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

Supporting Information

Gas-phase hydration of nopinone: the interplay between theoretical methods and experiments unveils the conformational landscape

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Tables of parameters of all observed conformers

Table S1

Monohydrate Conf. 1w(i)

Constants	Exp.	M06-2X/ 6-311++G(2df,p)	MP2/ 6- 311++G(d,p)	wB97X-D/ 6-311++G(d,p)	B3LYP-D3/ 6-311++G(2df,p)
A/MHz	1322.42948(26)	1334.7	1327.9	1328	1323
B/MHz	1005.490818(68)	1075.6	1037.6	1038	1038
C/MHz	756.541470(46)	797.2	774.2	774	773
D_J/kHz	0.30252(48)	0.2093	0.23643	-	0.14935
D_{JK}/kHz	-0.0376(24)	-0.1954	-0.1709	-	0.1671
D_K/kHz	-0.166(16)	0.059	-0.025	-	-0.201
d_1/kHz	-0.08892(24)	0.0188	-0.0424	-	-0.04169
d_2/*kHz*	-0.00518(20)	0.02145	0.01941	-	-0.00591
Std/kHz	1.2	-	-	-	-
Δ/amu.Å^2	-216.8	-214.6	-215	-214.5	-215.1
ΔE/kJoule.mol^{-1}	-	0	0	0	0
kappa	-0.12	0.04	-0.05	-0.05	-0.04
$\lvert\mu_a\rvert$/ D	Y	2.1	2.7	2.0	2.5
$\lvert\mu_b\rvert$/ D	Y	0.6	0.5	0.5	0.3
$\lvert\mu_c\rvert$/ D	N	0.1	0.2	0.1	0.05

N = **82**
J_{max} = 11
$K_{a\ max}$ = 7

Table S2

Monohydrate Conf. 1w(ii)

Constants	Exp.	M06-2X/ 6-311++G(2df,p)	MP2/ 6- 311++G(d,p)	wB97X-D/ 6-311++G(d,p)	B3LYP-D3/ 6-311++G(2df,p)
A/MHz	1442.1291(18)	1578	1636.7	-	-
B/MHz	768.49995(19)	836	769.1	-	-
C/MHz	719.00172(15)	772	720.4	-	-
D_J/kHz	1.93749(56)	0.20905	3.7413	-	-
D_{JK}/kHz	0.0808(30)	-0.5855	-18.09	-	-
D_K/kHz		0.8927	26.1	-	-
d_1/kHz	-0.67501(73)	-0.03298	-0.5419	-	-
d_2/*kHz*	-0.07650(43)	-0.000053	0.00956	-	-
Std/kHz	2.0		-	-	-
Δ/amu.Å^2	-305.1	-270.1	-264.1	-	-
kappa	-0.86	-0.84	-0.89	-	-
ΔE/kJoule.mol^{-1}	-	3.2	3.5	-	-
$\lvert\mu_a\rvert$/ D	Y	2.2	2.3	-	-
$\lvert\mu_b\rvert$/ D	Y	0.3	0.8	-	-
$\lvert\mu_c\rvert$/ D	N	0.5	0.0	-	-

N = **59**
J_{max} = 10
$K_{a\ max}$ = 5

Table S3

Monohydrate Conf. 1w(iii)

Constants	Exp.	M06-2X/ 6-311++G(2df,p)	MP2/ 6- 311++G(d,p)	wB97X-D/ 6-311++G(d,p)	B3LYP-D3 6-311++G(2df,p)
A/MHz	1748.772(10)	1791.6	1758.0	1792.5	1796
B/MHz	705.91270(13)	716.2	708.5	703.3	698
C/MHz	669.09363(11)	680.8	670.8	668.7	662
D_J/kHz	0.76314(25)	2.5502	0.6470	-	0.1368
D_{JK}/kHz	-3.0402(37)	-8.6211	-2.135	-	-0.16752
D_K/kHz		34.399	8.287	-	1.3773
d_1/kHz	-0.05412(35)	-0.22022	0.0587	-	-0.00749
d_2/*kHz*	0.00670(20)	0.03014	-1.115	-	0.00028
Std/kHz	1.3	-	-	-	-
Δ/amu.Å^2	-249.6	-245.6	-247.4	-239.3	-242.0
kappa	-0.93	-0.94	-0.93	-0.94	-0.94
ΔE/kJoule.mol^{-1}	-	3.8	3.8	2.0	2.0
$\lvert\mu_a\rvert$/ D	Y	3.0	3.2	3.4	3.4
$\lvert\mu_b\rvert$/ D	N	0.4	0.2	0.5	0.4
$\lvert\mu_c\rvert$/ D	N	0.2	0.1	0.1	0.2

N = **48**
J_{max} = 11
$K_{a\ max}$ = 4

Table S4

Dihydrate Conf. 2w(i)

Constants	Exp.	M06-2X/ 6-311++G(2df,p)	MP2/ 6- 311++G(d,p)	wB97X-D/ 6-311++G(d,p)	B3LYP-D3/ 6-311++G(2df,p)
A/MHz	1086.12505(96)	1099	1098.2	1096.0	1091
B/MHz	685.249819(87)	719	689.9	706.0	704
C/MHz	520.101739(56)	546	524.4	533.4	533
D_J/kHz	0.06498(41)	0.0681	-	-	0.0459
D_{JK}/kHz	0.7815(32)	0.4653	-	-	0.6512
D_K/kHz	-0.733(43)	-0.4446	-	-	-0.6119
d_1/kHz	-0.01398(19)	-0.01021	-	-	-0.0112
d_2/*kHz*	-0.01222(19)	-0.01011	-	-	-0.0117
Std/kHz	1.8	-	-	-	-
Δ/amu.Å^2	-231.1	-237.1	-228.2	-229.5	-232.9
Kappa	-0.42	-0.37	-0.42	-0.38	-0.39
ΔE/kJoule.mol^{-1}	-	0	0	0	0
$\lvert\mu_a\rvert$/ D	Y	1.6	2.1	1.9	1.9
$\lvert\mu_b\rvert$/ D	N	0.0	0.1	0.1	0.0
$\lvert\mu_c\rvert$/ D	N	0.3	0.3	0.3	0.3

N = **74**
J_{max} = 14
$K_{a\ max}$ = 6

Table S5

Dihydrate Conf. 2w(ii)

Constants	Exp.	M06-2X/ 6-311++G(2df,p)	MP2/ 6- 311++G(d,p)	wB97X-D/ 6-311++G(d,p))	B3LYP-D3/ 6-311++G(2df,p)
A/MHz	1263.5956(30)	1267	1277	1287.5	1285
B/MHz	561.264028(53)	599	569	570.3	564
C/MHz	529.294393(43)	564	541	541.1	533
D_J/kHz	0.13759(10)	0.14010	-	-	0.07436
D_{JK}/kHz	-0.1264(34)	-0.2844	-	-	0.0338
D_K/kHz		0.6929	-	-	0.2477
d_1/kHz	-0.00840(11)	-0.00557	-	-	-0.00309
d_2/*kHz*		-0.00016	-	-	-0.00157
Std/kHz	0.6	-	-	-	-
Δ/amu.Å^2	-345.5	-346.5	-349.8	-344.7	-341.2
Kappa	-0.91	-0.90	-0.92	-0.92	-0.92
ΔE/kJoule.mol^{-1}	-	1.0	1.3	1.5	1.4
$\lvert\mu_a\rvert$/ D	Y	1.2	1.6	1.6	1.8
$\lvert\mu_b\rvert$/ D	N	0.5	0.4	0.2	0.04
$\lvert\mu_c\rvert$/ D	N	0.4	0.4	0.7	0.7

N = **39**
J_{max} = 12
$K_{a\ max}$ = 3

Table S6

Trihydrate Conf. 3w(i)

Constants	Exp.	M06-2X/ 6-311++G(2df,p)	MP2/ 6-311++G(d,p)	wB97X-D/ 6-311++G(d,p)	B3LYP-D3/ 6-311++G(2df,p)
A/MHz	872.0385(11)	892	885	875.7	879
B/MHz	501.860939(57)	537	504	523.9	514
C/MHz	446.355960(53)	482	451	463.1	455
D_J/kHz	0.14100(12)	0.09372	-	-	0.0949
D_{JK}/kHz	-0.0541(14)	-0.1123	-	-	0.0100
D_K/kHz		0.1479	-	-	0.0504
d_1/kHz	-0.01360(13)	-0.01880	-	-	-0.01259
d_2/*kHz*	-0.002691(95)	-0.0020	-	-	-0.00171
Std/kHz	0.8	-	-	-	-
Δ/amu.Å^2	-454.4	-459	-453.2	-450.5	-447.5
kappa	-0.74	-0.73	-0.76	-0.71	-0.72
ΔE/kJoule.mol^{-1}	0	0	0	0	0
$\lvert\mu_a\rvert$/ D	Y	1.3	1.2	1.2	1.5
$\lvert\mu_b\rvert$/ D	N	0.8	0.7	0.8	0.5
$\lvert\mu_c\rvert$/ D	N	0.8	0.4	0.6	0.6

N = 60
J_{max} = 11
$K_{a\ max}$ = 5

Table S7

Trihydrate Conf. 3w(ii)

Constants	Exp.	M06-2X/ 6-311++G(2df,p)	MP2/ 6-311++G(d,p)	wB97X-D/ 6-311++G(d,p)	B3LYP-D3/ 6-311++G(2df,p)
A/MHz	1106.17164(22)	1149	1147	1112.7	1129
B/MHz	410.527409(34)	448	414	421.2	417
C/MHz	359.971675(23)	404	370	367.2	368
D_J/kHz	0.098855(53)	0.0420	-	-	0.07153
D_{JK}/kHz	0.1371(11)	-0.05491	-	-	0.0753
D_K/kHz	0.756(19)	0.2805	-	-	0.5738
d_1/kHz	-0.000192(55)	-0.00616	-	-	-0.00443
d_2/*kHz*	-0.000524(28)	-0.00033	-	-	-0.00013
Std/kHz	0.6	-	-	-	-
Δ/amu.Å^2	-284.16	-342.2	-295.4	-276.3	-286.3
kappa	-0.86	-0.88	-0.89	-0.86	-0.87
ΔE/kJoule.mol^{-1}	-	1.1	2.2	1.3	0.9
$\lvert\mu_a\rvert$/ D	Y	1.2	1.4	1.3	1.6
$\lvert\mu_b\rvert$/ D	N	0.6	0.03	0.5	0.3
$\lvert\mu_c\rvert$/ D	Y	0.7	1.0	0.5	0.7
		N = **66**			
		J_{max} = 14			
		$K_{a\ max}$ = 4			

MP2/6-311++G(d,p) structures of the observed conformers:

Conformer 1w(i)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.238247	-1.312454	-0.253724
2	6	0	1.075063	-1.817794	0.327725
3	6	0	2.059930	-0.678161	0.694742
4	6	0	1.710845	0.613493	-0.050041
5	6	0	0.238552	1.048450	0.231456
6	6	0	-0.155179	0.034687	-0.910926
7	6	0	1.268742	0.251373	-1.491189
8	6	0	-0.353050	0.830525	1.620074
9	6	0	-0.038527	2.487346	-0.203024
10	8	0	-1.281915	-1.949272	-0.157161
11	1	0	-1.432997	1.011047	1.589228
12	1	0	0.099314	1.532433	2.331605
13	1	0	-0.197118	-0.182044	2.004172
14	1	0	0.417127	3.182107	0.512947
15	1	0	-1.118988	2.667165	-0.218937
16	1	0	0.362082	2.714380	-1.194920
17	1	0	-1.043182	0.256174	-1.507599
18	1	0	1.758013	-0.602991	-1.970994
19	1	0	2.485353	1.377974	0.083465
20	1	0	3.081133	-0.979575	0.434959
21	1	0	1.514473	-2.454137	-0.451771
22	1	0	0.847791	-2.471960	1.174095
23	1	0	2.044356	-0.496782	1.774724
24	1	0	1.292566	1.102521	-2.172631
25	8	0	-3.283561	0.129894	-0.084875
26	1	0	-4.203075	-0.144805	-0.082888
27	1	0	-2.791800	-0.701264	-0.159714

Rotational constants (GHz): 1.3279391 1.0376245 0.7741537

Conformer 1w(ii)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.764929	-0.332094	0.829163
2	6	0	1.003733	-1.272201	-0.345533
3	6	0	-0.172058	-1.308589	-1.353333
4	6	0	-1.461007	-0.780526	-0.719016
5	6	0	-1.260950	0.659879	-0.152644
6	6	0	-0.679664	-0.050725	1.127770
7	6	0	-1.543171	-1.283843	0.745647
8	6	0	-0.359690	1.635372	-0.902817
9	6	0	-2.592778	1.344231	0.154548
10	8	0	1.680753	0.171466	1.470279
11	1	0	-0.196308	2.534151	-0.296247
12	1	0	-0.841862	1.944460	-1.838424
13	1	0	0.623146	1.225362	-1.151270
14	1	0	-3.074545	1.648868	-0.782300
15	1	0	-2.425676	2.243392	0.758633
16	1	0	-3.287046	0.695368	0.695385
17	1	0	-0.798767	0.442345	2.097145
18	1	0	-1.132317	-2.275495	0.962200
19	1	0	-2.327342	-0.934201	-1.373105
20	1	0	-0.332915	-2.338291	-1.692388
21	1	0	1.136929	-2.263775	0.108020
22	1	0	1.955607	-1.013118	-0.816417
23	1	0	0.073402	-0.714498	-2.240051
24	1	0	-2.546811	-1.215010	1.167145
25	8	0	3.718036	0.679892	-0.478031
26	1	0	4.571198	0.999169	-0.177675
27	1	0	3.216928	0.541372	0.338649

Rotational constants (GHz): 1.6367413 0.7691699 0.7204132

Conformer 1w(iii)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.800736	0.020185	-0.736091
2	6	0	1.061422	1.129926	0.275420
3	6	0	-0.177027	1.491552	1.132826
4	6	0	-1.467626	0.981595	0.487563
5	6	0	-1.398283	-0.555191	0.225438
6	6	0	-0.642430	-0.177929	-1.102272
7	6	0	-1.378595	1.189537	-1.046572
8	6	0	-0.677471	-1.448198	1.229922
9	6	0	-2.775221	-1.148007	-0.072837
10	8	0	1.701203	-0.662554	-1.211550
11	1	0	-0.577801	-2.462053	0.824238
12	1	0	-1.257718	-1.512668	2.158546
13	1	0	0.325532	-1.094939	1.484908
14	1	0	-3.357785	-1.211002	0.854093
15	1	0	-2.671760	-2.160834	-0.478877
16	1	0	-3.345759	-0.551170	-0.789567
17	1	0	-0.746720	-0.837668	-1.968802
18	1	0	-0.835695	2.070207	-1.405371
19	1	0	-2.356442	1.349971	1.013133
20	1	0	-0.238538	2.579634	1.247581
21	1	0	1.368028	1.996177	-0.326070
22	1	0	1.930318	0.856862	0.880592
23	1	0	-0.077494	1.070585	2.139126
24	1	0	-2.348355	1.142206	-1.543546
25	8	0	4.058854	-0.392750	0.400421
26	1	0	4.662639	-1.131475	0.302432
27	1	0	3.374063	-0.562222	-0.263758

Rotational constants (GHz): 1.7579831 0.7085044 0.6708272

Conformer 2w(i)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.270676	-1.371473	-0.054612
2	6	0	1.668610	-1.686810	0.459008
3	6	0	2.582098	-0.442722	0.584652
4	6	0	2.041354	0.720244	-0.249922
5	6	0	0.575120	1.070413	0.151205
6	6	0	0.150227	-0.091695	-0.826338
7	6	0	1.482374	0.165979	-1.586000
8	6	0	0.149490	0.963203	1.611662
9	6	0	0.135203	2.429852	-0.393136
10	1	0	-0.810738	-0.007882	-1.341506
11	1	0	2.089343	-2.390163	-0.271905
12	1	0	1.570025	-2.239560	1.397646
13	1	0	3.593187	-0.694913	0.245165
14	1	0	2.663000	-0.135711	1.632857
15	1	0	2.751640	1.554396	-0.288694
16	1	0	1.358368	0.935139	-2.348792
17	1	0	1.989411	-0.698211	-2.028699
18	1	0	0.638369	1.749620	2.200231
19	1	0	-0.934158	1.105137	1.685253
20	1	0	0.400773	0.000463	2.067807
21	1	0	-0.951503	2.520632	-0.307222
22	1	0	0.604698	3.225141	0.198896
23	1	0	0.420761	2.577456	-1.438747
24	8	0	-0.673043	-2.126132	0.162443
25	8	0	-3.080329	1.375682	0.316930
26	1	0	-3.255152	0.449617	0.077890
27	1	0	-3.873206	1.836568	0.034755
28	8	0	-3.287787	-1.332381	-0.408667
29	1	0	-3.865322	-1.986952	-0.009313
30	1	0	-2.391138	-1.680063	-0.250385

Rotational constants (GHz): 1.0982995 0.6898891 0.5244275

Conformer 2w(ii)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.272142	-1.104970	-0.174358
2	6	0	-0.566735	-0.666427	1.250588
3	6	0	0.472132	0.337223	1.807233
4	6	0	1.783051	0.270174	1.018998
5	6	0	1.539670	0.529351	-0.500695
6	6	0	1.168200	-1.000938	-0.580975
7	6	0	2.077958	-1.209917	0.661095
8	6	0	0.485307	1.546571	-0.922553
9	6	0	2.841618	0.813853	-1.249765
10	8	0	-1.142594	-1.508588	-0.941000
11	1	0	1.359761	-1.534943	-1.516575
12	1	0	3.114803	-1.382903	0.370132
13	1	0	1.778188	-1.974274	1.385675
14	1	0	2.574878	0.859193	1.496623
15	1	0	0.672530	0.108685	2.860342
16	1	0	0.061037	1.350956	1.767346
17	1	0	-0.547758	-1.593466	1.840151
18	1	0	-1.582671	-0.270234	1.307199
19	1	0	0.849365	2.562001	-0.721678
20	1	0	0.303504	1.465436	-2.001487
21	1	0	-0.474476	1.436566	-0.412124
22	1	0	2.671779	0.768209	-2.331721
23	1	0	3.192628	1.823215	-1.003761
24	1	0	3.639421	0.108745	-1.000613
25	1	0	-2.903813	-1.021720	-0.753179
26	8	0	-3.760051	-0.570265	-0.644052
27	1	0	-4.213249	-0.722147	-1.476331
28	1	0	-3.250150	1.067109	0.080308
29	8	0	-2.727271	1.761879	0.514491
30	1	0	-3.380804	2.395863	0.816780

Rotational constants (GHz): 1.2775220 0.5689003 0.5414240

Conformer 3w(i)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.088486	0.199361	0.967272
2	6	0	-0.228628	-0.405679	-0.369590
3	6	0	-0.539371	0.718983	-1.395858
4	6	0	-1.956753	0.781008	-0.767752
5	6	0	-1.914266	1.709636	0.448927
6	6	0	-0.599390	1.520124	1.245651
7	6	0	-1.776072	-0.709500	-0.345642
8	6	0	-2.397323	-1.194318	0.960405
9	6	0	-2.160656	-1.675347	-1.466160
10	8	0	0.821713	-0.342404	1.791236
11	1	0	0.451002	-1.224473	-0.622944
12	1	0	-2.809645	1.005983	-1.419313
13	1	0	-2.782290	1.519540	1.090290
14	1	0	-1.987516	2.748912	0.109355
15	1	0	0.142802	2.264428	0.930682
16	1	0	-0.733485	1.626441	2.325911
17	1	0	-0.544613	0.330944	-2.415704
18	1	0	0.081232	1.616628	-1.349177
19	1	0	-1.743818	-1.385047	-2.434120
20	1	0	-1.808577	-2.686697	-1.231761
21	1	0	-3.252508	-1.709612	-1.564701
22	1	0	-2.042473	-2.206152	1.190936
23	1	0	-3.489299	-1.234377	0.862730
24	1	0	-2.159618	-0.557867	1.817256
25	1	0	1.989905	-1.565951	1.203988
26	8	0	2.656382	-2.093342	0.720302
27	1	0	3.193055	-2.496972	1.406357
28	1	0	3.299670	-0.962512	-0.514542
29	8	0	3.509885	-0.240611	-1.136711
30	1	0	3.469507	-0.646107	-2.005313
31	1	0	2.708411	1.346261	-0.699058
32	8	0	2.255793	2.157093	-0.407957
33	1	0	2.971922	2.705126	-0.079335

Rotational constants (GHz): 0.8848935 0.5039688 0.4511214

Conformer 3w(ii)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.124804	0.425155	-0.348992
2	6	0	1.053906	-0.295252	-0.929990
3	6	0	2.318189	0.260676	-0.169961
4	6	0	1.973715	-0.791176	0.929608
5	6	0	0.909139	-0.257379	1.891668
6	6	0	-0.373239	0.153676	1.124633
7	6	0	1.274201	-1.632083	-0.171359
8	6	0	3.605646	-0.089465	-0.915733
9	6	0	2.345602	1.740429	0.198858
10	8	0	-0.805147	1.208986	-1.005985
11	1	0	1.044001	-0.259394	-2.023252
12	1	0	0.377128	-2.192660	0.100920
13	1	0	1.964560	-2.283174	-0.709787
14	1	0	2.821301	-1.231600	1.468255
15	1	0	0.660502	-1.036398	2.621063
16	1	0	1.309567	0.593489	2.454170
17	1	0	-1.087670	-0.677959	1.135124
18	1	0	-0.873285	1.019852	1.568616
19	1	0	3.648184	-1.140949	-1.211573
20	1	0	3.697956	0.523119	-1.820151
21	1	0	4.471419	0.117525	-0.274970
22	1	0	2.431558	2.351423	-0.707737
23	1	0	1.451382	2.070804	0.734656
24	1	0	3.215461	1.952359	0.832887
25	1	0	-2.388800	1.777884	-0.403985
26	8	0	-3.289617	1.942101	-0.061354
27	1	0	-3.643479	2.623366	-0.637747
28	1	0	-4.032024	0.324680	0.096801
29	8	0	-4.268553	-0.620429	0.160761
30	1	0	-4.705080	-0.704571	1.010991
31	1	0	-2.853088	-1.656911	-0.362986
32	8	0	-2.027777	-2.109466	-0.611371
33	1	0	-2.274968	-2.627908	-1.380102

Rotational constants (GHz): 1.1471891 0.4139780 0.3701498

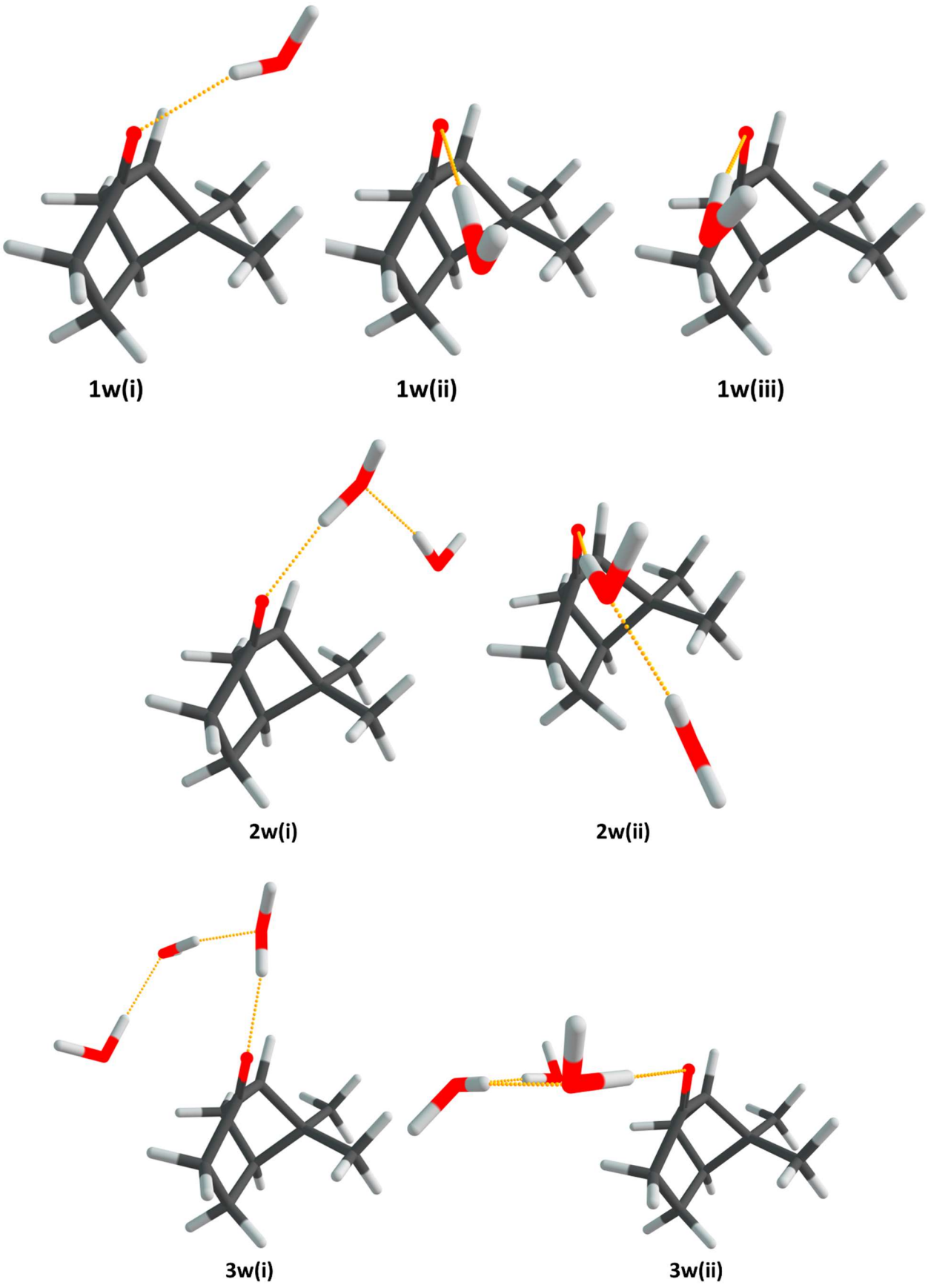


Figure S1. Structure of the all observed conformer of NOP···(H_2O)n (n=1,2,3). The position of NOP is fixed to help visualization and to easily compare them.

Modified structure of conformer 1w(ii)

As it was mentioned in the main text, the error on the *A* constant is slightly high for the conformer 1w(ii) at MP2/6-311++G(d,p). The rotational constants depend on the mass distribution of the atoms. In order to decrease the error on the *A* constant, the position of the water molecule was modified by scanning both the dihedral angle O-O-C-C and the angle O-O-C.

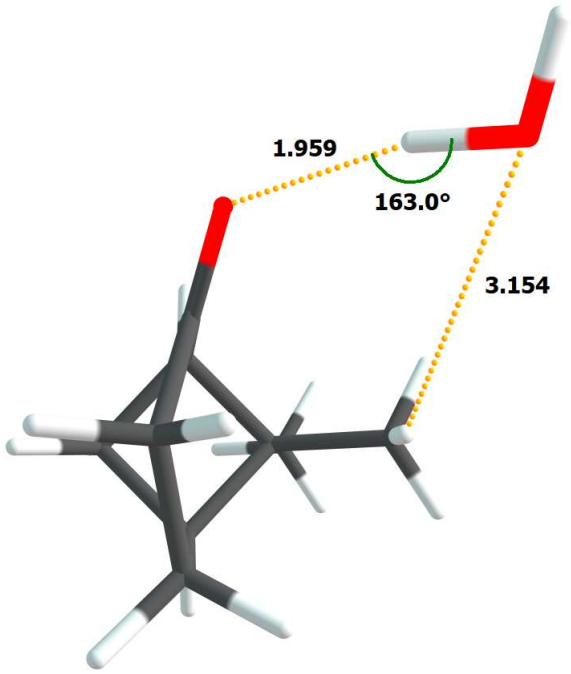


Figure S2. Modified structure of 1w(ii) to match better the experimental rotational parameters calculated at MP2/6-311++G(d,p) level of theory. This structure shows that the water molecule is closer to the methyl group. Bond distances are given in Å.

Table S8

Rotational constants	Exp.	Modified structure MP2/6-311++G(d,p)	MN15-L/6-311++G(d,p)
A	1442.1529(20)	1489	1534
B	768.51947(23)	798	817
C	718.98298(20)	693	752

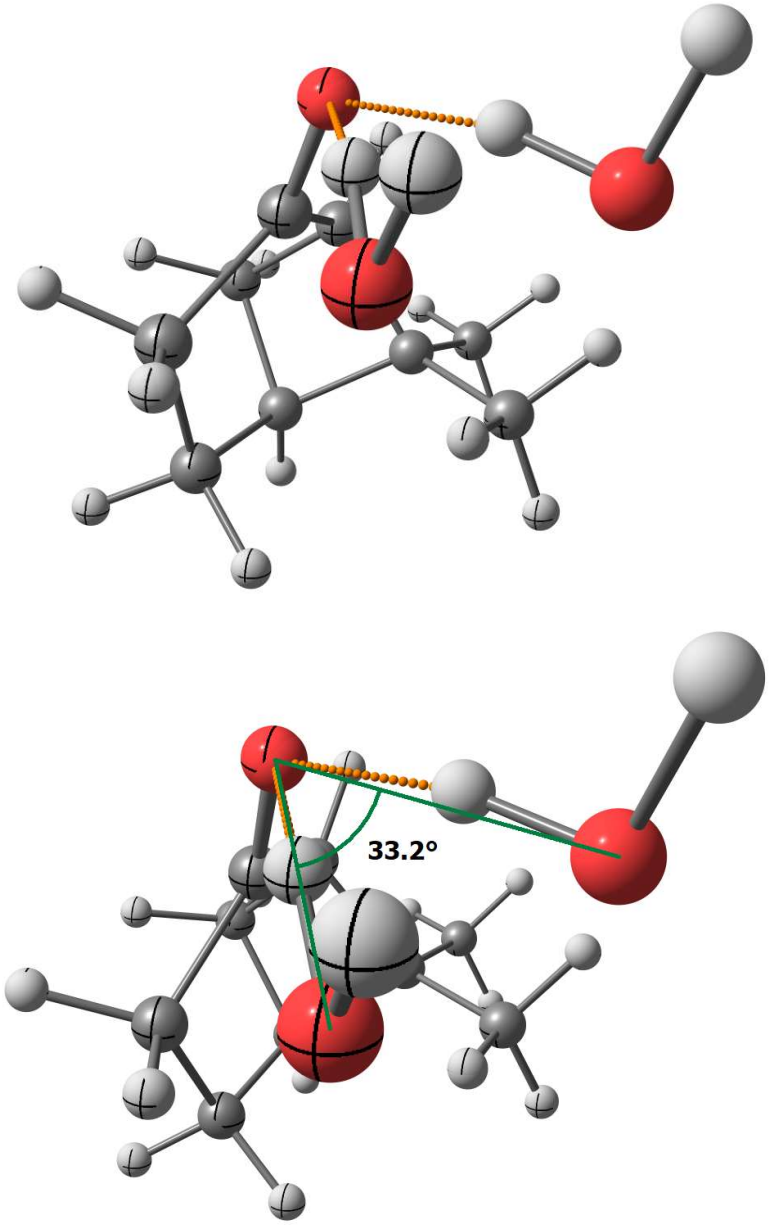


Figure S3. comparison between the calculated structure of conformer 1w(ii) at MP2/6-311++G(d,p) (water with black lines, on the left) with that obtained by scanning the position of water molecule (on the right) to match the experimental rotational constants.

Modified geometry of 1w(ii)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.689945	-0.730796	-0.684727
2	6	0	-0.499477	-1.688311	0.485114
3	6	0	0.730492	-1.351056	1.365193
4	6	0	1.716254	-0.453641	0.612861
5	6	0	1.020118	0.847903	0.105630
6	6	0	0.556774	-0.020151	-1.125736
7	6	0	1.794897	-0.920288	-0.864088
8	6	0	-0.053819	1.503422	0.967345
9	6	0	2.033308	1.909149	-0.323350
10	8	0	-1.785042	-0.530417	-1.193894
11	1	0	-0.564869	2.289169	0.399049
12	1	0	0.406876	1.967843	1.847870
13	1	0	-0.822713	0.810060	1.318209
14	1	0	2.495423	2.356367	0.564863
15	1	0	1.530635	2.706509	-0.882525
16	1	0	2.831425	1.503838	-0.951307
17	1	0	0.414593	0.477502	-2.089561
18	1	0	1.691274	-1.992592	-1.060927
19	1	0	2.651659	-0.325001	1.169934
20	1	0	1.237607	-2.277285	1.658414
21	1	0	-0.373531	-2.679851	0.030101
22	1	0	-1.432030	-1.722808	1.055789
23	1	0	0.411228	-0.854378	2.287520
24	1	0	2.678174	-0.547697	-1.384212
25	8	0	-3.820984	0.842842	0.340406
26	1	0	-4.667343	0.909789	-0.105938
27	1	0	-3.291810	0.301744	-0.258830

Rotational constants (GHz): 1.4890350 0.7978645 0.6934465

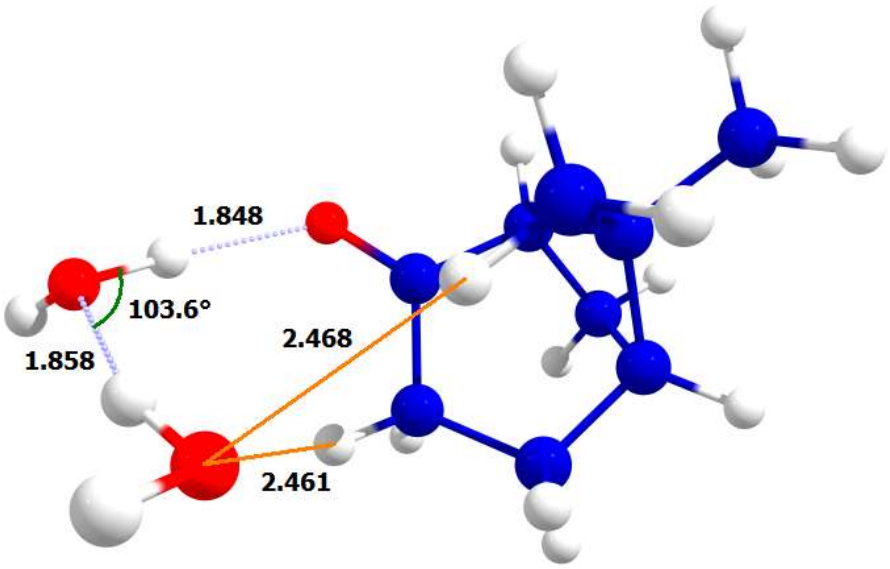
MN15-L/6-311++G(d,p) geometry of 1w(ii)

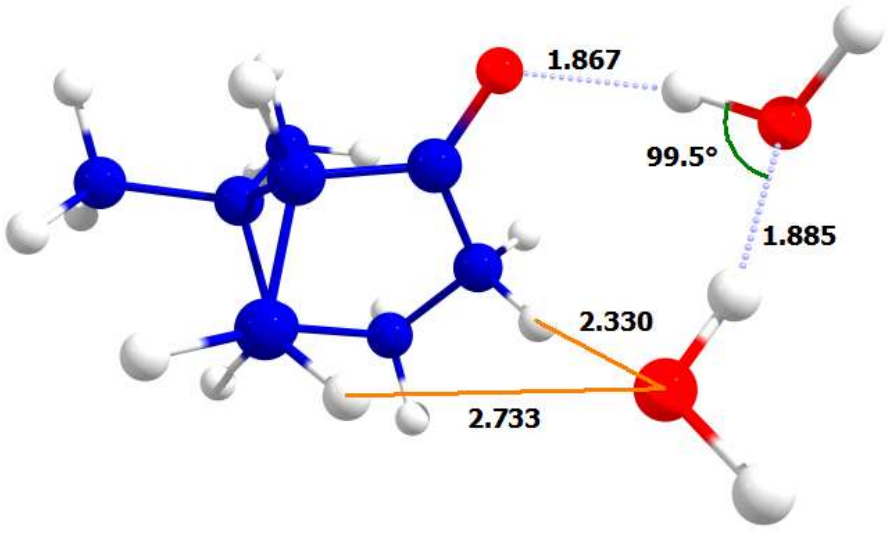
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.721751	-0.544757	-0.869946
2	6	0	-0.960680	-1.369530	0.396285
3	6	0	0.145126	-1.187050	1.475136
4	6	0	1.434091	-0.624889	0.853188
5	6	0	1.155662	0.721514	0.097028
6	6	0	0.727482	-0.196745	-1.125208
7	6	0	1.656647	-1.297030	-0.532277
8	6	0	0.121493	1.705532	0.661166
9	6	0	2.451292	1.485770	-0.215112
10	8	0	-1.632124	-0.165228	-1.594727
11	1	0	-0.064219	2.513843	-0.072591
12	1	0	0.515850	2.177470	1.582449
13	1	0	-0.857552	1.256109	0.903576
14	1	0	2.839052	1.953404	0.710899
15	1	0	2.254724	2.294035	-0.944963
16	1	0	3.246791	0.840275	-0.625827
17	1	0	0.874991	0.190354	-2.150254
18	1	0	1.333541	-2.350043	-0.641106
19	1	0	2.270721	-0.619802	1.580158
20	1	0	0.362914	-2.159341	1.956991
21	1	0	-0.972829	-2.422296	0.044903
22	1	0	-1.973756	-1.157417	0.778246
23	1	0	-0.213422	-0.508144	2.272165
24	1	0	2.689246	-1.204781	-0.903750
25	8	0	-3.488688	0.806528	0.489012
26	1	0	-4.234454	1.383564	0.293309
27	1	0	-3.161270	0.525476	-0.380056

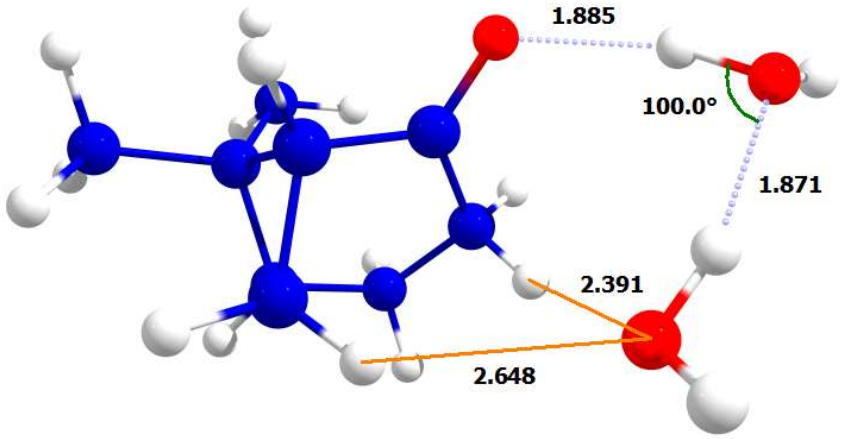
Rotational constants (GHz): 1.5345854 0.8174347 0.7526292

Parameters of the non-observed NOP-Water dihydrates:

MP2/6-311++G(d,p) equilibrium geometry of Nopinone-$(H2O)_2$ conformer 2w(iii), ΔE=2.4 kJ/mol		
		
A=1271	B=571	C=543
μ_a=1.5	μ_b=0.2	μ_c=1.7

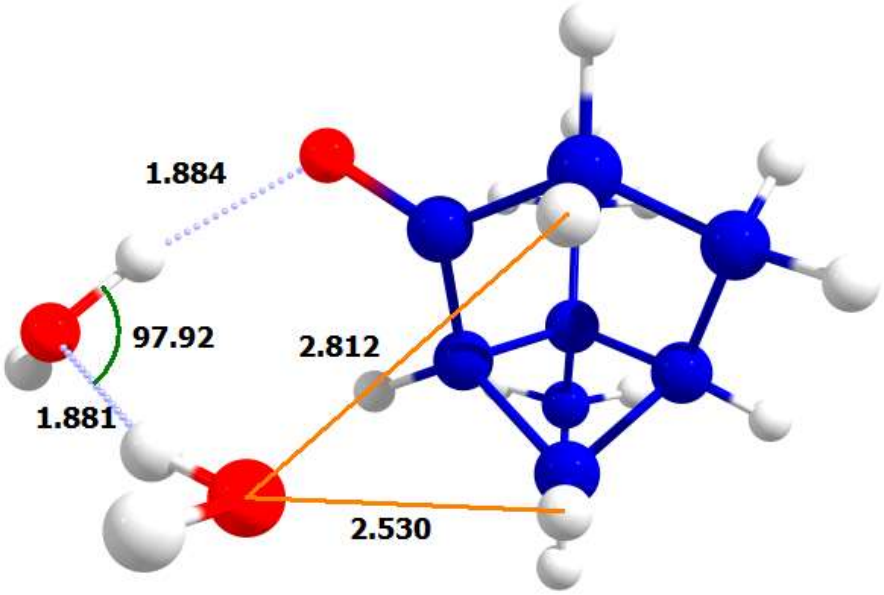
MP2/6-311++G(d,p) equilibrium geometry of Nopinone-$(H2O)_2$ conformer 2w(iv), ΔE= 3.3 kJ/mol		
		
A=1441	B=538	C=496
μ_a=1.2	μ_b=1.0	μ_c=0.1

MP2/6-311++G(d,p) equilibrium geometry of Nopinone-$(H2O)_2$ conformer 2w(v), ΔE=3.4 kJ/mol



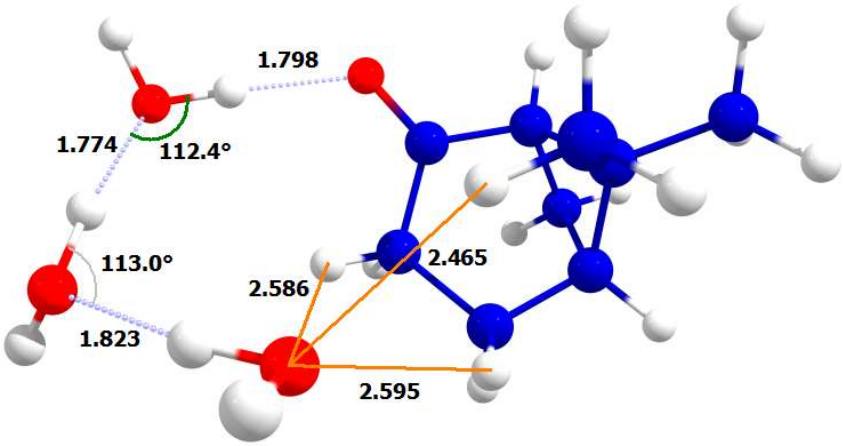
A=1428	B=542	C=503
μ_a=1.6	μ_b=0.9	μ_c=1.5

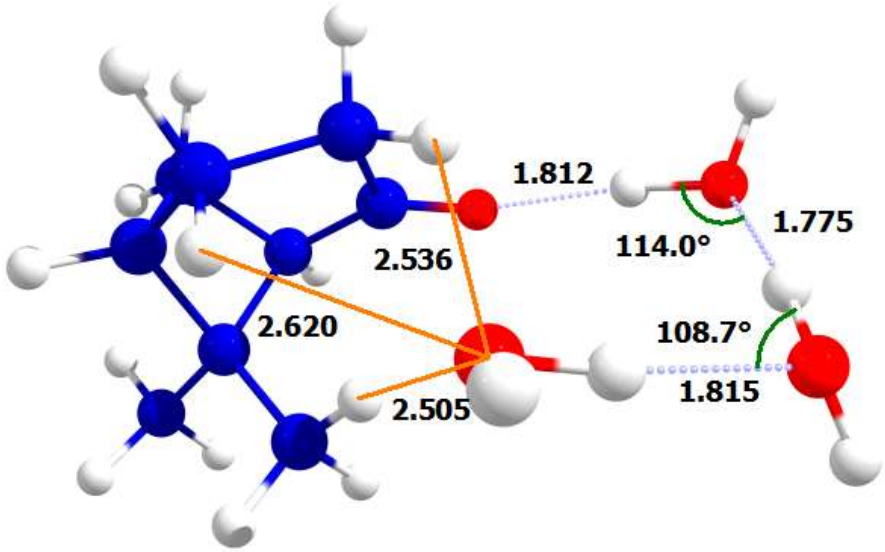
MP2/6-311++G(d,p) equilibrium geometry of Nopinone-$(H2O)_2$ conformer 2w(vi), ΔE=4.9 kJ/mol



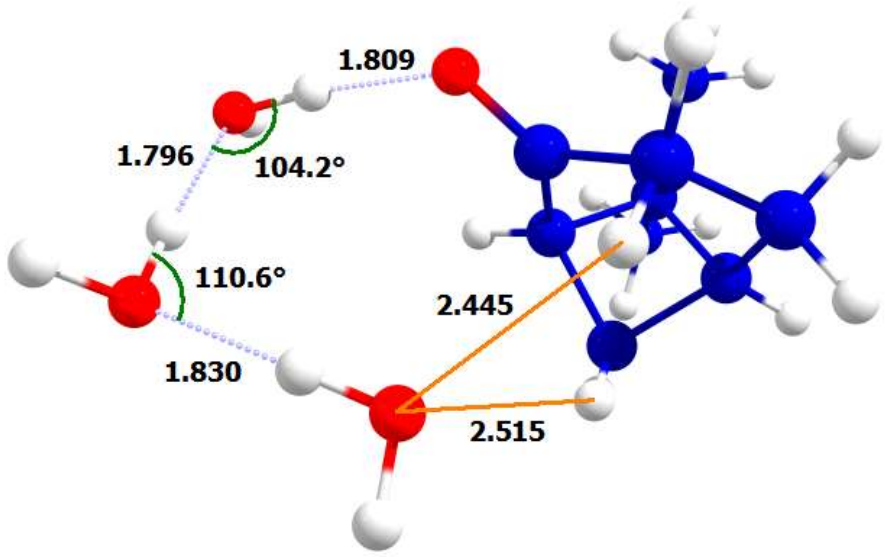
A=1216	B=600	C=567
μ_a=2.2	μ_b=0.1	μ_c=1.2

Parameters of the non-observed NOP-Water trihydrates:

MP2/6-311++G(d,p) equilibrium geometry of Nopinone-$(H2O)_3$ conformer 3w(iii), ΔE=3.4kJ/mol		
		
A=1023	B=424	C=374
μ_a=1.4	μ_b=0.0	μ_c=1.0

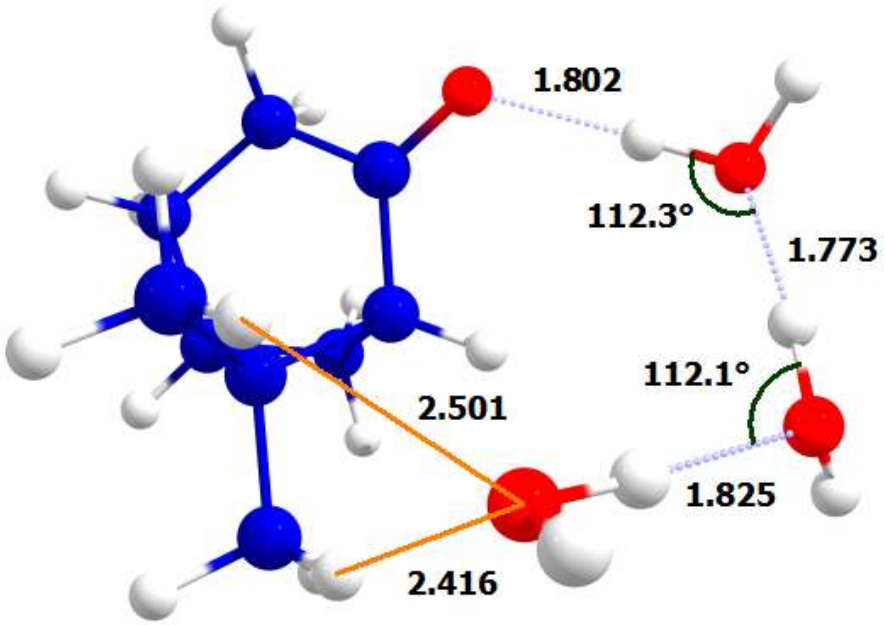
MP2/ 6-311++G(d,p) equilibrium geometry of Nopinone-$(H_2O)_3$ conformer 3w(iv), ΔE=5.3kJ/mol		
		
A=984	B=418	C=376
μ_a=1.6	μ_b=1.6	μ_c=0.8

MP2/6-311++G(d,p) equilibrium geometry of Nopinone-$(H2O)_3$ conformer 3w(v), ΔE=5.6kJ/mol



A=979	B=438	C=386
μ_a=3.0	μ_b=0.1	μ_c=0.5

MP2/6-311++G(d,p) equilibrium geometry of Nopinone-$(H2O)_3$ conformer 3w(vi), ΔE=6.0kJ/mol



A=858	B=487	C=381
μ_a=0.4	μ_b=1.5	μ_c=2.0

Measured rotational transitions for all conformers NOP-water

Nopinone-water 1w(i)

J	K_a	K_c	J'	K'_a	K'_c	ν_{EXP} (MHz)	$\Delta\nu$ (MHz)*
5	1	5	4	1	4	7934.7327	0.0001
4	1	4	3	1	3	6407.5272	0.0003
6	0	6	5	0	5	9456.8198	0.0000
4	2	3	3	2	2	6967.3871	0.0008
4	0	4	3	0	3	6451.9410	-0.0006
3	1	2	2	1	1	5578.3776	-0.0007
4	0	4	3	1	3	6386.5584	0.0007
5	1	5	4	0	4	7955.6998	-0.0018
4	2	2	3	2	1	7557.2922	-0.0010
4	1	3	3	1	2	7259.3075	0.0015
5	1	4	4	1	3	8797.2499	0.0000
5	3	3	4	3	2	8962.7342	0.0005
5	3	2	4	3	1	9343.6165	0.0021
5	2	4	4	2	3	8591.6828	0.0000
6	1	6	5	1	5	9452.4148	0.0003
6	2	5	5	2	4	10165.9302	0.0002
6	1	5	5	1	4	10268.1671	0.0000
6	3	4	5	3	3	10680.5823	0.0003
6	5	2	5	5	1	10836.0461	0.0009
6	5	1	5	5	0	10847.8740	0.0016
6	4	3	5	4	2	10859.7832	-0.0001
7	1	7	6	1	6	10966.6969	0.0001
7	6	1	6	6	0	12636.9294	-0.0003
7	0	7	6	0	6	10967.8993	0.0003
6	4	2	5	4	1	11032.4240	-0.0004
6	2	4	5	2	3	11108.1533	0.0004
6	3	3	5	3	2	11346.5436	-0.0009
7	2	6	6	2	5	11706.4607	-0.0001
7	1	6	6	1	5	11746.1983	0.0000
7	3	5	6	3	4	12334.5565	0.0001
5	3	2	4	1	3	12365.6729	-0.0012
8	1	8	7	1	7	12479.9439	0.0008
8	0	8	7	0	7	12480.2551	0.0000
8	1	8	7	0	7	12480.3541	-0.0041
7	0	7	6	1	6	10966.2818	0.0002
7	1	7	6	0	6	10968.3145	0.0003
7	5	3	6	5	2	12693.1476	0.0011
8	3	6	7	3	5	13929.7660	-0.0002
9	1	9	8	1	8	13992.9050	0.0009
9	0	9	8	0	8	13992.9825	0.0002

8	2	6	7	2	5	14100.7650	0.0001
8	4	5	7	4	4	14406.9729	0.0000
8	5	3	7	5	2	14738.5300	0.0001
8	5	4	7	5	3	14547.0082	0.0000
8	6	2	7	6	1	14513.3245	0.0013
8	6	3	7	6	2	14496.9926	-0.0001
7	2	5	6	2	4	12648.4490	0.0006
7	4	4	6	4	3	12660.8099	0.0000
7	4	3	6	4	2	13081.9882	-0.0010
9	2	8	8	2	7	14745.1750	0.0000
9	1	8	8	1	7	14749.2654	0.0008
8	3	5	7	3	4	14966.0484	0.0004
8	4	4	7	4	3	15134.6809	0.0000
9	3	7	8	3	6	15482.3001	-0.0003
10	1	10	9	1	9	15505.7842	-0.0005
10	0	10	9	0	9	15505.8052	0.0014
11	1	11	10	1	10	17018.6334	0.0021
11	0	11	10	0	10	17018.6334	-0.0023
9	2	7	8	2	6	15555.7296	-0.0008
10	1	9	9	1	8	16259.6193	-0.0008
10	2	9	9	2	8	16258.4410	0.0000
9	3	6	8	3	5	16512.8455	-0.0004
9	5	5	8	5	4	16371.8593	0.0003
7	6	2	6	6	1	12634.1990	0.0003
3	0	3	2	0	2	4961.2812	-0.0012
3	1	3	2	1	2	4858.9996	-0.0003
2	1	1	1	1	0	3773.0031	0.0015
2	0	2	1	0	1	3424.3809	-0.0004
3	2	2	2	2	1	5286.0644	-0.0011
4	1	4	3	0	3	6472.9109	0.0001
4	3	1	3	3	0	7334.6719	-0.0044
5	4	2	4	4	1	9028.3445	-0.0031
5	4	1	4	4	0	9073.9223	0.0044
4	3	1	3	1	2	10281.3664	0.0006
7	5	2	6	5	1	12751.3211	-0.0007
8	2	7	7	2	6	13229.4488	0.0004
7	3	4	6	3	3	13239.2379	0.0007
8	1	7	7	1	6	13242.7866	0.0002
8	7	2	7	7	1	14430.2724	-0.0001
8	7	1	7	7	0	14430.8554	-0.0011
9	6	4	8	6	3	16372.7261	0.0000
9	6	3	8	6	2	16439.5560	-0.0005

* $\Delta\nu = \nu_{CALC} - \nu_{EXP}$

Nopinone-water 1w(ii)

J	K_a	K_c	J'	K'_a	K'_c	ν_{EXP} (MHz)	$\Delta\nu$ (MHz)*
2	0	2	1	0	1	2972.3132	-0.0011
3	0	3	2	0	2	4451.8430	-0.0022
4	0	4	3	0	3	5923.7251	-0.0003
5	0	5	4	0	4	7386.2649	-0.0018
6	0	6	5	0	5	8838.9912	-0.0015
7	0	7	6	0	6	10282.9480	-0.0021
8	0	8	7	0	7	11720.4139	-0.0019
4	1	4	3	1	3	5845.6920	0.0000
5	1	5	4	1	4	7302.5473	0.0001
6	1	6	5	1	5	8756.8080	0.0006
8	1	8	7	1	7	11657.2277	0.0013
7	1	7	6	1	6	10208.3561	0.0010
7	1	6	6	1	5	10542.4119	-0.0039
4	1	3	3	1	2	6042.8194	-0.0013
5	1	4	4	1	3	7547.5567	-0.0016
6	1	5	5	1	4	9047.8605	-0.0015
3	1	2	2	1	1	4534.7818	-0.0015
6	2	5	5	2	4	8911.6570	0.0024
5	2	4	4	2	3	7430.7553	0.0011
4	2	3	3	2	2	5947.4848	-0.0001
4	2	2	3	2	1	5973.2306	-0.0004
5	2	3	4	2	2	7480.9343	-0.0004
7	2	6	6	2	5	10389.7601	0.0022
6	2	4	5	2	3	8995.7860	0.0011
7	2	5	6	2	4	10516.1750	-0.0010
8	2	7	7	2	6	11864.6788	0.0023
4	3	1	3	3	0	5955.0178	0.0000
4	3	2	3	3	1	5954.5001	0.0009
5	3	2	4	3	1	7446.4622	0.0008
6	3	3	5	3	2	8940.1674	0.0029
5	3	3	4	3	2	7444.6571	0.0006
6	3	4	5	3	3	8935.3987	0.0019
7	3	5	6	3	4	10426.4484	0.0015
7	3	4	6	3	3	10437.0220	0.0035
8	3	6	7	3	5	11917.3874	0.0005
8	3	5	7	3	4	11938.0779	0.0033
6	4	3	5	4	2	8932.1826	0.0021
6	4	2	5	4	1	8932.2651	0.0002
7	4	4	6	4	3	10422.7110	0.0022
7	4	3	6	4	2	10422.9901	0.0018
8	4	4	7	4	3	11914.7446	0.0029
9	2	8	8	2	7	13336.0799	-0.0002
9	4	6	8	4	5	13405.9930	0.0001
9	4	5	8	4	4	13407.7983	0.0014
9	3	7	8	3	6	13407.6724	-0.0043

9	3	6	8	3	5	13444.4310	-0.0004
10	1	10	9	1	9	14547.6888	-0.0005
6	1	6	5	0	5	9156.5105	-0.0015
6	0	6	5	1	5	8439.2896	0.0014
7	0	7	6	1	6	9965.4307	-0.0002
7	1	7	6	0	6	10525.8743	0.0000
8	0	8	7	1	7	11477.4879	-0.0038
8	1	8	7	0	7	11900.1529	0.0024
8	5	4	7	5	3	11908.7507	0.0021
8	5	3	7	5	2	11908.7566	-0.0044
7	5	3	6	5	2	10419.0935	-0.0012
7	5	2	6	5	1	10419.0953	-0.0026
6	5	2	5	5	1	8929.8552	-0.0033
6	5	1	5	5	0	8929.8565	-0.0026

* $\Delta\nu = \nu_{CALC} - \nu_{EXP}$

Nopinone-water 1w(iii)

J	K_a	K_c	J'	K'_a	K'_c	ν_{EXP} (MHz)	$\Delta\nu$ (MHz)*
3	0	3	2	0	2	4121.1107	0.0003
4	0	4	3	0	3	5490.2945	0.0005
4	1	4	3	1	3	5424.3626	0.0016
4	1	3	3	1	2	5571.5162	0.0002
4	2	3	3	2	2	5499.1809	0.0001
4	2	2	3	2	1	5508.7210	0.0012
5	1	5	4	1	4	6778.6329	0.0005
5	0	5	4	0	4	6855.6975	0.0000
5	2	4	4	2	3	6872.6424	0.0012
5	1	4	4	1	3	6962.3460	-0.0006
5	2	3	4	2	2	6891.5995	0.0009
5	3	2	4	3	1	6878.3806	0.0002
5	3	3	4	3	2	6878.0558	0.0023
6	2	5	5	2	4	8245.2143	0.0003
6	3	4	5	3	3	8254.5453	0.0018
6	3	3	5	3	2	8255.4139	0.0004
6	1	6	5	1	5	8131.7751	0.0006
6	0	6	5	0	5	8216.5744	-0.0006
6	1	5	5	1	4	8351.7246	-0.0007
6	2	4	5	2	3	8278.0212	0.0000
7	0	7	6	0	6	9572.4186	-0.0004
7	1	6	6	1	5	9739.2767	0.0017
7	4	4	6	4	3	9629.4260	-0.0053
7	2	6	6	2	5	9616.7239	-0.0012
8	1	7	7	1	6	11124.5705	-0.0015
8	2	6	7	2	5	11062.3871	-0.0015
8	3	5	7	3	4	11012.3986	-0.0007
8	3	6	7	3	5	11008.5155	0.0005
8	4	4	7	4	3	11006.0249	0.0012
8	4	5	7	4	4	11005.9567	0.0022
8	2	7	7	2	6	10987.0036	-0.0005
8	1	8	7	1	7	10834.1253	-0.0008
8	0	8	7	0	7	10923.0597	-0.0013
9	0	9	8	0	8	12268.7333	-0.0007
9	1	8	8	1	7	12507.1418	-0.0006
9	2	7	8	2	6	12459.8550	-0.0012
9	3	7	8	3	6	12385.8621	-0.0003
9	2	8	8	2	7	12355.8852	-0.0005
9	1	9	8	1	8	12183.1605	-0.0010
10	0	10	9	0	9	13610.0536	-0.0006
10	1	9	9	1	8	13886.4634	0.0015
10	1	10	9	1	9	13530.7216	0.0002
10	2	8	9	2	7	13859.8654	0.0013
10	3	7	9	3	6	13775.3075	0.0003
10	3	8	9	3	7	13763.2944	-0.0007

10	2	9	9	2	8	13723.2131	0.0008
11	1	11	10	1	10	14876.8162	0.0000
11	0	11	10	0	10	14947.9119	0.0018
3	0	3	2	0	2	4121.1107	0.0003

* $\Delta\nu = \nu_{CALC} - \nu_{EXP}$

Nopinone-water 2w(i)

J	K_a	K_c	J'	K'_a	K'_c	ν_{EXP} (MHz)	Δν (MHz)*
7	1	7	6	1	6	7584.3687	-0.0002
5	1	5	4	1	4	5487.4794	-0.0007
6	1	6	5	1	5	6539.0888	-0.0003
8	1	8	7	1	7	8626.5772	0.0001
10	1	10	9	1	9	10707.7976	0.0003
11	1	11	10	1	10	11747.9440	0.0008
9	1	8	8	1	7	10305.2404	0.0000
7	1	6	6	1	5	8278.1867	-0.0005
12	1	12	11	1	11	12788.0177	0.0015
12	0	12	11	0	11	12788.0676	-0.0001
13	1	13	12	1	12	13828.0602	0.0008
10	1	9	9	1	8	11333.1607	0.0004
14	1	14	13	1	13	14868.0877	0.0023
7	0	7	6	0	6	7592.3666	-0.0003
5	0	5	4	0	4	5530.5679	-0.0007
6	0	6	5	0	5	6558.5328	-0.0005
8	0	8	7	0	7	8629.6808	0.0005
10	0	10	9	0	9	10708.2163	0.0002
11	0	11	10	0	10	11748.0910	-0.0004
13	0	13	12	0	12	13828.0773	0.0002
14	0	14	13	0	13	14868.0890	-0.0023
11	1	10	10	1	9	12367.1569	0.0011
10	5	6	9	5	5	12363.6440	0.0024
4	2	2	3	2	1	5102.8631	-0.0022
6	3	4	5	3	3	7323.2882	0.0003
5	2	3	4	2	2	6424.2585	-0.0002
5	3	2	4	3	1	6235.2634	-0.0020
4	0	4	3	0	3	4506.2561	-0.0011
10	2	8	9	2	7	12050.7207	0.0009
9	4	6	8	4	5	11067.0099	0.0016
6	3	3	5	3	2	7592.9533	-0.0014
6	2	5	5	2	4	7053.2938	-0.0008
7	3	5	6	3	4	8509.0284	0.0004
7	2	6	6	2	5	8144.8413	-0.0001
5	1	4	4	1	3	6190.9450	0.0028
6	1	5	5	1	4	7259.2116	-0.0021
6	2	4	5	2	3	7696.7835	-0.0005
9	4	5	8	4	4	11459.2121	0.0024
9	5	5	8	5	4	11104.9335	0.0010
9	5	4	8	5	3	11168.6116	0.0015
10	3	8	9	3	7	11882.3443	0.0024
10	4	7	9	4	6	12257.4875	0.0030
9	3	7	8	3	6	10787.8523	0.0017
9	2	7	8	2	6	11053.7582	0.0000
9	3	6	8	3	5	11572.5011	0.0025

10	2	9	9	2	8	11318.0263	0.0004
5	2	4	4	2	3	5935.1529	0.0009
6	4	3	5	4	2	7363.7466	0.0010
6	4	2	5	4	1	7393.7431	-0.0001
11	2	10	10	2	9	12360.8665	0.0015
8	4	5	7	4	4	9848.2980	0.0015
9	0	9	8	0	8	9668.6098	0.0004
9	1	9	8	1	8	9667.4532	0.0006
8	1	7	7	1	6	9287.2034	-0.0005
8	3	6	7	3	5	9664.3903	0.0007
7	3	4	6	3	3	8965.5158	-0.0002
5	3	3	4	3	2	6113.1140	0.0036
4	1	3	3	1	2	5046.5297	-0.0012
4	2	3	3	2	2	4788.6433	-0.0005
4	1	4	3	1	3	4424.5984	-0.0006
3	1	2	2	1	1	3833.7014	-0.0010
3	0	3	2	0	2	3465.0595	0.0004
3	1	3	2	1	2	3345.0052	0.0000
6	5	2	5	5	1	7338.0270	0.0056
6	5	1	5	5	0	7339.0962	0.0017
5	4	1	4	4	0	6125.1946	0.0080
7	5	3	6	5	2	8586.4536	-0.0052
7	5	2	6	5	1	8592.1501	0.0009
8	5	3	7	5	2	9864.8615	-0.0007
10	3	7	9	3	6	12753.0235	0.0034
10	5	5	9	5	4	12518.2672	0.0055
11	2	9	10	2	8	13046.0112	0.0023
10	6	5	9	6	4	12324.3733	0.0000
10	6	4	9	6	3	12339.0314	0.0002

* $\Delta\nu = \nu_{CALC} - \nu_{EXP}$

Nopinone-water 2w(ii)

J	K_a	K_c	J'	K'_a	K'_c	ν_{EXP} (MHz)	$\Delta\nu$ (MHz)*
6	3	4	5	3	3	6548.5063	0.0008
4	0	4	3	0	3	4351.6014	-0.0009
5	0	5	4	0	4	5431.7416	0.0012
6	0	6	5	0	5	6507.1452	0.0002
7	0	7	6	0	6	7577.5313	0.0007
7	1	7	6	1	6	7509.1889	0.0013
6	1	6	5	1	5	6439.4033	0.0003
5	1	5	4	1	4	5368.3668	0.0007
3	0	3	2	0	2	3267.4019	0.0005
4	1	4	3	1	3	4296.1939	-0.0002
8	0	8	7	0	7	8643.1054	0.0016
8	1	8	7	1	7	8577.6531	0.0003
9	0	9	8	0	8	9704.5580	0.0020
9	1	9	8	1	8	9644.7833	0.0008
10	0	10	9	0	9	10762.9111	0.0021
10	1	10	9	1	9	10710.6086	0.0016
11	0	11	10	0	10	11819.2747	0.0018
11	1	11	10	1	10	11775.1991	0.0021
12	1	12	11	1	11	12838.6550	0.0019
8	2	7	7	2	6	8711.2065	0.0008
8	1	7	7	1	6	8827.8593	0.0015
9	1	8	8	1	7	9922.4498	0.0011
11	2	9	10	2	8	12134.2939	0.0007
9	2	7	8	2	6	9905.3221	0.0013
9	2	8	8	2	7	9795.5570	0.0010
6	2	5	5	2	4	6538.4412	-0.0001
4	1	3	3	1	2	4423.9352	0.0002
5	1	4	4	1	3	5527.7398	0.0004
6	1	5	5	1	4	6629.9661	0.0003
7	1	6	6	1	5	7730.1741	0.0005
7	2	5	6	2	4	7681.5900	-0.0001
6	2	4	5	2	3	6574.5137	-0.0001
5	2	3	4	2	2	5471.3380	0.0001
7	2	6	6	2	5	7625.4475	0.0004
7	3	5	6	3	4	7641.2518	0.0000
5	2	4	4	2	3	5450.3593	0.0012
8	3	5	7	3	4	8739.8553	0.0005
6	3	3	5	3	2	6549.7452	-0.0005
11	1	10	10	1	9	12099.8525	0.0057

* $\Delta\nu = \nu_{CALC} - \nu_{EXP}$

Nopinone-water 3w(i)

J	K_a	K_c	J'	K'_a	K'_c	ν_{EXP} (MHz)	Δν (MHz)*
5	1	5	4	1	4	4580.5974	0.0007
5	0	5	4	0	4	4640.4361	-0.0029
5	2	4	4	2	3	4728.1742	0.0004
5	1	4	4	1	3	4850.3173	-0.0017
6	1	6	5	1	5	5485.8418	0.0004
6	0	6	5	0	5	5532.3988	-0.0007
6	2	4	5	2	3	5819.3914	-0.0010
7	1	7	6	1	6	6387.4791	0.0003
7	0	7	6	0	6	6419.9820	0.0016
7	2	6	6	2	5	6593.1627	0.0004
7	3	5	6	3	4	6664.9635	0.0005
8	0	8	7	0	7	7307.1264	-0.0007
8	1	8	7	1	7	7286.1810	-0.0007
8	1	7	7	1	6	7650.1594	0.0004
6	2	5	5	2	4	5663.3500	0.0007
6	3	4	5	3	3	5711.4895	0.0000
6	3	3	5	3	2	5731.6645	-0.0008
6	1	5	5	1	4	5798.6628	0.0009
7	3	4	6	3	3	6708.1554	-0.0002
7	1	6	6	1	5	6732.7292	0.0007
7	2	5	6	2	4	6808.0922	0.0001
8	2	7	7	2	6	7517.1686	0.0003
8	3	6	7	3	5	7616.2654	-0.0004
8	3	5	7	3	4	7696.0544	0.0001
8	2	6	7	2	5	7788.9978	0.0001
9	1	9	8	1	8	8182.6835	-0.0002
9	0	9	8	0	8	8195.4372	-0.0004
9	2	8	8	2	7	8435.2412	-0.0003
10	1	10	9	1	9	9077.6454	0.0000
10	0	10	9	0	9	9085.1046	0.0000
11	1	11	10	1	10	9971.5891	0.0006
11	0	11	10	0	10	9975.8246	0.0000
9	3	7	8	3	6	8563.9911	0.0010
9	3	6	8	3	5	8694.1029	-0.0010
9	2	7	8	2	6	8758.2765	-0.0007
10	2	9	9	2	8	9347.6131	-0.0001
10	1	9	9	1	8	9440.2150	0.0009
10	3	7	9	3	6	9697.3227	0.0001
10	2	8	9	2	7	9712.9997	0.0004
11	2	10	10	2	9	10254.8447	0.0000
11	1	10	10	1	9	10322.7831	-0.0003
11	3	9	10	3	8	10443.9398	-0.0001
11	2	9	10	2	8	10650.5731	-0.0007
11	3	8	10	3	7	10698.4582	0.0000
9	4	6	8	4	5	8583.0130	0.0002

9	4	5	8	4	4	8598.0481	0.0000
10	3	8	9	3	7	9506.8768	-0.0003
9	5	5	8	5	4	8571.5472	-0.0004
9	5	4	8	5	3	8572.2481	-0.0003
10	5	5	9	5	4	9533.0976	-0.0001
10	4	7	9	4	6	9542.9025	-0.0015
10	4	6	9	4	5	9573.9345	-0.0004
11	4	8	10	4	7	10502.0314	0.0005
11	4	7	10	4	6	10559.8892	0.0017
5	2	3	4	2	2	4828.5821	0.0001
7	4	4	6	4	3	6665.2289	0.0009
7	4	3	6	4	2	6667.6366	0.0017
8	4	5	7	4	4	7623.5111	-0.0005
8	4	4	7	4	3	7629.9867	-0.0002
4	1	3	3	1	2	3891.0619	0.0012

* $\Delta\nu = \nu_{CALC} - \nu_{EXP}$

Nopinone-water 3w(ii)

J	K_a	K_c	J'	K'_a	K'_c	ν_{EXP} (MHz)	Δν (MHz)*
6	1	6	5	1	5	4452.3126	0.0000
6	0	6	5	0	5	4537.0675	-0.0002
7	1	7	6	1	6	5186.6804	0.0004
7	0	7	6	0	6	5263.8531	0.0005
8	1	8	7	1	7	5918.4583	0.0000
8	0	8	7	0	7	5984.0343	-0.0010
9	1	9	8	1	8	6647.8193	-0.0001
9	0	9	8	0	8	6700.3504	0.0000
10	1	10	9	1	9	7375.0297	0.0000
10	0	10	9	0	9	7415.1243	0.0003
11	1	11	10	1	10	8100.4070	-0.0005
11	0	11	10	0	10	8129.8580	-0.0001
12	1	12	11	1	11	8824.2851	-0.0001
12	0	12	11	0	11	8845.2798	0.0005
13	1	13	12	1	12	9546.9769	0.0002
13	0	13	12	0	12	9561.5958	-0.0007
14	1	14	13	1	13	10268.7580	0.0001
14	0	14	13	0	13	10278.7529	0.0002
6	1	5	5	1	4	4750.8123	-0.0008
8	2	6	7	2	5	6310.5828	0.0004
5	1	4	4	1	3	3966.2675	-0.0006
6	2	5	5	2	4	4610.9714	0.0000
7	1	6	6	1	5	5529.8179	0.0004
7	2	5	6	2	4	5502.0061	-0.0005
6	2	4	5	2	3	4696.7270	0.0006
9	2	7	8	2	6	7119.1027	-0.0004
8	3	5	7	3	4	6206.7061	0.0000
8	2	7	7	2	6	6131.6076	0.0004
6	3	4	5	3	3	4635.1730	0.0008
7	3	4	6	3	3	5421.0188	-0.0005
9	1	8	8	1	7	7065.1234	0.0000
6	3	3	5	3	2	4640.0031	-0.0020
7	2	6	6	2	5	5372.7878	0.0009
8	1	7	7	1	6	6301.7814	0.0002
10	2	9	9	2	8	7639.0234	0.0005
10	3	8	9	3	7	7734.8107	-0.0004
10	1	9	9	1	8	7818.4227	0.0000
10	4	6	9	4	5	7740.8204	-0.0012
10	4	7	9	4	6	7736.8548	0.0007
9	2	8	8	2	7	6887.1047	-0.0002
10	2	8	9	2	7	7924.5208	0.0000
11	2	10	10	2	9	8387.1935	0.0002
11	1	10	10	1	9	8560.8056	0.0003
11	2	9	10	2	8	8724.4711	0.0001
11	3	9	10	3	8	8507.4581	0.0009

12	2	11	11	2	10	9131.5543	0.0000
12	1	11	11	1	10	9292.3857	0.0002
13	2	12	12	2	11	9872.1588	-0.0008
13	2	11	12	2	10	10301.2798	-0.0003
14	2	13	13	2	12	10609.1770	-0.0001
14	1	13	13	1	12	10729.6302	0.0003
13	3	11	12	3	10	10045.6502	-0.0006
12	3	9	11	3	8	9415.8487	0.0001
9	3	6	8	3	5	6998.2985	0.0005
9	4	5	8	4	4	6960.7578	0.0003
9	3	7	8	3	6	6960.6436	0.0005
9	4	6	8	4	5	6958.9060	0.0000
7	3	5	6	3	4	5410.2697	-0.0007
5	3	3	4	2	3	7473.9749	-0.0003
8	4	5	7	4	4	6182.0979	0.0005
8	4	4	7	4	3	6182.8745	-0.0002
7	2	5	6	1	5	7333.7751	0.0000
8	2	6	7	1	6	8114.5412	0.0013
6	2	4	5	1	4	6582.5807	-0.0007
7	3	5	6	2	5	9061.9081	0.0003
9	2	7	8	1	7	8931.8613	-0.0006

* $\Delta\nu = \nu_{CALC} - \nu_{EXP}$