	0	7112.8796	0.0076
5	3	2	3	←	4	2	2	3	7113.7744	-0.0040
5	3	2	2	←	4	2	2	2	7114.6497	0.0129
9	1	9	0	←	8	1	8	1	7117.5854	-0.0005
9	1	9	2	←	8	1	8	3	7117.6682	0.0011
9	1	9	1	←	8	1	8	0	7118.7890	0.0106
9	1	9	3	←	8	1	8	2	7119.0411	0.0179
5	3	3	1	←	4	2	3	1	7144.0181	0.0003
5	3	3	0	←	4	2	3	0	7145.1091	-0.0014
5	3	3	3	←	4	2	3	3	7145.4766	0.0006
5	3	3	2	←	4	2	3	2	7146.7524	0.0082
9	0	9	0	←	8	0	8	1	7161.9963	0.0095
9	0	9	1	←	8	0	8	0	7162.1120	-0.0003
9	0	9	2	←	8	0	8	3	7162.2700	0.0062
9	0	9	3	←	8	0	8	2	7162.3854	0.0073
9	2	8	1	←	8	2	7	0	7319.1666	0.0113
9	2	8	0	←	8	2	7	1	7326.5589	-0.0159
9	2	8	2	←	8	2	7	3	7326.8947	-0.0281
9	1	8	3	←	8	1	7	2	7469.2201	-0.0070
9	1	8	1	←	8	1	7	0	7470.3289	-0.0257
9	1	8	0	←	8	1	7	1	7478.4491	0.0308
9	1	8	2	←	8	1	7	3	7478.6357	0.0347
9	1	8	2	←	8	1	7	3	7478.6357	0.0347
9	2	7	3	←	8	2	6	2	7519.0801	0.0315
9	2	7	1	←	8	2	6	0	7520.4969	0.0199
9	2	7	0	←	8	2	6	1	7525.7232	-0.0030
4	4	0	1	←	3	3	0	1	7527.2999	0.0069
4	4	1	1	←	3	3	1	1	7527.3783	0.0104
4	4	0	0	←	3	3	0	0	7527.5986	-0.0260
4	4	1	0	←	3	3	1	0	7527.6770	-0.0228
4	4	0	3	←	3	3	0	3	7529.7090	0.0110
4	4	1	3	←	3	3	1	3	7529.7872	0.0150
4	4	0	2	←	3	3	0	2	7530.0598	-0.0340
4	4	1	2	←	3	3	1	2	7530.1385	-0.0300

Table S79 Measured frequencies and residuals (in MHz) for the rotational transitions of the Phe-$(H_2O)_2$ complex.

J'	K_a'	K_c'	←	J''	K_a''	K_c''	ν_{obs}	ν_{obs}-ν_{calc}
3	0	3	←	2	1	2	2068.0567	0.0061
3	1	3	←	2	0	2	2122.1452	-0.0041
2	2	1	←	1	1	0	2135.8093	-0.0028
2	2	0	←	1	1	0	2236.8613	0.0002
2	2	1	←	1	1	1	2313.3831	0.0031
2	2	0	←	1	1	1	2414.4329	0.0041
4	0	4	←	3	1	3	2710.4892	0.0009

4	1	4	←	3	0	3	2723.2702	0.0001
3	2	2	←	2	1	1	2757.3977	0.0019
4	1	3	←	3	2	2	3043.3405	-0.0056
3	1	2	←	2	0	2	3144.1124	0.0027
3	2	1	←	2	1	1	3144.4151	0.0027
3	2	2	←	2	1	2	3290.0989	-0.0001
4	2	3	←	3	1	2	3300.8593	-0.0029
5	0	5	←	4	1	4	3336.8826	0.0026
5	1	5	←	4	0	4	3339.4068	0.0001
3	3	1	←	2	2	0	3392.6415	-0.0021
3	3	0	←	2	2	0	3436.0875	-0.0025
3	3	1	←	2	2	1	3493.6938	0.0013
3	3	0	←	2	2	1	3537.1360	-0.0029
5	1	4	←	4	2	3	3759.6711	-0.0024
5	2	4	←	4	1	3	3845.9005	-0.0011
5	2	3	←	4	3	2	3872.8893	0.0115
6	0	6	←	5	1	5	3959.3525	-0.0027
6	1	6	←	5	0	5	3959.8110	0.0027
4	3	2	←	3	2	1	4034.6760	-0.0059
4	2	2	←	3	1	2	4147.9563	-0.0022
4	3	1	←	3	2	1	4268.2334	-0.0016
4	2	3	←	3	1	3	4322.8247	0.0021
10	2	9	←	10	1	10	4347.7302	0.0059
6	1	5	←	5	2	4	4411.2365	0.0002
4	3	2	←	3	2	2	4421.7008	0.0022
6	2	5	←	5	1	4	4433.4688	0.0021
7	0	7	←	6	1	6	4581.0565	0.0055
7	1	7	←	6	0	6	4581.1349	0.0075
4	4	1	←	3	3	0	4647.2523	0.0037
4	3	1	←	3	2	2	4655.2544	0.0027
4	4	0	←	3	3	0	4662.6722	0.0034
4	4	1	←	3	3	1	4690.6826	-0.0123
4	4	0	←	3	3	1	4706.1126	-0.0025
6	2	4	←	5	3	3	4736.2230	-0.0061
7	1	6	←	6	2	5	5040.1100	-0.0068
7	2	6	←	6	1	5	5045.0105	-0.0009
6	3	4	←	5	2	3	5045.6644	-0.0027
5	3	2	←	4	2	2	5190.2236	-0.0010
8	0	8	←	7	1	7	5202.6216	0.0052
8	1	8	←	7	0	7	5202.6227	-0.0060
5	2	3	←	4	1	3	5251.2231	-0.0071
5	1	4	←	4	0	4	5372.0038	-0.0040
5	2	4	←	4	1	4	5388.0298	0.0035
5	3	3	←	4	2	3	5411.3031	0.0034
5	4	1	←	4	3	1	5459.2924	-0.0042
7	2	5	←	6	3	4	5461.4330	0.0008
7	3	5	←	6	2	4	5565.3912	-0.0045
5	4	2	←	4	3	2	5578.8959	-0.0016
8	2	7	←	7	1	6	5663.9383	-0.0123
5	4	1	←	4	3	2	5692.8561	0.0063
9	0	9	←	8	1	8	5824.1644	-0.0004

9	1	9	←	8	0	8	5824.1644	-0.0023
5	5	1	←	4	4	0	5883.2698	0.0045
5	5	1	←	4	4	0	5883.2698	0.0045
5	5	0	←	4	4	0	5888.1632	0.0036
6	4	3	←	5	3	2	5896.0775	0.0133
5	5	1	←	4	4	1	5898.6841	-0.0014
5	5	0	←	4	4	1	5903.5775	-0.0023
8	2	6	←	7	3	5	6115.8684	-0.0035
8	3	6	←	7	2	5	6143.9689	0.0022
6	3	3	←	5	3	4	6225.6301	-0.0028
6	3	3	←	5	2	3	6225.6376	0.0046
9	1	8	←	8	2	7	6284.5626	-0.0017
9	2	8	←	8	1	7	6284.7496	0.0029
6	4	2	←	5	3	2	6294.6992	0.0024
7	4	4	←	6	3	3	6343.8850	0.0048
6	2	4	←	5	1	4	6387.8476	-0.0076
8	3	5	←	7	4	4	6445.0560	-0.0004
10	0	10	←	9	1	9	6445.7175	0.0060
10	1	10	←	9	0	9	6445.7175	0.0057
6	3	4	←	5	2	4	6450.9982	0.0025
6	1	5	←	5	0	5	6462.3749	-0.0077
6	2	5	←	5	1	5	6466.0706	0.0028
6	4	3	←	5	3	3	6522.0901	0.0047
6	5	2	←	5	4	1	6646.0853	0.0030
6	5	2	←	5	4	1	6646.0853	0.0030
6	5	1	←	5	4	1	6692.4631	-0.0023
9	2	7	←	8	3	6	6745.2781	0.0025
9	3	7	←	8	2	6	6751.8907	0.0076
6	5	2	←	5	4	2	6760.0329	-0.0016
8	4	5	←	7	3	4	6778.1572	0.0082
6	5	1	←	5	4	2	6806.4150	-0.0026
6	4	2	←	5	3	3	6920.7156	-0.0023
5	3	3	←	4	0	4	7023.6343	0.0004
11	1	11	←	10	0	10	7067.2615	0.0053
11	0	11	←	10	1	10	7067.2619	0.0058
6	6	1	←	5	5	0	7107.2280	0.0003
6	6	0	←	5	5	0	7108.6762	-0.0024
6	6	1	←	5	5	1	7112.1245	0.0025
6	6	0	←	5	5	1	7113.5723	-0.0006
7	4	3	←	6	3	3	7238.4430	-0.0045
9	4	6	←	8	3	5	7281.8250	-0.0039
7	3	4	←	6	2	4	7358.9405	0.0150
7	3	4	←	6	3	5	7358.9419	0.0164
10	2	8	←	9	3	7	7367.8451	-0.0098
10	3	8	←	9	2	7	7369.2672	-0.0039
7	5	2	←	6	4	2	7474.6630	-0.0045
7	5	2	←	6	4	2	7474.6630	-0.0045
7	2	5	←	6	1	5	7501.1897	-0.0018
7	3	5	←	6	2	5	7519.7745	-0.0098
7	4	4	←	6	3	4	7523.8460	0.0000
11	2	10	←	10	1	9	7527.3739	-0.0149

11	1	10	←	10	2	9	7527.3741	-0.0092
7	1	6	←	6	0	6	7546.8243	-0.0050
7	2	6	←	6	1	6	7547.5875	0.0016
7	5	3	←	6	4	3	7661.0491	0.0039
12	0	12	←	11	1	11	7688.7897	-0.0072
12	1	12	←	11	0	11	7688.8026	0.0056
7	5	2	←	6	4	3	7873.2884	-0.0117
7	6	2	←	6	5	1	7912.4958	0.0000
7	6	1	←	6	5	1	7929.1871	0.0022
7	6	2	←	6	5	2	7958.8747	-0.0042
7	6	1	←	6	5	2	7975.5659	-0.0020
11	2	9	←	10	3	8	7989.0434	0.0156
11	3	9	←	10	2	8	7989.3123	0.0007

Table S80 Measured frequencies and residuals (in MHz) for the rotational transitions of the (1) ^{18}O singly-substituted isotopologue of the Phe-$(H_2O)_2$ complex.

J'	K_a'	K_c'	←	J''	K_a''	K_c''	ν_{obs}	ν_{obs}-ν_{calc}
3	1	3	←	2	0	2	2102.9338	-0.0044
4	0	4	←	3	1	3	2691.9667	0.0015
4	1	4	←	3	0	3	2702.7060	0.0021
3	2	2	←	2	1	1	2714.2440	-0.0010
4	1	3	←	3	2	2	3028.5878	-0.0075
3	2	2	←	2	1	2	3239.9786	-0.0010
3	2	2	←	2	1	2	3239.9786	-0.0020
4	2	3	←	3	1	2	3256.7617	-0.0008
5	0	5	←	4	1	4	3314.1877	-0.0014
5	1	5	←	4	0	4	3316.2158	0.0028
3	3	1	←	2	2	0	3325.5436	-0.0098
3	3	1	←	2	2	1	3428.1078	0.0036
3	3	0	←	2	2	1	3473.9148	0.0056
5	1	4	←	4	2	3	3731.5047	0.0003
5	2	4	←	4	1	3	3804.3783	0.0017
6	0	6	←	5	1	5	3933.0520	-0.0019
6	1	6	←	5	0	5	3933.4054	0.0055
4	3	2	←	3	2	1	3962.0880	0.0010
4	3	1	←	3	2	1	4203.9402	-0.0018
4	1	3	←	3	0	3	4213.2965	-0.0012
4	2	3	←	3	1	3	4262.4301	0.0043
4	3	2	←	3	2	2	4350.9255	-0.0027
6	1	5	←	5	2	4	4375.1803	-0.0002
6	2	5	←	5	1	4	4393.0618	0.0038
5	3	3	←	4	2	2	4489.1469	0.0013
7	0	7	←	6	1	6	4551.2801	-0.0049
7	1	7	←	6	0	6	4551.3156	-0.0250
4	4	1	←	3	3	1	4600.1778	-0.0025
4	4	0	←	3	3	1	4617.1064	0.0017
6	2	4	←	5	3	3	4709.6415	-0.0093
6	3	4	←	5	2	3	4974.1381	-0.0015
7	1	6	←	6	2	5	4999.1953	0.0050

7	2	6	←	6	1	5	5002.9444	0.0049
5	3	2	←	4	2	2	5126.4795	0.0026
8	1	8	←	7	0	7	5169.4205	-0.0046
8	0	8	←	7	1	7	5169.4205	0.0039
5	4	2	←	4	3	1	5243.0432	0.0059
5	1	4	←	4	0	4	5301.9667	0.0025
5	3	3	←	4	2	3	5333.7089	0.0065
5	4	1	←	4	3	1	5365.9372	-0.0025
7	2	5	←	6	3	4	5417.0342	0.0042
5	4	2	←	4	3	2	5484.8901	0.0008
7	3	5	←	6	2	4	5501.3677	-0.0004
5	4	1	←	4	3	2	5607.7926	0.0009
8	1	7	←	7	2	6	5618.2617	0.0005
8	2	7	←	7	1	6	5618.9762	0.0020
5	5	1	←	4	4	0	5765.7628	-0.0007
5	5	0	←	4	4	0	5771.3575	0.0048
5	5	1	←	4	4	1	5782.6843	-0.0041
6	4	3	←	5	3	2	5786.9339	-0.0043
9	1	9	←	8	0	8	5787.5373	-0.0003
9	0	9	←	8	1	8	5787.5373	0.0009
5	5	0	←	4	4	1	5788.2825	0.0037
8	3	6	←	7	2	5	6083.5255	-0.0032
6	3	3	←	5	2	3	6159.4623	-0.0058
6	4	2	←	5	3	2	6206.0713	0.0000
6	3	4	←	5	2	4	6363.8235	0.0017
6	1	5	←	5	0	5	6375.9688	0.0064
10	0	10	←	9	1	9	6405.6605	0.0059
10	1	10	←	9	0	9	6405.6608	0.0060
6	4	3	←	5	3	3	6424.2688	0.0032
6	5	2	←	5	4	2	6640.8754	-0.0039
8	4	5	←	7	3	4	6679.1577	0.0046
9	2	7	←	8	3	6	6685.8894	0.0003
9	3	7	←	8	2	6	6690.7370	0.0032
6	5	1	←	5	4	2	6693.1210	-0.0064
6	6	1	←	5	5	0	6965.0028	0.0002
6	6	0	←	5	5	0	6966.7203	-0.0013
6	6	1	←	5	5	1	6970.5841	-0.0035
6	6	0	←	5	5	1	6972.3123	-0.0034
11	1	11	←	10	0	10	7023.7643	-0.0061
11	0	11	←	10	1	10	7023.7643	-0.0061
7	4	3	←	6	3	3	7154.6669	-0.0074
9	4	6	←	8	3	5	7195.5075	-0.0053
7	5	2	←	6	4	2	7353.8003	0.0081
7	5	3	←	6	4	3	7539.8855	0.0050
12	0	12	←	11	1	11	7641.8713	-0.0056
7	6	2	←	6	5	1	7761.5035	-0.0031

Table S81 Measured frequencies and residuals (in MHz) for the rotational transitions of the (2) ^{18}O singly-substituted isotopologue of the Phe-$(H_2O)_2$ complex.

J'	K_a'	K_c'	←	J''	K_a''	K_c''	ν_{obs}	ν_{obs}-ν_{calc}

3	0	3	←	2	1	2	2039.6638	0.0016
2	2	0	←	1	1	0	2179.8788	0.0053
4	0	4	←	3	1	3	2664.0597	0.0005
4	1	4	←	3	0	3	2671.1864	-0.0018
3	2	2	←	2	1	1	2674.5387	-0.0048
3	2	1	←	2	1	1	3100.1580	0.0101
3	1	2	←	2	0	2	3119.1045	0.0107
4	2	3	←	3	1	2	3210.0543	-0.0013
3	2	2	←	2	1	2	3224.6356	0.0036
3	3	1	←	2	2	0	3273.2007	-0.0009
5	0	5	←	4	1	4	3276.7825	-0.0132
5	1	5	←	4	0	4	3277.9670	-0.0015
3	3	0	←	2	2	0	3330.1583	-0.0132
3	3	1	←	2	2	1	3388.5208	0.0045
3	3	0	←	2	2	1	3445.4910	0.0003
5	1	4	←	4	2	3	3710.9901	-0.0062
5	2	4	←	4	1	3	3760.0225	-0.0073
6	0	6	←	5	1	5	3887.1746	-0.0080
6	1	6	←	5	0	5	3887.3546	-0.0030
4	3	2	←	3	2	1	3897.8551	-0.0058
4	3	1	←	3	2	1	4183.5232	-0.0017
4	3	2	←	3	2	2	4323.4679	0.0010
6	1	5	←	5	2	4	4338.4640	0.0019
6	2	5	←	5	1	4	4348.9145	-0.0008
5	3	3	←	4	2	2	4412.8847	0.0051
4	4	1	←	3	3	0	4485.0804	0.0023
7	0	7	←	6	1	6	4497.1801	-0.0099
7	1	7	←	6	0	6	4497.2089	-0.0057
4	4	0	←	3	3	0	4508.5405	0.0053
4	4	1	←	3	3	1	4542.0423	-0.0055
4	4	0	←	3	3	1	4565.5036	-0.0058
6	3	3	←	5	4	2	4677.5995	-0.0033
6	2	4	←	5	3	3	4716.9120	-0.0100
7	2	6	←	6	1	5	4953.7139	-0.0031
8	0	8	←	7	1	7	5107.1513	0.0028
8	1	8	←	7	0	7	5107.1513	-0.0004
5	3	2	←	4	2	2	5132.4673	-0.0029
5	1	4	←	4	0	4	5300.1990	-0.0019
5	4	1	←	4	3	1	5316.3870	-0.0044
5	3	3	←	4	2	3	5318.2776	0.0017
7	2	5	←	6	3	4	5389.6421	0.0114
7	3	5	←	6	2	4	5439.9286	-0.0031
5	4	2	←	4	3	2	5440.7056	0.0018
8	1	7	←	7	2	6	5562.1350	-0.0018
8	2	7	←	7	1	6	5562.4548	0.0012
5	4	1	←	4	3	2	5602.0619	0.0036
5	5	1	←	4	4	0	5681.7634	-0.0014
5	5	1	←	4	4	0	5681.7637	-0.0027
5	5	0	←	4	4	0	5690.3917	0.0027
5	5	1	←	4	4	1	5705.2224	-0.0016
5	5	0	←	4	4	1	5713.8468	-0.0030

9	0	9	←	8	1	8	5717.1077	0.0052
9	1	9	←	8	0	8	5717.1077	0.0048
8	2	6	←	7	3	5	6015.4685	0.0065
9	2	8	←	8	1	7	6172.0344	-0.0056
6	3	3	←	5	2	3	6191.1063	0.0081
6	2	4	←	5	1	4	6324.1958	-0.0025
10	0	10	←	9	1	9	6327.0551	0.0000
10	1	10	←	9	0	9	6327.0551	0.0000
6	3	4	←	5	2	4	6356.3582	0.0068
6	1	5	←	5	0	5	6369.6576	-0.0074
6	2	5	←	5	1	5	6371.1499	0.0022
6	4	3	←	5	3	3	6396.9216	0.0061
6	5	1	←	5	4	1	6492.3569	-0.0093
9	2	7	←	8	3	6	6628.0731	0.0029
6	5	1	←	5	4	2	6653.7171	-0.0008
10	2	9	←	9	1	8	6781.8240	-0.0020
6	6	0	←	5	5	1	6876.9339	0.0037
11	0	11	←	10	1	10	6937.0075	0.0029
11	1	11	←	10	0	10	6937.0075	0.0029
7	4	3	←	6	3	3	7177.2505	-0.0050
7	5	2	←	6	4	2	7300.3805	0.0015
7	2	5	←	6	1	5	7407.5103	-0.0095
7	4	4	←	6	3	4	7407.8764	-0.0021
8	5	4	←	7	4	3	7409.8807	0.0007
7	5	3	←	6	4	3	7494.7393	0.0017
12	0	12	←	11	1	11	7546.9485	-0.0007
7	6	2	←	6	5	1	7651.0375	0.0002
7	6	1	←	6	5	2	7760.6046	-0.0016

Table S82 Measured frequencies and residuals (in MHz) for the rotational transitions of the Phe-$(H_2O)_3$ complex.

J'	K_a'	K_c'	←	J''	K_a''	K_c''	ν_{obs}	ν_{obs}-ν_{calc}
3	1	3	←	2	0	2	2173.0324	-0.0082
3	1	2	←	2	0	2	2617.1497	0.0061
4	1	4	←	3	0	3	2780.1573	0.0004
3	2	1	←	2	1	1	2819.7769	0.0073
3	2	2	←	2	1	2	2960.2065	0.0015
3	3	1	←	2	2	0	3300.5453	-0.0020
3	3	0	←	2	2	0	3303.2820	-0.0018
3	3	1	←	2	2	1	3318.2885	-0.0103
3	3	0	←	2	2	1	3321.0404	0.0050
4	2	3	←	3	1	2	3343.4461	0.0042
5	1	5	←	4	0	4	3396.3390	-0.0013
4	1	3	←	3	0	3	3506.3856	-0.0060
4	2	2	←	3	1	2	3563.8932	0.0008
4	2	3	←	3	1	3	3787.5452	0.0004
5	2	4	←	4	1	3	3919.3755	-0.0036
4	3	2	←	3	2	1	3983.6610	-0.0082
6	0	6	←	5	1	5	4000.4636	-0.0016
4	3	1	←	3	2	1	4002.1639	-0.0028

6	1	6	←	5	0	5	4025.2488	-0.0017
4	3	2	←	3	2	2	4066.6535	0.0000
4	3	1	←	3	2	2	4085.1580	0.0069
5	2	3	←	4	1	3	4356.4230	0.0037
6	2	5	←	5	1	4	4481.3492	0.0022
4	4	1	←	3	3	0	4488.8447	-0.0032
4	4	0	←	3	3	0	4489.1972	0.0013
4	4	1	←	3	3	1	4491.5810	-0.0034
4	4	0	←	3	3	1	4491.9313	-0.0010
5	2	4	←	4	1	4	4645.6136	-0.0003
7	0	7	←	6	1	6	4652.6515	0.0041
7	1	7	←	6	0	6	4662.7480	0.0057
5	3	2	←	4	2	2	4686.6178	-0.0017
5	3	3	←	4	2	3	4838.2158	0.0023
7	2	6	←	6	1	5	5051.3175	-0.0003
5	4	2	←	4	3	1	5203.0828	0.0015
5	4	1	←	4	3	1	5206.1450	0.0022
6	2	4	←	5	1	4	5206.4600	0.0049
5	4	2	←	4	3	2	5221.5744	-0.0043
5	4	1	←	4	3	2	5224.6394	-0.0008
8	0	8	←	7	1	7	5300.6499	-0.0011
8	1	8	←	7	0	7	5304.5865	0.0019
6	3	3	←	5	2	3	5383.2567	0.0006
6	1	5	←	5	0	5	5406.6512	0.0016
6	2	5	←	5	1	5	5529.5514	0.0024
6	3	4	←	5	2	4	5638.1882	-0.0006
8	2	7	←	7	1	6	5643.7570	0.0030
5	5	1	←	4	4	0	5669.6921	0.0319
5	5	0	←	4	4	0	5669.6921	-0.0079
5	5	1	←	4	4	1	5670.0310	0.0229
5	5	0	←	4	4	1	5670.0310	-0.0170
6	4	3	←	5	3	2	5891.0976	0.0053
6	4	2	←	5	3	2	5905.7876	-0.0019
9	0	9	←	8	1	8	5946.8616	-0.0058
9	1	9	←	8	0	8	5948.3463	-0.0055
6	4	3	←	5	3	3	5959.9490	0.0002
6	4	2	←	5	3	3	5974.6415	-0.0045
7	2	5	←	6	1	5	6118.2010	-0.0066
7	3	4	←	6	2	4	6121.8247	-0.0002
9	2	8	←	8	1	7	6258.6394	-0.0037
7	1	6	←	6	0	6	6367.3436	-0.0047
6	5	2	←	5	4	1	6392.5741	0.0047
6	5	1	←	5	4	1	6393.0059	0.0049
6	5	2	←	5	4	2	6395.6173	-0.0135
6	5	1	←	5	4	2	6396.0672	0.0048
7	2	6	←	6	1	6	6432.7222	0.0053
7	3	5	←	6	2	5	6468.8014	-0.0047
7	4	3	←	6	3	3	6581.8565	0.0006
10	0	10	←	9	1	9	6592.3698	0.0056
10	1	10	←	9	0	9	6592.9118	0.0007
7	4	4	←	6	3	4	6713.6615	-0.0087

6	6	1	←	5	5	0	6849.2106	0.0207
6	6	0	←	5	5	0	6849.2106	0.0164
6	6	1	←	5	5	1	6849.2106	-0.0192
6	6	0	←	5	5	1	6849.2106	-0.0235
8	3	5	←	7	2	5	6920.2566	0.0024
7	5	3	←	6	4	2	7107.4832	-0.0001
7	5	2	←	6	4	2	7109.9972	-0.0031
7	5	3	←	6	4	3	7122.1827	0.0020
7	5	2	←	6	4	3	7124.7038	0.0061
8	4	4	←	7	3	4	7246.7269	0.0029
8	3	6	←	7	2	6	7328.9663	0.0005
8	4	5	←	7	3	5	7489.9561	0.0020
7	6	1	←	6	5	1	7573.8504	-0.0061
7	6	2	←	6	5	2	7574.2333	0.0002

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