

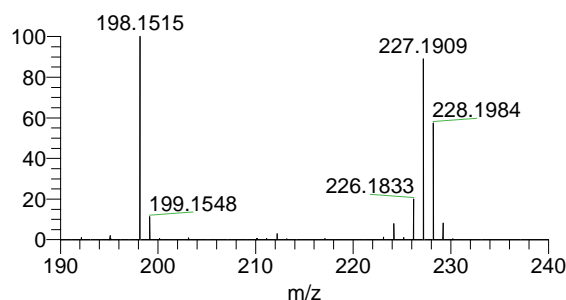
## Supplementary material

## Unexpected rapid aerobic transformation of 2,2,6,6-tetraethyl-4-oxo(piperidin-1-yloxy) radical by cytochrome P450 in the presence of NADPH: evidence against a simple reduction of the nitroxide moiety to the hydroxylamine.

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## 1. HRMS analysis of pure TEEPONE and TEEPOL

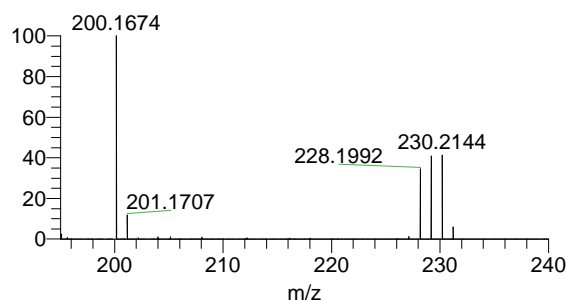
**Supplementary Figure S1:** HRMS spectrum of TEEPONE (peak eluted at 16.4 min, Figure 4A). The corresponding observed and calculated m/z values for the indicated elemental composition are reported in Supplementary Table T1.



**Supplementary table T1:** HRMS characteristics of TEEPONE as observed in Supplementary Figure S1.

m/z (Da)		chemical formula
observed	calculated	
198.1515	198.1489	C <sub>11</sub> H <sub>20</sub> NO <sub>2</sub> <sup>+</sup> [MH <sup>+</sup> -C <sub>2</sub> H <sub>5</sub> ]
226.1833	226.1802	C <sub>13</sub> H <sub>24</sub> NO <sub>2</sub> <sup>+</sup> [M <sup>+</sup> ]
227.1909	227.1880	C <sub>13</sub> H <sub>25</sub> NO <sub>2</sub> <sup>+</sup> [MH <sup>+</sup> ]
228.1984	228.1958	C <sub>13</sub> H <sub>26</sub> NO <sub>2</sub> <sup>+</sup> [MH <sub>2</sub> <sup>+</sup> ]

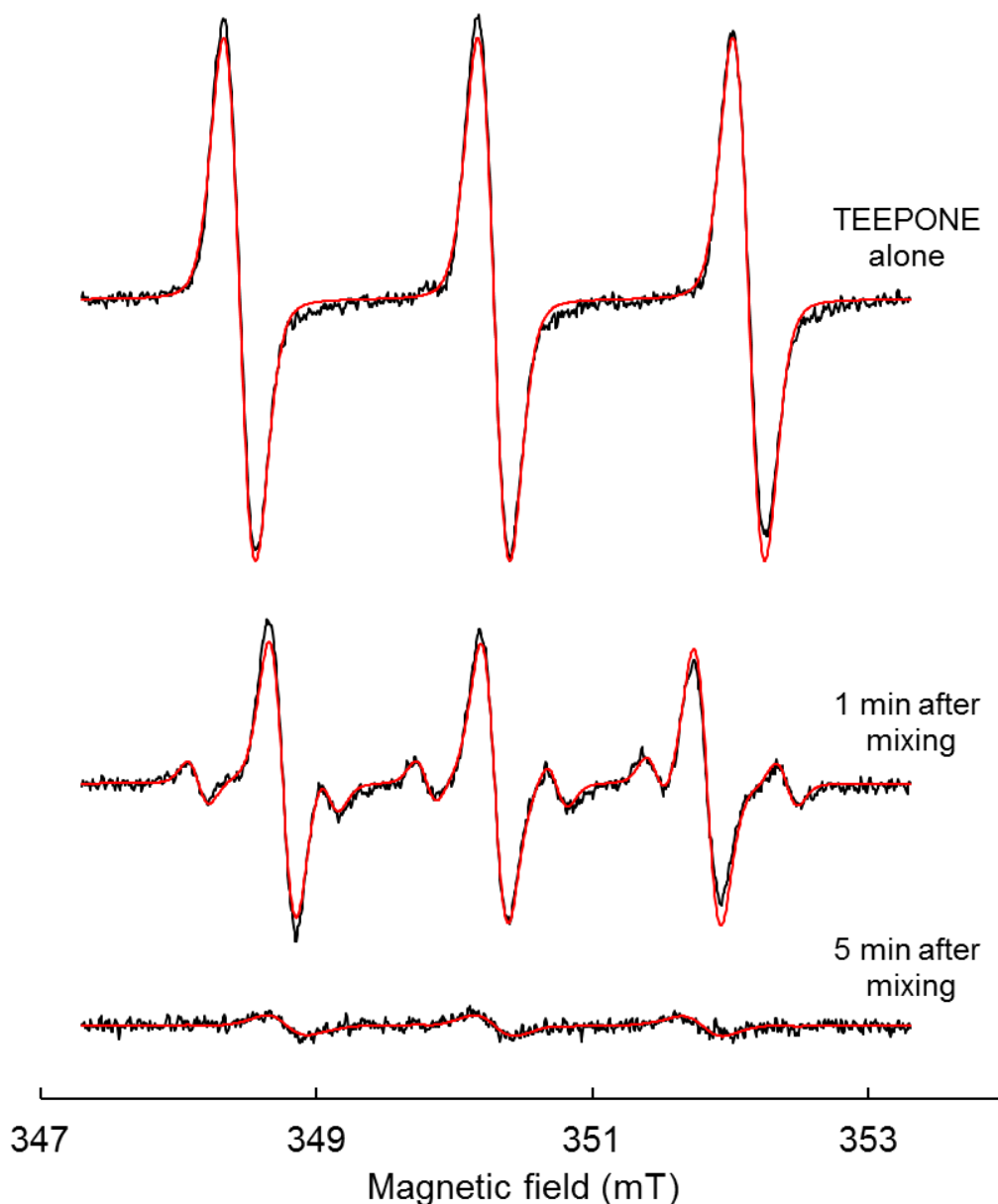
**Supplementary Figure S2:** HRMS spectrum of TEEPOL (peak eluted at 15.6 min, Figure 4B). The corresponding observed and calculated m/z values for the indicated elemental composition are reported in Supplementary Table T2.



**Supplementary Table T2:** HRMS characteristics of TEEPOL as observed in Supplementary Figure S2.

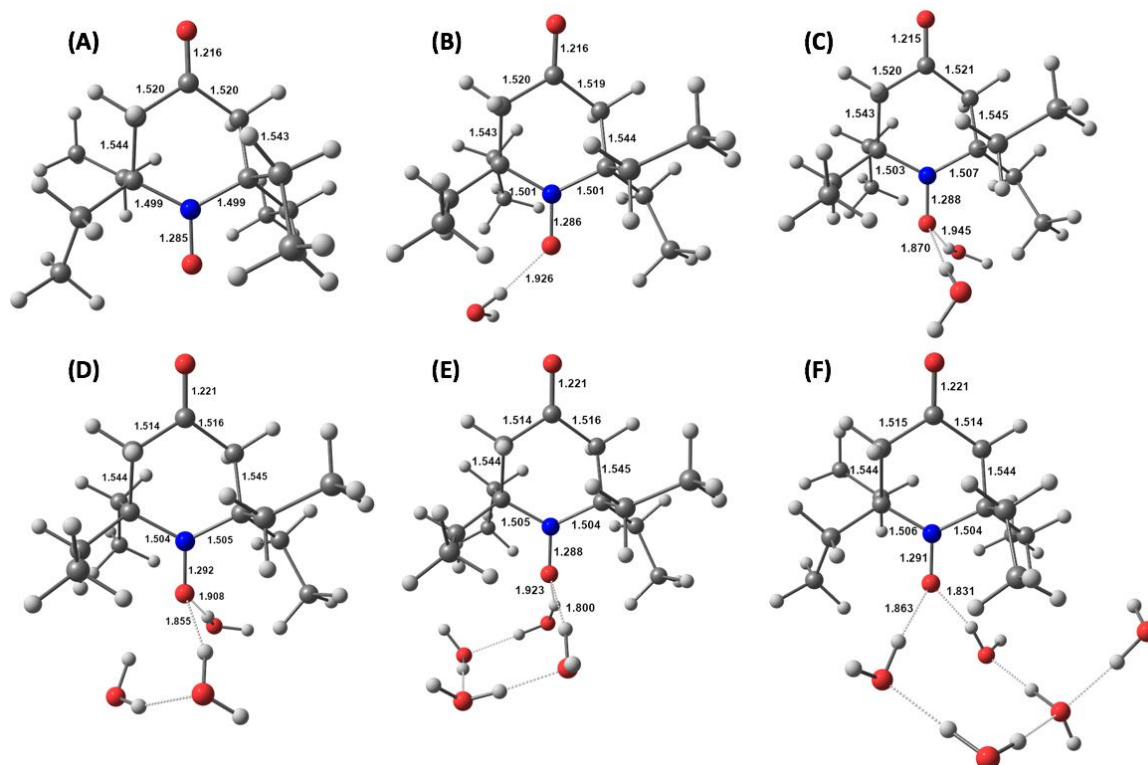
m/z (Da)		chemical formula
observed	calculated	
200.1674	200.1645	C <sub>11</sub> H <sub>22</sub> NO <sub>2</sub> <sup>+</sup> [MH <sup>+</sup> -C <sub>2</sub> H <sub>5</sub> ]
228.1992	228.1958	C <sub>13</sub> H <sub>26</sub> NO <sub>2</sub> <sup>+</sup> [M <sup>+</sup> ]
229.2067	229.2036	C <sub>13</sub> H <sub>27</sub> NO <sub>2</sub> <sup>+</sup> [MH <sup>+</sup> ]
230.2144	230.2115	C <sub>13</sub> H <sub>28</sub> NO <sub>2</sub> <sup>+</sup> [MH <sub>2</sub> <sup>+</sup> ]

## 2. EasySpin simulations



**Supplementary Figure S3:** Superimposition of experimental (black) and calculated (red) spectra of TEEPONE alone and 1 or 5 min after mixing with RLM and NADPH. The parameters used in the simulation are given in Table 1. See legend of Figure 2 and experimental section for experimental details.

### 3. DFT calculations



**Supplementary Figure S4:** DFT-optimized structures with selected metrical parameters (Å) for TEEPONE without (A) and with 1 (B), 2 (C), 3 (D), 4 (E), and 5 (F) water molecules.

**Supplementary Table T3:** DFT-calculated  $^{14}\text{N}$  hyperfine coupling constants (hfc, MHz) for the geometry-optimized TEEPONE with explicit solvent molecules.

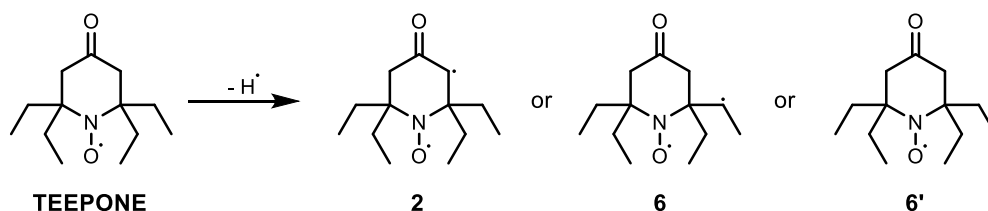
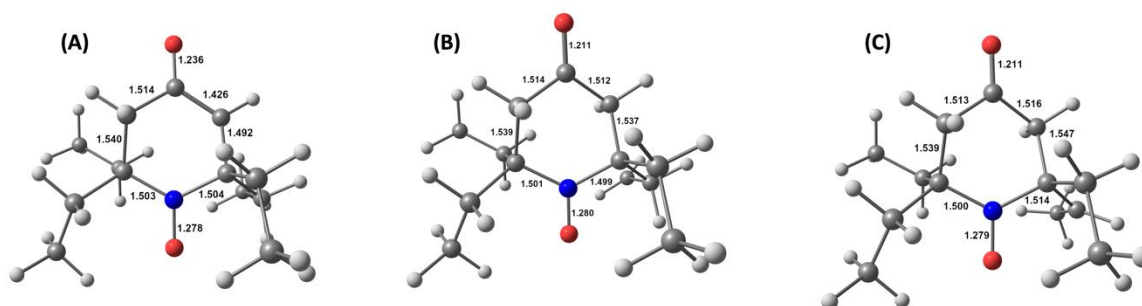
Model	$A_{\text{min}}$	$A_{\text{mid}}$	$A_{\text{max}}$	$A_{\text{iso}}$
No $\text{H}_2\text{O}$	11.8	12.5	82.9	35.7
1 $\text{H}_2\text{O}$	13.7	13.9	90.6	39.4
2 $\text{H}_2\text{O}$	15.6	15.6	97.4	42.9
3 $\text{H}_2\text{O}$	16.5	16.5	101.1	44.7
4 $\text{H}_2\text{O}$	16.1	16.1	98.5	43.6
5 $\text{H}_2\text{O}$	16.0	16.1	99.0	43.7
Experimental	-	-	-	43.2

**Supplementary Table T4:** DFT-calculated hyperfine coupling constants (hfc, MHz) for the geometry-optimized structure  $3' + 4 \text{H}_2\text{O}$ . (The proton hfc refers to atom 24 in Figure 9C.)

	$A_{\text{min}}$	$A_{\text{mid}}$	$A_{\text{max}}$	$A_{\text{iso}}$
$^{14}\text{N}$ A	16.7	16.9	99.0	44.2
$^1\text{H}$ A	35.9	37.6	49.6	41.0

**Supplementary Table T5:** DFT-calculated hyperfine coupling constants (hfc, MHz) for the geometry-optimized structure **3'** + 4 H<sub>2</sub>O. (The proton hfc refers to atom 32 in Figure 9F.)

	<b>A<sub>min</sub></b>	<b>A<sub>mid</sub></b>	<b>A<sub>max</sub></b>	<b>A<sub>iso</sub></b>
<sup>14</sup> N <b>A</b>	8.3	8.9	62.5	26.5
<sup>1</sup> H <b>A</b>	-11.3	-27.3	-38.0	-25.5

**Supplementary Figure S5:** Structures **2**, **6** and **6'** resulting of H-abstraction at different positions on TEEPONE.**Supplementary Figure S6:** DFT-optimized structures for **2** (A), **6** (B), and **6'** (C) with selected metrical parameters (Å).**Supplementary Table T6:** Gibbs free energy calculations for the H-atom abstraction.

	<b>G (E<sub>h</sub>)</b>	<b>ΔG (kcal.mol<sup>-1</sup>)</b>	<b>ΔΔG (kcal.mol<sup>-1</sup>)</b>
<b>TEEPONE</b>	-714.87235996	0	-
<b>2</b>	-714.23765823	-	-
<b>6</b>	-714.22389014	-	-
<b>6'</b>	-714.21846439	-	-
<b>H<sup>•</sup></b>	-0.5	-	-
<b>2 + H<sup>•</sup></b>	-714.73765823	+84.5	0
<b>6 + H<sup>•</sup></b>	-714.72389014	+93.2	8.7
<b>6' + H<sup>•</sup></b>	-714.71846439	+96.6	12.1

**Supplementary Table T7:** Cartesian coordinates for the DFT-optimized structure of TEEPONE

Atomic number	X	Y	Z
6	-2.903959000	1.334763000	2.185364000
6	-3.026805000	1.391378000	0.658763000
1	-2.945422000	2.349299000	2.597182000
1	-1.958090000	0.888584000	2.507494000
1	-3.712074000	0.749638000	2.633424000
6	-3.072383000	0.022349000	-0.089766000
1	-2.180750000	1.955459000	0.242403000
1	-3.922916000	1.969672000	0.398792000
6	-3.357016000	0.279991000	-1.584188000
6	-5.842631000	0.328318000	-0.894771000
6	-5.547581000	-0.940276000	-0.065039000
7	-4.158593000	-0.832886000	0.488367000
6	-1.713418000	-0.704068000	0.078354000
6	-1.591534000	-2.094789000	-0.553491000
1	-1.502834000	-0.793962000	1.145655000
1	-0.949851000	-0.037845000	-0.345212000
1	-2.327668000	-2.781773000	-0.127702000
1	-0.595674000	-2.504868000	-0.348951000
1	-1.713269000	-2.081387000	-1.643163000
6	-5.604655000	-2.230749000	-0.929248000
6	-6.946579000	-2.528837000	-1.610797000
1	-5.322026000	-3.063533000	-0.276855000
1	-4.824942000	-2.173930000	-1.699038000
1	-7.772296000	-2.592471000	-0.894322000
1	-6.891544000	-3.490220000	-2.133759000
1	-7.207157000	-1.770150000	-2.356902000
8	-3.857591000	-1.568590000	1.497618000
6	-6.572460000	-0.967444000	1.108673000
6	-6.746974000	-2.263077000	1.910335000
1	-7.113077000	-3.087700000	1.289215000
1	-7.488567000	-2.101504000	2.701704000
1	-5.806674000	-2.568374000	2.369311000
1	-6.296721000	-0.155180000	1.792176000
1	-7.543934000	-0.685314000	0.681543000
8	-5.046003000	1.335648000	-2.917979000
6	-4.776996000	0.716783000	-1.906627000
1	-3.175988000	-0.632230000	-2.167369000
1	-2.666072000	1.033192000	-1.977427000
1	-5.957455000	1.180584000	-0.208580000
1	-6.797323000	0.235624000	-1.419303000

**Supplementary Table T8:** Cartesian coordinates for the DFT-optimized structure of 2

Atomic number	X	Y	Z
6	-2.732057277	1.290342425	2.296580591
6	-3.034841112	1.422137681	0.805301986

1	-2.785449367	2.276766950	2.762857183
1	-1.733002163	0.896977362	2.482366479
1	-3.445153879	0.637725261	2.797604877
6	-3.111632179	0.079218213	-0.010175780
1	-2.274803939	2.046461919	0.327037183
1	-3.983774587	1.946430697	0.676347073
6	-3.409763220	0.445225455	-1.425028655
6	-5.845218715	0.291652869	-0.954151464
6	-5.575145282	-0.927984829	-0.052966280
7	-4.211226496	-0.774371122	0.558389342
6	-1.764289834	-0.673929783	0.078123455
6	-1.677162781	-1.954987971	-0.746401832
1	-1.567830046	-0.907550614	1.121339256
1	-0.992407980	0.031185915	-0.244736556
1	-2.397027746	-2.695096654	-0.397495738
1	-0.681845338	-2.393984577	-0.651591308
1	-1.856226312	-1.778219931	-1.809613305
6	-5.562170405	-2.243831229	-0.868646114
6	-6.857812598	-2.596486676	-1.600364967
1	-5.291495245	-3.046444252	-0.181573819
1	-4.751506601	-2.186605429	-1.600660545
1	-7.714541426	-2.655006548	-0.927269173
1	-6.755133252	-3.571896662	-2.079853824
1	-7.096329687	-1.878579192	-2.386035398
8	-3.909011918	-1.529440261	1.544758449
6	-6.645663283	-0.921433252	1.071413781
6	-6.839770900	-2.178085744	1.919276078
1	-7.163361169	-3.032153490	1.322524990
1	-7.619225248	-1.993281571	2.662367237
1	-5.927724425	-2.454333163	2.440688973
1	-6.415579590	-0.076996120	1.726303541
1	-7.597334548	-0.674103172	0.591747693
8	-4.953670179	0.926125465	-3.105424149
6	-4.732798937	0.581521667	-1.938866477
1	-2.585476314	0.694895474	-2.082888333
1	-5.982623587	1.176918815	-0.323772202
1	-6.773793253	0.156208789	-1.504157047

**Supplementary Table T9:** Cartesian coordinates for the DFT-optimized structure of **3**

Atomic number / X / Y / Z

6	-2.328023000	-1.350385000	2.840040000
6	-1.697375000	-0.305376000	1.904352000
1	-1.962480000	-2.362375000	2.634885000
1	-3.418924000	-1.367636000	2.756924000
1	-2.079546000	-1.117744000	3.880307000
6	-1.912515000	-0.566485000	0.390451000
1	-0.615846000	-0.258459000	2.089240000
1	-2.090467000	0.688067000	2.134763000
6	-3.404030000	-0.710868000	-0.011557000
6	-4.343801000	0.431367000	0.410412000
1	-3.766521000	-1.658184000	0.407821000

1	-3.431049000	-0.823476000	-1.101176000
1	-4.407280000	0.529111000	1.498955000
1	-5.354909000	0.236753000	0.037336000
1	-4.006015000	1.390477000	0.011416000
6	-1.084897000	-1.777706000	-0.106656000
6	0.158024000	-1.210246000	-0.776793000
1	-1.623789000	-2.333873000	-0.882721000
1	-0.802990000	-2.475351000	0.684719000
6	-0.128874000	0.234240000	-1.207698000
7	-1.286050000	0.579594000	-0.363797000
8	1.217208000	-1.789642000	-0.916479000
6	-0.380283000	0.357215000	-2.749592000
1	0.706942000	0.891114000	-0.941600000
6	0.978088000	0.111066000	-3.483948000
6	0.878354000	-0.635503000	-4.828987000
1	1.636254000	-0.470288000	-2.833165000
1	1.463230000	1.082955000	-3.634902000
1	0.506969000	-1.653696000	-4.682984000
1	1.871094000	-0.709163000	-5.283237000
1	0.227933000	-0.132043000	-5.551541000
6	-0.987770000	1.744452000	-3.069526000
6	-1.257794000	2.029546000	-4.558741000
1	-0.311317000	2.512378000	-2.676501000
1	-1.920456000	1.843951000	-2.508682000
1	-0.339025000	2.051660000	-5.151746000
1	-1.740035000	3.006362000	-4.663110000
1	-1.936587000	1.294574000	-5.009968000
8	-1.334694000	-0.686220000	-3.033653000
1	-1.569128000	-0.632578000	-3.966867000
8	-1.506912000	1.795307000	-0.029530000

**Supplementary Table T10:** Cartesian coordinates for the DFT-optimized structure of **4**

Atomic number / X / Y / Z

6	0.051975381	3.727317112	1.995550684
6	0.977846556	2.509403362	1.834392904
1	0.646656549	4.607090043	2.261952331
1	-0.689772429	3.578889203	2.785158647
1	-0.487617199	3.951089435	1.071345878
6	0.312407663	1.179767453	1.362644926
1	1.464966339	2.290405307	2.792428357
1	1.783310502	2.760646314	1.134880257
6	1.404868973	0.102385220	1.194675210
6	1.733723459	0.949654059	-1.152101241
6	0.427932980	1.393310513	-1.161776743
7	-0.321568617	1.427926350	0.011008894
6	-0.778956093	0.725649281	2.359041560
6	-1.500663758	-0.594596369	2.033603713
1	-1.524475245	1.518129473	2.440498980
1	-0.287893665	0.644993855	3.336537887
1	-1.972644351	-0.554556672	1.048472004
1	-2.289728847	-0.771459432	2.770805400

1	-0.830544214	-1.458962479	2.063695200
6	-0.256921195	1.885029867	-2.416086151
6	-0.399326871	3.422880284	-2.475934266
1	-1.249583747	1.428430787	-2.473492767
1	0.326929712	1.533890177	-3.271714846
1	-1.017891071	3.788426664	-1.653031124
1	-0.876550383	3.716894584	-3.416081487
1	0.579816899	3.910063571	-2.425762062
8	-1.541349609	1.817301164	-0.026861030
8	3.550849344	0.060240160	0.083458425
6	2.362389224	0.373616775	0.037796364
1	0.945015649	-0.870920140	0.984666544
1	1.982412599	0.004327544	2.117861799
1	2.321842796	0.995068906	-2.062950899

**Supplementary Table T11:** Cartesian coordinates for the DFT-optimized structure of **6**

Atomic number / X / Y / Z

6	-2.886410044	1.350551007	2.177993887
6	-3.042042987	1.419500376	0.660710379
1	-2.928796979	2.357011003	2.599088649
1	-1.934304929	0.912558206	2.478141021
1	-3.677011520	0.759010517	2.639109274
6	-3.073584358	0.066773850	-0.102212540
1	-2.221584209	2.005604864	0.234223418
1	-3.951981245	1.978533007	0.426308086
6	-3.372868550	0.319659226	-1.587989100
6	-5.840284326	0.311178462	-0.884443921
6	-5.522352314	-0.950378171	-0.061894968
7	-4.126518910	-0.830123748	0.476257926
6	-1.691577112	-0.640078092	0.021341421
6	-1.570021773	-1.950902171	-0.667276930
1	-1.487166077	-0.775769892	1.085308441
1	-0.949694499	0.063210851	-0.364882562
1	-2.123803162	-2.805793414	-0.306316126
1	-0.869725763	-2.102302999	-1.477472963
6	-5.574638023	-2.234845665	-0.927290494
6	-6.912181580	-2.539040297	-1.603033848
1	-5.284658087	-3.065847555	-0.283055062
1	-4.799959595	-2.171893985	-1.695664491
1	-7.735198089	-2.604389285	-0.890044097
1	-6.854133076	-3.498728917	-2.120333567
1	-7.177003679	-1.789472198	-2.350442577
8	-3.787615023	-1.609606081	1.433039551
6	-6.532040464	-0.987642377	1.119624617
6	-6.691924301	-2.278440365	1.921788195
1	-7.060707176	-3.103190695	1.309950415
1	-7.424333905	-2.118742171	2.716818510
1	-5.754368856	-2.585007056	2.376262110
1	-6.258215224	-0.175372980	1.797681834
1	-7.506257923	-0.712399432	0.705042988
8	-5.088540954	1.313432622	-2.916215243



6	-4.797595426	0.712305876	-1.905589144
1	-3.160826405	-0.592242621	-2.156992644
1	-2.705808302	1.086348903	-1.985445799
1	-5.955392887	1.161074495	-0.202059017
1	-6.797412053	0.206788502	-1.392631430

**Supplementary Table T12:** Cartesian coordinates for the DFT-optimized structure of **6'**

Atomic number / X / Y / Z

6	-2.891843075	1.297147323	2.127934481
6	-3.039062863	1.383097352	0.611602137
1	-2.852800656	2.300606477	2.556228389
1	-1.981333217	0.773640761	2.421619772
1	-3.727530647	0.767629329	2.584692514
6	-3.080657137	0.027087721	-0.142732873
1	-2.201029486	1.948034196	0.190705184
1	-3.934486378	1.961344387	0.370293138
6	-3.397843674	0.272228173	-1.636586704
6	-5.860486689	0.314047630	-0.896604295
6	-5.563210647	-0.950941334	-0.071227150
7	-4.156409798	-0.863599372	0.440982420
6	-1.758364744	-0.670953839	-0.020367919
6	-1.464693792	-1.999011227	-0.617076545
1	-0.954220249	-0.139674123	0.472357889
1	-2.368038082	-2.589081082	-0.777344293
1	-0.806781423	-2.579827812	0.034641412
1	-0.947170344	-1.917631731	-1.584569964
6	-5.662947842	-2.236278134	-0.931132731
6	-7.022131810	-2.518096908	-1.572444463
1	-5.370089714	-3.071211350	-0.293236016
1	-4.909526105	-2.185698356	-1.721992494
1	-7.826816570	-2.571162119	-0.838047376
1	-6.993437117	-3.477743568	-2.092242812
1	-7.293987425	-1.762655386	-2.311403849
8	-3.814899228	-1.645933121	1.393924551
6	-6.555159400	-0.956339663	1.125514419
6	-6.725266571	-2.235435625	1.944155835
1	-7.115479285	-3.060844083	1.346615599
1	-7.444281880	-2.055143828	2.746929773
1	-5.786488252	-2.552164435	2.388949890
1	-6.255964353	-0.142204136	1.790593184
1	-7.530691740	-0.667433251	0.723243545
8	-5.123314539	1.243778618	-2.968440156
6	-4.828147538	0.670476949	-1.943523433
1	-3.197978075	-0.637562194	-2.210194386
1	-2.732544548	1.036136476	-2.041089490
1	-5.930667630	1.171688111	-0.218161225
1	-6.831599377	0.237883613	-1.382609268

**Supplementary Table T13:** Cartesian coordinates for the DFT-optimized structure of TEEPONE + 1H<sub>2</sub>O

Atomic number	X	Y	Z
1	-2.367048440	3.454889807	-0.265019794
8	-2.558650732	4.409770250	-0.314110243
1	-2.928361875	4.620229722	0.556327439
6	-0.012031022	3.681200208	2.147859348
6	0.940632626	2.514078432	1.861310385
1	0.575804495	4.555716678	2.448791542
1	-0.698233680	3.454365964	2.970572589
1	-0.608061689	3.971229998	1.277389139
6	0.311234544	1.169277981	1.390333054
1	1.513834365	2.285324614	2.769496545
1	1.677089925	2.825910694	1.110855217
6	1.435672341	0.135933823	1.182743818
6	1.666421239	1.013426919	-1.152975887
6	0.352009758	1.409817130	-1.132206762
7	-0.362000826	1.413873483	0.058303806
6	-0.736157946	0.659676089	2.403072499
6	-1.438429459	-0.661129303	2.065740832
1	-1.496051107	1.431441262	2.536679845
1	-0.210383351	0.564558756	3.362094197
1	-1.961901644	-0.596141999	1.107333412
1	-2.185263611	-0.885478694	2.835293725
1	-0.749446067	-1.511968039	2.030161372
6	-0.361410828	1.888247489	-2.371312509
6	-0.250576314	3.411523124	-2.583452567
1	-1.413657442	1.598646422	-2.311311210
1	0.080312517	1.367503452	-3.227139543
1	-0.726633454	3.971995985	-1.774988984
1	-0.747923502	3.689851814	-3.518792724
1	0.798483264	3.719035681	-2.653597623
8	-1.603294215	1.737806951	0.072052702
8	3.540471376	0.162893771	0.005178640
6	2.348430487	0.446074130	0.003787055
1	1.003426725	-0.853677655	0.987808425
1	2.039067523	0.051992529	2.091191218
1	2.227040852	1.085299790	-2.079399392

**Supplementary Table T14:** Cartesian coordinates for the DFT-optimized structure of TEEPONE + 2H<sub>2</sub>O

Atomic number	X	Y	Z
6	-0.565925000	1.565997000	-3.040064000
6	-0.124889000	0.266546000	-2.359042000
1	-0.500911000	1.440328000	-4.127438000
1	0.072366000	2.412792000	-2.771108000
1	-1.598488000	1.832485000	-2.804374000
6	0.007270000	0.262529000	-0.801225000
1	0.862856000	-0.025514000	-2.739764000

1	-0.806805000	-0.538053000	-2.659562000
6	0.318602000	-1.180282000	-0.351725000
6	-2.232172000	-1.541511000	-0.434956000
6	-2.342705000	-0.219759000	0.357304000
7	-1.281147000	0.710452000	-0.170524000
6	1.146676000	1.222610000	-0.372737000
6	1.453999000	1.322838000	1.126640000
1	0.912498000	2.219942000	-0.750629000
1	2.044994000	0.886150000	-0.906803000
1	0.600870000	1.695980000	1.701434000
1	2.283721000	2.023223000	1.277898000
1	1.767480000	0.365801000	1.558456000
6	-2.085531000	-0.426492000	1.878202000
6	-3.031290000	-1.414178000	2.575542000
1	-2.137420000	0.550676000	2.367117000
1	-1.056259000	-0.773907000	2.023504000
1	-4.084815000	-1.141632000	2.453365000
1	-2.818196000	-1.425857000	3.650116000
1	-2.904947000	-2.438931000	2.209545000
8	-1.468226000	1.980548000	-0.069889000
6	-3.749686000	0.381805000	0.064860000
6	-4.317788000	1.436483000	1.025896000
1	-4.489811000	1.037189000	2.029813000
1	-5.289664000	1.776003000	0.647732000
1	-3.664159000	2.303688000	1.129387000
1	-3.727784000	0.799940000	-0.947599000
1	-4.447721000	-0.464543000	0.033892000
8	-0.668891000	-3.348106000	-0.631429000
6	-0.841054000	-2.153604000	-0.490847000
1	0.618051000	-1.195420000	0.702688000
1	1.169478000	-1.570300000	-0.918907000
1	-2.550183000	-1.359947000	-1.471442000
1	-2.921512000	-2.289057000	-0.034543000
1	-2.751852000	2.896170000	-1.208995000
8	-3.415750000	3.148181000	-1.877403000
1	-4.220594000	3.309347000	-1.363696000
8	-1.446602000	2.905390000	2.612151000
1	-0.970617000	3.746789000	2.671981000
1	-1.452517000	2.692912000	1.658747000

**Supplementary Table T15:** Cartesian coordinates for the DFT-optimized structure of TEEPONE + 3H<sub>2</sub>O

Atomic number / X / Y / Z			
6	-0.761978000	1.380504000	-3.163543000
6	-0.282364000	0.107147000	-2.459517000
1	-0.793837000	1.199486000	-4.244177000
1	-0.089289000	2.227658000	-2.994566000
1	-1.767678000	1.674004000	-2.850970000
6	-0.064245000	0.167503000	-0.914032000
1	0.682775000	-0.197342000	-2.883101000
1	-0.981978000	-0.704994000	-2.689319000
6	0.312047000	-1.246351000	-0.422048000

6	-2.220886000	-1.696730000	-0.326887000
6	-2.338604000	-0.332014000	0.388233000
7	-1.337925000	0.599528000	-0.240710000
6	1.069498000	1.169023000	-0.576559000
6	1.461927000	1.309254000	0.899024000
1	0.793955000	2.154526000	-0.954912000
1	1.941844000	0.842334000	-1.155377000
1	0.626363000	1.653857000	1.515799000
1	2.259442000	2.055568000	0.987888000
1	1.844276000	0.377011000	1.327492000
6	-2.000216000	-0.428451000	1.903814000
6	-2.884562000	-1.383790000	2.716335000
1	-2.062126000	0.579617000	2.329395000
1	-0.956145000	-0.738947000	2.020074000
1	-3.946936000	-1.126340000	2.654953000
1	-2.591642000	-1.338189000	3.770857000
1	-2.771030000	-2.423238000	2.390439000
8	-1.565435000	1.868530000	-0.162115000
6	-3.781213000	0.195101000	0.129556000
6	-4.344972000	1.314387000	1.016190000
1	-4.369754000	1.033215000	2.073136000
1	-5.378070000	1.519425000	0.712461000
1	-3.780352000	2.245047000	0.930942000
1	-3.836903000	0.499805000	-0.922438000
1	-4.442790000	-0.673380000	0.225550000
8	-0.612635000	-3.450668000	-0.582056000
6	-0.817127000	-2.253632000	-0.458402000
1	0.658963000	-1.209894000	0.617482000
1	1.150633000	-1.628041000	-1.011789000
1	-2.619917000	-1.600484000	-1.346298000
1	-2.849257000	-2.440293000	0.170117000
1	-2.929653000	2.719395000	-1.190231000
8	-3.553642000	3.162851000	-1.794284000
1	-4.413264000	3.085925000	-1.351586000
8	-1.267729000	3.407800000	2.148902000
1	-2.115572000	3.783722000	2.437918000
1	-1.503896000	2.737515000	1.475241000
8	-0.335020000	4.596864000	-0.265561000

**Supplementary Table T16:** Cartesian coordinates for the DFT-optimized structure of TEEPONE + 4H<sub>2</sub>O

Atomic number / X / Y / Z

6	-0.826079000	1.367076000	-3.089579000
6	-0.449761000	0.062284000	-2.379149000
1	-1.030169000	1.154989000	-4.145053000
1	-0.007900000	2.094778000	-3.058006000
1	-1.715038000	1.843303000	-2.666211000
6	-0.233368000	0.124528000	-0.833757000
1	0.488090000	-0.316125000	-2.805207000
1	-1.209257000	-0.695815000	-2.600734000
6	0.279830000	-1.247535000	-0.347281000
6	-2.193545000	-1.963917000	-0.336195000

6	-2.480928000	-0.630305000	0.390000000
7	-1.540946000	0.413059000	-0.147218000
6	0.781535000	1.241151000	-0.488217000
6	1.187181000	1.382725000	0.983043000
1	0.367977000	2.193806000	-0.824844000
1	1.673026000	1.047492000	-1.097302000
1	0.320489000	1.573165000	1.622942000
1	1.871615000	2.232678000	1.090925000
1	1.710253000	0.501434000	1.368177000
6	-2.223596000	-0.735909000	1.920991000
6	-3.087118000	-1.756545000	2.672439000
1	-2.374578000	0.258960000	2.353317000
1	-1.168080000	-0.980946000	2.086981000
1	-4.158220000	-1.555848000	2.566668000
1	-2.846130000	-1.718698000	3.740504000
1	-2.901570000	-2.781490000	2.333229000
8	-1.844886000	1.648558000	0.051936000
6	-3.949992000	-0.236901000	0.051493000
6	-4.653195000	0.849891000	0.875745000
1	-4.689552000	0.602009000	1.941686000
1	-5.688817000	0.941047000	0.528418000
1	-4.175116000	1.825061000	0.773162000
1	-3.977769000	0.034347000	-1.011152000
1	-4.534973000	-1.160247000	0.138957000
8	-0.402354000	-3.533263000	-0.573411000
6	-0.735181000	-2.366866000	-0.434265000
1	0.576608000	-1.188305000	0.707324000
1	1.177430000	-1.531442000	-0.904641000
1	-2.572135000	-1.902326000	-1.366226000
1	-2.751350000	-2.777696000	0.134354000
1	-2.297420000	4.158352000	-1.530488000
8	-3.137151000	3.640390000	-1.536721000
1	-2.888819000	2.848290000	-1.028977000
8	-1.910501000	3.180695000	2.352486000
1	-1.511423000	2.711327000	3.103195000
1	-1.943241000	2.526315000	1.620238000
8	-0.706784000	5.010656000	-1.392476000
1	-0.034367000	4.490473000	-1.859361000
1	-0.452438000	4.951664000	-0.433358000
8	-0.080092000	4.908192000	1.259975000
1	-0.727957000	4.305293000	1.706511000
1	0.784050000	4.485197000	1.387137000

**Supplementary Table T17:** Cartesian coordinates for the DFT-optimized structure of TEEPONE + 5H<sub>2</sub>O

Atomic number / X / Y / Z

6	-0.805499000	1.802249000	-2.543996000
6	-0.385398000	0.407604000	-2.064428000
1	-0.971209000	1.767902000	-3.627115000
1	-0.029663000	2.551128000	-2.355838000
1	-1.734243000	2.145635000	-2.082730000
6	-0.224454000	0.184294000	-0.526102000

1	0.585033000	0.155723000	-2.510699000
1	-1.095013000	-0.333910000	-2.450612000
6	0.281412000	-1.255728000	-0.292063000
6	-2.187703000	-1.967258000	-0.420175000
6	-2.473933000	-0.783276000	0.529164000
7	-1.561897000	0.350847000	0.141672000
6	0.785844000	1.199287000	0.060157000
6	1.049308000	1.121034000	1.569040000
1	0.454055000	2.208087000	-0.190437000
1	1.724960000	1.042935000	-0.484700000
1	0.131263000	1.253763000	2.150967000
1	1.747467000	1.913993000	1.860824000
1	1.503181000	0.171237000	1.869176000
6	-2.174243000	-1.122425000	2.017326000
6	-2.949623000	-2.314708000	2.593581000
1	-2.385843000	-0.222093000	2.603762000
1	-1.102367000	-1.314005000	2.137080000
1	-4.033659000	-2.200941000	2.486742000
1	-2.728935000	-2.407872000	3.662568000
1	-2.661831000	-3.259017000	2.119425000
8	-1.943916000	1.545352000	0.446691000
6	-3.958298000	-0.367326000	0.306336000
6	-4.664655000	0.483626000	1.370753000
1	-4.720826000	-0.031509000	2.334543000
1	-5.693144000	0.676724000	1.045654000
1	-4.173513000	1.445032000	1.525468000
1	-4.014884000	0.134315000	-0.667311000
1	-4.523012000	-1.299528000	0.187023000
8	-0.390775000	-3.468708000	-0.914996000
6	-0.729643000	-2.344802000	-0.579792000
1	0.583993000	-1.392086000	0.753767000
1	1.177124000	-1.433091000	-0.894056000
1	-2.561910000	-1.717759000	-1.423638000
1	-2.748082000	-2.850911000	-0.105177000
1	-3.310557000	2.496766000	-0.389310000
8	-3.972634000	3.091563000	-0.798928000
1	-4.494314000	2.516930000	-1.382597000
8	-0.951038000	4.014667000	1.301321000
1	-0.227479000	3.936478000	1.944244000
1	-1.166756000	3.095416000	1.034753000
8	1.970101000	4.101568000	-1.955835000
1	2.347402000	3.654978000	-1.182963000
1	1.198011000	4.594354000	-1.592455000
8	-0.275311000	5.371075000	-0.940020000
1	-0.501178000	4.919767000	-0.082500000
1	-0.134648000	6.305157000	-0.711672000

**Supplementary Table T18:** Cartesian coordinates for the DFT-optimized structure of **3** + 1H<sub>2</sub>O

Atomic number / X / Y / Z

6	-0.965384000	1.556682000	-2.861786000
6	-0.201235000	0.375127000	-2.254560000

1	-0.871667000	1.531455000	-3.953869000
1	-0.592630000	2.521957000	-2.508457000
1	-2.031913000	1.507367000	-2.617469000
6	-0.109015000	0.321577000	-0.696049000
1	0.832103000	0.376237000	-2.625698000
1	-0.646590000	-0.558640000	-2.621740000
6	0.366027000	-1.085265000	-0.274643000
6	-2.114701000	-1.754126000	-0.467582000
6	-2.435107000	-0.467011000	0.323185000
7	-1.456791000	0.592120000	-0.094369000
6	0.909473000	1.381742000	-0.199733000
6	1.043031000	1.551546000	1.317813000
1	0.671878000	2.351422000	-0.641477000
1	1.879701000	1.083441000	-0.619372000
1	0.097466000	1.871348000	1.763552000
1	1.789808000	2.323271000	1.533876000
1	1.370948000	0.635137000	1.822586000
6	-2.276050000	-0.669486000	1.856246000
6	-3.174383000	-1.739571000	2.488820000
1	-2.457678000	0.300317000	2.331110000
1	-1.229866000	-0.917687000	2.073263000
1	-4.238295000	-1.547187000	2.314528000
1	-3.017884000	-1.759566000	3.573280000
1	-2.947998000	-2.743127000	2.112274000
8	-1.800184000	1.813817000	0.115576000
6	-3.876486000	-0.029818000	-0.074625000
6	-4.605780000	1.010714000	0.785336000
1	-4.758710000	0.664892000	1.813185000
1	-5.598039000	1.198757000	0.359059000
1	-4.056974000	1.951882000	0.817383000
1	-3.828604000	0.328898000	-1.110206000
1	-4.482207000	-0.945021000	-0.103227000
8	-0.340193000	-3.364410000	-0.501917000
6	-0.661823000	-2.194676000	-0.425062000
1	0.671032000	-1.082527000	0.779229000
1	1.257960000	-1.361978000	-0.846728000
1	-2.370735000	-1.593220000	-1.525184000
1	-2.739289000	-2.583359000	-0.126241000
1	-1.089412000	3.528456000	-0.403822000
8	-0.702631000	4.341749000	-0.781699000
1	-1.370289000	4.642907000	-1.415594000

**Supplementary Table T19:** Cartesian coordinates for the DFT-optimized structure of **3** + 2H<sub>2</sub>O

Atomic number	X	Y	Z
6	-2.512242000	-0.544474000	2.361328000
6	-1.945222000	0.535168000	1.431968000
1	-2.012496000	-1.510961000	2.230386000
1	-3.584864000	-0.697500000	2.203836000
1	-2.371039000	-0.240206000	3.404538000
6	-1.995543000	0.177697000	-0.073887000
1	-0.896518000	0.727831000	1.694184000

1	-2.481964000	1.472531000	1.598138000
6	-3.412848000	-0.173412000	-0.594664000
6	-4.516110000	0.864650000	-0.364797000
1	-3.698683000	-1.121454000	-0.122772000
1	-3.317258000	-0.376689000	-1.666849000
1	-4.674403000	1.072364000	0.698821000
1	-5.461479000	0.487898000	-0.770416000
1	-4.292616000	1.809875000	-0.868240000
6	-0.990123000	-0.946443000	-0.423994000
6	0.156728000	-0.309153000	-1.183266000
1	-1.437875000	-1.693314000	-1.090755000
1	-0.610348000	-1.474015000	0.454159000
6	-0.279974000	1.059601000	-1.708082000
7	-1.438402000	1.340066000	-0.850418000
8	1.257640000	-0.799657000	-1.337384000
6	-0.587542000	1.017947000	-3.246848000
1	0.479797000	1.826258000	-1.528024000
6	0.777812000	0.911621000	-3.994988000
6	0.758722000	0.063901000	-5.275292000
1	1.520951000	0.472876000	-3.322170000
1	1.124184000	1.927771000	-4.219037000
1	0.480725000	-0.971551000	-5.053341000
1	1.759846000	0.050854000	-5.720616000
1	0.068079000	0.446067000	-6.034282000
6	-1.395173000	2.267479000	-3.658456000
6	-1.718448000	2.389430000	-5.153517000
1	-0.835862000	3.152742000	-3.333413000
1	-2.332505000	2.263737000	-3.093893000
1	-0.820437000	2.530699000	-5.762605000
1	-2.367559000	3.257009000	-5.316997000
1	-2.255550000	1.512197000	-5.535677000
8	-1.376454000	-0.171868000	-3.405190000
1	-1.674692000	-0.223802000	-4.327672000
8	-1.804266000	2.551754000	-0.621392000
1	-2.956921000	3.328580000	0.666500000
8	-3.528343000	3.775321000	1.321059000
1	-4.425024000	3.519774000	1.053387000
8	0.244332000	4.434263000	-1.276599000
1	-0.522263000	3.871217000	-1.044205000
1	-0.133308000	5.112442000	-1.859085000

**Supplementary Table T20:** Cartesian coordinates for the DFT-optimized structure of **3** + 3H<sub>2</sub>O

Atomic number	X	Y	Z
6	-2.728921000	-0.719429000	2.366593000
6	-2.138353000	0.403544000	1.505130000
1	-2.200943000	-1.669984000	2.228643000
1	-3.788219000	-0.889139000	2.147792000
1	-2.648875000	-0.448946000	3.425466000
6	-2.100380000	0.095454000	-0.011903000
1	-1.109605000	0.608622000	1.829511000
1	-2.705280000	1.322515000	1.673089000



6	-3.482837000	-0.256291000	-0.619885000
6	-4.610723000	0.762281000	-0.424304000
1	-3.781905000	-1.219535000	-0.188922000
1	-3.327376000	-0.430651000	-1.690180000
1	-4.823024000	0.947761000	0.633796000
1	-5.529664000	0.380937000	-0.882768000
1	-4.376718000	1.720663000	-0.897482000
6	-1.062022000	-1.004011000	-0.343223000
6	0.094576000	-0.337553000	-1.062958000
1	-1.474329000	-1.756222000	-1.026378000
1	-0.695535000	-1.529943000	0.541822000
6	-0.332461000	1.046886000	-1.550488000
7	-1.518540000	1.289004000	-0.719768000
8	1.198291000	-0.823860000	-1.212745000
6	-0.593531000	1.053454000	-3.099583000
1	0.429358000	1.806316000	-1.329295000
6	0.795795000	0.999300000	-3.805122000
6	0.829468000	0.241180000	-5.140341000
1	1.512767000	0.515982000	-3.135158000
1	1.149491000	2.028067000	-3.938128000
1	0.543854000	-0.807141000	-5.003219000
1	1.849175000	0.254223000	-5.541967000
1	0.173970000	0.675776000	-5.901617000
6	-1.421598000	2.297108000	-3.491738000
6	-1.710423000	2.466070000	-4.989330000
1	-0.899789000	3.189025000	-3.124024000
1	-2.373813000	2.248938000	-2.954939000
1	-0.802644000	2.659935000	-5.568257000
1	-2.384471000	3.317226000	-5.137350000
1	-2.207447000	1.585979000	-5.416154000
8	-1.352233000	-0.145869000	-3.328040000
1	-1.594464000	-0.183142000	-4.267600000
8	-1.914713000	2.485958000	-0.461864000
1	-3.161164000	3.198563000	0.771394000
8	-3.781882000	3.621762000	1.395613000
1	-4.654374000	3.415074000	1.025714000
8	-0.379194000	4.795070000	-0.947965000
1	-0.959705000	4.010933000	-0.828135000
1	-0.707616000	5.227831000	-1.752864000
8	1.995474000	3.444584000	-1.375747000
1	1.197690000	4.011686000	-1.251441000
1	2.307234000	3.286543000	-0.470047000

**Supplementary Table T21:** Cartesian coordinates for the DFT-optimized structure of **3** + 4H<sub>2</sub>O

Atomic number / X / Y / Z

6	-2.623330000	0.047480000	2.211205000
6	-2.155323000	1.027080000	1.129263000
1	-1.959115000	-0.819592000	2.297712000
1	-3.635864000	-0.322620000	2.020080000
1	-2.635084000	0.550913000	3.184493000
6	-2.012081000	0.404137000	-0.279381000

1	-1.177369000	1.442735000	1.394040000
1	-2.848210000	1.871454000	1.081572000
6	-3.315588000	-0.239157000	-0.819916000
6	-4.557733000	0.655721000	-0.866241000
1	-3.521702000	-1.118323000	-0.196745000
1	-3.096691000	-0.614641000	-1.825075000
1	-4.849886000	1.006613000	0.130130000
1	-5.404080000	0.091075000	-1.272556000
1	-4.405747000	1.529268000	-1.508249000
6	-0.839836000	-0.604204000	-0.341786000
6	0.211871000	-0.045419000	-1.282826000
1	-1.154751000	-1.578991000	-0.730241000
1	-0.381144000	-0.775910000	0.635530000
6	-0.338497000	1.188672000	-2.003302000
7	-1.546847000	1.478335000	-1.225213000
8	1.318986000	-0.516759000	-1.442291000
6	-0.585959000	0.912615000	-3.525430000
1	0.347221000	2.034248000	-1.902534000
6	0.807517000	0.863279000	-4.227213000
6	0.927857000	-0.144551000	-5.378571000
1	1.568300000	0.605803000	-3.485205000
1	1.045447000	1.873427000	-4.582749000
1	0.761863000	-1.166753000	-5.022043000
1	1.938738000	-0.101367000	-5.799132000
1	0.225938000	0.048264000	-6.195999000
6	-1.515076000	1.990663000	-4.125710000
6	-1.795103000	1.864971000	-5.629685000
1	-1.078248000	2.976702000	-3.924540000
1	-2.465733000	1.956232000	-3.585627000
1	-0.899130000	2.035702000	-6.235001000
1	-2.539838000	2.611646000	-5.926686000
1	-2.204136000	0.882088000	-5.895486000
8	-1.233638000	-0.371021000	-3.534814000
1	-1.453005000	-0.599280000	-4.452588000
8	-2.026067000	2.672524000	-1.205944000
1	-2.243451000	4.160567000	2.799639000
8	-2.230633000	4.823837000	2.091080000
1	-2.977750000	4.570439000	1.492200000
8	-0.235582000	4.369052000	0.251876000
1	-0.790684000	3.959685000	-0.441048000
1	-0.879906000	4.536944000	0.986421000
8	-4.040419000	4.039643000	0.184750000
1	-4.787481000	3.498170000	0.485913000
1	-3.463500000	3.431327000	-0.326796000
8	1.171721000	2.045941000	0.702889000
1	0.702233000	2.914112000	0.633291000
1	1.199782000	1.862894000	1.654954000

**Supplementary Table T22:** Cartesian coordinates for the DFT-optimized structure of **4** + 1H<sub>2</sub>O

Atomic number / X / Y / Z

1	-2.367048000	3.454890000	-0.265020000
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8	-2.558651000	4.409770000	-0.314110000
1	-2.928362000	4.620230000	0.556327000
6	-0.012031000	3.681200000	2.147859000
6	0.940633000	2.514078000	1.861310000
1	0.575804000	4.555717000	2.448792000
1	-0.698234000	3.454366000	2.970573000
1	-0.608062000	3.971230000	1.277389000
6	0.311235000	1.169278000	1.390333000
1	1.513834000	2.285325000	2.769497000
1	1.677090000	2.825911000	1.110855000
6	1.435672000	0.135934000	1.182744000
6	1.666421000	1.013427000	-1.152976000
6	0.352010000	1.409817000	-1.132207000
7	-0.362001000	1.413873000	0.058304000
6	-0.736158000	0.659676000	2.403072000
6	-1.438429000	-0.661129000	2.065741000
1	-1.496051000	1.431441000	2.536680000
1	-0.210383000	0.564559000	3.362094000
1	-1.961902000	-0.596142000	1.107333000
1	-2.185264000	-0.885479000	2.835294000
1	-0.749446000	-1.511968000	2.030161000
6	-0.361411000	1.888247000	-2.371313000
6	-0.250576000	3.411523000	-2.583453000
1	-1.413657000	1.598646000	-2.311311000
1	0.080313000	1.367503000	-3.227140000
1	-0.726633000	3.971996000	-1.774989000
1	-0.747924000	3.689852000	-3.518793000
1	0.798483000	3.719036000	-2.653598000
8	-1.603294000	1.737807000	0.072053000
8	3.540471000	0.162894000	0.005179000
6	2.348430000	0.446074000	0.003787000
1	1.003427000	-0.853678000	0.987808000
1	2.039068000	0.051993000	2.091191000
1	2.227041000	1.085300000	-2.079399000

**Supplementary Table T23:** Cartesian coordinates for the DFT-optimized structure of **4** + 2H<sub>2</sub>O

Atomic number / X / Y / Z

1	-3.169670000	2.088779000	1.763985000
8	-3.437491000	2.864525000	2.279646000
1	-3.182617000	3.598438000	1.686959000
6	0.119516000	3.692538000	2.081054000
6	1.030976000	2.460414000	2.087712000
1	0.644675000	4.529137000	2.555515000
1	-0.816848000	3.536049000	2.624026000
1	-0.136110000	4.008983000	1.066339000
6	0.418917000	1.110087000	1.607462000
1	1.390673000	2.274275000	3.107682000
1	1.924601000	2.673420000	1.487368000
6	1.545171000	0.063700000	1.495188000
6	1.911239000	0.863716000	-0.852310000
6	0.600301000	1.266970000	-0.916944000

7	-0.174977000	1.319128000	0.231052000
6	-0.681264000	0.634140000	2.581215000
6	-1.408059000	-0.668172000	2.221332000
1	-1.417957000	1.429334000	2.710229000
1	-0.184031000	0.515353000	3.552305000
1	-1.904557000	-0.594600000	1.248871000
1	-2.179367000	-0.873477000	2.971524000
1	-0.740074000	-1.536418000	2.201565000
6	-0.050016000	1.681178000	-2.213598000
6	-0.037494000	3.202409000	-2.462137000
1	-1.079928000	1.312707000	-2.224766000
1	0.488956000	1.179345000	-3.023358000
1	-0.641466000	3.745206000	-1.730136000
1	-0.446617000	3.415272000	-3.455961000
1	0.983475000	3.597298000	-2.428875000
8	-1.413267000	1.656600000	0.150883000
8	3.710992000	0.038922000	0.430833000
6	2.523235000	0.328674000	0.360264000
1	1.119159000	-0.931684000	1.314897000
1	2.096943000	0.012050000	2.438189000
1	2.522317000	0.895500000	-1.748331000
8	-2.505281000	4.272294000	-0.055523000
1	-3.285082000	4.239107000	-0.631572000
1	-2.103608000	3.384172000	-0.132582000

**Supplementary Table T24:** Cartesian coordinates for the DFT-optimized structure of **4** + 3H<sub>2</sub>O

Atomic number	X	Y	Z
1	-2.281893000	3.200113000	0.987369000
8	-2.734116000	4.044852000	0.822143000
1	-3.220054000	3.874914000	-0.019980000
6	0.338486000	3.424435000	2.637142000
6	1.293451000	2.274454000	2.299124000
1	0.925553000	4.291583000	2.959296000
1	-0.344043000	3.168489000	3.453470000
1	-0.262958000	3.737234000	1.779008000
6	0.663358000	0.931930000	1.821396000
1	1.891183000	2.027758000	3.185199000
1	2.005284000	2.612602000	1.536286000
6	1.795947000	-0.066990000	1.512398000
6	1.880812000	0.917567000	-0.792974000
6	0.556703000	1.272698000	-0.688742000
7	-0.088736000	1.194560000	0.533691000
6	-0.308552000	0.365818000	2.877119000
6	-0.985050000	-0.971083000	2.549460000
1	-1.079321000	1.111836000	3.078220000
1	0.277058000	0.264516000	3.799172000
1	-1.560599000	-0.912798000	1.620093000
1	-1.681160000	-1.231598000	3.354553000
1	-0.269112000	-1.795152000	2.460832000
6	-0.229818000	1.784979000	-1.867349000
6	-0.417520000	3.314942000	-1.868903000

1	-1.208155000	1.297026000	-1.888125000
1	0.302194000	1.479456000	-2.772442000
1	-1.023979000	3.651080000	-1.023223000
1	-0.921461000	3.616965000	-2.794176000
1	0.549122000	3.827902000	-1.833362000
8	-1.342635000	1.469931000	0.617139000
8	3.823432000	0.037345000	0.211289000
6	2.624146000	0.306416000	0.298492000
1	1.377998000	-1.059998000	1.304534000
1	2.446625000	-0.165294000	2.385592000
1	2.391311000	1.054619000	-1.740562000
8	-4.096035000	3.315158000	-1.494956000
1	-3.991399000	2.339482000	-1.358111000
1	-3.529293000	3.518524000	-2.256120000
8	-3.630006000	0.685667000	-0.858757000
1	-2.769948000	0.785636000	-0.400660000
1	-3.448903000	0.106494000	-1.617289000

**Supplementary Table T25:** Cartesian coordinates for the DFT-optimized structure of **4** + 4H<sub>2</sub>O

Atomic number / X / Y / Z

1	-3.299716000	3.253921000	1.578945000
8	-3.560627000	2.818460000	2.421661000
1	-3.701125000	1.896376000	2.134623000
6	-0.007944000	3.626525000	1.938101000
6	1.035255000	2.515581000	2.087057000
1	0.392757000	4.552967000	2.364137000
1	-0.948603000	3.401735000	2.448894000
1	-0.236775000	3.826733000	0.886736000
6	0.619131000	1.076832000	1.652462000
1	1.338072000	2.429683000	3.137508000
1	1.937980000	2.801176000	1.532781000
6	1.859040000	0.163649000	1.710969000
6	2.374904000	0.906157000	-0.628581000
6	1.037818000	1.142287000	-0.846914000
7	0.148861000	1.135157000	0.213585000
6	-0.517526000	0.539276000	2.545564000
6	-0.947357000	-0.914732000	2.305815000
1	-1.384318000	1.196180000	2.449218000
1	-0.163536000	0.643025000	3.578447000
1	-1.199023000	-1.103816000	1.257161000
1	-1.836031000	-1.137189000	2.906001000
1	-0.171620000	-1.630276000	2.596075000
6	0.480098000	1.423022000	-2.217804000
6	0.189829000	2.912908000	-2.484929000
1	-0.438254000	0.841896000	-2.346782000
1	1.208055000	1.058718000	-2.948354000
1	-0.598724000	3.298195000	-1.832411000
1	-0.142543000	3.037330000	-3.520838000
1	1.088370000	3.522471000	-2.341344000
8	-1.102301000	1.324117000	-0.019599000
8	4.109713000	0.328737000	0.859284000

6	2.904157000	0.489185000	0.661179000
1	1.569976000	-0.881261000	1.541067000
1	2.308818000	0.218389000	2.706484000
1	3.066105000	0.982273000	-1.461367000
8	-2.832648000	3.657019000	-0.186067000
1	-3.597202000	3.202167000	-0.623650000
1	-2.123184000	2.989342000	-0.218344000
8	-3.690697000	0.472862000	0.776526000
1	-2.754761000	0.501843000	0.490344000
1	-3.926957000	-0.468970000	0.819761000
8	-4.883566000	2.078863000	-1.125204000
1	-4.591434000	1.379722000	-0.492058000
1	-4.655070000	1.727457000	-2.001446000