Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information

Open-[60]fullerenols with water adsorbed both inside and outside

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1. General

Fullerene C_{60} was purchased from SES Research Co. Compounds H_2O@**1**–**3** and **1** were synthesized according to literature procedures.[1] The powdery samples were obtained from evaporation of corresponding CS_2 or toluene solutions.

IR measurements were carried out at SPring-8 (BL43IR). Prior to measurements, the powdery samples were pressed by two BaF_2 disks and the samples attached on the disk was used for the measurements. The powder shapes were confirmed by microscopy.

2. Computational Methods

All calculations were conducted using the Gaussian 09 program. All structures at the stationary states were optimized at the B3LYP-D3/6-31G(d,p) level of theory without any symmetry assumptions and confirmed by the frequency analyses at the same level of theory. For hydrogen halides, effective core potentials were incorporated in the calculations at the B3LYP-D3 level of theory with basis sets of LanL2DZ for halogens and 6-31G(d,p) for the rest.

Using the geometries optimized at the B3LYP-D3/6-31G(d,p) level of theory, natural bond orbital (NBO) analyses were performed at the same level of theory. The atoms-in-molecules (AIM) analyses and reduced density gradient (RDG) isosurface analyses were conducted by the use of Multiwfn[2] and the results were visualized by VMD.[3]

3. IR Spectra

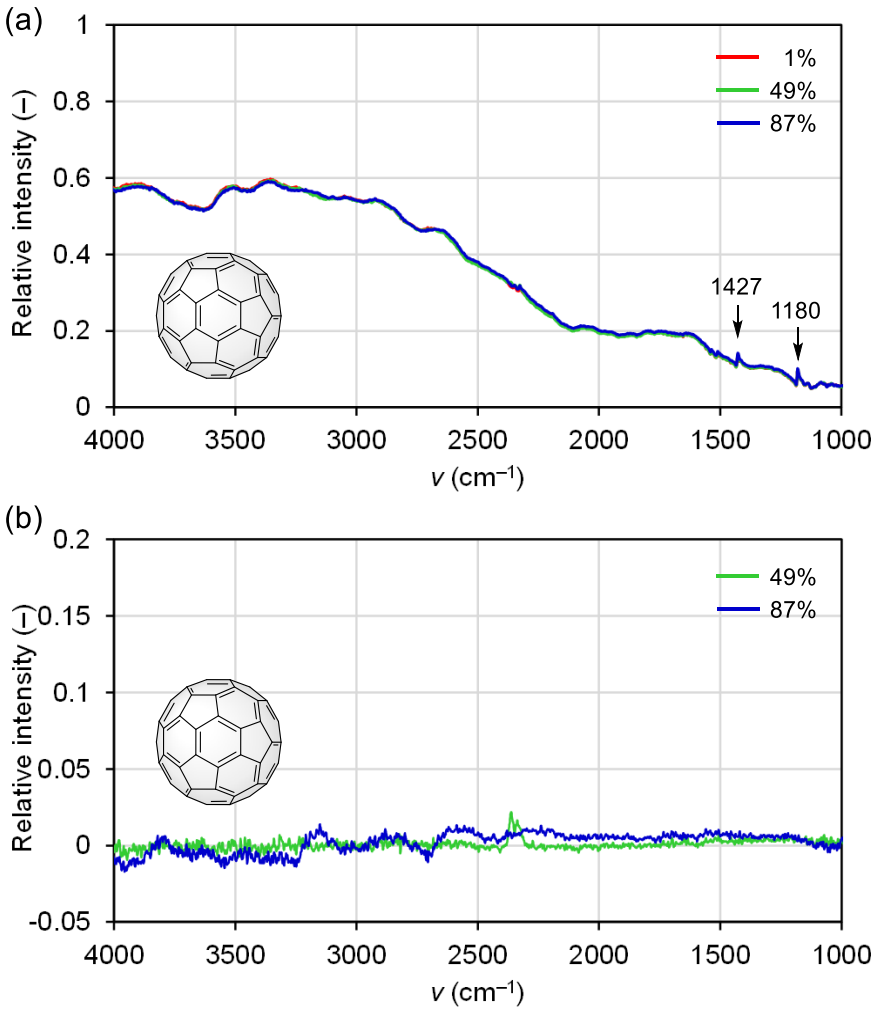


Figure S1. (a) Original and (b) differential IR spectra of C_{60} at variable relative humidities.

Though the spectral feature of H_2O@**1** (Figure S2) showed close resemblance to that of **1** (Figure 2), both OH stretching modes became sharpened. Likewise, the band observed at 1261 cm^{-1} became sharpened. This band was assigned to be a C–OH stretching mode adjacent to carbonyl **b** (1288 cm^{-1}) according to theoretical calculations (Figure S8). Furthermore, the vibration band of carbonyl **b** became broadened. These feature strongly supports that the encapsulated H_2O is adsorbed from inside toward the central oxygen in the bis(hemiketal) moiety through a hydrogen-bonding.

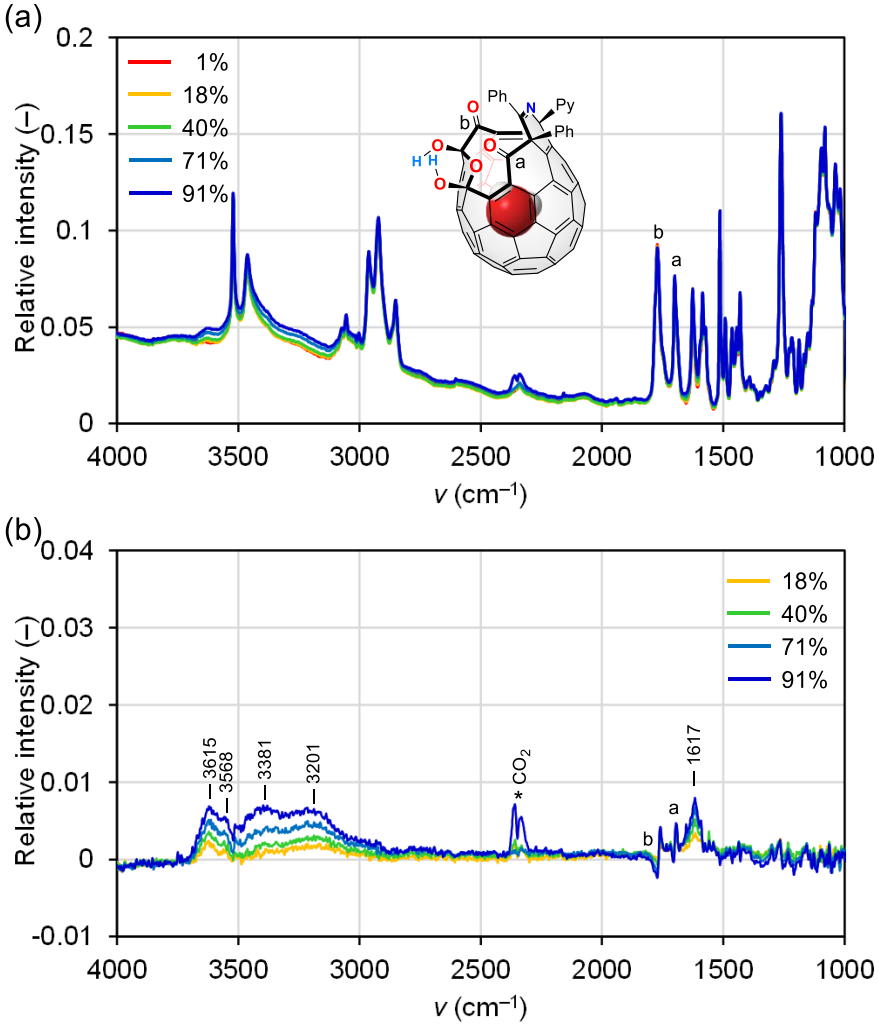


Figure S2. (a) Original and (b) differential IR spectra of H_2O@**1** at variable relative humidities.

For [60]fullerenol **1**, carbonyl **b** is largely influenced by adsorbed water while carbonyl **a** has a larger influence in **2** upon water adsorption. The structural difference is only one substituent, OH (for **1**) or H (for **2**), at the same locant. Considering the significant decrease in relative amount of adsorbed water for **2** compared to **1**, carbonyl groups **a** and **b** are considered to play a secondary role for water adsorption whereas each carbonyl group has a different effect on water adsorption depending presumably upon their surrounding stereoenvironment as well as distance to hydroxy groups which should be an actual initiator for the adsorption event.

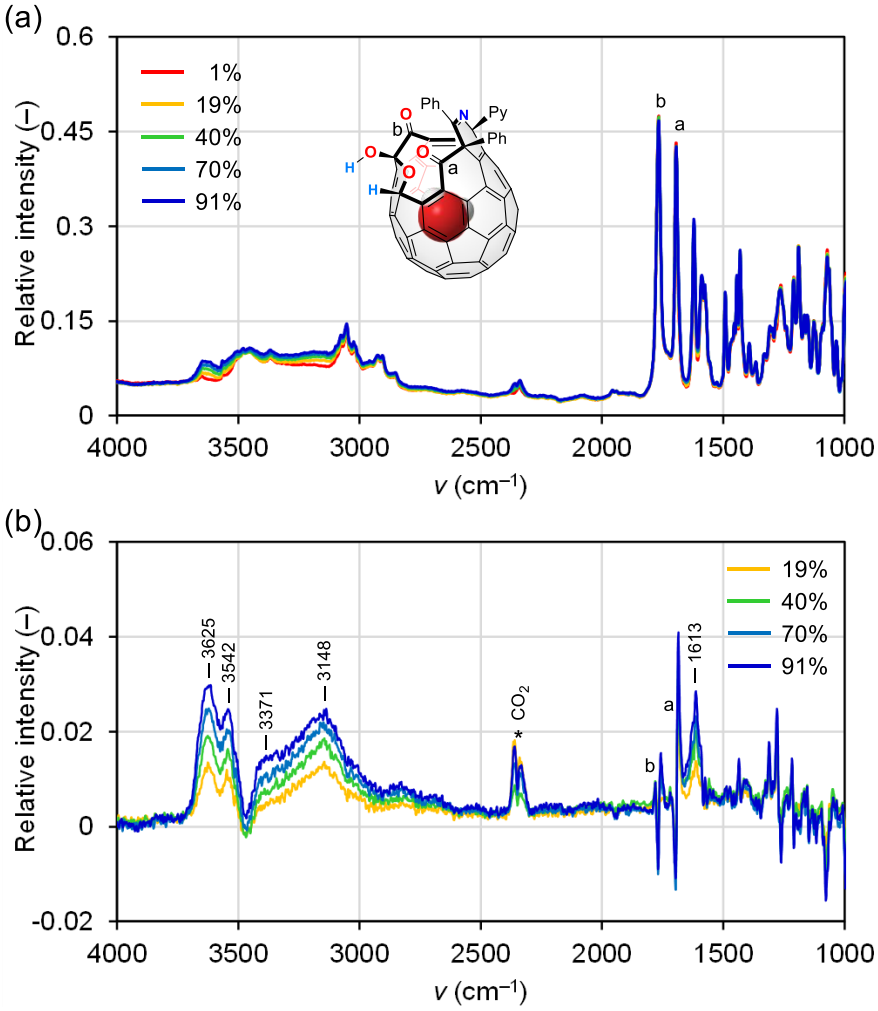


Figure S3. (a) Original and (b) differential IR spectra of H_2O@**2** at variable relative humidities.

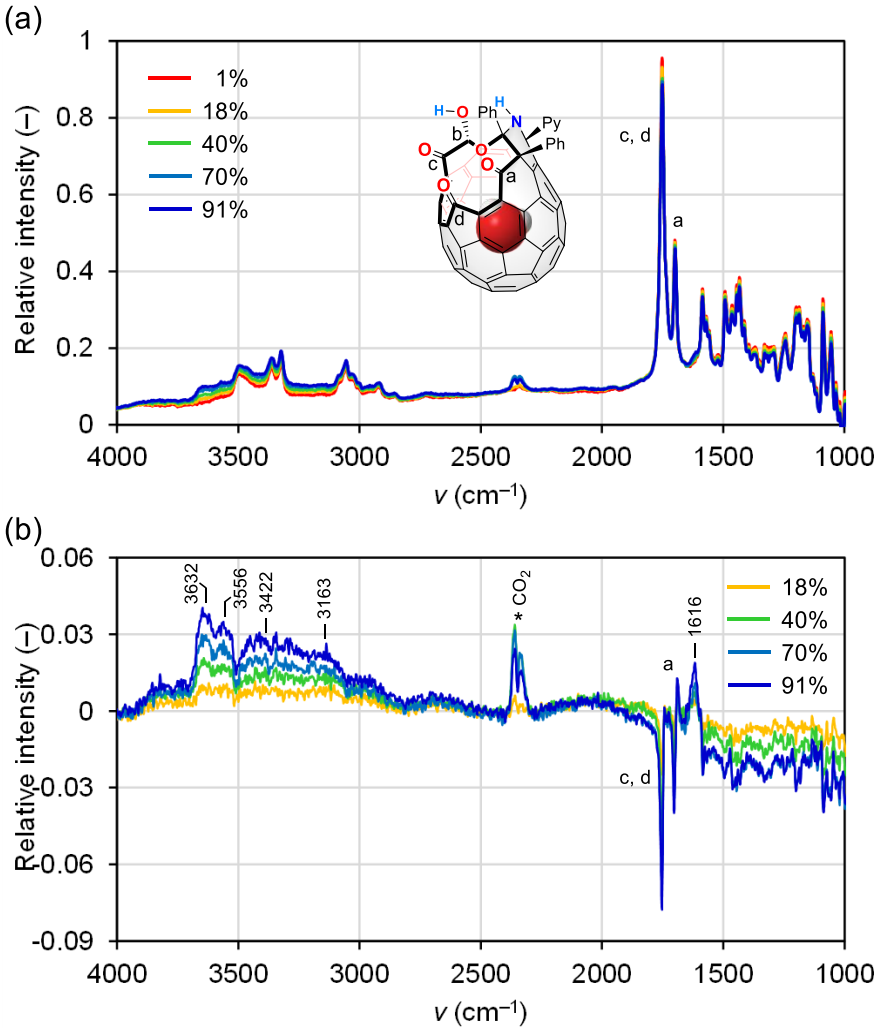


Figure S4. (a) Original and (b) differential IR spectra of H_2O@**3** at variable relative humidities.

4. DFT Calculations

4.1. Simulated IR Spectra of 1–3

The remained sharpness in the spectral feature for OH stretching modes of hydroxy substituents (Figures S2–4) indicates that the free form of [60]fullerenol still exists even at high RHs. In other words, water adsorption is favored on already-wetted surface of [60]fullerenols than dry surface. Therefore, the spectra are obtained as a results of an average between the two states, i.e., dry and wet [60]fullereonls. As shown in Figure S5, under dry conditions, **1** shows OH stretching modes at 3743 and 3665 cm^{-1} while under wet conditions, they are shifted to 2041 and 1995 cm^{-1} (Figure S11). If all molecules of [60]fullerenol adsorbs water, significant broadening of the bands would be expected.

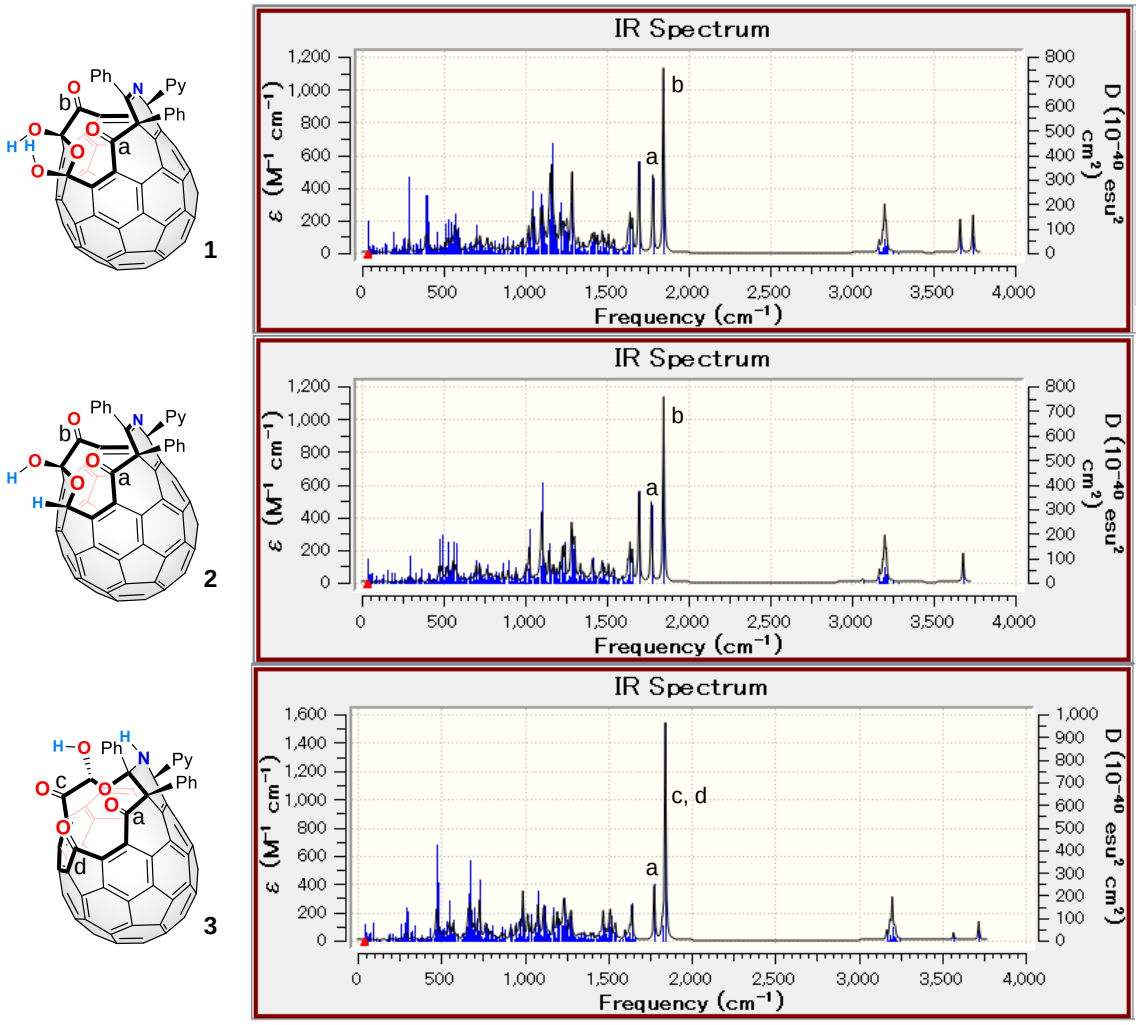
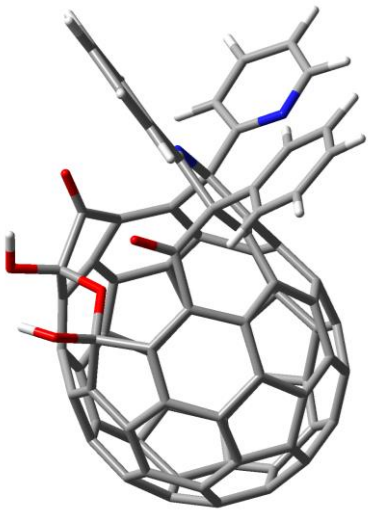


Figure S5. Simulated IR spectra of **1**–**3** (B3LYP-D3/6-31G(d,p)).

Table S1. Optimized structure of **1** (B3LYP-D3/6-31G(d,p))



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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3	6	0	1.572907	2.248265	2.755381
4	6	0	2.213341	1.171993	3.491125
5	6	0	3.558509	0.880274	3.268572
6	6	0	4.320358	1.679512	2.323523
7	6	0	1.693323	3.361299	0.571895
8	6	0	0.230453	1.848678	2.429626
9	6	0	1.243038	0.106603	3.612026
10	6	0	3.981337	-0.503335	3.137228
11	6	0	5.221529	0.789573	1.611428
12	6	0	4.000292	2.970397	0.245481
13	6	0	3.038086	-1.530139	3.245552
14	6	0	1.642558	-1.218913	3.495863
15	6	0	3.072721	-2.644878	2.319230
16	6	0	0.815701	-2.135407	2.736985
17	6	0	0.392203	2.940018	0.219484
18	6	0	0.009836	0.529590	2.984605
19	6	0	1.703011	-3.006790	2.012312
20	6	0	-0.844922	-0.360110	2.337345
21	6	0	-0.372815	2.196913	1.215574
22	6	0	4.999632	-0.560990	2.103360
23	6	0	5.493977	1.006329	0.258975
24	6	0	0.100182	2.641103	-1.193818
25	6	0	4.889640	2.130912	-0.435916
26	6	0	2.773471	3.396598	-0.398867
27	6	0	5.536197	-0.115413	-0.663253
28	6	0	4.595187	1.718891	-1.793443
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32	6	0	-1.496415	1.402386	0.792019
33	6	0	4.966178	0.317381	-1.925362
34	6	0	3.453197	2.193477	-2.434445
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39	6	0	-2.225389	-2.081694	0.430310
40	6	0	2.663822	1.312150	-3.266612
41	6	0	2.971209	-0.052196	-3.329354
42	6	0	1.930202	-1.061166	-3.296055
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45	6	0	-1.723755	-0.321922	-2.962238
46	6	0	5.290442	-1.407212	-0.200694
47	6	0	4.435579	-2.301256	-0.963232
48	6	0	-0.970665	0.917474	-2.575656
49	6	0	-0.861043	-2.394992	0.953887
50	6	0	0.067271	-3.095804	0.191821
51	6	0	0.298573	0.730582	-3.238544
52	6	0	0.614313	-0.662076	-3.413821
53	6	0	3.829923	-1.869040	-2.143678
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55	6	0	-0.624508	-1.442913	-3.066059
56	6	0	3.669254	-3.084526	-0.036521
57	6	0	1.352239	-3.378637	0.713540
58	6	0	0.158866	-3.078429	-1.356452
59	6	0	2.342321	-3.376354	-0.344565
60	6	0	1.710637	-2.961249	-1.571386
61	6	0	-2.196179	1.811150	-0.489468
62	6	0	-2.873135	-0.728287	0.880395
63	6	0	-3.657609	-0.106081	-0.304199
64	7	0	-3.288344	0.964791	-0.900881
65	6	0	-3.789038	-0.914060	2.112544
66	6	0	-2.855248	3.198942	-0.318637
67	8	0	-2.815765	-2.880248	-0.267946
68	8	0	-2.861733	-0.538945	-3.300966
69	6	0	-2.901095	4.133751	-1.354649
70	6	0	-3.576185	5.333607	-1.139215
71	6	0	-4.183794	5.552553	0.096224
72	6	0	-4.092967	4.549105	1.061441
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74	6	0	-4.494280	0.206683	2.571379
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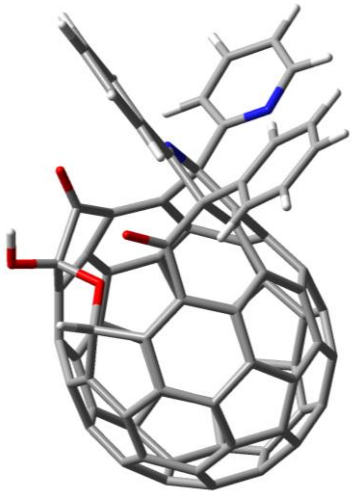
95	1	0	-4.765969	-3.154321	4.480485	101	1	0	-8.263252	-2.129784	-2.280341
96	1	0	-3.351951	-2.999426	2.470430	102	1	0	-7.202679	-0.111253	-3.287248
97	1	0	-1.948377	-2.485373	-3.939865	103	1	0	-5.084490	0.765777	-2.353618
98	1	0	-0.380635	-4.100208	-2.878061						
99	1	0	-5.072377	-2.386535	0.555915						

The total electronic energy was calculated to be –3543.7628178 Hartree.

Table S2. Optimized structure of **2** (B3LYP-D3/6-31G(d,p))



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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71	6	0	4.212575	4.990440	-2.247455
72	6	0	4.110349	3.687226	-2.735138
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76	6	0	5.410411	-2.851768	-3.499716
77	6	0	4.685574	-3.683969	-2.647207
78	6	0	3.875683	-3.136317	-1.650422
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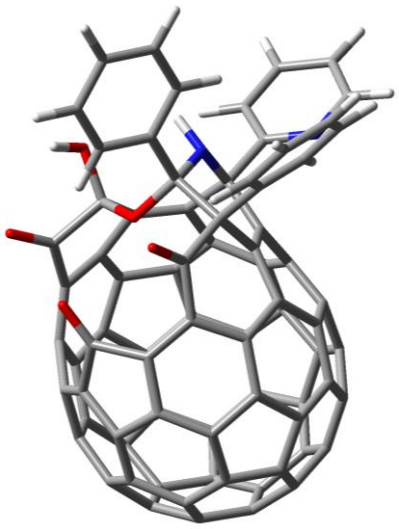
80	8	0	0.983081	-0.754479	4.598179
81	6	0	4.920635	-0.395815	1.108228
82	6	0	5.504006	-1.672281	1.086296
83	6	0	6.697852	-1.925098	1.759810
84	6	0	7.334382	-0.912025	2.474919
85	6	0	6.762768	0.362160	2.511824
86	6	0	5.575709	0.617139	1.835735
87	1	0	0.280215	-2.837219	3.314635
88	1	0	2.451828	4.460284	0.605739
89	1	0	3.670239	6.282907	-0.602368

90	1	0	4.751180	5.746553	-2.809059
91	1	0	4.572450	3.412978	-3.681221
92	1	0	4.408536	0.163836	-2.273246
93	1	0	5.870079	-0.809148	-4.019071
94	1	0	6.042032	-3.279036	-4.272757
95	1	0	4.748553	-4.762994	-2.752694
96	1	0	3.329172	-3.798221	-0.986399
97	1	0	1.955692	-0.827804	4.579948
98	1	0	5.032733	-2.482359	0.554232
99	1	0	7.126889	-2.922093	1.724144
100	1	0	8.264297	-1.112248	2.999790
101	1	0	7.243240	1.160213	3.070461
102	1	0	5.123510	1.599251	1.866340

The total electronic energy was calculated to be –34 68.5391888 Hartree.

Table S3. Optimized structure of **3** (B3LYP-D3/6-31G(d,p))

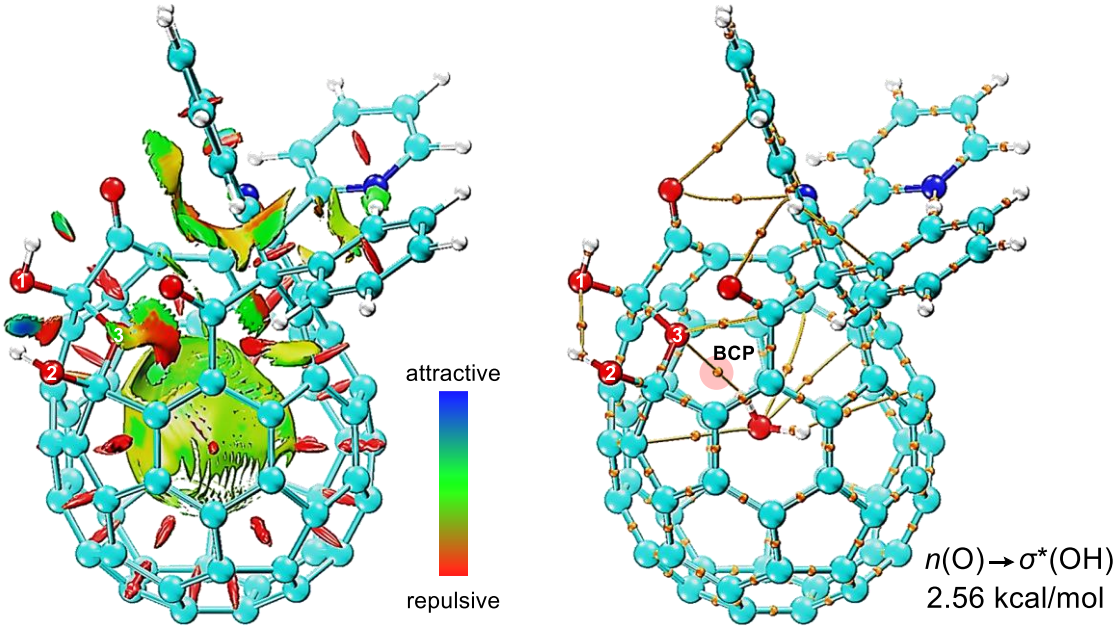


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.846074	2.916541	0.977073
2	6	0	2.446640	3.241675	1.195315
3	6	0	1.769564	2.664204	2.256658
4	6	0	2.445967	1.745415	3.152729
5	6	0	3.782610	1.410228	2.932446
6	6	0	4.494619	2.004421	1.814198
7	6	0	1.785082	3.375077	-0.088934
8	6	0	0.416077	2.210363	2.068615
9	6	0	1.486097	0.727067	3.516846
10	6	0	4.207578	0.026406	3.057736
11	6	0	5.354962	0.983454	1.241069
12	6	0	4.067607	2.882100	-0.453081
13	6	0	3.281138	-0.953387	3.424198
14	6	0	1.894621	-0.591586	3.665594
15	6	0	3.281260	-2.236828	2.750681
16	6	0	1.042837	-1.639644	3.154806
17	6	0	0.461329	2.925709	-0.292068
18	6	0	0.226476	1.017513	2.861316
19	6	0	1.902618	-2.657547	2.602870
20	6	0	-0.642301	0.015659	2.420243
21	6	0	-0.250846	2.345255	0.849111
22	6	0	5.167356	-0.241997	2.001193
23	6	0	5.546313	0.928763	-0.141094
24	6	0	0.092182	2.409409	-1.616402
25	6	0	4.909577	1.907853	-1.005864
26	6	0	2.814515	3.211974	-1.104488
27	6	0	5.519941	-0.353186	-0.824994
28	6	0	4.524613	1.240827	-2.232476
29	6	0	2.486252	2.622505	-2.313953
30	6	0	-0.206114	-1.372187	2.564481
31	6	0	5.152291	-1.476516	1.340663
32	6	0	-1.391788	1.484717	0.625292
33	6	0	4.859154	-0.168649	-2.101928
34	6	0	3.357129	1.608066	-2.890822
35	6	0	1.116761	2.252482	-2.567579
36	6	0	1.150097	1.052059	-3.358060
37	6	0	-1.098923	1.583586	-1.742016
38	6	0	-1.590852	0.344401	1.371245
39	6	0	-2.134677	-2.111667	1.157560
40	6	0	2.497587	0.595876	-3.466682
41	6	0	2.748224	-0.763046	-3.239951
42	6	0	1.692695	-1.731921	-2.970206
43	6	0	3.962027	-1.136496	-2.563002
44	6	0	4.187946	-2.486983	1.720681
45	6	0	-1.944606	-0.758332	-2.514608
46	6	0	5.308906	-1.526275	-0.105882
47	6	0	4.401095	-2.538536	-0.618368
48	6	0	-1.082035	0.484300	-2.573319
49	6	0	-0.718949	-2.291580	1.576943
50	6	0	0.156365	-3.178884	0.962795
51	6	0	0.135722	0.126225	-3.239633
52	6	0	0.378708	-1.299559	-3.174986
53	6	0	3.688861	-2.330192	-1.803946
54	6	0	2.282633	-2.715574	-1.975501
55	6	0	-1.009382	-1.859804	-3.147304
56	6	0	3.735095	-3.141048	0.500056
57	6	0	1.485748	-3.303145	1.444953
58	6	0	0.197733	-3.513077	-0.521654
59	6	0	2.407529	-3.507444	0.343674
60	6	0	1.677943	-3.368679	-0.896905
61	6	0	-2.171820	1.757665	-0.649265
62	6	0	-2.702797	-0.664941	1.070924
63	6	0	-3.202237	-0.512553	-0.430218
64	7	0	-3.326518	0.876161	-0.750421
65	6	0	-3.859363	-0.426100	2.070575
66	6	0	-2.755259	3.182563	-0.655594
67	8	0	-2.816965	-3.095350	0.945707
68	8	0	-3.109310	-0.618605	-3.261559
69	6	0	-2.958049	3.866828	-1.856771
70	6	0	-3.572377	5.118034	-1.817779
71	6	0	-3.955679	5.639689	-0.584136
72	6	0	-3.709409	4.877321	0.559344
73	7	0	-3.125888	3.675241	0.532802
74	6	0	-4.207383	0.894268	2.398137
75	6	0	-5.285126	1.155547	3.243429
76	6	0	-6.028829	0.108081	3.787028
77	6	0	-5.687292	-1.205105	3.467774
78	6	0	-4.616380	-1.472613	2.614186
79	8	0	-0.717833	-3.778619	-1.261695
80	8	0	-1.455402	-2.826446	-3.716903
81	6	0	-5.784544	-3.120591	-1.518605
82	6	0	-4.565742	-2.500358	-1.249624
83	6	0	-4.536566	-1.206984	-0.712256

84	6	0	-5.743677	-0.552701	-0.439246	95	1	0	-4.395632	-2.498182	2.352647
85	6	0	-6.961693	-1.178938	-0.706262	96	1	0	-5.791754	-4.123332	-1.935590
86	6	0	-6.986771	-2.462954	-1.249582	97	1	0	-3.634422	-3.018706	-1.443405
87	1	0	-2.636497	3.429055	-2.795832	98	1	0	-5.727074	0.439881	-0.004719
88	1	0	-3.744020	5.674437	-2.734311	99	1	0	-7.889782	-0.659592	-0.485975
89	1	0	-4.431902	6.611246	-0.503945	100	1	0	-7.934892	-2.949720	-1.459539
90	1	0	-3.992666	5.248430	1.542115	101	8	0	-2.139462	-1.182657	-1.179724
91	1	0	-3.658914	1.729458	1.979363	102	1	0	-3.828744	1.004567	-1.622067
92	1	0	-5.539620	2.185990	3.475164	103	1	0	-3.425234	-1.518713	-3.454393
93	1	0	-6.865938	0.312833	4.448301	---					
94	1	0	-6.260431	-2.033159	3.874557	The total electronic energy was calculated to be –3543.7729827 Hartree.					

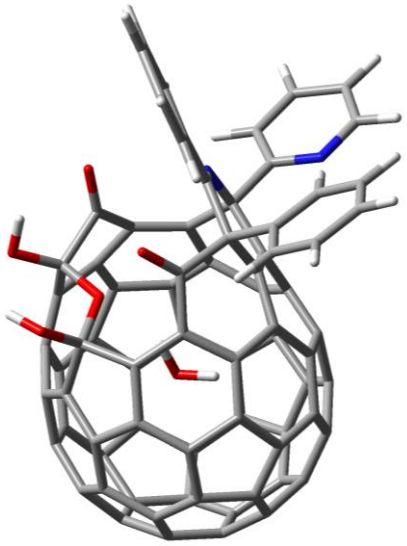
4.2. Topological Analysis of H_2O@1



Compd.	LUMO	$q_{O(1)}$	$q_{H(1)}$	Δq_1	$q_{O(2)}$	$q_{H(2)}$	Δq_2
1	–3.170	–0.7544	+0.5103	+1.2647	–0.7342	+0.5038	+1.2380
H_2O@**1**	–3.134	–0.7520	+0.5115	+1.2635	–0.7313	+0.5051	+1.2364
1'	–3.165	–0.7539	+0.5113	+1.2651	–0.7328	+0.5046	+1.2374

Figure S6. Topological analysis of electron densities for H_2O@1 with selected natural charges (units in au) and LUMO levels (units in eV) (B3LYP-D3/6-31G(d,p)). The geometry of **1'** is generated by subtracting a coordinate of H_2O from that of H_2O@**1**.

Table S4. Optimized structure of H_2O@**1** (B3LYP-D3/6-31G(d,p))



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.672626	2.727462	1.656163
2	6	0	2.259745	2.998931	1.860106
3	6	0	1.540657	2.239539	2.768885
4	6	0	2.181632	1.159300	3.499162
5	6	0	3.526864	0.868062	3.274051
6	6	0	4.288477	1.671574	2.332962
7	6	0	1.661162	3.360442	0.588154
8	6	0	0.197715	1.841650	2.440317
9	6	0	1.212328	0.092372	3.614131
10	6	0	3.950359	-0.514588	3.136469
11	6	0	5.190464	0.785406	1.617894
12	6	0	3.967987	2.971307	0.261184
13	6	0	3.008418	-1.542603	3.240332
14	6	0	1.612834	-1.232568	3.490067
15	6	0	3.044419	-2.653784	2.310054
16	6	0	0.786983	-2.146681	2.727493
17	6	0	0.360355	2.943593	0.233574
18	6	0	-0.022098	0.517863	2.989007
19	6	0	1.676372	-3.014900	2.000490
20	6	0	-0.875353	-0.370814	2.336561
21	6	0	-0.403959	2.195174	1.226209
22	6	0	4.969017	-0.566991	2.103026
23	6	0	5.461139	1.007724	0.266672
24	6	0	0.070143	2.649871	-1.180415
25	6	0	4.856831	2.134648	-0.423024
26	6	0	2.741793	3.399540	-0.381051
27	6	0	5.504700	-0.109380	-0.660302
28	6	0	4.563316	1.728149	-1.781608
29	6	0	2.488592	3.052813	-1.695287
30	6	0	-0.441129	-1.756985	2.163139
31	6	0	4.999990	-1.640319	1.206413
32	6	0	-1.525887	1.399888	0.798411
33	6	0	4.934227	0.328134	-1.919482
34	6	0	3.422170	2.204712	-2.419611
35	6	0	1.145654	2.702324	-2.087205
36	6	0	1.259714	1.706405	-3.119127
37	6	0	-1.095422	1.840984	-1.525288
38	6	0	-1.785703	0.177734	1.355581
39	6	0	-2.249988	-2.082182	0.415318
40	6	0	2.634239	1.327615	-3.255363
41	6	0	2.942119	-0.035574	-3.325119
42	6	0	1.902532	-1.045487	-3.300140
43	6	0	4.109269	-0.534248	-2.644037
44	6	0	4.009188	-2.692043	1.305531
45	6	0	-1.750456	-0.304180	-2.959851
46	6	0	5.259747	-1.402670	-0.204347
47	6	0	4.405221	-2.292844	-0.970450
48	6	0	-0.998780	0.933089	-2.571589
49	6	0	-0.889104	-2.400868	0.944340
50	6	0	0.043673	-3.096317	0.181344
51	6	0	0.271082	0.748905	-3.235509
52	6	0	0.587973	-0.642490	-3.424006
53	6	0	3.799748	-1.856863	-2.148350
54	6	0	2.415223	-2.184579	-2.480695
55	6	0	-0.648363	-1.419548	-3.069952
56	6	0	3.641267	-3.081268	-0.048086
57	6	0	1.328107	-3.381470	0.700054
58	6	0	0.137568	-3.070916	-1.364554
59	6	0	2.317269	-3.377438	-0.358505
60	6	0	1.687041	-2.961505	-1.585035
61	6	0	-2.225304	1.814314	-0.481277
62	6	0	-2.900971	-0.733307	0.875710
63	6	0	-3.686181	-0.104662	-0.304983
64	7	0	-3.316951	0.969081	-0.896419
65	6	0	-3.815780	-0.927453	2.107078
66	6	0	-2.885444	3.200485	-0.303445
67	8	0	-2.833692	-2.869439	-0.301271
68	8	0	-2.888786	-0.528390	-3.293910
69	6	0	-2.929955	4.141015	-1.334235
70	6	0	-3.607227	5.338631	-1.113466
71	6	0	-4.217735	5.549738	0.121936
72	6	0	-4.127407	4.541195	1.081852
73	7	0	-3.478974	3.388814	0.880945
74	6	0	-4.522379	0.189754	2.572389
75	6	0	-5.330658	0.086328	3.702483
76	6	0	-5.433395	-1.126363	4.387822
77	6	0	-4.718437	-2.235265	3.936096
78	6	0	-3.910728	-2.137203	2.801547
79	8	0	-0.552727	-1.863463	-1.712211
80	8	0	-1.009585	-2.414959	-3.964248
81	8	0	-0.418241	-4.207134	-1.932166
82	6	0	-4.946725	-0.724432	-0.826202
83	6	0	-5.548542	-1.871428	-0.284769
84	6	0	-6.742491	-2.366924	-0.805997
85	6	0	-7.361138	-1.733649	-1.882460
86	6	0	-6.771905	-0.594451	-2.436183
87	6	0	-5.585194	-0.095155	-1.913227
88	1	0	-2.445904	3.936610	-2.282301
89	1	0	-3.657291	6.092472	-1.893488
90	1	0	-4.753496	6.467950	0.338776
91	1	0	-4.595678	4.661895	2.056504
92	1	0	-4.420704	1.141802	2.057221
93	1	0	-5.878376	0.957206	4.050446

94	1	0	-6.063207	-1.205014	5.268874	102	1	0	-7.238488	-0.093115	-3.279255
95	1	0	-4.788053	-3.182355	4.462875	103	1	0	-5.120447	0.781904	-2.342865
96	1	0	-3.374863	-3.014052	2.453089	104	8	0	1.700020	-0.060137	-0.156311
97	1	0	-1.984379	-2.464986	-3.916607	105	1	0	1.436855	0.142944	0.749130
98	1	0	-0.412185	-4.074019	-2.894020	106	1	0	0.895939	-0.417201	-0.559241
99	1	0	-5.092777	-2.395898	0.538940	---					
100	1	0	-7.185177	-3.255563	-0.366011	The total electronic energy was calculated to be –3620.2157964 Hartree.					
101	1	0	-8.290882	-2.123311	-2.287482						

4.3. Gas-Phase Acidity

Gas-phase acidity was calculated by the equation:

$$\Delta H = H(A^-) + H(H^+) - H(HA)$$

where $H(H^+)$ is +1.48121 kcal/mol.

Gas-phase acidity ΔH (kcal/mol)	
O(1)H	334
O(2)H	335
PhOH	361
t-BuOH	392
HCl	343
HBr	328
HI	317

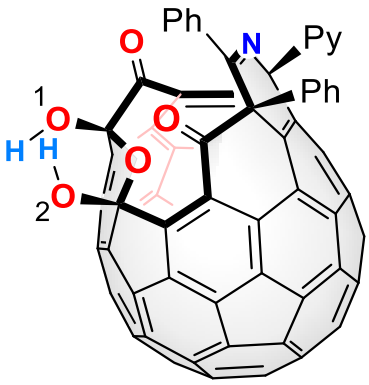
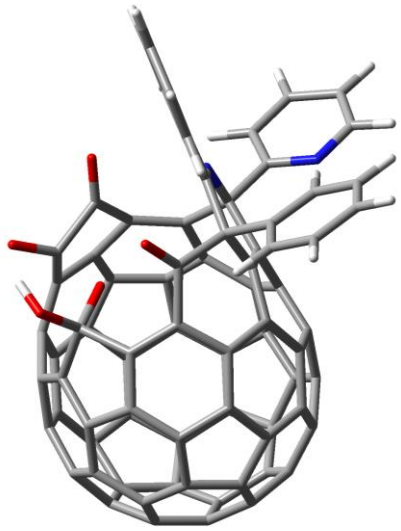


Figure S7. Gas-phase acidity of **1** and selected alcohols and hydrogen halides (B3LYP-D3 with basis sets of LanL2DZ for halogens and 6-31G(d,p) for the rest).

Table S5. Optimized structure of **1–O(1)**$^{-}$ (B3LYP-D3/6-31G(d,p))



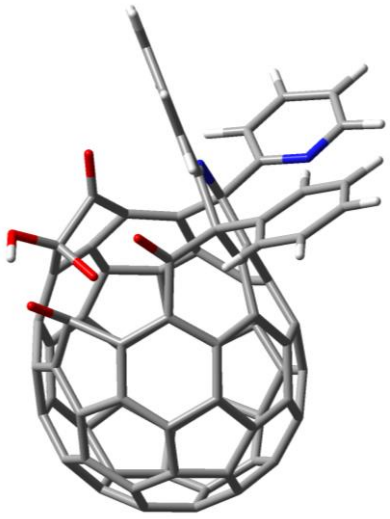
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.699115	2.558901	1.895802
2	6	0	2.284036	2.807369	2.119833
3	6	0	1.564434	1.967060	2.954680
4	6	0	2.205297	0.827752	3.589327
5	6	0	3.552031	0.559845	3.341190
6	6	0	4.314936	1.445706	2.476670
7	6	0	1.688227	3.279359	0.882534
8	6	0	0.223946	1.596130	2.588919
9	6	0	1.236459	-0.245822	3.609516
10	6	0	3.976114	-0.804773	3.079788
11	6	0	5.218517	0.628162	1.685159
12	6	0	3.997306	2.929316	0.528581
13	6	0	3.033498	-1.838807	3.087776
14	6	0	1.637528	-1.554556	3.366722
15	6	0	3.068637	-2.862224	2.061151
16	6	0	0.810989	-2.400793	2.530296
17	6	0	0.390914	2.883194	0.485190
18	6	0	0.003087	0.232162	3.021754
19	6	0	1.699143	-3.195717	1.722086
20	6	0	-0.848903	-0.596009	2.292494
21	6	0	-0.374795	2.052521	1.408138
22	6	0	4.995454	-0.763216	2.045961
23	6	0	5.490935	0.971816	0.358418
24	6	0	0.101848	2.712229	-0.948918
25	6	0	4.888560	2.158210	-0.229179
26	6	0	2.771137	3.412369	-0.075795
27	6	0	5.536327	-0.056742	-0.666982
28	6	0	4.601019	1.878374	-1.621692
29	6	0	2.518638	3.182669	-1.417312
30	6	0	-0.419399	-1.964032	2.003150
31	6	0	5.025146	-1.751205	1.054431
32	6	0	-1.497792	1.301493	0.910832
33	6	0	4.969938	0.494865	-1.883618
34	6	0	3.455556	2.406119	-2.217520
35	6	0	1.176980	2.866156	-1.845699
36	6	0	1.294598	1.973448	-2.967757
37	6	0	-1.060806	1.932128	-1.376373
38	6	0	-1.756526	0.036063	1.360595
39	6	0	-2.240218	-2.157187	0.257344
40	6	0	2.671809	1.616267	-3.140252
41	6	0	2.973758	0.258122	-3.324751
42	6	0	1.936107	-0.747097	-3.402859
43	6	0	4.139691	-0.298426	-2.681990
44	6	0	4.032148	-2.807847	1.055153
45	6	0	-1.746261	-0.063945	-3.056432
46	6	0	5.285640	-1.386913	-0.329706
47	6	0	4.433018	-2.205851	-1.174058
48	6	0	-0.967497	1.129831	-2.506172
49	6	0	-0.870212	-2.504106	0.738158
50	6	0	0.058649	-3.111621	-0.097329
51	6	0	0.305226	1.026664	-3.175129
52	6	0	0.614758	-0.342438	-3.474468
53	6	0	3.823223	-1.659115	-2.306100
54	6	0	2.437579	-1.948976	-2.671138
55	6	0	-0.641960	-1.195687	-3.328775
56	6	0	3.664871	-3.073039	-0.329072
57	6	0	1.346523	-3.434544	0.390632
58	6	0	0.120312	-2.891074	-1.640928
59	6	0	2.332735	-3.322347	-0.666876
60	6	0	1.695617	-2.793341	-1.845346
61	6	0	-2.190158	1.822884	-0.333096
62	6	0	-2.871842	-0.827622	0.801382
63	6	0	-3.651065	-0.102070	-0.323929
64	7	0	-3.296597	1.027223	-0.806855
65	6	0	-3.796514	-1.098455	2.012295
66	6	0	-2.844632	3.194862	-0.051135
67	8	0	-2.874856	-2.929001	-0.430588
68	8	0	-2.899733	-0.120977	-3.399706
69	6	0	-2.893241	4.199654	-1.021856
70	6	0	-3.560523	5.384727	-0.725071
71	6	0	-4.160446	5.526098	0.526426
72	6	0	-4.069369	4.459983	1.420720
73	7	0	-3.430705	3.317301	1.146506
74	6	0	-4.503645	-0.012801	2.547899
75	6	0	-5.315898	-0.184239	3.666615
76	6	0	-5.424109	-1.436917	4.275230
77	6	0	-4.709097	-2.515576	3.755715
78	6	0	-3.898035	-2.348351	2.631508
79	8	0	-0.508252	-1.656918	-1.831125
80	8	0	-0.872487	-2.120814	-4.178807
81	8	0	-0.433561	-3.931081	-2.370166
82	6	0	-4.915932	-0.672321	-0.898030
83	6	0	-5.556187	-1.825046	-0.418264
84	6	0	-6.761591	-2.257462	-0.969747
85	6	0	-7.351263	-1.555952	-2.019416
86	6	0	-6.717389	-0.415650	-2.518338
87	6	0	-5.519656	0.021171	-1.964766
88	1	0	-2.415984	4.043762	-1.982172
89	1	0	-3.611492	6.184374	-1.458747
90	1	0	-4.688092	6.433425	0.803374
91	1	0	-4.530504	4.524034	2.404968
92	1	0	-4.396367	0.969778	2.095307
93	1	0	-5.862020	0.665688	4.066638

94	1	0	-6.056857	-1.569419	5.148442	100	1	0	-8.288299	-1.898277	-2.451368
95	1	0	-4.780626	-3.494432	4.221738	101	1	0	-7.152988	0.132087	-3.349626
96	1	0	-3.362893	-3.201052	2.228206	102	1	0	-5.010699	0.888903	-2.360609
97	1	0	-0.691261	-3.484620	-3.226955						
98	1	0	-5.118861	-2.404339	0.377815						
99	1	0	-7.233155	-3.153851	-0.576621						

The total electronic energy was calculated to be –3543.21 75641 Hartree.

Table S6. Optimized structure of **1–O(2)**$^{-}$ (B3LYP-D3/6-31G(d,p))



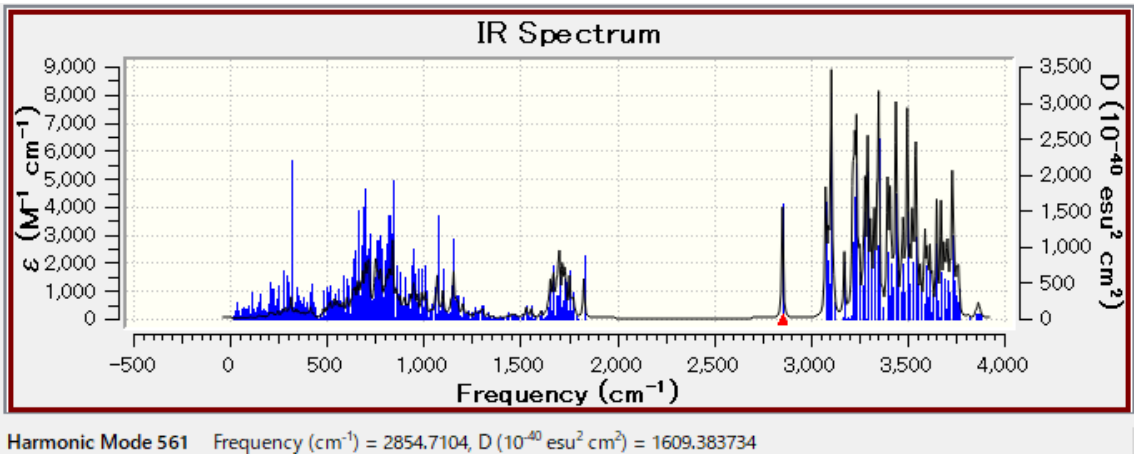
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.697459	2.648736	1.778050
2	6	0	2.282652	2.905125	1.992876
3	6	0	1.564572	2.100269	2.863148
4	6	0	2.207110	0.989375	3.544691
5	6	0	3.554234	0.713174	3.308493
6	6	0	4.314521	1.561536	2.404900
7	6	0	1.684456	3.325069	0.738064
8	6	0	0.224336	1.712004	2.513881
9	6	0	1.239566	-0.083533	3.611509
10	6	0	3.980179	-0.660954	3.106503
11	6	0	5.219451	0.711747	1.649463
12	6	0	3.992731	2.957947	0.395213
13	6	0	3.038964	-1.695013	3.159374
14	6	0	1.641999	-1.400747	3.423253
15	6	0	3.075751	-2.763138	2.179314
16	6	0	0.817787	-2.284508	2.624336
17	6	0	0.385294	2.915328	0.360973
18	6	0	0.007457	0.365909	3.001113
19	6	0	1.707298	-3.114935	1.854219
20	6	0	-0.838185	-0.495332	2.302897
21	6	0	-0.378287	2.120529	1.317897
22	6	0	4.999780	-0.662993	2.071762
23	6	0	5.489617	0.996566	0.308466
24	6	0	0.093784	2.687871	-1.064574
25	6	0	4.883422	2.154758	-0.328704
26	6	0	2.765434	3.414382	-0.227750
27	6	0	5.537066	-0.076104	-0.671100
28	6	0	4.591795	1.811899	-1.706090
29	6	0	2.511489	3.126702	-1.558135
30	6	0	-0.409289	-1.873087	2.071326
31	6	0	5.030602	-1.693646	1.125384
32	6	0	-1.498621	1.344723	0.853504
33	6	0	4.964265	0.419004	-1.908146
34	6	0	3.446802	2.313676	-2.322921
35	6	0	1.168473	2.792503	-1.969121
36	6	0	1.284672	1.846782	-3.049009
37	6	0	-1.070579	1.889805	-1.452434
38	6	0	-1.749649	0.094657	1.349075
39	6	0	-2.231473	-2.153300	0.340981
40	6	0	2.659621	1.478330	-3.202998
41	6	0	2.961828	0.114070	-3.325339
42	6	0	1.923441	-0.897507	-3.343606
43	6	0	4.133618	-0.411491	-2.668356
44	6	0	4.042209	-2.753278	1.174511
45	6	0	-1.743807	-0.184453	-3.018776
46	6	0	5.288393	-1.391015	-0.274811
47	6	0	4.441502	-2.251537	-1.080664
48	6	0	-0.971780	1.033625	-2.537372
49	6	0	-0.863172	-2.482305	0.835477
50	6	0	0.058442	-3.140186	0.030058
51	6	0	0.297503	0.888479	-3.203498
52	6	0	0.601658	-0.496598	-3.434189
53	6	0	3.825489	-1.757079	-2.234488
54	6	0	2.443251	-2.073834	-2.583007
55	6	0	-0.649159	-1.319100	-3.127358
56	6	0	3.675407	-3.082392	-0.194904
57	6	0	1.352773	-3.420130	0.537663
58	6	0	0.137155	-3.102200	-1.562396
59	6	0	2.345764	-3.356799	-0.519409
60	6	0	1.708288	-2.882537	-1.718520
61	6	0	-2.198217	1.816040	-0.405164
62	6	0	-2.862854	-0.796088	0.829940
63	6	0	-3.647790	-0.116821	-0.319507
64	7	0	-3.299868	0.995471	-0.847112
65	6	0	-3.784642	-1.020262	2.052994
66	6	0	-2.858311	3.194082	-0.171655
67	8	0	-2.870467	-2.943140	-0.321727
68	8	0	-2.888714	-0.280184	-3.378687
69	6	0	-2.895270	4.173792	-1.167940
70	6	0	-3.566378	5.366009	-0.909587
71	6	0	-4.181936	5.538783	0.330038
72	6	0	-4.101588	4.495656	1.252305
73	7	0	-3.459023	3.347264	1.015272
74	6	0	-4.490404	0.084324	2.550493
75	6	0	-5.302140	-0.046762	3.675137
76	6	0	-5.411237	-1.277027	4.327621
77	6	0	-4.697488	-2.374018	3.846108
78	6	0	-3.887184	-2.247488	2.716116
79	8	0	-0.542161	-1.749181	-1.783507
80	8	0	-0.952762	-2.298316	-4.039987
81	8	0	-0.334641	-4.063249	-2.271794
82	6	0	-4.911718	-0.711904	-0.870415
83	6	0	-5.546104	-1.849720	-0.349102
84	6	0	-6.749932	-2.307236	-0.883546
85	6	0	-7.344419	-1.646594	-1.956708
86	6	0	-6.717482	-0.520842	-2.495826
87	6	0	-5.521493	-0.058933	-1.959173

88	1	0	-2.405811	3.995387	-2.118142	97	1	0	-0.813484	-3.160475	-3.540193
89	1	0	-3.607928	6.146866	-1.663783	98	1	0	-5.104967	-2.398761	0.465962
90	1	0	-4.713119	6.452562	0.577347	99	1	0	-7.216312	-3.191604	-0.458435
91	1	0	-4.574874	4.584364	2.228817	100	1	0	-8.280111	-2.008829	-2.375086
92	1	0	-4.382803	1.050344	2.063540	101	1	0	-7.157615	-0.003835	-3.344274
93	1	0	-5.847228	0.817275	4.045308	102	1	0	-5.019897	0.799318	-2.384182
94	1	0	-6.043580	-1.378069	5.205352	---					
95	1	0	-4.769550	-3.335778	4.346381	The total electronic energy was calculated to be –3543.2163087 Hartree.					
96	1	0	-3.353163	-3.114393	2.342920						

4.4. Simulated IR Spectra of 1•$(H_2O)_{39}$

The four local minimum structures of **1**•$(H_2O)_{39}$, i.e., **A**, **B**, **C**, and **D**, were computed with the use of different initial coordinates. The presence of acidic water was suggested for all cases with elongated OH bond lengths, showing their absorption bands at around 2000–3000 cm^{-1}. For model structures of water adsorbed [60]fullerenes, 60–70 water molecules are usually employed.[4] In our cases, nearly one third of [60]fullerene sphere is covered by the aryl functional groups which are not participate in the water adsorption since experimental results did not show any change in band intensity and wavenumbers. Thus, ca. 40 water molecules are considered to be enough to describe the adsorbed physical picture. To suppress the calculations cost, we then computed some local minimum structures for **1**•$(H_2O)_{39}$.



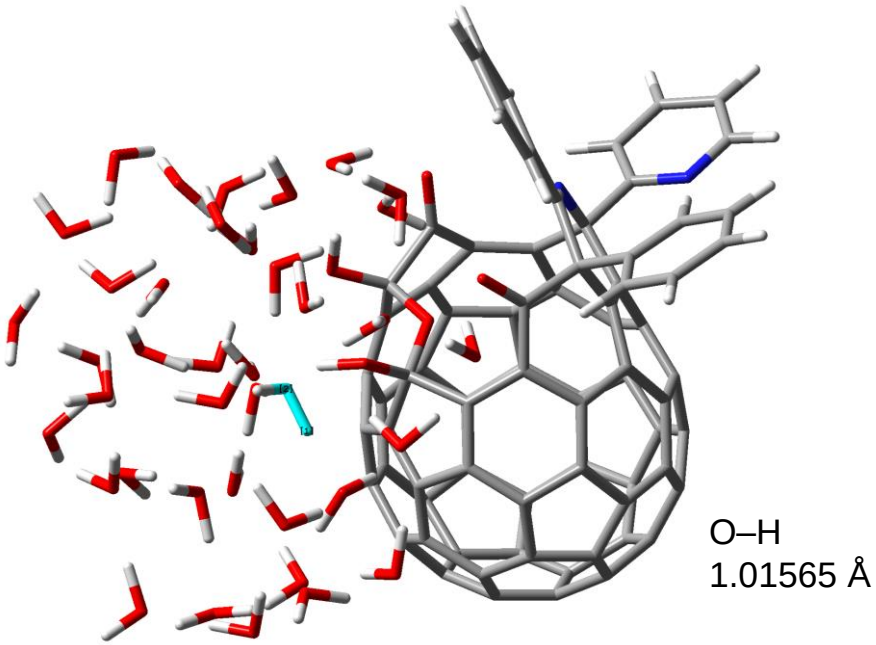


Figure S8. Simulated IR spectra of **1**•$(H_2O)_{39}$-**A** (B3LYP-D3/6-31G(d,p)).

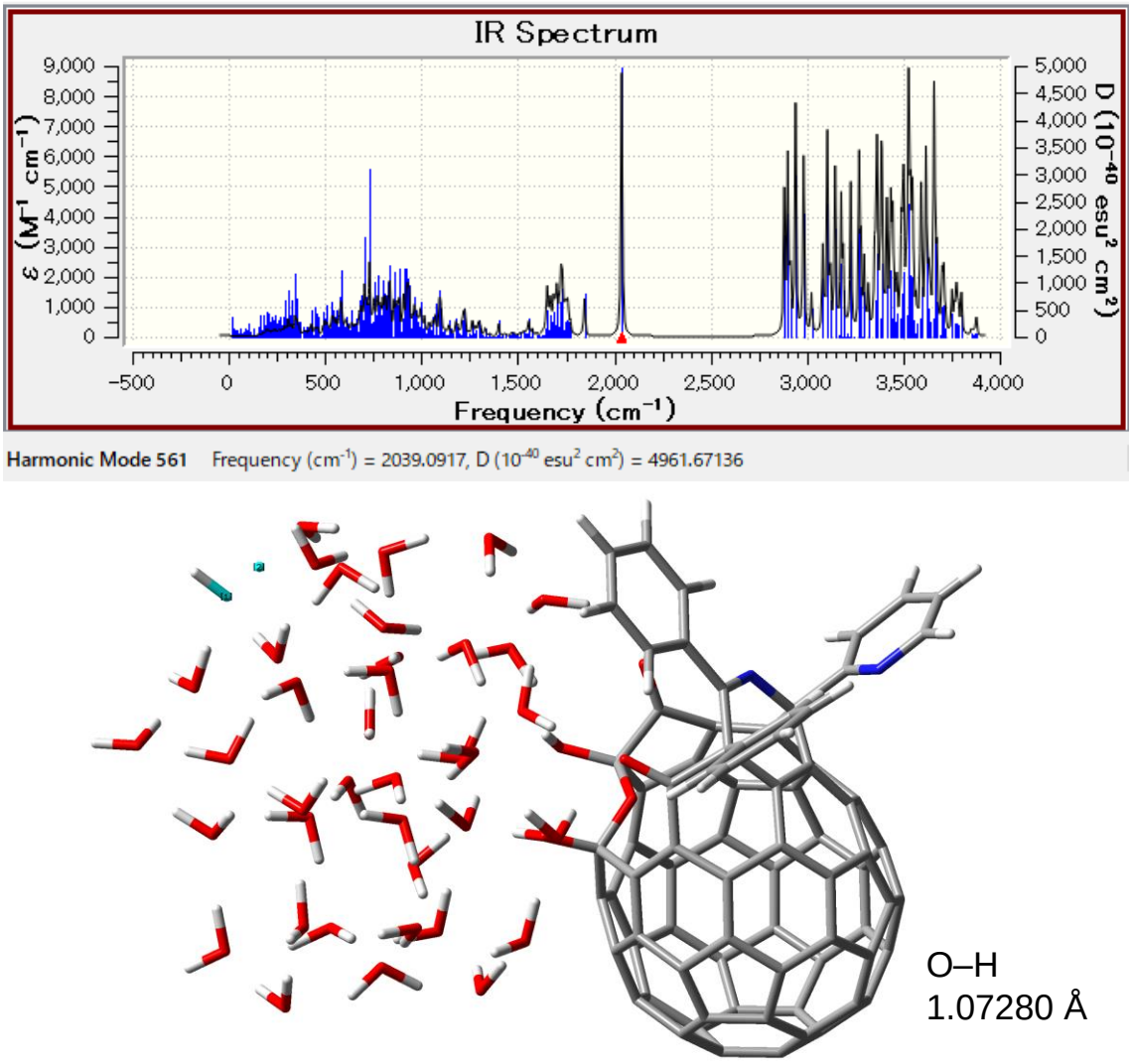


Figure S9. Simulated IR spectra of **1**•$(H_2O)_{39}$-**B** (B3LYP-D3/6-31G(d,p)).

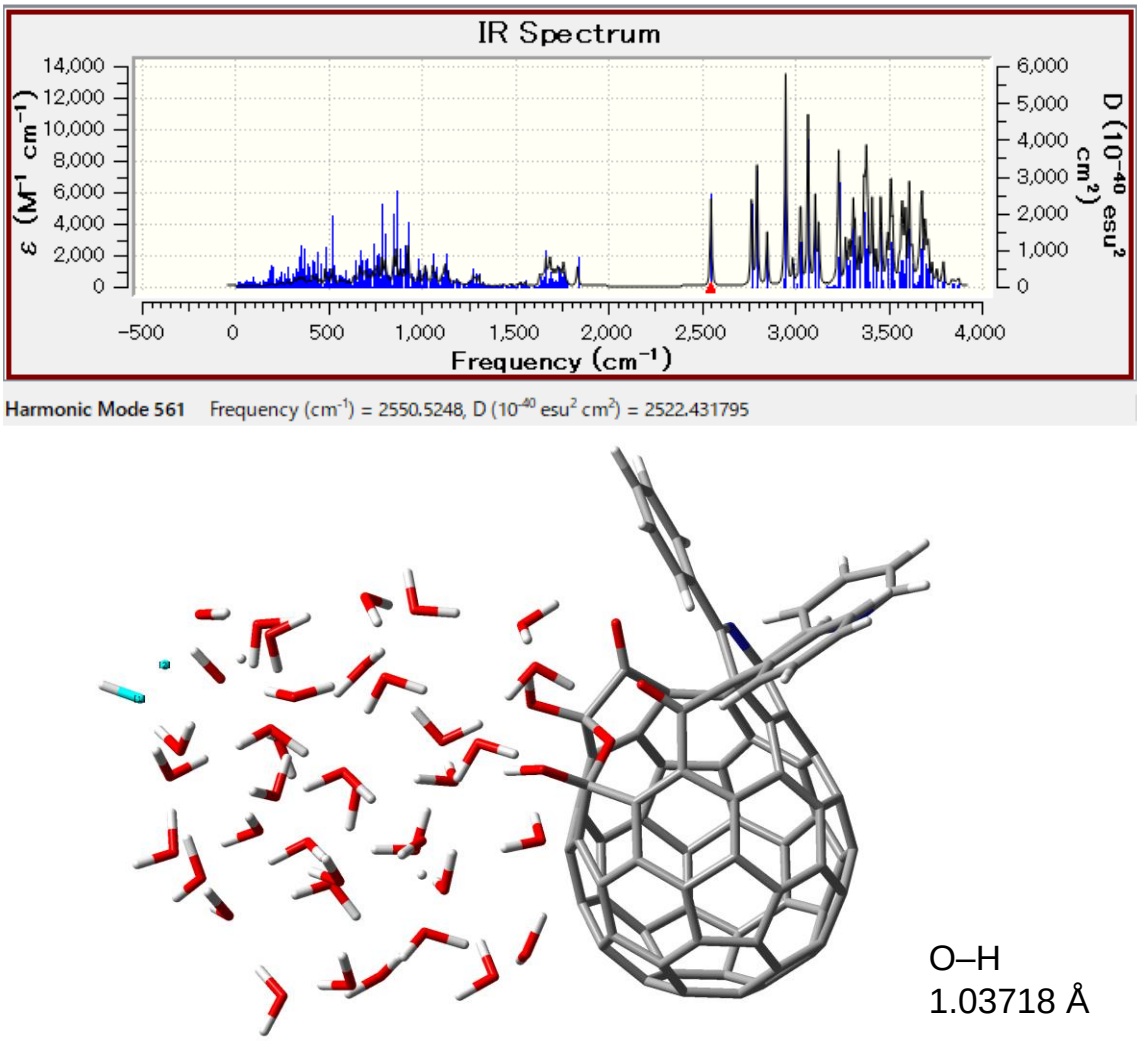
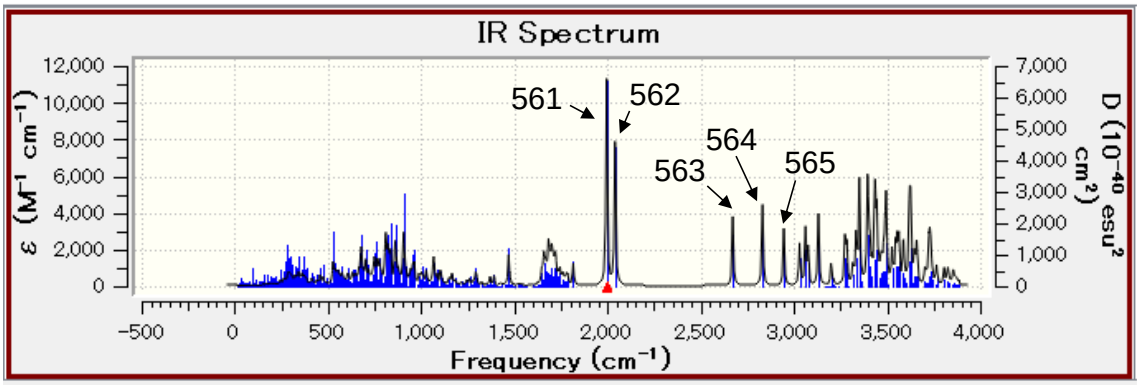


Figure S10. Simulated IR spectra of **1**•$(H_2O)_{39}$-**C** (B3LYP-D3/6-31G(d,p)).



Harmonic Mode 561 Frequency (cm^{-1}) = 1995.34, D (10^{-40} esu^2 cm^2) = 6508.907965
Harmonic Mode 562 Frequency (cm^{-1}) = 2040.6555, D (10^{-40} esu^2 cm^2) = 4414.621067
Harmonic Mode 563 Frequency (cm^{-1}) = 2672.2179, D (10^{-40} esu^2 cm^2) = 1641.183382
Harmonic Mode 564 Frequency (cm^{-1}) = 2832.3188, D (10^{-40} esu^2 cm^2) = 1813.491282
Harmonic Mode 565 Frequency (cm^{-1}) = 2946.2859, D (10^{-40} esu^2 cm^2) = 1227.273579

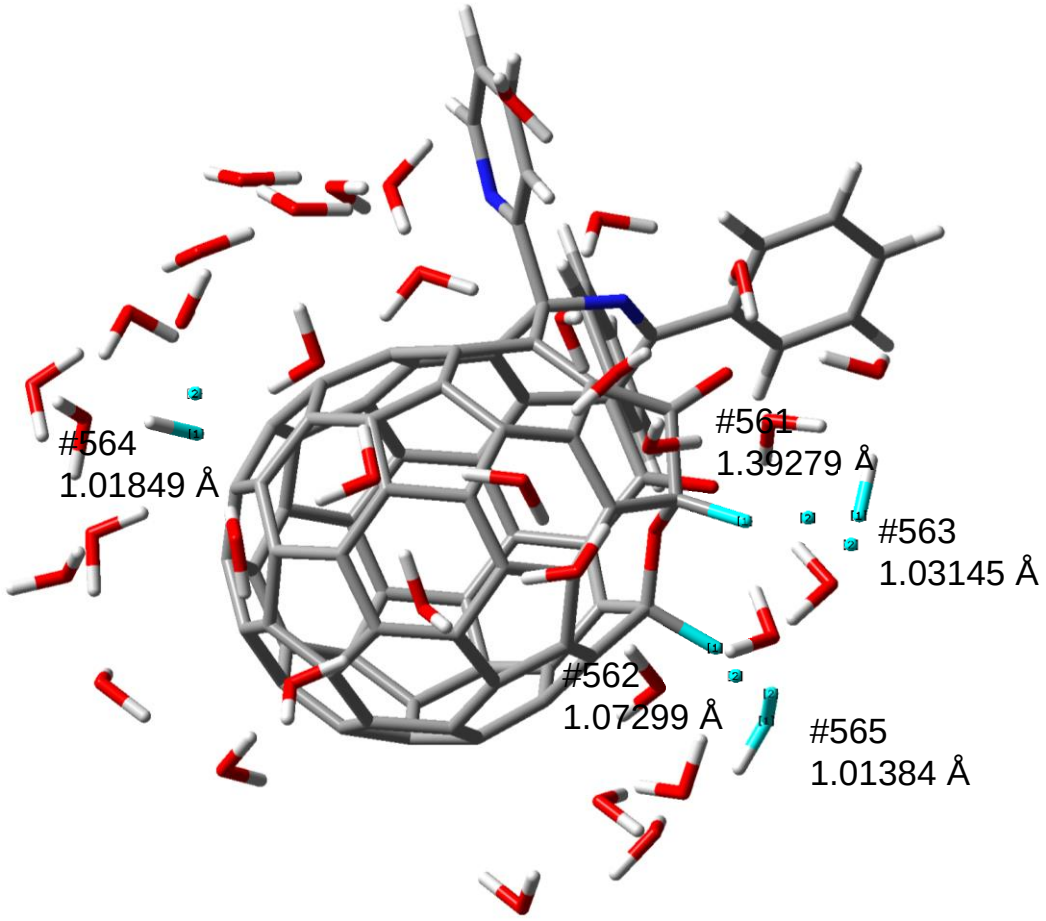
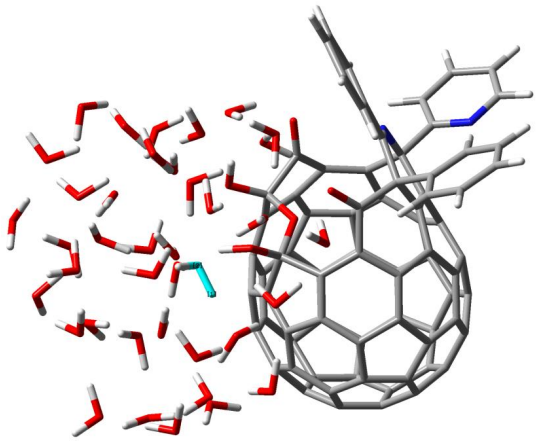


Figure S11. Simulated IR spectra of **1**•$(H_2O)_{39}$-**D** (B3LYP-D3/6-31G(d,p)).

Table S7. Optimized structure of **1**•$(H_2O)_{39}$-**A** (B3LYP-D3/6-31G(d,p))



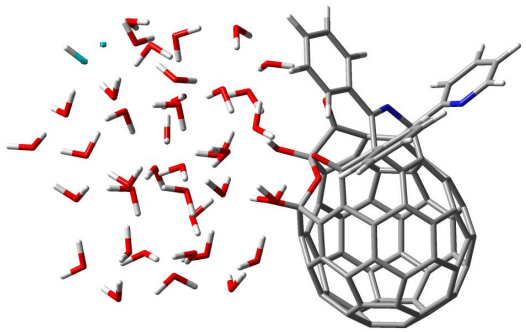
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.799982	-3.387635	-0.375703
2	6	0	-7.010290	-1.960866	-0.558002
3	6	0	-6.602885	-1.352600	-1.733928
4	6	0	-5.946404	-2.123937	-2.775345
5	6	0	-5.701252	-3.483415	-2.585408
6	6	0	-6.138922	-4.128616	-1.359280
7	6	0	-6.799692	-1.288272	0.710994
8	6	0	-6.000024	-0.047282	-1.677124
9	6	0	-4.933083	-1.272210	-3.357513
10	6	0	-4.411856	-4.041824	-2.955549
11	6	0	-5.122904	-5.093172	-0.974602
12	6	0	-6.510284	-3.612818	1.023955
13	6	0	-3.429908	-3.213914	-3.506890
14	6	0	-3.700235	-1.802660	-3.718784
15	6	0	-2.052099	-3.333454	-3.067727
16	6	0	-2.500765	-1.049624	-3.418676
17	6	0	-6.167408	-0.027560	0.787085
18	6	0	-4.983665	0.019509	-2.706463
19	6	0	-1.495651	-1.998689	-3.008227
20	6	0	-3.846898	0.800001	-2.503770
21	6	0	-5.803301	0.627320	-0.465929
22	6	0	-4.048028	-5.026964	-1.951879
23	6	0	-4.829902	-5.298850	0.375120
24	6	0	-5.327560	0.274766	1.958874
25	6	0	-5.550794	-4.561672	1.398808
26	6	0	-6.553750	-2.328540	1.695167
27	6	0	-3.449251	-5.428411	0.809062
28	6	0	-4.630149	-4.270583	2.479441
29	6	0	-5.707949	-2.071888	2.759528
30	6	0	-2.547538	0.226460	-2.834640
31	6	0	-2.718294	-5.139955	-1.530863
32	6	0	-4.815058	1.677795	-0.451847
33	6	0	-3.319580	-4.778727	2.100000
34	6	0	-4.727738	-3.066557	3.172339
35	6	0	-5.119135	-0.761016	2.892559
36	6	0	-3.817730	-0.947950	3.477616
37	6	0	-4.351743	1.360178	1.889423
38	6	0	-3.890533	1.792689	-1.452529
39	6	0	-1.422226	2.021303	-1.471726
40	6	0	-3.533313	-2.348816	3.559781
41	6	0	-2.277111	-2.790461	3.124682
42	6	0	-1.270667	-1.861359	2.646878
43	6	0	-2.178003	-4.024524	2.385863
44	6	0	-1.706780	-4.265251	-2.089528
45	6	0	-1.778900	1.833367	2.397669
46	6	0	-2.415376	-5.330959	-0.120214
47	6	0	-1.229259	-4.550216	0.190111
48	6	0	-3.123697	1.189980	2.513112
49	6	0	-1.452426	0.639626	-1.977203
50	6	0	-0.608857	-0.331660	-1.456431
51	6	0	-2.808785	-0.064910	3.146413
52	6	0	-1.486312	-0.509405	2.811761
53	6	0	-1.125035	-3.868599	1.404117
54	6	0	-0.585233	-2.511795	1.494161
55	6	0	-0.766504	0.638307	2.146649
56	6	0	-0.800149	-3.897473	-1.011747
57	6	0	-0.643339	-1.649627	-1.962481
58	6	0	-0.006367	-0.365930	-0.026278
59	6	0	-0.309995	-2.597710	-0.922780
60	6	0	-0.164234	-1.889595	0.323501
61	6	0	-4.637599	2.451890	0.840294
62	6	0	-2.756854	2.808171	-1.423105
63	6	0	-2.805314	3.688880	-0.147068
64	7	0	-3.605177	3.463016	0.825016
65	6	0	-2.929582	3.664296	-2.702619
66	6	0	-5.920779	3.249952	1.163263
67	8	0	-0.349371	2.541560	-1.175940
68	8	0	-1.443235	2.977722	2.609982
69	6	0	-6.393641	3.406784	2.467419
70	6	0	-7.522063	4.197656	2.675247
71	6	0	-8.130775	4.804986	1.578107
72	6	0	-7.571756	4.597607	0.316546
73	7	0	-6.490152	3.840002	0.105513
74	6	0	-4.068924	4.475922	-2.779890
75	6	0	-4.306144	5.240787	-3.920084
76	6	0	-3.417359	5.194656	-4.996330
77	6	0	-2.289917	4.376896	-4.924694
78	6	0	-2.042313	3.610102	-3.784044
79	8	0	-0.850514	0.509180	0.721174
80	8	0	0.498992	0.828251	2.629868
81	8	0	1.323675	0.033910	-0.036502
82	6	0	-1.875908	4.854746	0.033640
83	6	0	-0.966078	5.305466	-0.937492
84	6	0	-0.087266	6.354701	-0.671166
85	6	0	-0.112453	6.995252	0.566467
86	6	0	-1.034031	6.583030	1.532394
87	6	0	-1.905261	5.531502	1.269280
88	1	0	-5.889863	2.919533	3.294238
89	1	0	-7.917872	4.336198	3.676948
90	1	0	-9.013020	5.426095	1.692531
91	1	0	-8.011015	5.059163	-0.565413
92	1	0	-4.775185	4.490421	-1.953231
93	1	0	-5.189703	5.870483	-3.968253
94	1	0	-3.604112	5.790003	-5.885089
95	1	0	-1.593196	4.331341	-5.756268
96	1	0	-1.143950	3.000309	-3.749455
97	1	0	0.819905	1.738739	2.421174

98	1	0	1.789421	-0.386944	0.743684	161	8	0	3.878849	2.928208	-3.154651
99	1	0	-0.915001	4.832210	-1.904547	162	1	0	4.323143	2.183885	-2.665064
100	1	0	0.636932	6.641766	-1.426999	163	1	0	4.592205	3.224723	-3.744608
101	1	0	0.578077	7.806777	0.777815	164	8	0	7.544385	-2.383766	2.313371
102	1	0	-1.069776	7.077178	2.499051	165	1	0	6.916625	-3.112073	2.487030
103	1	0	-2.604734	5.194114	2.021708	166	1	0	6.950651	-1.610097	2.138359
104	8	0	2.533524	-1.192798	1.934999	167	8	0	7.036888	-1.052261	4.823409
105	1	0	3.202857	-0.581939	2.302127	168	1	0	7.483271	-1.578662	4.135468
106	1	0	2.001360	-1.432763	2.742775	169	1	0	7.025879	-0.151633	4.451218
107	8	0	2.201413	-4.767401	-0.916829	170	8	0	7.277028	1.704303	3.727659
108	1	0	3.075946	-5.184776	-0.983312	171	1	0	7.577586	2.203720	4.498753
109	1	0	2.127304	-4.493170	0.016421	172	1	0	6.443550	2.166781	3.439535
110	8	0	1.807127	-3.359765	-3.285008	173	8	0	7.937900	1.810650	1.093264
111	1	0	1.868910	-3.796304	-2.404670	174	1	0	8.002927	1.869749	2.072469
112	1	0	1.768535	-2.403831	-3.097668	175	1	0	7.267507	2.479937	0.809029
113	8	0	2.088313	-0.532449	-2.714698	176	8	0	8.939393	0.240135	-0.790192
114	1	0	2.158520	-0.386980	-1.751397	177	1	0	9.893267	0.132118	-0.686643
115	1	0	1.668077	0.299166	-3.055436	178	1	0	8.646227	0.824388	-0.042581
116	8	0	1.275390	1.932676	-3.387461	179	8	0	7.758680	-2.293034	-0.411340
117	1	0	2.152517	2.358609	-3.486792	180	1	0	7.890078	-2.434725	0.557321
118	1	0	0.953263	2.193662	-2.507334	181	1	0	8.123913	-1.405567	-0.612799
119	8	0	1.606256	-2.225815	4.183028	182	8	0	5.074763	-3.609267	2.427483
120	1	0	2.480825	-2.267408	4.610841	183	1	0	4.280951	-4.176312	2.420957
121	1	0	1.093095	-1.542714	4.682121	184	1	0	5.043233	-3.211087	1.517433
122	8	0	0.394809	-0.116645	5.409226	185	8	0	4.491891	-2.100384	4.603471
123	1	0	0.536659	-0.067410	6.362843	186	1	0	5.382127	-1.849669	4.943841
124	1	0	0.909059	0.639610	5.047856	187	1	0	4.692094	-2.622175	3.785093
125	8	0	2.239534	1.874832	4.713590	188	8	0	4.231650	0.303850	3.611779
126	1	0	2.808470	1.300355	4.159167	189	1	0	4.269918	-0.599027	4.044107
127	1	0	1.916148	2.561639	4.091842	190	1	0	4.999257	0.298829	2.993755
128	8	0	2.415968	-3.929947	1.791840	191	8	0	6.102280	-0.176106	1.727293
129	1	0	1.755104	-3.908713	2.500732	192	1	0	6.756518	0.493109	1.438412
130	1	0	2.615192	-2.976859	1.663210	193	1	0	5.434145	-0.249125	0.987152
131	8	0	1.257370	3.453090	2.686942	194	8	0	4.248451	-0.284970	-0.128404
132	1	0	1.557091	3.788095	1.809928	195	1	0	4.245321	-1.269189	-0.219210
133	1	0	0.299068	3.628562	2.722502	196	1	0	4.697870	0.099800	-0.932741
134	8	0	7.616223	-4.382663	-2.152131	197	8	0	5.050767	-2.759635	-0.103664
135	1	0	8.430431	-4.899810	-2.149676	198	1	0	5.973333	-2.498564	-0.321307
136	1	0	7.776068	-3.619463	-1.548099	199	1	0	4.904573	-3.615214	-0.605165
137	8	0	6.731217	-3.584424	-4.819181	200	8	0	5.896762	3.503392	0.482630
138	1	0	7.138987	-3.814710	-3.963994	201	1	0	5.753146	3.830760	1.395631
139	1	0	6.926891	-2.628526	-4.948399	202	1	0	5.095309	2.904515	0.393114
140	8	0	4.960995	-4.991593	-1.474805	203	8	0	5.913151	5.256276	-1.505968
141	1	0	5.920392	-5.143165	-1.566818	204	1	0	5.920645	4.627465	-0.731273
142	1	0	4.738783	-4.504317	-2.317504	205	1	0	6.465937	6.003378	-1.245260
143	8	0	4.447772	-3.461663	-3.535752	206	8	0	1.816577	3.775926	0.112344
144	1	0	5.092816	-3.647315	-4.268906	207	1	0	0.973152	3.493452	-0.280866
145	1	0	3.485442	-3.553998	-3.762500	208	1	0	2.243913	4.417112	-0.523321
146	8	0	6.932242	-0.807484	-5.113518	209	8	0	3.067388	5.141318	-1.761309
147	1	0	5.978378	-0.656635	-4.987831	210	1	0	3.952664	5.484765	-1.549817
148	1	0	7.349329	-0.216092	-4.463256	211	1	0	3.285268	4.349655	-2.306294
149	8	0	7.751656	1.170419	-3.107349	212	8	0	3.708485	2.104221	0.876221
150	1	0	8.357834	1.023394	-2.354523	213	1	0	3.654528	1.176876	0.560304
151	1	0	7.631925	2.126883	-3.274952	214	1	0	2.923577	2.595668	0.520008
152	8	0	6.630054	3.674677	-3.625290	215	8	0	4.773802	2.441835	5.571711
153	1	0	6.940066	4.232431	-4.349248	216	1	0	4.933328	1.548650	5.219578
154	1	0	6.440659	4.286747	-2.873686	217	1	0	3.794428	2.438225	5.620365
155	8	0	4.442099	-0.845558	-3.895053	218	8	0	5.104329	3.122366	3.010926
156	1	0	4.577545	-1.795550	-3.636512	219	1	0	4.843430	3.115364	3.966746
157	1	0	3.497318	-0.693178	-3.648043	220	1	0	4.422272	2.616305	2.518634
158	8	0	5.263376	0.871342	-2.197467						
159	1	0	6.224498	0.994076	-2.394131						
160	1	0	4.983787	0.177840	-2.884796						

The total electronic energy was calculated to be –6525.3114175 Hartree.

Table S8. Optimized structure of **1**•$(H_2O)_{39}$-**B** (B3LYP-D3/6-31G(d,p))

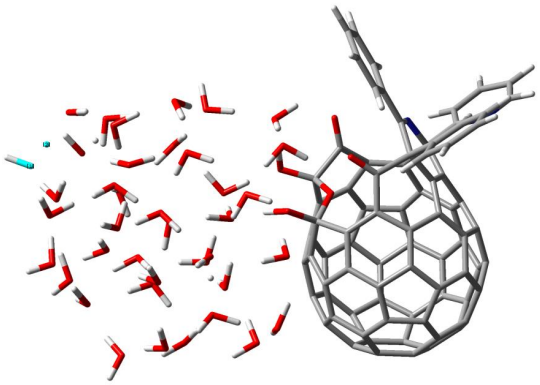


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	7.873856	-2.059039	-0.546642
2	6	0	7.728515	-0.642147	-0.255998
3	6	0	7.365011	-0.237764	1.018356
4	6	0	7.106689	-1.217296	2.059024
5	6	0	7.203035	-2.578815	1.773248
6	6	0	7.595523	-3.008083	0.441266
7	6	0	7.151027	0.018436	-1.412474
8	6	0	6.439702	0.853039	1.172438
9	6	0	6.008965	-0.711128	2.852956
10	6	0	6.181314	-3.489727	2.259837
11	6	0	6.820975	-4.190989	0.106970
12	6	0	7.434642	-2.274424	-1.908848
13	6	0	5.116076	-2.995825	3.018433
14	6	0	5.031806	-1.578671	3.325308
15	6	0	3.767995	-3.466118	2.764744
16	6	0	3.643326	-1.169979	3.266494
17	6	0	6.207609	1.060996	-1.277980
18	6	0	5.614046	0.579200	2.330261
19	6	0	2.873874	-2.337603	2.915214
20	6	0	4.293744	1.027143	2.360098
21	6	0	5.886980	1.516978	0.071475
22	6	0	5.936368	-4.478926	1.224633
23	6	0	6.380909	-4.391316	-1.203265
24	6	0	5.142337	1.187695	-2.287626
25	6	0	6.709921	-3.426499	-2.238690
26	6	0	7.031897	-0.991100	-2.450457
27	6	0	5.032016	-4.869964	-1.453484
28	6	0	5.583870	-3.336786	-3.146289
29	6	0	5.988793	-0.915628	-3.357035
30	6	0	3.256987	0.100782	2.805527
31	6	0	4.633947	-4.930137	0.981578
32	6	0	4.670425	2.256502	0.295739
33	6	0	4.531416	-4.207087	-2.642488
34	6	0	5.249621	-2.114825	-3.723727
35	6	0	5.064313	0.189450	-3.278944
36	6	0	3.779303	-0.311522	-3.690155
37	6	0	3.941636	1.959968	-1.978774
38	6	0	3.913588	2.056672	1.417192
39	6	0	1.504174	1.579341	1.733273
40	6	0	3.862391	-1.730426	-3.866609
41	6	0	2.852216	-2.524515	-3.309065
42	6	0	1.723546	-1.936592	-2.610184
43	6	0	3.201407	-3.779229	-2.690229
44	6	0	3.530243	-4.402395	1.758059
45	6	0	1.286633	1.735996	-2.038649
46	6	0	4.170561	-5.114205	-0.385631
47	6	0	2.786693	-4.675798	-0.450906
48	6	0	2.713598	1.500258	-2.435615
49	6	0	1.972526	0.239462	2.145424
50	6	0	1.345227	-0.904210	1.670385
51	6	0	2.639694	0.243537	-3.140555
52	6	0	1.544346	-0.567204	-2.680693
53	6	0	2.315317	-3.977106	-1.563981
54	6	0	1.423858	-2.823785	-1.443696
55	6	0	0.689407	0.293832	-1.782078
56	6	0	2.394984	-4.243190	0.859996
57	6	0	1.795180	-2.187931	2.045714
58	6	0	0.551823	-1.027124	0.349147
59	6	0	1.564145	-3.132738	0.972744
60	6	0	1.037528	-2.423121	-0.168451
61	6	0	4.102758	3.026801	-0.879520
62	6	0	2.556464	2.714213	1.627748
63	6	0	2.190370	3.663940	0.456376
64	7	0	2.865415	3.723523	-0.627977
65	6	0	2.648576	3.484623	2.965108
66	6	0	5.073091	4.155257	-1.295821
67	8	0	0.313771	1.801856	1.544228
68	8	0	0.613226	2.739064	-2.042041
69	6	0	5.271499	4.512653	-2.630889
70	6	0	6.110138	5.588872	-2.913974
71	6	0	6.712938	6.269574	-1.857262
72	6	0	6.438599	5.842894	-0.557356
73	7	0	5.636422	4.811065	-0.274033
74	6	0	3.538734	4.564459	3.026964
75	6	0	3.692616	5.276423	4.214676
76	6	0	2.969646	4.911094	5.352562
77	6	0	2.091103	3.829395	5.294169
78	6	0	1.927461	3.114043	4.106154
79	8	0	1.062290	0.069893	-0.431315
80	8	0	-0.662171	0.200194	-2.013447
81	8	0	-0.796857	-0.962526	0.589345
82	6	0	0.988199	4.561619	0.507177
83	6	0	0.076648	4.622267	1.573380
84	6	0	-1.047242	5.445892	1.510009
85	6	0	-1.281061	6.242314	0.390842
86	6	0	-0.370152	6.211764	-0.668860
87	6	0	0.748211	5.388439	-0.609796
88	1	0	4.781296	3.959225	-3.423550
89	1	0	6.288590	5.889675	-3.942094
90	1	0	7.375562	7.111061	-2.030898
91	1	0	6.882169	6.351244	0.296336
92	1	0	4.117926	4.831669	2.146119
93	1	0	4.381408	6.115357	4.251600
94	1	0	3.092270	5.465116	6.278509
95	1	0	1.525790	3.536218	6.173753
96	1	0	1.220751	2.288810	4.079753
97	1	0	-1.167246	0.711907	-1.295257
98	1	0	-1.304520	-1.365029	-0.170562
99	1	0	0.215861	4.016150	2.453323
100	1	0	-1.747178	5.452541	2.339864
101	1	0	-2.172037	6.856577	0.326494
102	1	0	-0.539259	6.825916	-1.548585
103	1	0	1.446919	5.345914	-1.434829
104	8	0	-2.327268	-1.983559	-1.266806

105	1	0	-3.113883	-1.477740	-0.935082	164	8	0	-10.377059	-1.701629	-0.406667
106	1	0	-2.169676	-1.683312	-2.194903	165	1	0	-11.278728	-1.979202	-0.607195
107	8	0	-2.227402	-4.650882	-1.110159	166	1	0	-9.980524	-1.406620	-1.264551
108	1	0	-3.109883	-4.953276	-0.820484	167	8	0	-9.150338	-0.909663	-2.702370
109	1	0	-2.311402	-3.665583	-1.126321	168	1	0	-9.569284	-1.141649	-3.541849
110	8	0	-1.281044	-4.650873	1.673705	169	1	0	-9.162607	0.092657	-2.658221
111	1	0	-1.358083	-4.577968	0.703409	170	8	0	-9.137115	1.672669	-2.318252
112	1	0	-1.052973	-3.764639	2.044323	171	1	0	-10.009850	2.080675	-2.253600
113	8	0	-0.884584	-2.500777	3.310585	172	1	0	-8.534336	2.365575	-2.872724
114	1	0	-1.572233	-2.670322	3.973748	173	8	0	-7.923274	1.482703	0.060700
115	1	0	-0.925100	-1.525351	3.223810	174	1	0	-8.387624	1.501816	-0.816208
116	8	0	-0.935228	0.308012	3.564483	175	1	0	-8.023669	2.406110	0.392138
117	1	0	-1.765782	0.795108	3.718792	176	8	0	-8.507945	-0.651299	1.526010
118	1	0	-0.666354	0.633138	2.689701	177	1	0	-9.433600	-0.813733	1.282211
119	8	0	-2.431621	-1.491184	-3.923543	178	1	0	-8.251033	0.142520	0.984826
120	1	0	-3.405332	-1.623863	-3.901741	179	8	0	-8.163632	-3.088231	0.345458
121	1	0	-2.267674	-0.613259	-4.300574	180	1	0	-9.065840	-2.909066	0.007237
122	8	0	-2.201180	1.520763	-3.894371	181	1	0	-8.010623	-2.286360	0.895729
123	1	0	-3.079642	1.215001	-3.574592	182	8	0	-4.902813	-2.630225	-3.692323
124	1	0	-1.548118	1.073130	-3.320395	183	1	0	-4.315492	-3.419730	-3.827672
125	8	0	-2.073886	3.647113	-2.110116	184	1	0	-5.231228	-2.683629	-2.767659
126	1	0	-2.158747	3.029808	-2.877556	185	8	0	-6.692253	-0.753049	-4.162464
127	1	0	-1.121059	3.814730	-2.037827	186	1	0	-7.372245	-0.970008	-3.500709
128	8	0	-2.837814	-4.343026	-3.867948	187	1	0	-6.135099	-1.561508	-4.262239
129	1	0	-2.279308	-3.579259	-4.087921	188	8	0	-4.744819	0.918597	-3.159488
130	1	0	-2.550322	-4.600998	-2.964741	189	1	0	-5.364740	0.188235	-3.377143
131	8	0	-2.029433	1.574141	-0.276340	190	1	0	-4.979341	1.222507	-2.259856
132	1	0	-1.397167	1.688669	0.451437	191	8	0	-5.261546	1.631522	-0.528620
133	1	0	-2.099695	2.442288	-0.732425	192	1	0	-6.197027	1.476875	-0.258145
134	8	0	-7.196621	-5.483090	1.183608	193	1	0	-4.797357	0.747352	-0.382805
135	1	0	-7.849587	-6.176994	1.034604	194	8	0	-4.402496	-0.769143	-0.168017
136	1	0	-7.630944	-4.630429	0.938741	195	1	0	-5.094221	-1.421151	-0.456663
137	8	0	-5.833763	-5.427802	3.687418	196	1	0	-4.293750	-0.851355	0.820701
138	1	0	-6.403832	-5.475831	2.896503	197	8	0	-5.914359	-2.681644	-1.153098
139	1	0	-6.045416	-4.568346	4.098433	198	1	0	-6.845967	-2.778999	-0.867026
140	8	0	-4.813204	-4.763195	-0.028225	199	1	0	-5.455786	-3.472882	-0.735376
141	1	0	-5.573178	-5.330496	0.203512	200	8	0	-7.800403	4.133979	0.410510
142	1	0	-4.423663	-4.527275	0.866665	201	1	0	-8.463257	4.818591	0.263215
143	8	0	-3.762886	-4.417871	2.331719	202	1	0	-7.131584	4.208164	-0.339644
144	1	0	-4.294681	-5.043471	2.881383	203	8	0	-6.175081	3.979475	2.667173
145	1	0	-2.808236	-4.710724	2.173805	204	1	0	-6.871309	4.102968	1.994041
146	8	0	-6.180632	-2.839942	4.927083	205	1	0	-5.344848	3.907596	2.132952
147	1	0	-6.522222	-2.837790	5.828822	206	8	0	-3.904079	5.304406	-0.934962
148	1	0	-6.494892	-2.000680	4.508080	207	1	0	-3.212703	4.883702	-1.492903
149	8	0	-6.818031	-0.540698	3.658882	208	1	0	-3.771459	4.855580	-0.073937
150	1	0	-7.568064	-0.530129	3.026595	209	8	0	-3.990410	3.454743	1.151941
151	1	0	-6.641229	0.386152	3.955759	210	1	0	-4.356746	2.765838	0.554504
152	8	0	-5.973754	1.959740	4.250641	211	1	0	-3.497417	2.932217	1.827735
153	1	0	-6.113289	2.352971	5.120953	212	8	0	-6.072333	4.049837	-1.558944
154	1	0	-6.158893	2.710516	3.593088	213	1	0	-5.674569	3.173475	-1.383710
155	8	0	-3.529353	-2.493752	4.138729	214	1	0	-5.281741	4.671077	-1.418208
156	1	0	-3.593162	-3.206524	3.447557	215	8	0	-6.332525	1.861022	-5.238398
157	1	0	-4.330625	-2.626779	4.681148	216	1	0	-6.661431	0.945545	-5.167814
158	8	0	-4.347038	-0.668721	2.440238	217	1	0	-5.537708	1.811041	-4.671752
159	1	0	-5.275137	-0.639979	2.764517	218	8	0	-7.781626	3.311909	-3.566036
160	1	0	-3.899670	-1.312410	3.064788	219	1	0	-7.264949	2.831252	-4.276515
161	8	0	-3.343226	1.717862	3.154155	220	1	0	-7.117893	3.719671	-2.964017
162	1	0	-3.630066	0.859699	2.750986	----------					
163	1	0	-4.086706	1.899740	3.761093	The total electronic energy was calculated to be –6525.2994634 Hartree.					

Table S9. Optimized structure of **1**•$(H_2O)_{39}$-**C** (B3LYP-D3/6-31G(d,p))



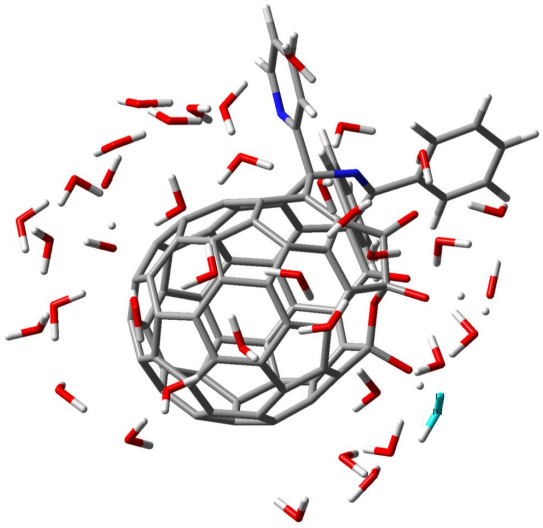
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.889914	-3.840461	-0.587555
2	6	0	7.309945	-2.459077	-0.419598
3	6	0	7.227432	-1.864923	0.829045
4	6	0	6.701666	-2.602612	1.965093
5	6	0	6.255081	-3.913030	1.798513
6	6	0	6.352608	-4.545027	0.493464
7	6	0	6.935018	-1.705403	-1.602395
8	6	0	6.793967	-0.496759	0.927057
9	6	0	5.939195	-1.666648	2.760728
10	6	0	5.007747	-4.332752	2.413382
11	6	0	5.168080	-5.364155	0.304255
12	6	0	6.297866	-3.961491	-1.902359
13	6	0	4.268463	-3.422240	3.174559
14	6	0	4.747806	-2.063799	3.355402
15	6	0	2.826904	-3.357417	3.024512
16	6	0	3.614488	-1.161841	3.323132
17	6	0	6.465545	-0.375517	-1.518471
18	6	0	6.018420	-0.360885	2.142469
19	6	0	2.437909	-1.965596	3.112484
20	6	0	4.970506	0.556046	2.193720
21	6	0	6.447038	0.254620	-0.202255
22	6	0	4.329208	-5.218761	1.483167
23	6	0	4.584787	-5.468158	-0.960427
24	6	0	5.449268	0.082077	-2.482781
25	6	0	5.170692	-4.770758	-2.092655
26	6	0	6.367064	-2.660309	-2.538249
27	6	0	3.139769	-5.414296	-1.103504
28	6	0	4.094435	-4.320005	-2.951758
29	6	0	5.361821	-2.253236	-3.397698
30	6	0	3.698266	0.126551	2.768813
31	6	0	2.938942	-5.154473	1.342369
32	6	0	5.619378	1.414602	0.011414
33	6	0	2.834208	-4.691508	-2.323415
34	6	0	4.201076	-3.103064	-3.620617
35	6	0	4.928841	-0.876362	-3.375392
36	6	0	3.522632	-0.878264	-3.677929
37	6	0	4.650931	1.272086	-2.186137
38	6	0	4.934604	1.587873	1.181759
39	6	0	2.567476	2.119013	1.718357
40	6	0	3.052824	-2.230821	-3.731662
41	6	0	1.864921	-2.547452	-3.060441
42	6	0	1.100875	-1.532531	-2.361080
43	6	0	1.761907	-3.795818	-2.347482
44	6	0	2.178972	-4.193972	2.117219
45	6	0	2.096787	2.066487	-2.100108
46	6	0	2.334682	-5.240094	0.020912
47	6	0	1.217851	-4.312172	-0.019321
48	6	0	3.307148	1.285715	-2.539823
49	6	0	2.511790	0.708198	2.167806
50	6	0	1.456390	-0.130468	1.825915
51	6	0	2.724132	0.102046	-3.122231
52	6	0	1.457048	-0.211012	-2.529644
53	6	0	0.956465	-3.565417	-1.167030
54	6	0	0.577614	-2.154118	-1.109497
55	6	0	1.025370	0.971288	-1.709212
56	6	0	1.125759	-3.671629	1.259787
57	6	0	1.432768	-1.468566	2.282588
58	6	0	0.567327	-0.034777	0.554143
59	6	0	0.784116	-2.323576	1.309659
60	6	0	0.474895	-1.544568	0.135892
61	6	0	5.285498	2.267542	-1.197839
62	6	0	3.967142	2.735247	1.414388
63	6	0	3.867496	3.664849	0.175470
64	7	0	4.417753	3.393520	-0.946362
65	6	0	4.530387	3.503450	2.632833
66	6	0	6.568593	2.917593	-1.762877
67	8	0	1.555442	2.798173	1.645718
68	8	0	1.838369	3.247017	-2.137537
69	6	0	6.789340	3.067907	-3.133174
70	6	0	7.943114	3.727219	-3.553034
71	6	0	8.827832	4.215628	-2.592950
72	6	0	8.509014	4.026751	-1.247669
73	7	0	7.405690	3.394649	-0.833774
74	6	0	5.728874	4.207649	2.457159
75	6	0	6.307182	4.883140	3.529738
76	6	0	5.705228	4.853398	4.789769
77	6	0	4.521667	4.138425	4.970943
78	6	0	3.936309	3.463675	3.897985
79	8	0	1.325158	0.788554	-0.326872
80	8	0	-0.271402	1.328298	-1.973532
81	8	0	-0.676273	0.507086	0.867536
82	6	0	3.097188	4.952472	0.220771
83	6	0	2.481426	5.469962	1.371788
84	6	0	1.772225	6.669132	1.328517
85	6	0	1.662007	7.382696	0.136212
86	6	0	2.277749	6.887105	-1.016028
87	6	0	2.990239	5.693755	-0.972969
88	1	0	6.075182	2.676656	-3.848467
89	1	0	8.146099	3.856852	-4.611947
90	1	0	9.739451	4.732398	-2.874275
91	1	0	9.167944	4.398754	-0.465778
92	1	0	6.214796	4.204992	1.484704
93	1	0	7.233466	5.430247	3.380981
94	1	0	6.158014	5.379783	5.624635
95	1	0	4.048054	4.103137	5.947522
96	1	0	3.009876	2.920762	4.053840
97	1	0	-0.492965	2.203807	-1.535598
98	1	0	-1.344078	0.287555	0.141211
99	1	0	2.536558	4.940948	2.309182

100	1	0	1.300489	7.039297	2.233585	162	1	0	-3.419703	1.116919	3.264107
101	1	0	1.103827	8.314104	0.104010	163	1	0	-2.158088	1.812574	3.776338
102	1	0	2.202892	7.431929	-1.952805	164	8	0	-8.191745	-3.062692	-2.969201
103	1	0	3.457599	5.298283	-1.864199	165	1	0	-8.640812	-3.698098	-3.540540
104	8	0	-2.448344	-0.223422	-0.836741	166	1	0	-8.482312	-2.160249	-3.310117
105	1	0	-3.402906	-0.055872	-0.629459	167	8	0	-8.770541	-0.788681	-4.113736
106	1	0	-2.342506	-0.114227	-1.812816	168	1	0	-7.878288	-0.452377	-4.332683
107	8	0	-1.760023	-4.676899	0.984191	169	1	0	-9.224021	-0.013575	-3.716567
108	1	0	-2.627485	-5.107721	1.058899	170	8	0	-9.859025	1.547367	-3.053403
109	1	0	-1.924836	-4.056385	0.229995	171	1	0	-10.694510	1.800895	-3.464929
110	8	0	-1.581042	-3.407661	3.359798	172	1	0	-9.203260	2.325161	-3.255274
111	1	0	-1.495686	-3.836198	2.466331	173	8	0	-9.451168	0.933798	-0.532951
112	1	0	-1.196937	-2.514006	3.301907	174	1	0	-9.776122	1.216709	-1.430585
113	8	0	-1.324732	-0.515844	3.460524	175	1	0	-9.364948	1.734889	0.041559
114	1	0	-2.270958	-0.609841	3.648231	176	8	0	-9.854772	-1.278851	0.701044
115	1	0	-1.270417	-0.175641	2.545793	177	1	0	-10.787870	-1.499259	0.805307
116	8	0	-1.123631	3.357719	1.592195	178	1	0	-9.802159	-0.431330	0.158927
117	1	0	-1.818608	2.718202	1.834375	179	8	0	-8.174224	-3.227073	-0.246370
118	1	0	-0.282316	2.890322	1.750725	180	1	0	-8.284251	-3.305826	-1.223684
119	8	0	-2.646105	-2.779924	-3.660544	181	1	0	-8.783667	-2.516000	0.051498
120	1	0	-3.615525	-2.754544	-3.756847	182	8	0	-5.454059	-2.351061	-3.283123
121	1	0	-2.372746	-1.847864	-3.757211	183	1	0	-6.299570	-2.819800	-3.418616
122	8	0	-2.084507	0.002209	-3.528602	184	1	0	-5.324765	-2.447825	-2.304796
123	1	0	-2.702053	0.709324	-3.833010	185	8	0	-6.141765	0.162887	-3.949159
124	1	0	-1.252362	0.459332	-3.311881	186	1	0	-6.540238	0.489993	-3.101264
125	8	0	-3.284533	3.837431	-1.996741	187	1	0	-5.797752	-0.748468	-3.742149
126	1	0	-3.335763	4.606888	-2.579536	188	8	0	-3.969419	1.923664	-3.912558
127	1	0	-2.343737	3.818285	-1.677679	189	1	0	-4.697940	1.288577	-3.740530
128	8	0	-2.589460	-2.994182	-0.923623	190	1	0	-3.827841	2.462636	-3.105839
129	1	0	-2.522207	-3.080644	-1.902796	191	8	0	-6.924670	1.078610	-1.603328
130	1	0	-2.457074	-2.039495	-0.768975	192	1	0	-7.778776	0.824949	-1.190537
131	8	0	-0.838904	3.656820	-0.946094	193	1	0	-6.191581	0.598920	-1.113571
132	1	0	0.007858	4.091999	-1.134500	194	8	0	-5.015065	-0.104562	-0.327861
133	1	0	-0.953506	3.591711	0.062473	195	1	0	-5.173039	-1.095332	-0.325941
134	8	0	-7.304059	-4.681533	1.881041	196	1	0	-5.301338	0.259006	0.550977
135	1	0	-7.763018	-5.525528	1.967058	197	8	0	-5.523013	-2.619257	-0.618400
136	1	0	-7.693439	-4.234846	1.092175	198	1	0	-6.462757	-2.803088	-0.395943
137	8	0	-6.219595	-3.729095	4.354764	199	1	0	-4.983771	-3.340775	-0.191501
138	1	0	-6.755663	-3.930667	3.564382	200	8	0	-8.869060	3.165501	0.892840
139	1	0	-6.550721	-2.886692	4.714806	201	1	0	-9.527314	3.873111	0.883051
140	8	0	-4.613466	-4.558129	0.971121	202	1	0	-8.176716	3.442322	0.196857
141	1	0	-5.478624	-4.866969	1.299507	203	8	0	-7.658596	3.388408	3.443168
142	1	0	-4.342028	-3.898109	1.654996	204	1	0	-8.068589	3.292760	2.558656
143	8	0	-4.075691	-2.866945	3.007050	205	1	0	-6.711455	3.562120	3.257127
144	1	0	-4.735008	-3.270734	3.631454	206	8	0	-5.042075	4.806683	-0.049580
145	1	0	-3.131906	-3.131508	3.273050	207	1	0	-4.324685	4.423864	-0.592715
146	8	0	-6.701368	-0.955680	4.743101	208	1	0	-4.948056	4.425720	0.851728
147	1	0	-7.175820	-0.240654	5.207665	209	8	0	-5.101773	3.473160	2.364163
148	1	0	-7.165776	-0.945106	3.877649	210	1	0	-5.417163	2.589988	2.057225
149	8	0	-8.226471	-0.226211	2.602224	211	1	0	-4.272690	3.261850	2.835768
150	1	0	-8.909223	-0.659607	2.046429	212	8	0	-7.182194	3.669551	-0.983682
151	1	0	-8.643823	0.333915	3.294304	213	1	0	-6.900920	2.744370	-1.191355
152	8	0	-8.393345	1.285481	4.785585	214	1	0	-6.362386	4.167785	-0.663461
153	1	0	-9.099001	1.608698	5.357723	215	8	0	-6.389255	2.650149	-5.246370
154	1	0	-8.019814	2.106899	4.332695	216	1	0	-6.474377	1.683441	-5.179480
155	8	0	-4.347276	-0.380331	3.519440	217	1	0	-5.463615	2.772194	-4.966831
156	1	0	-4.228542	-1.337616	3.189186	218	8	0	-8.303292	3.491929	-3.507373
157	1	0	-5.014289	-0.486997	4.236362	219	1	0	-7.573421	3.256288	-4.134953
158	8	0	-5.948388	0.958608	1.869758	220	1	0	-7.876579	3.755747	-2.664229
159	1	0	-6.876071	0.653242	2.016195						
160	1	0	-5.400332	0.443718	2.518835						
161	8	0	-2.917641	1.956077	3.194531						

The total electronic energy was calculated to be –6525.2969399 Hartree.

Table S10. Optimized structure of **1**•$(H_2O)_{39}$-**D** (B3LYP-D3/6-31G(d,p))



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.161595	-1.322119	-2.699739
2	6	0	2.041178	-2.239871	-2.580860
3	6	0	1.007615	-2.181486	-3.502513
4	6	0	1.021074	-1.188058	-4.564835
5	6	0	2.072464	-0.277792	-4.652199
6	6	0	3.167203	-0.349146	-3.699773
7	6	0	1.744275	-2.441981	-1.174821
8	6	0	-0.346637	-2.346031	-3.044456
9	6	0	-0.343394	-0.745830	-4.746595
10	6	0	1.789761	1.122736	-4.916234
11	6	0	3.570281	1.008544	-3.381558
12	6	0	3.599149	-0.990620	-1.361260
13	6	0	0.467585	1.546889	-5.085840
14	6	0	-0.621348	0.590715	-5.005138
15	6	0	0.016517	2.772903	-4.457408
16	6	0	-1.741148	1.214700	-4.329346
17	6	0	0.419802	-2.559913	-0.704532
18	6	0	-1.194174	-1.478125	-3.835672
19	6	0	-1.337293	2.553697	-3.989904
20	6	0	-2.337071	-0.920448	-3.265357
21	6	0	-0.650963	-2.559753	-1.695218
22	6	0	2.708398	1.917695	-4.119939
23	6	0	3.986553	1.332707	-2.088670
24	6	0	0.081843	-2.027690	0.629026
25	6	0	4.020666	0.308727	-1.057156
26	6	0	2.754206	-1.710985	-0.428827
27	6	0	3.532240	2.566572	-1.469384
28	6	0	3.636556	0.917105	0.202882
29	6	0	2.427403	-1.150279	0.791451
30	6	0	-2.597710	0.501084	-3.473257
31	6	0	2.272078	3.105984	-3.522564
32	6	0	-1.997201	-2.270733	-1.274472
33	6	0	3.299458	2.308352	-0.060138
34	6	0	2.882732	0.192157	1.125296
35	6	0	1.093167	-1.330166	1.316134
36	6	0	0.766229	-0.136139	2.044755
37	6	0	-1.311121	-1.759606	0.970355
38	6	0	-2.833789	-1.518639	-2.049352
39	6	0	-4.256289	0.455865	-1.574749
40	6	0	1.808879	0.830367	1.857229
41	6	0	1.435521	2.144746	1.550278
42	6	0	0.041588	2.542636	1.482359
43	6	0	2.198942	2.887202	0.577769
44	6	0	0.895648	3.528420	-3.682665
45	6	0	-2.844144	0.195716	1.921953
46	6	0	2.682400	3.428914	-2.164440
47	6	0	1.548102	4.034781	-1.485113
48	6	0	-1.614062	-0.626655	1.721749
49	6	0	-3.235133	1.197176	-2.364500
50	6	0	-2.719415	2.428203	-1.963177
51	6	0	-0.552783	0.276268	2.089925
52	6	0	-0.925630	1.646129	1.890226
53	6	0	1.278627	3.728918	-0.150277
54	6	0	-0.078255	3.496563	0.342541
55	6	0	-2.427851	1.716773	1.703834
56	6	0	0.453179	4.094468	-2.415575
57	6	0	-1.756779	3.088224	-2.770464
58	6	0	-2.577034	2.983834	-0.506976
59	6	0	-0.832668	3.840338	-1.944387
60	6	0	-1.128640	3.575795	-0.560251
61	6	0	-2.351169	-2.560247	0.168829
62	6	0	-4.224231	-1.101514	-1.610274
63	6	0	-4.569238	-1.676587	-0.210473
64	7	0	-3.703811	-2.228197	0.548331
65	6	0	-5.192362	-1.664953	-2.676577
66	6	0	-2.283628	-4.077094	0.451230
67	8	0	-5.144051	1.042092	-0.975256
68	8	0	-3.950054	-0.117767	2.316639
69	6	0	-1.945417	-4.570189	1.709859
70	6	0	-2.013070	-5.948763	1.915176
71	6	0	-2.417289	-6.767904	0.862800
72	6	0	-2.734528	-6.174511	-0.358740
73	7	0	-2.673991	-4.852691	-0.570699
74	6	0	-5.281237	-3.059456	-2.788034
75	6	0	-6.110592	-3.632662	-3.749268
76	6	0	-6.849841	-2.823812	-4.615817
77	6	0	-6.751590	-1.436567	-4.515963
78	6	0	-5.925049	-0.857598	-3.550602
79	8	0	-2.767725	1.846026	0.306414
80	8	0	-3.054910	2.573393	2.533063
81	8	0	-3.488302	4.013841	-0.274018
82	6	0	-5.967763	-1.656122	0.340978
83	6	0	-7.053252	-0.986148	-0.244755
84	6	0	-8.320515	-1.025803	0.341416
85	6	0	-8.537039	-1.745652	1.518184
86	6	0	-7.468589	-2.431296	2.104370
87	6	0	-6.206706	-2.389552	1.521649
88	1	0	-1.620033	-3.898623	2.497079
89	1	0	-1.730007	-6.357368	2.879256
90	1	0	-2.473123	-7.845338	0.976552
91	1	0	-3.044004	-6.780118	-1.207607
92	1	0	-4.685017	-3.690460	-2.132953
93	1	0	-6.175213	-4.713981	-3.824114
94	1	0	-7.494348	-3.272501	-5.365478
95	1	0	-7.318001	-0.798544	-5.187665

96	1	0	-5.870230	0.223883	-3.479437	160	1	0	6.948590	2.312042	-2.429039
97	1	0	-4.429644	2.743842	2.388482	161	8	0	7.083398	-3.791577	-1.818836
98	1	0	-3.162370	4.745109	0.440346	162	1	0	7.325911	-2.851951	-1.739583
99	1	0	-6.923194	-0.421534	-1.153170	163	1	0	6.466474	-3.965298	-1.082618
100	1	0	-9.140866	-0.495211	-0.132412	164	8	0	1.231670	-4.842233	2.166755
101	1	0	-9.524119	-1.775947	1.969560	165	1	0	1.510696	-3.965139	2.525672
102	1	0	-7.618601	-2.997617	3.018185	166	1	0	0.727382	-5.223703	2.926411
103	1	0	-5.377625	-2.923413	1.968753	167	8	0	-0.216634	-5.416447	4.402574
104	8	0	-2.882228	5.847669	1.233514	168	1	0	0.343338	-5.548589	5.176683
105	1	0	-2.526924	5.607029	2.152062	169	1	0	-0.616708	-4.512679	4.512359
106	1	0	-2.271569	6.463591	0.794026	170	8	0	-1.094485	-2.903489	4.395150
107	8	0	6.269918	3.175580	1.086194	171	1	0	-1.950056	-2.466338	4.608005
108	1	0	5.480033	3.145282	1.685446	172	1	0	-0.409217	-2.295100	4.736714
109	1	0	6.857880	3.845682	1.459217	173	8	0	0.610745	-5.641745	-0.348157
110	8	0	-1.130859	6.900397	-0.693683	174	1	0	0.660026	-5.283868	0.566415
111	1	0	-0.410647	7.330197	-1.198087	175	1	0	-0.166332	-5.238369	-0.751128
112	1	0	-1.787711	6.572990	-1.349590	176	8	0	3.147872	-5.274517	-1.240158
113	8	0	1.423921	7.437023	-1.625408	177	1	0	3.157233	-5.384329	-2.222143
114	1	0	1.573339	6.638743	-2.148812	178	1	0	2.198487	-5.326360	-0.981509
115	1	0	1.609909	7.148761	-0.711081	179	8	0	2.283560	-2.877150	3.589167
116	8	0	-6.118470	3.455458	-0.034018	180	1	0	1.788172	-2.242948	4.154487
117	1	0	-5.243447	3.844752	-0.253433	181	1	0	3.045422	-2.368044	3.237358
118	1	0	-6.038524	2.584931	-0.463061	182	8	0	1.626353	0.494009	7.129420
119	8	0	7.118450	-0.918230	-1.689499	183	1	0	2.497414	0.911364	6.845116
120	1	0	7.345767	0.023424	-1.910349	184	1	0	1.617579	0.512037	8.093190
121	1	0	6.493548	-0.889911	-0.945564	185	8	0	0.926448	6.498779	0.998856
122	8	0	-2.035592	4.938639	3.490933	186	1	0	0.084177	6.360545	0.506564
123	1	0	-1.052059	5.018725	3.558496	187	1	0	0.758296	7.289862	1.530933
124	1	0	-2.236331	4.022246	3.216217	188	8	0	4.723761	-1.853433	3.170594
125	8	0	-2.618503	1.464399	4.905239	189	1	0	4.945161	-2.749582	3.534154
126	1	0	-2.854782	1.924340	4.046889	190	1	0	5.177523	-1.782684	2.304445
127	1	0	-3.110120	1.934778	5.591196	191	8	0	0.890066	-1.144997	5.102887
128	8	0	0.620138	5.333275	3.505129	192	1	0	0.584281	-0.285836	4.742500
129	1	0	0.904240	5.455324	2.583273	193	1	0	1.215270	-0.885979	5.990454
130	1	0	1.214068	4.671577	3.911966	194	8	0	4.363602	2.857259	2.967077
131	8	0	-5.489708	2.922289	2.368744	195	1	0	4.567653	1.934556	3.310536
132	1	0	-5.972757	2.071193	2.622116	196	1	0	4.585977	3.433214	3.712499
133	1	0	-5.788623	3.173811	1.414137	197	8	0	3.730509	1.782000	6.251580
134	8	0	6.000737	-1.670279	0.747349	198	1	0	3.221196	2.400639	5.685192
135	1	0	5.463900	-2.453720	0.379452	199	1	0	4.333717	1.308678	5.644748
136	1	0	6.895331	-2.022634	0.863569	200	8	0	-6.562360	0.637862	2.932107
137	8	0	4.900240	-3.832259	0.009113	201	1	0	-5.760576	0.116108	2.757202
138	1	0	4.638398	-4.377641	0.787955	202	1	0	-7.215384	0.302378	2.300510
139	1	0	4.216739	-4.147987	-0.650858	203	8	0	-3.151101	5.958793	-2.281361
140	8	0	5.151436	0.629767	4.086851	204	1	0	-3.462062	5.262538	-1.669026
141	1	0	4.843568	-0.289327	3.891555	205	1	0	-2.930656	5.487698	-3.093965
142	1	0	6.005454	0.662431	3.586595	206	8	0	6.964644	0.649208	2.094056
143	8	0	4.602521	-4.409319	3.996934	207	1	0	6.887458	1.515105	1.647900
144	1	0	4.570180	-5.031366	3.247309	208	1	0	6.461827	0.038567	1.530434
145	1	0	3.667148	-4.165965	4.132178	209	8	0	6.145706	-0.866944	-4.229052
146	8	0	3.747502	-5.695606	1.605089	210	1	0	6.404053	-1.000245	-3.284102
147	1	0	3.706651	-6.139935	0.741663	211	1	0	6.975157	-0.982629	-4.712053
148	1	0	2.806472	-5.466291	1.813908	212	8	0	-3.335555	-1.370804	4.763848
149	8	0	5.026358	-3.379616	-3.585185	213	1	0	-3.086471	-0.434802	4.888563
150	1	0	5.304775	-2.586017	-4.074620	214	1	0	-3.746152	-1.373476	3.886290
151	1	0	5.809067	-3.644544	-3.048518	215	8	0	2.079057	3.189790	4.483897
152	8	0	3.071849	-5.150381	-3.956044	216	1	0	1.288018	2.601108	4.570479
153	1	0	2.310831	-4.565095	-4.061048	217	1	0	2.544938	2.920125	3.672448
154	1	0	3.843194	-4.529956	-3.977440	218	8	0	0.111260	1.472038	5.070054
155	8	0	6.355507	3.771226	-1.627189	219	1	0	-0.870375	1.565124	5.064972
156	1	0	5.475204	4.031325	-1.924717	220	1	0	0.403743	1.314714	5.993266
157	1	0	6.236751	3.542028	-0.681959						
158	8	0	7.281816	1.469749	-2.814092						
159	1	0	6.637131	1.192232	-3.481360						

The total electronic energy was calculated to be –6525.2291263 Hartree.

5 Microscope Images

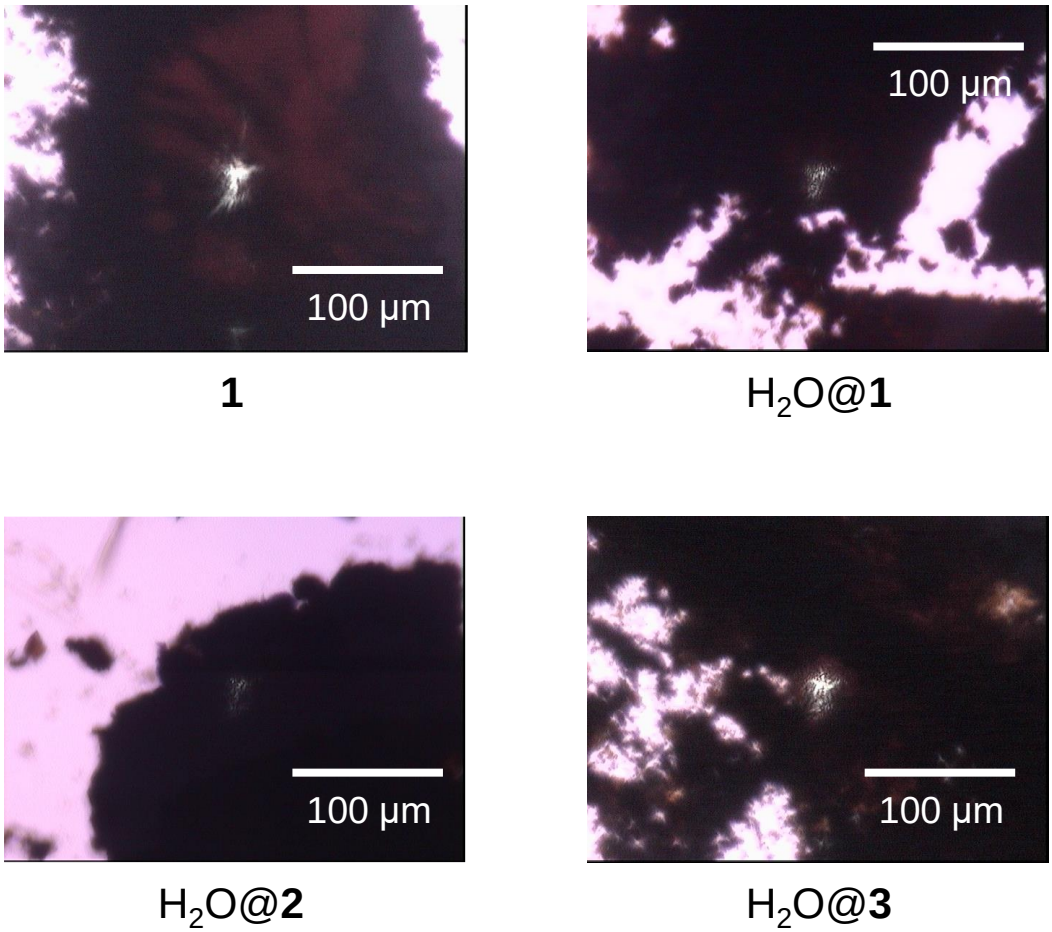


Figure S12. Microscope images of powdery [60]fullerenol samples used for synchrotron IR measurements.

6. References

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