Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

An Orifice Design: Water Insertion into C_{60}

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1. General

The ^{1}H and ^{13}C NMR measurements were carried out at room temperature unless otherwise noted with a JEOL JNM ECA500 instrument. The NMR chemical shifts were reported in ppm with reference to residual protons and carbons of $CDCl_3$ (δ 7.26 ppm in ^{1}H NMR, δ 77.00 ppm in ^{13}C NMR) and acetone-d_6 (δ 2.05 ppm in ^{1}H NMR, δ 29.92 ppm in ^{13}C NMR). APCI (atmospheric pressure chemical ionization) mass spectra were measured on a Bruker micrOTOF-Q II. The high-performance liquid chromatography (HPLC) was performed with the use of a Cosmosil Buckyprep column (250 mm in length, 4.6 mm in inner diameter) for analytical purpose. Thin layer chromatography (TLC) was performed on glass plates coated with 0.25 mm thick silica gel 60F-254 (Merck). Column chromatography was performed using PSQ 60B (Fuji Silysia).

Fullerene C_{60} was purchased from SES Research Co. Toluene and tetrahydrofuran were purchased from Kanto Chemical Co., Inc. *N*-Methylmorpholine *N*-oxide (NMO) and carbon disulfide were purchased from FUJIFILM Wako Pure Chemical Corporation. Ethyl acetate was purchased from Nacalai Tesque, Inc. Tri(*p*-tolyl)phosphine, triphenylphosphine, and triisopropyl phosphite were purchased from Tokyo Chemical Industry Co., Ltd. *o*-Dichlorobenzene (ODCB) and 1-chloronaphthalene were purchased from Sigma-Aldroch Co. LLC. **INT3f** was synthesized according to the literature.[1]

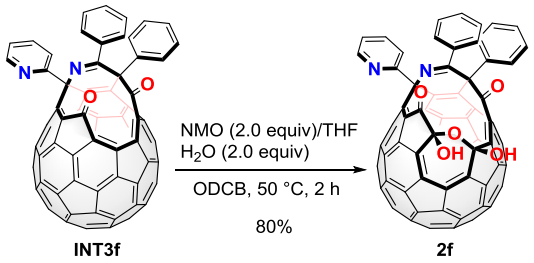
All reactions were carried out under Ar atmosphere. Unless otherwise noted, materials purchased from commercial suppliers were used without further purification.

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) level of theory without any symmetry assumptions and confirmed by the frequency analyses at the same level of theory. The natural population analyses were carried out at the B3LYP-D3/6-31G(d) level of theory.

3. Synthesis

3.1. Synthesis of 2f



INT3f (700 mg, 676 μmol) was placed into a 500-mL two-neck flask and degassed through three vacuum-Ar cycles. *o*-Dichlorobenzene (ODCB) (8.80 mL) and then distilled water (24.3 μL, 1.35 mmol, 2.00 equiv) were added. *N*-methylmorpholine *N*-oxide (NMO) (177 mg, 1.51 mmol, 2.23 equiv) dissolved in THF (62.0 mL) was further added to the flask at room temperature. The reaction mixture was then heated at 60 °C for 1.5 h. After passing through a silica gel pad (toluene/hexane (3:1)) for removal of unreacted NMO, the remaining THF was removed under reduced pressure. The crude mixture in ODCB was purified by silica gel column chromatography (CS_2/EtOAc (40:1) to (5:1)) to give unreacted **INT3f** (61.9 mg, 59.8 μmol, 9%) and **2f** (583 mg, 538 μmol, 80%).

2f: ^{1}H NMR (500 MHz, CS_2/acetone-d_6 (2:1)) δ 8.47 (d, 1H, J = 5.73 Hz), 8.26 (d, 2H, J = 8.02 Hz), 7.91 (d, 1H, J = 8.02 Hz), 7.87 (dt, 1H, J = 7.45, 1.72 Hz), 7.75 (br d, 1H, J = 7.45 Hz), 7.56 (br s, 1H), 7.45 (br t, 1H, J = 5.73 Hz), 7.39 (t, 1H, J = 7.45 Hz), 7.30–7.24 (m, 5H), 7.21 (br d, 1H, J = 7.45 Hz), 6.37 (br s, 1H); ^{13}C NMR (126 MHz, CS_2/acetone-d_6 (2:1)) δ 194.23, 191.30, 165.55, 159.77, 150.77, 150.75, 150.66, 150.28, 150.06, 149.98, 149.90, 149.72, 149.28, 149.19, 149.07, 149.03, 149.00, 148.62, 148.18, 148.12, 147.99, 147.79, 147.56, 147.33, 146.86, 146.71, 146.04, 146.02, 145.99, 145.97, 145.09, 144.82, 144.16, 143.60, 143.55, 142.87, 142.77, 142.09, 141.84, 141.74, 141.44, 141.39, 141.22, 140.85, 139.87, 139.26, 138.80, 138.65, 138.44, 137.73, 137.69, 137.66, 137.59, 136.74, 136.49, 135.45, 135.31, 135.11, 134.67, 134.17, 131.76, 131.70, 131.41, 130.70, 130.14, 130.05, 128.19, 127.13, 126.95, 125.55, 124.68, 123.38, 110.19, 96.76, 72.80, 60.02 (The sum of carbon signals must be 76 in theory. Observed 76.); HRMS (APCI, negative ion mode) calcd for $C_{80}H_{14}N_2O_4$ (**2f**–H_2O) 1066.0959, found 1066.0937.

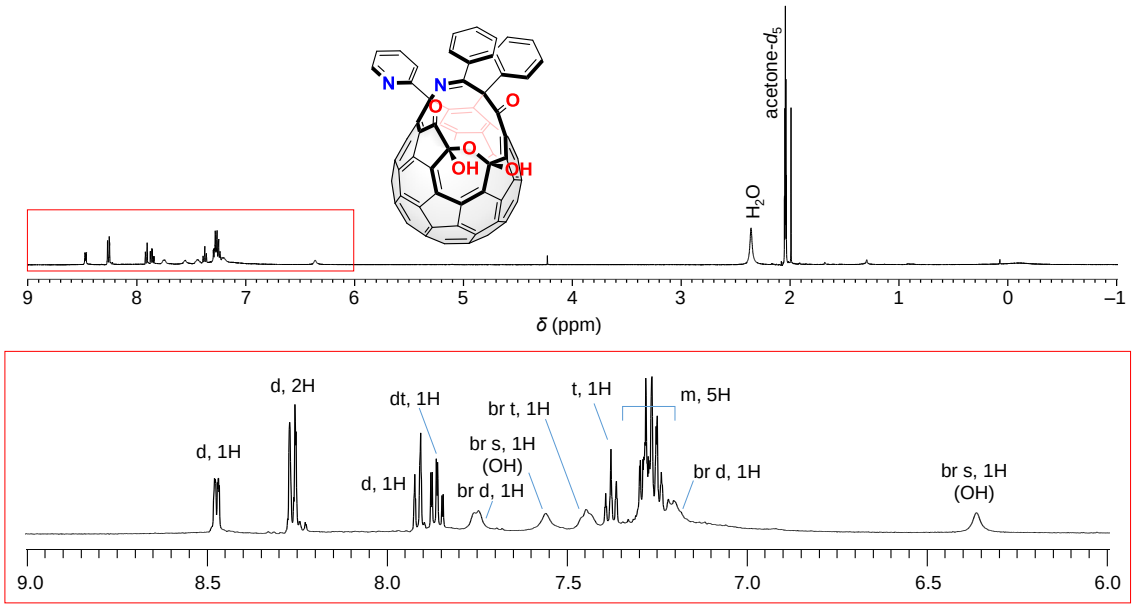


Figure S1. ^{1}H NMR spectra (500 MHz, CS_2/acetone-d_6 (2:1)) of **2f**.

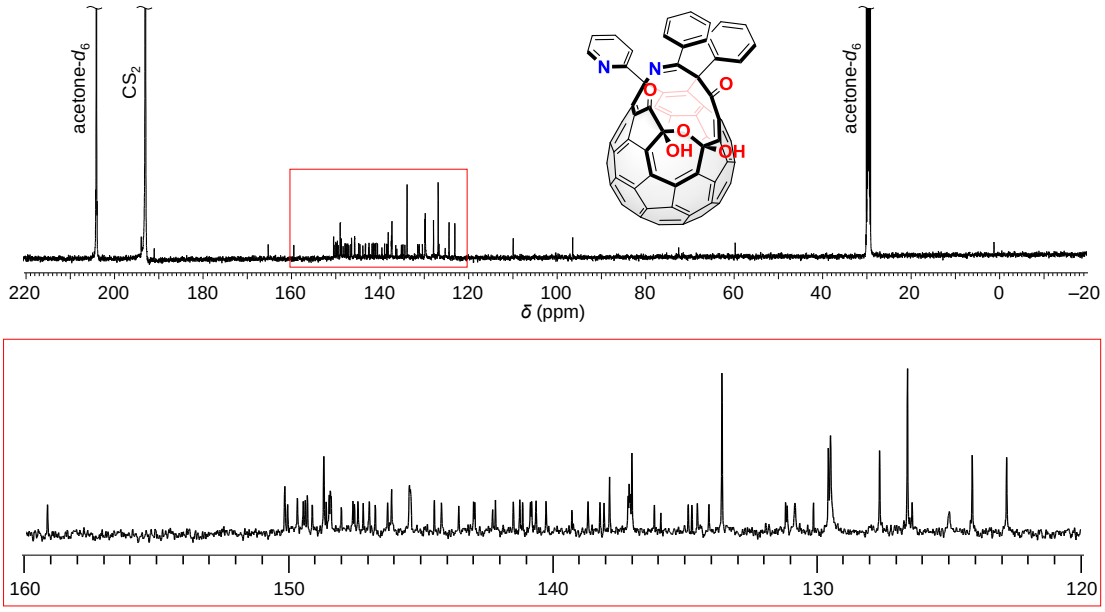


Figure S2. ^{13}C NMR spectra (126 MHz, CS_2/acetone-d_6 (2:1)) of **2f**.

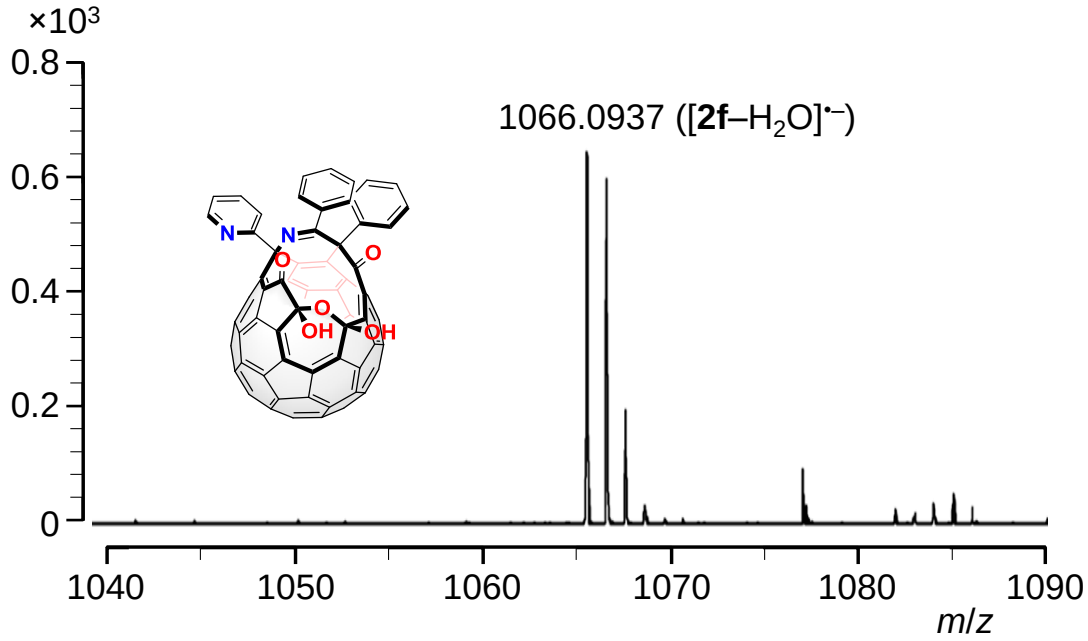
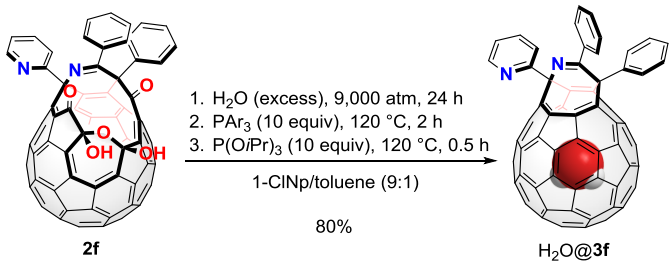


Figure S3. APCI mass spectrum (negative ion mode) of **2f**.

3.2. Synthesis of H_2O@3f from 2f



2f (160 mg, 147 μmol) was dissolved in a mixed solvent system including 1-chloronaphthalene and toluene (9:1, 3.5 mL). The reaction mixture was heated at 160 °C under 9,000 atm for 24 h. The resulting solution was then transferred into a 25-mL Schlenk tube containing P(*p*-tolyl)$_3$ (449 mg, 1.47 mmol, 9.99 equiv) and degassed under reduced pressure. After adding toluene (0.30 mL) for washing the reaction vessel, the reaction mixture was heated at 120 °C for 2 h. After cooling down to room temperature, P(O*i*Pr)$_3$ (340 μL distilled from CaH_2, ρ = 0.9035 g/mL, 1.48 mmol, 10.0 equiv) was further added and heated at 120 °C for 0.5 h. The crude mixture was purified by silica gel column chromatography (CS_2/EtOAc (30:1)) to give H_2O@**3f** (121 mg, 118 μmol, H_2O: 98%) in 80% isolated yield.

H_2@**3f** (H_2O: 98%): ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.82 (d, 1H, J = 5.15 Hz), 8.08 (d, 1H, J = 8.02 Hz), 7.94 (t, 1H, J = 7.45 Hz), 7.93 (t, 1H, J = 7.45 Hz), 7.45–7.40 (m, 2H), 7.25–7.12 (m, 7H), –6.11 (s, 1.96H); ^{13}C NMR (201 MHz, $CDCl_3$) δ 169.30, 164.86, 149.61, 148.18, 145.91, 145.86, 145.75, 145.66, 145.63, 145.18, 144.91, 144.88, 144.86, 144.74, 144.70, 144.67, 144.60, 144.56, 144.534, 144.527, 144.36, 4.31, 144.27, 144.26, 144.24, 144.21, 144.20, 144.14, 144.09, 143.89, 143.85, 143.84, 143.75, 143.70, 143.56, 143.26, 141.89, 141.28, 141.24, 141.15, 141.14, 140.99, 140.63, 140.48, 139.34, 139.23, 138.75, 138.65, 138.52, 137.32, 137.24, 137.20, 136.96, 136.95, 135.83, 135.53, 135.31, 135.16, 132.10, 132.02, 131.36, 131.28, 129.19, 129.09, 128.80, 128.73, 128.37, 127.72, 127.54, 127.38, 126.67, 125.83, 125.46, 123.36, 73.01, 56.81 (The sum of carbon signals must be 76 in theory. Observed 76.); HRMS (APCI, negative ion mode) calcd for $C_{80}H_{14}N_2$ (**3f**) 1002.1151, found 1002.1180 and calcd for $C_{80}H_{16}N_2O_1$ (H_2O@**3f**) 1020.1268, found 1020.1255.

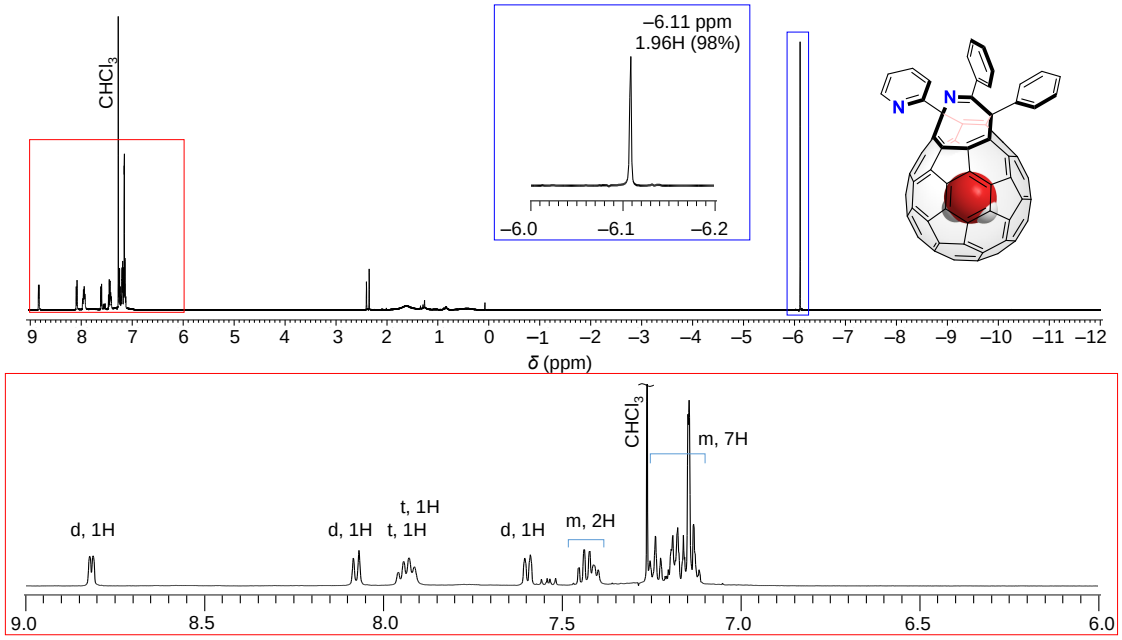


Figure S4. ^{1}H NMR spectra (500 MHz, $CDCl_3$) of H_2O@**3f** (H_2O: 98%).

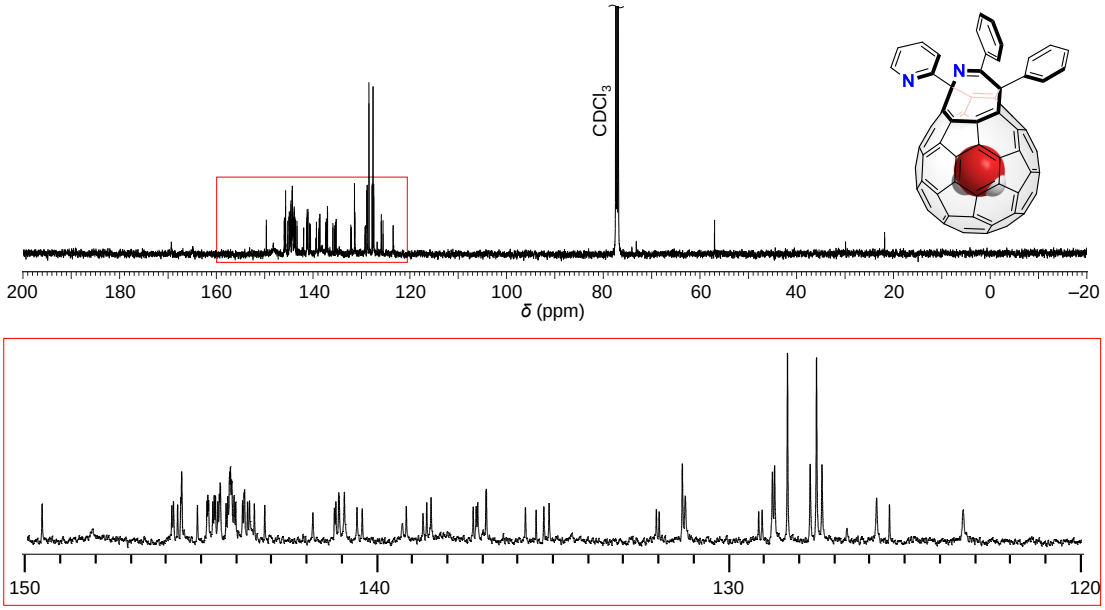


Figure S5. ^{13}C NMR spectra (126 MHz, $CDCl_3$) of H_2O@**3f** (H_2O: 98%).

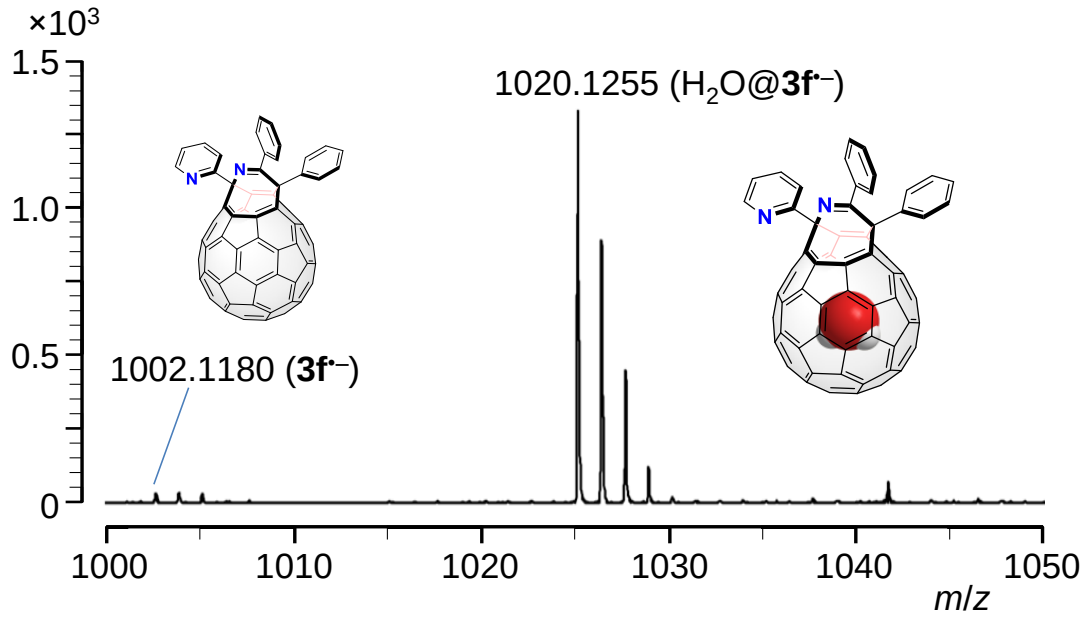
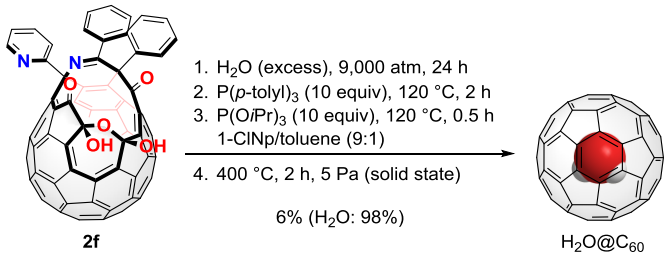


Figure S6. APCI mass spectrum (negative ion mode) of H_2O@**3f** (H_2O: 98%).

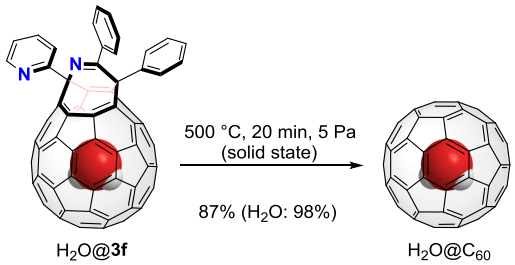
3.3. Synthesis of $H_2O@C_{60}$ from 2f



2f (160 mg, 147 μmol) was dissolved in a mixed solvent system including 1-chloronaphthalene and toluene (9:1, 3.5 mL). The reaction mixture was heated at 160 °C under 9,000 atm for 24 h. The resulting solution was then transferred into a 25-mL Schlenk tube containing P(*p*-tolyl)$_3$ (449 mg, 1.47 mmol, 10.0 equiv) and degassed under reduced pressure. The reaction mixture was heated at 120 °C for 2 h. After cooling down to room temperature, P(O*i*Pr)$_3$ (340 μL, ρ = 0.9035 g/mL, 1.48 mmol, 10.0 equiv) was further added and heated at 120 °C for 0.5 h. The crude mixture was reprecipitated by addition of methanol (80 mL). The resulting powder was placed into a 20-mL test tube and heated at 400 °C under 5 Pa for 2 h. The chromatographic purification using silica gel (toluene) gave $H_2O@C_{60}$ (6.2 mg, 8.4 μmol, H_2O: 98%) in 6% isolated yield.

$H_2O@C_{60}$: ^{1}H NMR (500 MHz, $CDCl_3/CS_2$ (1:1)) δ –4.64 (s, 2H); HRMS (APCI, negative ion mode) calcd for $C_{60}H_2O$ ($H_2O@C_{60}^{\bullet-}$) 738.0113, found 738.0140.

3.4. Synthesis of $H_2O@C_{60}$ from $H_2O@3f$



H_2O@**3f** (102 mg, 100 μmol, H_2O: 98%) wrapped with an aluminum foil was placed into a 20-mL test tube and heated at 500 °C under 5 Pa for 20 min. The chromatographic purification using silica gel (CS_2) gave $H_2O@C_{60}$ (64.1 mg, 86.8 μmol, H_2O: 98%) in 87% isolated yield.

4. Single Crystal X-Ray-Structure of $[(H_2O)_{0.593(8)}@\{(3f)_{0.854(2)}(3f)_{0.146(2)}\}]\bullet(C_6H_6)_{2.85}$

Single crystals of H_2O@**3f** were obtained from a benzene/hexane solution by slow evaporation. Intensity data were collected at 100 K on a Bruker Single Crystal CCD X-ray Diffractometer (SMART APEX II) with Mo Kα radiation (λ = 0.71073 Å) and graphite monochromator. A total of 13432 reflections were measured at the maximum 2θ angle of 50.08°, of which 9533 were independent reflections (R_{int} = 0.0188). The structure was solved by direct methods (SHELXS-97[2]) and refined by the full-matrix least-squares on F^2 (SHELXL-97[2]). A benzene molecule was disordered, which was solved using appropriate models. Thus, (C89–C90–C92–C94–C97–C98) and (C115–C116–C117–C118–C119–C120) were placed and their occupancies were refined to be 0.731(11) and 0.269(11), respectively. A part of orifice structure was disordered together with a benzene molecule, which was solved using appropriate models. Thus, [(C1–C2–C3–C5–C6–C8–C9–C64–C65–C66–C67–C68–C69–C70–C71–C72–C73–C74–C75) and (C85–C89–C91–C93–C95–C96)] and (C99–C100–C101–C102–C103–C104–C105–C106–C107–C108–C109–C110–C111–C112–C113–C114–C121–C122–C123) were placed and their occupancies were refined to be 0.854(2) and 0.146(2), respectively. The occupancy of the encapsulated water molecule was refined to be 0.593(8). All non-hydrogen atoms and a part of disordered moieties were refined anisotropically. All hydrogen atoms except for that of the encapsulated water molecule were placed using AFIX instructions. The crystal data are as follows: $C_{97.12}H_{32.31}N_2O_{0.59}$; FW = 1236.54, crystal size 0.19 × 0.07 × 0.04 mm^3, triclinic, *P*-1, *a* = 10.005(4) Å, *b* = 12.857(5) Å, *c* = 22.495(9) Å, α = 98.332(5)°, β = 97.908(5)°, γ = 104.389(6)°, *V* = 2727.2(18) Å^3, *Z* = 2, D_c = 1.506 g cm^{-3}. The refinement converged to R_1 = 0.0532, wR_2 = 0.1399 ($I > 2\sigma(I)$), GOF = 1.028. The data was deposited at the Cambridge Crystallographic Data Centre (CCDC 1999283).

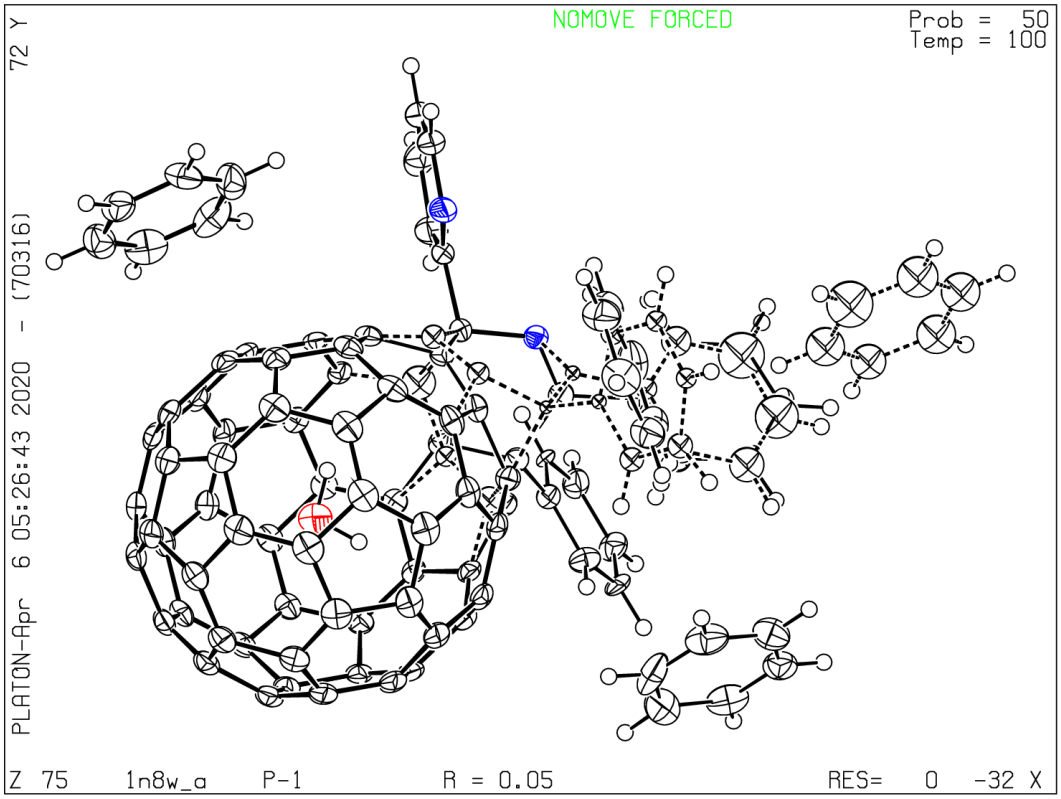
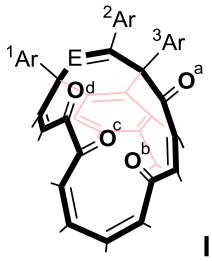


Figure S7. Single crystal X-ray structure of $[(H_2O)_{0.593(8)}@\{(\mathbf{3f})_{0.854(2)}(\mathbf{3f})_{0.146(2)}\}]\bullet(C_6H_6)_{2.85}$.

5. Natural Population Analyses of INT1 and INT3

The natural charges of carbonyl groups in **INT1** and **INT3** were calculated at the B3LYP-D3/6-31G(d) level of theory.

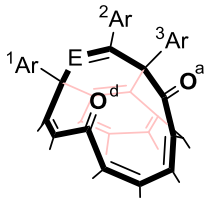
Table S1. Natural charges of **INT1** (B3LYP-D3/6-31G(d))



INT1

Addends	C(a)/O(a)	C(b)/O(b)	C(c)/O(c)	C(d)/O(d)
a	+0.588/–0.499	+0.557/–0.494	+0.490/–0.465	+0.500/–0.478
b	+0.586/–0.490	+0.557/–0.495	+0.491/–0.464	+0.501/–0.475
c	+0.589/–0.490	+0.559/–0.502	+0.491/–0.467	+0.501/–0.476
d	+0.589/–0.494	+0.556/–0.487	+0.489/–0.461	+0.499/–0.473
e	+0.583/–0.491	+0.557/–0.494	+0.488/–0.465	+0.494/–0.455
f	+0.575/–0.476	+0.557/–0.490	+0.489/–0.464	+0.496/–0.457

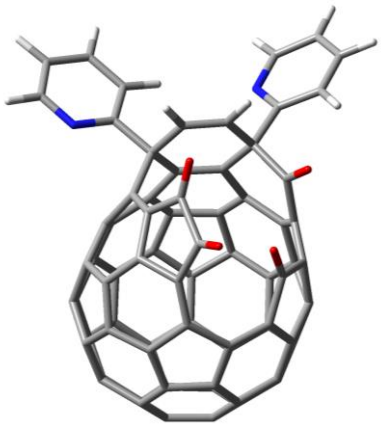
Table S2. Natural charges of **INT3** (B3LYP-D3/6-31G(d))



INT3

Addends	C(a)/O(a)	C(d)/O(d)
a	+0.583/–0.510	+0.561/–0.474
b	+0.579/–0.502	+0.563/–0.469
c	+0.584/–0.511	+0.560/–0.467
d	+0.576/–0.497	+0.562/–0.469
e	+0.577/–0.501	+0.561/–0.469
f	+0.574/–0.491	+0.559/–0.469

Table S3. Optimized structure of **INT1a** (B3LYP-D3/6-31G(d))

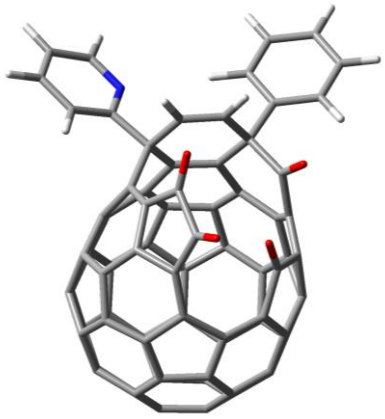


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.938394	-0.266728	1.294137
2	6	0	3.736868	1.034782	1.117629
3	6	0	2.782817	1.625838	0.112523
4	6	0	1.540318	2.263150	0.770907
5	6	0	1.195302	2.120592	2.115678
6	6	0	1.782211	1.506110	3.366633
7	6	0	0.543635	1.049145	4.239101
8	6	0	-0.665744	1.360764	3.414406
9	6	0	-1.975749	0.904768	3.224564
10	6	0	-2.527115	-0.490185	3.047784
11	6	0	-1.838041	-1.695186	2.854440
12	6	0	-0.342600	-1.950562	2.945843
13	6	0	-0.015680	-2.858780	1.766625
14	6	0	1.091538	-2.708773	0.933153
15	6	0	2.403564	-2.216045	1.442425
16	6	0	3.260282	-1.342372	0.480355
17	7	0	4.754571	-1.797619	-1.392810
18	8	0	2.917475	1.453886	3.772631
19	8	0	2.812654	-2.525505	2.544704
20	7	0	3.383874	3.948920	-0.442114
21	6	0	2.372858	-0.782112	-0.605560
22	6	0	1.253580	1.029621	-1.808844
23	8	0	0.604420	0.765625	5.408379
24	6	0	1.530746	-1.736227	-1.293936
25	6	0	0.536936	2.764910	-0.170517
26	8	0	0.443140	-1.403008	3.685217
27	6	0	-0.696664	2.443009	-2.307081
28	6	0	4.111331	4.845814	-1.123616
29	6	0	-1.884969	3.054671	-1.736563
30	6	0	3.584655	2.655482	-0.707442
31	6	0	0.473955	2.233985	-1.542048
32	6	0	0.781448	0.097623	-2.740987
33	6	0	2.197950	0.563394	-0.818941
34	6	0	-1.856702	3.481209	-0.421198
35	6	0	-0.436267	0.304231	-3.479092
36	6	0	-1.012127	3.100267	1.690765
37	6	0	-1.162316	1.465018	-3.273167
38	6	0	0.895781	-1.316697	-2.459551
39	6	0	0.897933	-2.792108	-0.501603
40	6	0	-0.634002	3.359364	0.332743
41	6	0	4.999656	-3.256028	0.502793
42	6	0	4.378646	-2.197855	-0.169738
43	6	0	-4.074666	2.485399	-0.015512
44	6	0	-0.286108	-3.377546	-0.991276
45	6	0	-0.286795	-1.965626	-2.981203
46	6	0	6.037125	-3.933269	-0.137077
47	6	0	-0.179033	2.362820	2.494074
48	6	0	-2.613544	1.403291	-3.223891
49	6	0	5.058815	4.498227	-2.084399
50	6	0	-4.624792	1.399109	0.781657
51	6	0	-3.268423	0.173289	-3.333212
52	6	0	-2.422433	2.887679	1.760339
53	6	0	6.423423	-3.532632	-1.414800
54	6	0	4.523160	2.199176	-1.643855
55	6	0	-2.873607	1.776731	2.480787
56	6	0	5.751484	-2.455791	-1.993837
57	6	0	-1.111496	-0.972377	-3.632005
58	6	0	-5.082685	0.367897	-0.128477
59	6	0	-4.318524	-1.329272	1.485769
60	6	0	-2.978742	3.196110	0.462245
61	6	0	-1.374711	-3.684542	-0.095980
62	6	0	-3.059841	2.385699	-2.258902
63	6	0	-4.364849	-0.141855	-2.433484
64	6	0	-4.001269	1.036847	1.979243
65	6	0	5.268425	3.141716	-2.344719
66	6	0	-1.252166	-3.308536	1.237864
67	6	0	-3.804711	-0.346334	2.336529
68	6	0	-4.781933	0.794274	-1.484996
69	6	0	-4.133945	2.093047	-1.407848
70	6	0	-2.360396	-2.676294	1.930840
71	6	0	-2.501291	-1.042364	-3.543302
72	6	0	-3.120304	-2.109438	-2.774315
73	6	0	-0.872903	-2.997314	-2.257950
74	6	0	-4.553843	-1.955742	-0.768638
75	6	0	-2.319429	-3.067121	-2.145448
76	6	0	-2.629508	-3.493992	-0.795353
77	6	0	-3.575187	-2.540083	1.277285
78	6	0	-4.951668	-0.972172	0.227759
79	6	0	-3.714434	-2.938869	-0.117139
80	6	0	-4.262578	-1.547585	-2.075626
81	1	0	4.605099	-0.620491	2.073185
82	1	0	4.244221	1.750398	1.753629
83	1	0	3.921954	5.890561	-0.883864
84	1	0	4.685273	-3.534827	1.501356
85	1	0	6.534660	-4.761751	0.359598
86	1	0	5.617460	5.267338	-2.609042
87	1	0	7.224550	-4.034025	-1.949000
88	1	0	4.656342	1.132221	-1.803416
89	1	0	6.023777	-2.101513	-2.986497
90	1	0	6.001768	2.825119	-3.081524

The total electronic energy was calculated to be –3236.212597 Hartree.

Table S4. Optimized structure of **INT1b** (B3LYP-D3/6-31G(d))

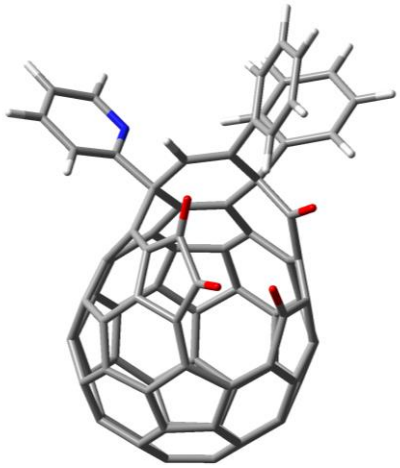


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.570674	1.255427	-3.314933
2	6	0	-1.118355	1.308106	-3.351751
3	6	0	-0.396209	0.134568	-3.487815
4	6	0	-1.076924	-1.144962	-3.584048
5	6	0	-2.467944	-1.203694	-3.508511
6	6	0	-3.231050	0.024732	-3.369168
7	6	0	-0.658339	2.329699	-2.429765
8	6	0	0.813102	-0.040205	-2.728282
9	6	0	-0.265170	-2.108059	-2.874662
10	6	0	-3.101408	-2.227661	-2.694334
11	6	0	-4.339021	-0.239377	-2.467039
12	6	0	-3.022700	2.286505	-2.405256
13	6	0	-2.312715	-3.155863	-2.008233
14	6	0	-0.864837	-3.098814	-2.106954
15	6	0	-2.640564	-3.513004	-0.642124
16	6	0	-0.294687	-3.417991	-0.816085
17	6	0	0.504211	2.153185	-1.643965
18	6	0	0.914740	-1.438764	-2.372757
19	6	0	-1.394682	-3.675241	0.080624
20	6	0	1.530707	-1.799693	-1.177936
21	6	0	1.283744	0.936081	-1.841899
22	6	0	-4.248721	-1.626139	-2.038252
23	6	0	-4.762480	0.744991	-1.571971
24	6	0	0.550705	2.748475	-0.297525
25	6	0	-4.107731	2.042268	-1.552671
26	6	0	-1.849961	2.973986	-1.902808
27	6	0	-5.081063	0.388593	-0.199410
28	6	0	-4.062592	2.504110	-0.181221
29	6	0	-1.835596	3.467970	-0.610966
30	6	0	0.886069	-2.813776	-0.342254
31	6	0	-4.557064	-1.966841	-0.715981
32	6	0	2.216252	0.518029	-0.820467
33	6	0	-4.627429	1.461735	0.663110
34	6	0	-2.969089	3.233568	0.272804
35	6	0	-0.622554	3.375196	0.162425
36	6	0	-1.017529	3.187262	1.527471
37	6	0	1.537509	2.284463	0.681866
38	6	0	2.367662	-0.815421	-0.525617
39	6	0	2.376671	-2.143926	1.585838
40	6	0	-2.429783	2.987614	1.591384
41	6	0	-2.893701	1.915327	2.360429
42	6	0	-2.009842	1.077670	3.159238
43	6	0	-4.019894	1.156909	1.884497
44	6	0	-3.730625	-2.919952	-0.005736
45	6	0	1.748194	1.673960	3.320948
46	6	0	-4.961012	-0.932448	0.225175
47	6	0	-4.344203	-1.229071	1.506875
48	6	0	1.176819	2.218387	2.029427
49	6	0	1.066145	-2.659171	1.087811
50	6	0	-0.051580	-2.761295	1.914470
51	6	0	-0.198807	2.487713	2.378476
52	6	0	-0.700829	1.537531	3.345225
53	6	0	-3.835654	-0.207207	2.313876
54	6	0	-2.567535	-0.321732	3.046468
55	6	0	0.497138	1.263095	4.199781
56	6	0	-3.604699	-2.452186	1.368230
57	6	0	-1.284722	-3.232288	1.394897
58	6	0	-0.386813	-1.790801	3.038862
59	6	0	-2.397945	-2.561275	2.041912
60	6	0	-1.881227	-1.536843	2.920208
61	6	0	2.791560	1.619798	0.069777
62	6	0	3.249004	-1.330605	0.590327
63	6	0	3.921140	-0.220735	1.356712
64	6	0	3.732815	1.071951	1.113503
65	6	0	4.351709	-2.225718	-0.032436
66	6	0	3.610946	2.607970	-0.783906
67	8	0	2.768517	-2.397186	2.707569
68	8	0	2.877991	1.658459	3.743304
69	6	0	3.667703	3.973030	-0.487965
70	6	0	4.486826	4.792798	-1.263230
71	6	0	5.219354	4.223320	-2.303372
72	6	0	5.101863	2.848275	-2.513335
73	7	0	4.322177	2.052172	-1.774852
74	6	0	5.097206	-1.689057	-1.093703
75	6	0	6.110964	-2.436146	-1.688934
76	6	0	6.396711	-3.726017	-1.232631
77	6	0	5.666224	-4.256478	-0.170700
78	6	0	4.649109	-3.509995	0.431539
79	8	0	0.392303	-1.201116	3.752718
80	8	0	0.543410	1.041288	5.382655
81	1	0	4.581022	-0.541943	2.155097
82	1	0	4.244788	1.813256	1.715928
83	1	0	3.080482	4.381917	0.327797
84	1	0	4.548841	5.857886	-1.057559
85	1	0	5.866894	4.823178	-2.935277
86	1	0	5.659551	2.360563	-3.310787
87	1	0	4.884031	-0.681534	-1.443719
88	1	0	6.680743	-2.008685	-2.509858
89	1	0	7.186701	-4.309067	-1.698275
90	1	0	5.885679	-5.254499	0.199172
91	1	0	4.107192	-3.932920	1.270019

The total electronic energy was calculated to be –3220.1735974 Hartree.

Table S5. Optimized structure of **INT1c** (B3LYP-D3/6-31G(d))



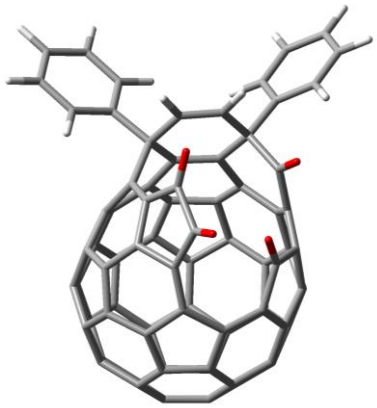
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.736453	1.784894	-2.525682
2	6	0	-2.325163	2.007726	-2.791417
3	6	0	-1.565360	0.989953	-3.343149
4	6	0	-2.164419	-0.297711	-3.647136
5	6	0	-3.508428	-0.529218	-3.355223
6	6	0	-4.310834	0.536453	-2.779971
7	6	0	-1.767304	2.824457	-1.730030
8	6	0	-0.225156	0.775335	-2.867377
9	6	0	-1.168879	-1.304913	-3.356078
10	6	0	-3.904277	-1.782088	-2.733639
11	6	0	-5.205480	-0.057937	-1.801193
12	6	0	-4.074846	2.512884	-1.321135
13	6	0	-2.938620	-2.752833	-2.452152
14	6	0	-1.543926	-2.512072	-2.778865
15	6	0	-2.971557	-3.457663	-1.185559
16	6	0	-0.715546	-3.064781	-1.730039
17	6	0	-0.468458	2.593662	-1.220119
18	6	0	0.039103	-0.646669	-2.907772
19	6	0	-1.601608	-3.646410	-0.751740
20	6	0	0.897180	-1.211443	-1.969238
21	6	0	0.336194	1.552650	-1.848557
22	6	0	-4.941975	-1.487595	-1.761469
23	6	0	-5.514682	0.631403	-0.627003
24	6	0	-0.205261	2.854568	0.205035
25	6	0	-4.958479	1.952723	-0.388894
26	6	0	-2.876806	3.188637	-0.864706
27	6	0	-5.539669	-0.074474	0.642910
28	6	0	-4.684155	2.077749	1.027302
29	6	0	-2.649713	3.360329	0.488853
30	6	0	0.492123	-2.461728	-1.328926
31	6	0	-4.965956	-2.165230	-0.536428
32	6	0	1.471616	1.007934	-1.138489
33	6	0	-5.004348	0.807332	1.661321
34	6	0	-3.576656	2.798055	1.461757
35	6	0	-1.308211	3.222478	0.998757
36	6	0	-1.423676	2.677182	2.319172
37	6	0	0.977108	2.281887	0.854801
38	6	0	1.777471	-0.325825	-1.230846
39	6	0	2.283264	-2.107325	0.421325
40	6	0	-2.781162	2.310136	2.565915
41	6	0	-3.014938	1.040337	3.104226
42	6	0	-1.938502	0.143258	3.503390
43	6	0	-4.154850	0.292438	2.644979
44	6	0	-3.955134	-3.159690	-0.243110
45	6	0	1.726947	1.106964	3.172910
46	6	0	-5.249803	-1.436217	0.690828
47	6	0	-4.378929	-1.956057	1.730921
48	6	0	0.883903	1.869789	2.183791
49	6	0	0.931948	-2.621533	0.039614
50	6	0	0.005900	-3.037476	0.993955
51	6	0	-0.412739	1.895680	2.818794
52	6	0	-0.653550	0.692691	3.583412
53	6	0	-3.796456	-1.104054	2.673404
54	6	0	-2.406195	-1.241990	3.126895
55	6	0	0.703645	0.355789	4.119206
56	6	0	-3.597495	-3.018610	1.162412
57	6	0	-1.269098	-3.512468	0.592701
58	6	0	-0.170052	-2.392333	2.359975
59	6	0	-2.277898	-3.142748	1.569087
60	6	0	-1.671934	-2.301363	2.576287
61	6	0	2.130375	1.916144	-0.106290
62	6	0	2.910061	-0.995704	-0.473239
63	6	0	3.704930	-0.015868	0.394104
64	6	0	3.313895	1.251667	0.553241
65	6	0	3.864139	-1.629273	-1.518423
66	6	0	2.702439	3.168366	-0.805303
67	8	0	2.876605	-2.604395	1.356595
68	8	0	2.917051	1.128217	3.373983
69	6	0	2.765786	4.407095	-0.160311
70	6	0	3.364315	5.477071	-0.823665
71	6	0	3.878006	5.273667	-2.103516
72	6	0	3.772408	3.997378	-2.658712
73	7	0	3.203388	2.963017	-2.030956
74	6	0	4.218158	-0.856034	-2.634957
75	6	0	5.115845	-1.350953	-3.578531
76	6	0	5.671606	-2.623512	-3.421266
77	6	0	5.330499	-3.388636	-2.307151
78	6	0	4.434578	-2.894043	-1.355875
79	8	0	0.691807	-1.880540	3.039918
80	8	0	0.997349	-0.140492	5.176794
81	6	0	6.262328	-1.257646	2.926858
82	6	0	5.043930	-0.895798	2.352713
83	6	0	4.991857	-0.460921	1.021635
84	6	0	6.182030	-0.388605	0.282822
85	6	0	7.398856	-0.756309	0.857847
86	6	0	7.441818	-1.193750	2.182319
87	1	0	3.911597	1.901462	1.182803
88	1	0	2.353653	4.527423	0.836364
89	1	0	3.426633	6.451799	-0.347667
90	1	0	4.350167	6.078076	-2.658883
91	1	0	4.163099	3.793012	-3.653915
92	1	0	3.809015	0.145085	-2.746853
93	1	0	5.384162	-0.739275	-4.435959
94	1	0	6.370533	-3.010242	-4.158007
95	1	0	5.767411	-4.373496	-2.166175
96	1	0	4.209577	-3.488930	-0.478256
97	1	0	6.286553	-1.590595	3.961039

98	1	0	4.132776	-0.950334	2.934017
99	1	0	6.150475	-0.047075	-0.747154
100	1	0	8.311410	-0.696560	0.270129
101	1	0	8.388983	-1.479341	2.633127

The total electronic energy was calculated to be –3451.2397105 Hartree.

Table S6. Optimized structure of **INT1d** (B3LYP-D3/6-31G(d))

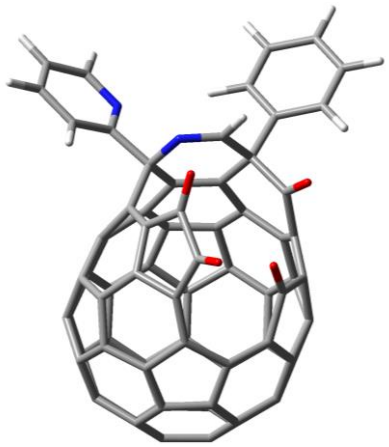


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.985309	-0.262778	1.213529
2	6	0	3.772566	1.042078	1.076406
3	6	0	2.795823	1.659733	0.106792
4	6	0	1.537667	2.238179	0.798397
5	6	0	1.202433	2.057790	2.141065
6	6	0	1.804623	1.413093	3.369633
7	6	0	0.574663	0.939513	4.246890
8	6	0	-0.645647	1.265897	3.441141
9	6	0	-1.958693	0.816387	3.252839
10	6	0	-2.514624	-0.574212	3.051068
11	6	0	-1.825689	-1.772114	2.826017
12	6	0	-0.330687	-2.029293	2.918898
13	6	0	0.004449	-2.882402	1.699602
14	6	0	1.105336	-2.696510	0.863473
15	6	0	2.404131	-2.174720	1.382481
16	6	0	3.279496	-1.326408	0.408769
17	6	0	5.014208	-3.218167	0.540026
18	8	0	2.945394	1.354439	3.756780
19	8	0	2.787186	-2.437836	2.505121
20	6	0	3.532905	4.089987	-0.274820
21	6	0	2.378859	-0.739109	-0.652356
22	6	0	1.246019	1.092525	-1.813946
23	8	0	0.648776	0.640086	5.410996
24	6	0	1.524705	-1.679493	-1.348364
25	6	0	0.526157	2.767824	-0.121426
26	8	0	0.436880	-1.523816	3.704200
27	6	0	-0.721454	2.502328	-2.255393
28	6	0	4.292418	5.047339	-0.950516
29	6	0	-1.907859	3.092223	-1.658248
30	6	0	3.563502	2.749401	-0.671502
31	6	0	0.458236	2.280961	-1.508594
32	6	0	0.764987	0.177829	-2.758050
33	6	0	2.208470	0.613105	-0.845716
34	6	0	-1.871320	3.484807	-0.332534
35	6	0	-0.460745	0.394376	-3.480426
36	6	0	-1.008798	3.045906	1.761387
37	6	0	-1.190784	1.546461	-3.241504
38	6	0	0.884496	-1.241746	-2.504095
39	6	0	0.903438	-2.752640	-0.571893
40	6	0	-0.642685	3.343362	0.408071
41	6	0	4.741880	-2.070937	-1.563029
42	6	0	4.353426	-2.250609	-0.228542
43	6	0	-4.082294	2.472217	0.064693
44	6	0	-0.277576	-3.336367	-1.069838
45	6	0	-0.298077	-1.884884	-3.031791
46	6	0	5.753658	-2.851463	-2.122014
47	6	0	-0.168431	2.287671	2.537684
48	6	0	-2.641387	1.476269	-3.181029
49	6	0	5.095629	4.673829	-2.028082
50	6	0	-4.624189	1.365124	0.838570
51	6	0	-3.291144	0.246064	-3.313848
52	6	0	-2.418272	2.832905	1.837853
53	6	0	6.397655	-3.822759	-1.354513
54	6	0	4.386038	2.379278	-1.742809
55	6	0	-2.862501	1.704536	2.535215
56	6	0	6.025849	-3.998787	-0.021274
57	6	0	-1.131536	-0.881922	-3.655394
58	6	0	-5.085580	0.355440	-0.093567
59	6	0	-4.309024	-1.378875	1.475475
60	6	0	-2.985252	3.174038	0.552412
61	6	0	-1.358926	-3.673571	-0.177407
62	6	0	-3.084285	2.432409	-2.188613
63	6	0	-4.380010	-0.095349	-2.414431
64	6	0	-3.993396	0.975664	2.023726
65	6	0	5.142785	3.333853	-2.419928
66	6	0	-1.231655	-3.330836	1.164364
67	6	0	-3.794031	-0.415090	2.347764
68	6	0	-4.794708	0.815835	-1.440984
69	6	0	-4.150551	2.114617	-1.336685
70	6	0	-2.344124	-2.729459	1.878111
71	6	0	-2.520240	-0.960768	-3.557947
72	6	0	-3.128793	-2.048152	-2.809527
73	6	0	-0.873679	-2.933616	-2.325529
74	6	0	-4.552124	-1.949896	-0.793205
75	6	0	-2.318904	-3.015200	-2.207008
76	6	0	-2.619022	-3.475524	-0.865791
77	6	0	-3.562242	-2.581556	1.233010
78	6	0	-4.948293	-0.992603	0.229202
79	6	0	-3.705089	-2.945152	-0.170061
80	6	0	-4.269834	-1.508765	-2.091246
81	1	0	4.683779	-0.627970	1.958189
82	1	0	4.303664	1.743143	1.709354
83	1	0	4.742874	-3.360855	1.580333
84	1	0	2.912013	4.391747	0.563551
85	1	0	4.253599	6.085510	-0.631857
86	1	0	4.253567	-1.317582	-2.172983
87	1	0	6.037974	-2.696642	-3.159471
88	1	0	5.683933	5.419058	-2.556267
89	1	0	7.183986	-4.433054	-1.790077
90	1	0	4.438247	1.335851	-2.041618
91	1	0	6.522820	-4.747155	0.590097
92	1	0	5.771680	3.030244	-3.252554

The total electronic energy was calculated to be –3204.1341752 Hartree.

Table S7. Optimized structure of **INT1e** (B3LYP-D3/6-31G(d))

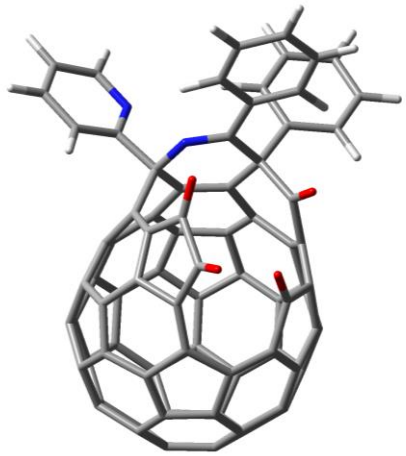


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.619027	1.357917	-3.262014
2	6	0	-1.167090	1.391988	-3.323494
3	6	0	-0.463882	0.212907	-3.505834
4	6	0	-1.163672	-1.054848	-3.619722
5	6	0	-2.553528	-1.096740	-3.519207
6	6	0	-3.297074	0.137837	-3.335915
7	6	0	-0.677820	2.383574	-2.382699
8	6	0	0.757365	0.003243	-2.774979
9	6	0	-0.352541	-2.045449	-2.948019
10	6	0	-3.186141	-2.131949	-2.718753
11	6	0	-4.393402	-0.134126	-2.422199
12	6	0	-3.041312	2.371385	-2.318680
13	6	0	-2.398112	-3.086286	-2.068603
14	6	0	-0.951451	-3.044995	-2.190982
15	6	0	-2.707925	-3.471936	-0.706189
16	6	0	-0.363905	-3.400356	-0.916665
17	6	0	0.495048	2.170931	-1.622383
18	6	0	0.846425	-1.405254	-2.454011
19	6	0	-1.452228	-3.664615	-0.008362
20	6	0	1.479270	-1.805470	-1.279458
21	6	0	1.254605	0.953100	-1.874075
22	6	0	-4.314387	-1.532037	-2.029070
23	6	0	-4.788976	0.833158	-1.496197
24	6	0	0.573070	2.721777	-0.257076
25	6	0	-4.115647	2.120530	-1.454887
26	6	0	-1.850772	3.028943	-1.818149
27	6	0	-5.091036	0.446943	-0.128005
28	6	0	-4.041858	2.547038	-0.073268
29	6	0	-1.806450	3.486693	-0.513799
30	6	0	0.832651	-2.822005	-0.449297
31	6	0	-4.605861	-1.901242	-0.710795
32	6	0	2.194289	0.495254	-0.882220
33	6	0	-4.610145	1.492429	0.753483
34	6	0	-2.929555	3.247637	0.381561
35	6	0	-0.582830	3.354067	0.237827
36	6	0	-0.958749	3.138005	1.603544
37	6	0	1.561756	2.212359	0.697879
38	6	0	2.332755	-0.843294	-0.622491
39	6	0	2.354121	-2.192519	1.475242
40	6	0	-2.373975	2.961688	1.685005
41	6	0	-2.846578	1.880666	2.436034
42	6	0	-1.965283	1.012328	3.202347
43	6	0	-3.990331	1.149688	1.958432
44	6	0	-3.780136	-2.881495	-0.037819
45	6	0	1.804251	1.508303	3.323008
46	6	0	-4.982064	-0.885800	0.261825
47	6	0	-4.350378	-1.222306	1.526209
48	6	0	1.227708	2.114657	2.051524
49	6	0	1.035739	-2.694241	0.981529
50	6	0	-0.069912	-2.807962	1.823680
51	6	0	-0.137792	2.406152	2.426056
52	6	0	-0.647279	1.446459	3.379489
53	6	0	-3.818292	-0.227368	2.351304
54	6	0	-2.541677	-0.376145	3.062638
55	6	0	0.552670	1.127944	4.212402
56	6	0	-3.627539	-2.450107	1.345251
57	6	0	-1.315841	-3.255319	1.314243
58	6	0	-0.378649	-1.867972	2.981942
59	6	0	-2.411744	-2.589904	1.996530
60	6	0	-1.871099	-1.595109	2.893982
61	6	0	2.793828	1.541367	0.053529
62	6	0	3.207499	-1.350400	0.492316
63	6	0	3.833130	-0.205793	1.280258
64	7	0	3.682332	1.037577	1.089753
65	6	0	4.376947	-2.176304	-0.098021
66	6	0	3.650571	2.543765	-0.743062
67	8	0	2.764136	-2.467382	2.585969
68	8	0	2.934503	1.411288	3.724715
69	6	0	3.854062	3.847285	-0.283318
70	6	0	4.695214	4.684681	-1.011666
71	6	0	5.305277	4.189089	-2.164744
72	6	0	5.049495	2.867893	-2.530285
73	7	0	4.240910	2.055010	-1.838978
74	6	0	5.082763	-1.620860	-1.177056
75	6	0	6.156692	-2.306427	-1.741131
76	6	0	6.541466	-3.550932	-1.236559
77	6	0	5.850938	-4.097655	-0.155668
78	6	0	4.776153	-3.413188	0.417719
79	8	0	0.418418	-1.312055	3.702930
80	8	0	0.603582	0.886850	5.391629
81	1	0	4.478462	-0.516158	2.101524
82	1	0	3.369288	4.186045	0.626085
83	1	0	4.873704	5.704905	-0.683577
84	1	0	5.966836	4.806673	-2.764381
85	1	0	5.511967	2.437905	-3.416691
86	1	0	4.795347	-0.647747	-1.568346
87	1	0	6.694913	-1.864679	-2.575474
88	1	0	7.377418	-4.086214	-1.678526
89	1	0	6.147249	-5.060519	0.251600
90	1	0	4.266124	-3.845568	1.270639

The total electronic energy was calculated to be –3236.2105932 Hartree.

Table S8. Optimized structure of **INT1f** (B3LYP-D3/6-31G(d))



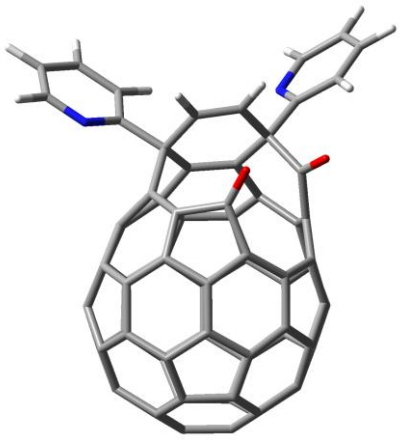
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.690557	1.119115	-2.925423
2	6	0	-2.276658	1.196985	-3.252778
3	6	0	-1.567681	0.032425	-3.499608
4	6	0	-2.221232	-1.261912	-3.415266
5	6	0	-3.567665	-1.343156	-3.061541
6	6	0	-4.317912	-0.124627	-2.810829
7	6	0	-1.668617	2.256938	-2.469247
8	6	0	-0.226945	-0.093333	-2.995553
9	6	0	-1.260387	-2.182883	-2.849669
10	6	0	-4.001972	-2.348565	-2.105820
11	6	0	-5.220038	-0.377233	-1.700207
12	6	0	-3.978619	2.172634	-1.975186
13	6	0	-3.069557	-3.235331	-1.559656
14	6	0	-1.671460	-3.154222	-1.945151
15	6	0	-3.113136	-3.548378	-0.145026
16	6	0	-0.850871	-3.411069	-0.781102
17	6	0	-0.370355	2.125812	-1.924856
18	6	0	-0.020099	-1.475552	-2.617934
19	6	0	-1.745502	-3.655231	0.322669
20	6	0	0.827507	-1.780655	-1.555895
21	6	0	0.382445	0.921931	-2.249928
22	6	0	-5.013365	-1.746099	-1.255351
23	6	0	-5.482238	0.629893	-0.769494
24	6	0	-0.072129	2.753653	-0.625260
25	6	0	-4.868743	1.939092	-0.918734
26	6	0	-2.746641	2.896762	-1.734509
27	6	0	-5.518513	0.316042	0.648526
28	6	0	-4.566234	2.448233	0.402473
29	6	0	-2.487702	3.430237	-0.484630
30	6	0	0.381083	-2.762117	-0.570492
31	6	0	-5.049009	-2.046357	0.111710
32	6	0	1.501739	0.553385	-1.421386
33	6	0	-4.932046	1.426534	1.372347
34	6	0	-3.420958	3.209440	0.611486
35	6	0	-1.144670	3.378030	0.038296
36	6	0	-1.260020	3.230794	1.459008
37	6	0	1.090208	2.327032	0.160067
38	6	0	1.748914	-0.755384	-1.115046
39	6	0	2.193259	-1.953169	1.015556
40	6	0	-2.628967	3.017746	1.805826
41	6	0	-2.913810	1.969361	2.686725
42	6	0	-1.874103	1.175940	3.326560
43	6	0	-4.093353	1.175880	2.461877
44	6	0	-4.074253	-2.957336	0.674463
45	6	0	1.833660	1.790425	2.716842
46	6	0	-5.287266	-0.987573	1.082038
47	6	0	-4.426495	-1.228230	2.227524
48	6	0	1.008250	2.301147	1.552133
49	6	0	0.830516	-2.531043	0.787604
50	6	0	-0.096866	-2.637902	1.823986
51	6	0	-0.275989	2.573773	2.156034
52	6	0	-0.563028	1.657905	3.236480
53	6	0	-3.797405	-0.169270	2.888888
54	6	0	-2.410765	-0.234912	3.367366
55	6	0	0.785346	1.425732	3.846297
56	6	0	-3.696179	-2.440848	1.982983
57	6	0	-1.392025	-3.162921	1.574429
58	6	0	-0.237407	-1.656550	2.981691
59	6	0	-2.378525	-2.501008	2.410020
60	6	0	-1.731795	-1.439408	3.144421
61	6	0	2.211860	1.658935	-0.660057
62	6	0	2.859015	-1.192438	-0.176347
63	6	0	3.668809	0.019516	0.358490
64	7	0	3.312337	1.233099	0.165895
65	6	0	3.753201	-2.123540	-1.028514
66	6	0	2.866323	2.651810	-1.647827
67	8	0	2.756401	-2.121638	2.076607
68	8	0	3.023175	1.767984	2.901224
69	6	0	3.011507	4.006437	-1.339309
70	6	0	3.682147	4.826002	-2.244381
71	6	0	4.185943	4.263858	-3.417564
72	6	0	4.000594	2.896976	-3.625224
73	7	0	3.357333	2.100782	-2.763115
74	6	0	3.828194	-3.504932	-0.826726
75	6	0	4.615098	-4.297279	-1.665135
76	6	0	5.329085	-3.717502	-2.713717
77	6	0	5.247341	-2.338833	-2.924183
78	6	0	4.460039	-1.545770	-2.091934
79	8	0	0.643631	-1.046288	3.542055
80	8	0	1.063621	1.266287	5.007259
81	6	0	6.726078	-1.508968	2.096537
82	6	0	5.509121	-1.418339	1.423016
83	6	0	4.947789	-0.169373	1.113278
84	6	0	5.648730	0.986365	1.510907
85	6	0	6.859497	0.894498	2.186562
86	6	0	7.408811	-0.356026	2.480777
87	1	0	2.612496	4.401557	-0.411286
88	1	0	3.810497	5.884628	-2.036088
89	1	0	4.713111	4.865064	-4.151897
90	1	0	4.384655	2.415192	-4.522465
91	1	0	3.293835	-3.971276	-0.004466
92	1	0	4.669389	-5.368724	-1.492657
93	1	0	5.942995	-4.334819	-3.363690
94	1	0	5.795763	-1.877795	-3.741152
95	1	0	4.376643	-0.476865	-2.274471
96	1	0	7.135685	-2.489481	2.323444
97	1	0	5.003732	-2.332078	1.154687

98	1	0	5.213299	1.951922	1.291058
99	1	0	7.374812	1.802475	2.488260
100	1	0	8.356706	-0.429767	3.007724

The total electronic energy was calculated to be –3467.2768334 Hartree.

Table S9. Optimized structure of **INT3a** (B3LYP-D3/6-31G(d))

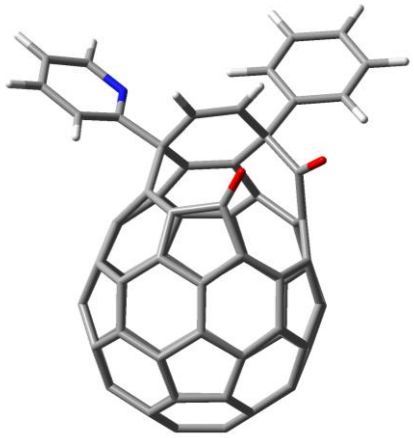


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.475033	2.088672	1.150925
2	6	0	1.005758	1.578195	2.351995
3	6	0	1.354924	0.293110	3.118020
4	6	0	2.547187	-2.113810	1.508136
5	6	0	1.205522	-2.488200	0.985407
6	6	0	0.048225	-2.596924	1.768782
7	6	0	-0.481755	-1.659621	2.846186
8	6	0	-0.002714	-0.412632	3.242692
9	6	0	-0.930201	0.683846	3.399772
10	6	0	-0.337991	1.851918	2.774188
11	6	0	-1.139275	2.762436	2.111157
12	6	0	-0.707616	3.199290	0.802747
13	6	0	0.504874	2.734764	0.263981
14	6	0	-1.896061	3.387535	0.007633
15	6	0	-3.059250	3.018493	0.799727
16	6	0	-2.581023	2.604342	2.101242
17	6	0	-3.161633	1.507378	2.740858
18	6	0	-2.307467	0.526010	3.387480
19	6	0	-2.831240	-0.785679	3.125299
20	6	0	-1.938729	-1.825866	2.838678
21	6	0	-2.314044	-2.789601	1.835961
22	6	0	-3.515245	-2.690952	1.137420
23	6	0	-4.395021	-1.563845	1.383691
24	6	0	-4.058473	-0.631177	2.362822
25	6	0	-4.249509	0.790254	2.106606
26	6	0	-4.737452	1.212983	0.865826
27	6	0	-4.128319	2.353545	0.198807
28	6	0	-5.082812	0.236012	-0.151277
29	6	0	-4.926989	-1.128228	0.106803
30	6	0	-4.700511	0.774604	-1.446641
31	6	0	-4.200498	-0.071451	-2.438160
32	6	0	-4.057352	-1.495350	-2.178766
33	6	0	-4.401912	-2.010030	-0.925363
34	6	0	-3.540675	-2.984953	-0.286604
35	6	0	-2.384382	-3.427395	-0.927148
36	6	0	-2.042092	-2.918006	-2.242862
37	6	0	-2.858821	-1.960424	-2.852222
38	6	0	-2.255953	-0.819905	-3.525967
39	6	0	-3.076595	0.348588	-3.257675
40	6	0	-2.471815	1.586223	-3.018960
41	6	0	-2.989461	2.463453	-1.987595
42	6	0	-4.096076	2.077151	-1.226541
43	6	0	-1.856674	3.106289	-1.348753
44	6	0	-0.631409	2.600191	-1.938025
45	6	0	-1.025549	1.700588	-3.009225
46	6	0	-0.247603	0.589476	-3.297040
47	6	0	-0.869308	-0.694400	-3.563267
48	6	0	-0.026289	-1.704605	-2.955796
49	6	0	-0.598028	-2.786714	-2.300179
50	6	0	-0.047910	-3.197061	-1.023171
51	6	0	-1.147977	-3.567155	-0.177554
52	6	0	-1.107892	-3.217072	1.173288
53	6	0	1.091065	-2.598638	-0.464781
54	6	0	1.751599	-1.535116	-1.222574
55	6	0	1.125463	-1.058847	-2.372260
56	6	0	0.964847	0.370999	-2.553110
57	6	0	1.381685	1.241665	-1.539582
58	6	0	0.526477	2.369481	-1.163162
59	6	0	2.581263	-0.615968	-0.484432
60	6	0	2.349906	0.732205	-0.594809
61	6	0	2.807698	1.708072	0.477026
62	6	0	3.453920	-1.230870	0.582398
63	6	0	4.133461	-0.190936	1.442031
64	6	0	3.481938	2.952352	-0.128590
65	7	0	3.311444	4.101792	0.534119
66	6	0	3.934773	5.191192	0.067175
67	6	0	4.751422	5.186826	-1.063362
68	6	0	4.938784	3.978174	-1.735819
69	6	0	4.550786	-2.108369	-0.068913
70	6	0	5.266560	-3.055097	0.674998
71	6	0	6.279068	-3.771055	0.040008
72	6	0	6.547738	-3.519048	-1.305219
73	6	0	5.785035	-2.548753	-1.954178
74	7	0	4.810077	-1.853227	-1.357168
75	6	0	4.297902	2.837409	-1.260070
76	6	0	3.821852	1.100667	1.414787
77	8	0	2.372832	-0.041984	3.667870
78	8	0	2.948663	-2.543991	2.572590
79	1	0	4.845064	-0.571154	2.166874
80	1	0	3.770579	6.109515	0.628234
81	1	0	5.228599	6.101814	-1.400838
82	1	0	5.573744	3.924737	-2.616015
83	1	0	5.028052	-3.222927	1.718772
84	1	0	6.847897	-4.515921	0.589895
85	1	0	7.326496	-4.055814	-1.838364
86	1	0	5.961626	-2.314048	-3.002519
87	1	0	4.422159	1.874239	-1.745288
88	1	0	4.290189	1.793597	2.107509

The total electronic energy was calculated to be –3085.7598656 Hartree.

Table S10. Optimized structure of **INT3b** (B3LYP-D3/6-31G(d))

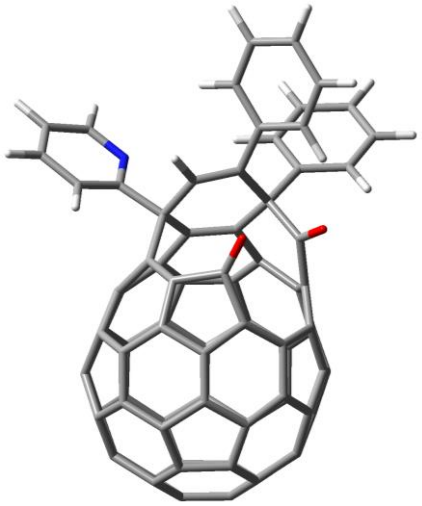


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.465148	2.070604	1.197940
2	6	0	0.966791	1.567814	2.392309
3	6	0	1.287130	0.278122	3.170491
4	6	0	2.492843	-2.138807	1.576930
5	6	0	1.154812	-2.502194	1.029700
6	6	0	-0.019547	-2.599723	1.788156
7	6	0	-0.562463	-1.655501	2.853372
8	6	0	-0.079383	-0.413790	3.261458
9	6	0	-0.998624	0.692161	3.398845
10	6	0	-0.382196	1.854811	2.785865
11	6	0	-1.160634	2.772601	2.104852
12	6	0	-0.698464	3.205541	0.805826
13	6	0	0.520504	2.729166	0.290602
14	6	0	-1.868484	3.407942	-0.013036
15	6	0	-3.050908	3.050538	0.755358
16	6	0	-2.603740	2.631413	2.066374
17	6	0	-3.207077	1.539411	2.693011
18	6	0	-2.376624	0.549094	3.357368
19	6	0	-2.908530	-0.756868	3.084379
20	6	0	-2.020717	-1.805949	2.815653
21	6	0	-2.385151	-2.766048	1.805517
22	6	0	-3.570700	-2.654774	1.082571
23	6	0	-4.443550	-1.518538	1.310845
24	6	0	-4.118143	-0.589553	2.297071
25	6	0	-4.289574	0.833589	2.037226
26	6	0	-4.747503	1.261318	0.786743
27	6	0	-4.113788	2.395842	0.132500
28	6	0	-5.082508	0.288124	-0.237454
29	6	0	-4.945036	-1.077560	0.023542
30	6	0	-4.668303	0.822872	-1.524582
31	6	0	-4.155719	-0.028230	-2.505301
32	6	0	-4.032590	-1.453674	-2.243625
33	6	0	-4.408145	-1.964895	-0.997755
34	6	0	-3.570366	-2.948755	-0.341485
35	6	0	-2.405586	-3.402864	-0.957824
36	6	0	-2.030953	-2.896516	-2.265979
37	6	0	-2.825078	-1.930766	-2.892093
38	6	0	-2.196879	-0.796472	-3.552860
39	6	0	-3.011145	0.380300	-3.301577
40	6	0	-2.398883	1.611698	-3.050847
41	6	0	-2.928995	2.493903	-2.030307
42	6	0	-4.054682	2.118778	-1.291874
43	6	0	-1.803095	3.124347	-1.367812
44	6	0	-0.570497	2.607616	-1.933489
45	6	0	-0.951793	1.712344	-3.012626
46	6	0	-0.179245	0.592828	-3.282087
47	6	0	-0.808666	-0.684951	-3.561087
48	6	0	0.010862	-1.703415	-2.936226
49	6	0	-0.584871	-2.779915	-2.293142
50	6	0	-0.065574	-3.197421	-1.005181
51	6	0	-1.186393	-3.556965	-0.182927
52	6	0	-1.170025	-3.207013	1.168589
53	6	0	1.066799	-2.610645	-0.422154
54	6	0	1.750408	-1.549722	-1.163433
55	6	0	1.156194	-1.068258	-2.328006
56	6	0	1.015729	0.362922	-2.514032
57	6	0	1.424286	1.232098	-1.495670
58	6	0	0.570908	2.366531	-1.137625
59	6	0	2.565570	-0.636416	-0.402424
60	6	0	2.365559	0.714744	-0.530340
61	6	0	2.811192	1.682399	0.554296
62	6	0	3.420346	-1.265115	0.675130
63	6	0	4.084103	-0.236246	1.554947
64	6	0	3.525566	2.899063	-0.063197
65	6	0	3.445116	4.173778	0.506523
66	6	0	4.179571	5.210806	-0.066305
67	6	0	4.968848	4.939959	-1.183093
68	6	0	4.990409	3.632184	-1.670618
69	6	0	4.520132	-2.116480	-0.003119
70	6	0	4.765167	-3.455312	0.312533
71	6	0	5.780726	-4.157022	-0.343887
72	6	0	6.561734	-3.528361	-1.312325
73	6	0	6.328112	-2.185299	-1.620548
74	6	0	5.315923	-1.483393	-0.970404
75	7	0	4.292437	2.629081	-1.128016
76	6	0	3.796363	1.060267	1.515279
77	8	0	2.286644	-0.060061	3.749545
78	8	0	2.870277	-2.575191	2.647297
79	1	0	4.772714	-0.630906	2.293705
80	1	0	2.815032	4.348373	1.372707
81	1	0	4.132969	6.212506	0.352133
82	1	0	5.554315	5.716876	-1.664955
83	1	0	5.596546	3.375114	-2.537502
84	1	0	4.181339	-3.956467	1.076236
85	1	0	5.958550	-5.198809	-0.090662
86	1	0	7.349610	-4.077463	-1.820877
87	1	0	6.935445	-1.682639	-2.368671
88	1	0	5.137170	-0.437107	-1.206834
89	1	0	4.267744	1.744328	2.215433

The total electronic energy was calculated to be –3069.7210172 Hartree.

Table S11. Optimized structure of **INT3c** (B3LYP-D3/6-31G(d))

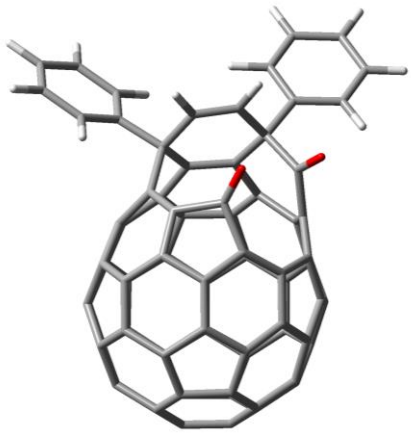


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.958109	2.132824	1.020202
2	6	0	0.679259	1.519539	2.231654
3	6	0	1.201359	0.206950	2.825964
4	6	0	2.266129	-1.975835	0.899062
5	6	0	0.897595	-2.405852	0.501657
6	6	0	-0.133584	-2.650389	1.417371
7	6	0	-0.558426	-1.831110	2.629378
8	6	0	-0.090294	-0.593850	3.070330
9	6	0	-1.046845	0.427017	3.437212
10	6	0	-0.606986	1.676228	2.842980
11	6	0	-1.534504	2.581252	2.360867
12	6	0	-1.302049	3.137850	1.047273
13	6	0	-0.150271	2.786592	0.319742
14	6	0	-2.592705	3.315195	0.428657
15	6	0	-3.620906	2.818722	1.330181
16	6	0	-2.955028	2.338429	2.522505
17	6	0	-3.386100	1.160508	3.135414
18	6	0	-2.404539	0.186920	3.585055
19	6	0	-2.892074	-1.129934	3.283007
20	6	0	-1.992981	-2.086937	2.797032
21	6	0	-2.449904	-2.994045	1.774852
22	6	0	-3.736695	-2.917051	1.247208
23	6	0	-4.631462	-1.867714	1.697013
24	6	0	-4.215958	-0.993667	2.699499
25	6	0	-4.510822	0.428280	2.588431
26	6	0	-5.179913	0.912982	1.459918
27	6	0	-4.723785	2.135829	0.817187
28	6	0	-5.608574	-0.003117	0.418044
29	6	0	-5.350387	-1.370669	0.539664
30	6	0	-5.429007	0.653895	-0.866553
31	6	0	-5.022955	-0.082544	-1.981059
32	6	0	-4.775470	-1.510996	-1.861576
33	6	0	-4.923835	-2.138695	-0.620901
34	6	0	-3.937486	-3.105030	-0.181087
35	6	0	-2.855989	-3.426866	-0.999464
36	6	0	-2.717658	-2.800495	-2.301954
37	6	0	-3.654844	-1.850373	-2.719370
38	6	0	-3.204076	-0.627626	-3.367074
39	6	0	-4.039733	0.465494	-2.899919
40	6	0	-3.471002	1.715551	-2.638997
41	6	0	-3.890900	2.478793	-1.480383
42	6	0	-4.865759	1.969609	-0.618396
43	6	0	-2.717255	3.137964	-0.940225
44	6	0	-1.556907	2.753749	-1.722692
45	6	0	-2.043759	1.916064	-2.805642
46	6	0	-1.255498	0.878913	-3.280559
47	6	0	-1.842240	-0.416226	-3.569827
48	6	0	-0.876811	-1.416813	-3.162319
49	6	0	-1.302391	-2.579092	-2.533906
50	6	0	-0.568135	-3.051108	-1.376467
51	6	0	-1.525388	-3.548662	-0.429269
52	6	0	-1.323577	-3.297058	0.929431
53	6	0	0.602114	-2.427037	-0.922242
54	6	0	1.105489	-1.271305	-1.662749
55	6	0	0.310057	-0.748225	-2.680103
56	6	0	0.054517	0.678554	-2.719976
57	6	0	0.557063	1.491640	-1.698645
58	6	0	-0.296620	2.533471	-1.125070
59	6	0	1.974348	-0.364045	-0.950511
60	6	0	1.661445	0.969646	-0.928016
61	6	0	2.205500	1.877438	0.157220
62	6	0	3.035712	-1.017767	-0.073191
63	6	0	3.863710	0.025535	0.687744
64	6	0	2.747839	3.184730	-0.460535
65	6	0	2.664922	4.412312	0.203829
66	6	0	3.250377	5.532492	-0.384408
67	6	0	3.899192	5.388482	-1.609751
68	6	0	3.937786	4.118077	-2.187140
69	6	0	3.967630	-1.830743	-1.003061
70	6	0	4.268927	-3.179535	-0.806750
71	6	0	5.133137	-3.841608	-1.683615
72	6	0	5.707021	-3.161925	-2.756299
73	6	0	5.415583	-1.808627	-2.949583
74	6	0	4.551267	-1.148426	-2.080620
75	6	0	5.247962	-0.280498	1.153002
76	6	0	5.587339	-1.376288	1.960928
77	6	0	6.910483	-1.583611	2.348886
78	6	0	7.920454	-0.713280	1.934337
79	6	0	7.596877	0.375142	1.123481
80	6	0	6.274472	0.586181	0.735807
81	7	0	3.382748	3.036206	-1.631260
82	6	0	3.401989	1.272862	0.848637
83	8	0	2.310191	-0.092904	3.185901
84	8	0	2.763173	-2.457405	1.899534
85	1	0	2.149021	4.487599	1.155404
86	1	0	3.198248	6.500226	0.106911
87	1	0	4.366176	6.233360	-2.106397
88	1	0	4.438419	3.958878	-3.140583
89	1	0	3.851129	-3.720262	0.035080
90	1	0	5.358739	-4.891755	-1.518587
91	1	0	6.380079	-3.679031	-3.434780
92	1	0	5.863362	-1.265707	-3.777701
93	1	0	4.328294	-0.094101	-2.226069
94	1	0	4.807730	-2.046495	2.294780
95	1	0	7.151695	-2.432363	2.983854

96	1	0	8.950533	-0.884914	2.236062	99	1	0	3.988379	1.969698	1.440114
97	1	0	8.373451	1.055192	0.782629						
98	1	0	6.027135	1.416482	0.080085	The total electronic energy was calculated to be –3300.7870091 Hartree.					

Table S12. Optimized structure of **INT3d** (B3LYP-D3/6-31G(d))

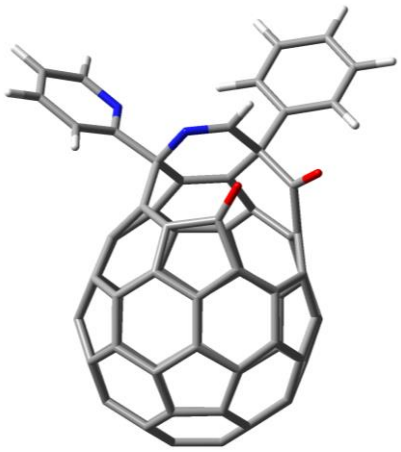


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.490380	2.071707	1.138890
2	6	0	0.993278	1.600831	2.345893
3	6	0	1.307226	0.328862	3.152039
4	6	0	2.483989	-2.123720	1.608210
5	6	0	1.141845	-2.487313	1.073559
6	6	0	-0.029660	-2.563307	1.838640
7	6	0	-0.560678	-1.594747	2.887024
8	6	0	-0.065192	-0.349218	3.266847
9	6	0	-0.974853	0.767090	3.383111
10	6	0	-0.351390	1.909457	2.740305
11	6	0	-1.124765	2.819040	2.043547
12	6	0	-0.664456	3.219270	0.733455
13	6	0	0.547687	2.721746	0.223380
14	6	0	-1.836263	3.414709	-0.084353
15	6	0	-3.018380	3.084297	0.696396
16	6	0	-2.569183	2.689659	2.014413
17	6	0	-3.179315	1.616771	2.667210
18	6	0	-2.354381	0.634391	3.349640
19	6	0	-2.898067	-0.672760	3.106753
20	6	0	-2.019990	-1.734613	2.857610
21	6	0	-2.395745	-2.712975	1.869306
22	6	0	-3.582877	-2.607627	1.148113
23	6	0	-4.446044	-1.460102	1.355402
24	6	0	-4.108951	-0.512586	2.319966
25	6	0	-4.269909	0.905921	2.030400
26	6	0	-4.729575	1.310570	0.772932
27	6	0	-4.089448	2.425668	0.091941
28	6	0	-5.076347	0.318269	-0.228762
29	6	0	-4.948833	-1.042588	0.060846
30	6	0	-4.663329	0.821925	-1.528727
31	6	0	-4.162399	-0.053921	-2.493605
32	6	0	-4.048883	-1.474140	-2.201519
33	6	0	-4.422961	-1.955450	-0.943362
34	6	0	-3.590092	-2.931581	-0.269549
35	6	0	-2.431237	-3.407381	-0.880617
36	6	0	-2.058391	-2.932444	-2.200812
37	6	0	-2.847753	-1.974400	-2.844390
38	6	0	-2.213977	-0.859678	-3.532710
39	6	0	-3.017965	0.328511	-3.303048
40	6	0	-2.395200	1.560160	-3.081399
41	6	0	-2.913567	2.468166	-2.077405
42	6	0	-4.038788	2.117771	-1.326367
43	6	0	-1.779730	3.103310	-1.433326
44	6	0	-0.554018	2.564853	-1.992834
45	6	0	-0.947240	1.649660	-3.051200
46	6	0	-0.184517	0.519311	-3.301638
47	6	0	-0.824936	-0.759160	-3.549647
48	6	0	-0.010492	-1.770220	-2.906540
49	6	0	-0.611623	-2.826791	-2.236167
50	6	0	-0.090177	-3.218724	-0.940937
51	6	0	-1.210195	-3.553071	-0.107213
52	6	0	-1.186340	-3.175831	1.236798
53	6	0	1.048760	-2.627654	-0.375268
54	6	0	1.739612	-1.591599	-1.145508
55	6	0	1.142546	-1.130969	-2.316987
56	6	0	1.012391	0.296818	-2.533633
57	6	0	1.432415	1.184692	-1.535781
58	6	0	0.588311	2.331971	-1.196733
59	6	0	2.570584	-0.669933	-0.411718
60	6	0	2.377603	0.682653	-0.563953
61	6	0	2.837909	1.673297	0.497899
62	6	0	3.419989	-1.286059	0.678998
63	6	0	4.100536	-0.243311	1.528645
64	6	0	3.539324	2.903158	-0.112054
65	6	0	3.498022	4.142071	0.537857
66	6	0	4.200410	5.234814	0.028649
67	6	0	4.958018	5.100888	-1.136079
68	6	0	5.012939	3.865209	-1.783516
69	6	0	4.490588	-2.187671	0.020890
70	6	0	4.573442	-3.566747	0.231247
71	6	0	5.555711	-4.320613	-0.417026
72	6	0	6.465778	-3.706545	-1.276195
73	6	0	6.393385	-2.326486	-1.483127
74	6	0	5.413403	-1.575172	-0.839043
75	6	0	4.311028	2.773663	-1.271854
76	6	0	3.819250	1.054498	1.466289
77	8	0	2.308113	-0.004910	3.731423
78	8	0	2.865640	-2.541333	2.683747
79	1	0	4.792919	-0.626511	2.269925
80	1	0	2.908921	4.255207	1.444020
81	1	0	4.152568	6.191305	0.542195
82	1	0	5.502199	5.952296	-1.535397
83	1	0	5.601942	3.749061	-2.689345
84	1	0	3.887871	-4.062701	0.909166
85	1	0	5.607210	-5.391956	-0.242612
86	1	0	7.228502	-4.295848	-1.777730
87	1	0	7.100796	-1.834690	-2.145532
88	1	0	5.361088	-0.500758	-0.994358
89	1	0	4.354997	1.815172	-1.781491
90	1	0	4.301474	1.748087	2.148806

The total electronic energy was calculated to be –3053.6822825 Hartree.

Table S13. Optimized structure of **INT3e** (B3LYP-D3/6-31G(d))

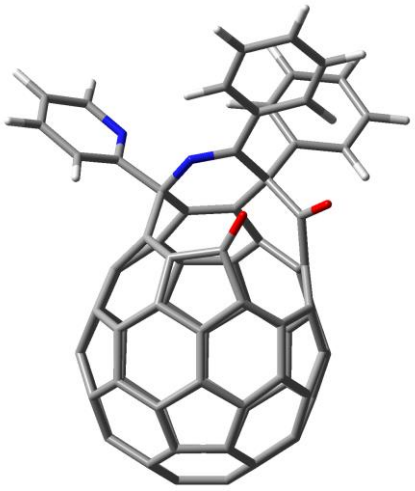


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.495022	1.995730	1.204885
2	6	0	1.007740	1.476114	2.397198
3	6	0	1.309005	0.156720	3.134370
4	6	0	2.465358	-2.222004	1.480542
5	6	0	1.110452	-2.549273	0.945695
6	6	0	-0.056080	-2.650211	1.717128
7	6	0	-0.574621	-1.724874	2.811214
8	6	0	-0.068935	-0.499976	3.239160
9	6	0	-0.964066	0.618440	3.411654
10	6	0	-0.331294	1.780541	2.813555
11	6	0	-1.102051	2.724793	2.160055
12	6	0	-0.649107	3.177271	0.864626
13	6	0	0.555594	2.693128	0.322685
14	6	0	-1.825935	3.417855	0.065427
15	6	0	-3.004540	3.064146	0.841135
16	6	0	-2.548390	2.609529	2.137032
17	6	0	-3.164656	1.516269	2.748624
18	6	0	-2.344407	0.498679	3.383410
19	6	0	-2.900758	-0.792833	3.088971
20	6	0	-2.034366	-1.851524	2.787427
21	6	0	-2.424525	-2.782196	1.759909
22	6	0	-3.616172	-2.635607	1.053800
23	6	0	-4.467684	-1.490728	1.317169
24	6	0	-4.115748	-0.588576	2.319122
25	6	0	-4.266300	0.842470	2.091243
26	6	0	-4.731771	1.303922	0.855820
27	6	0	-4.086644	2.441287	0.218154
28	6	0	-5.095525	0.358504	-0.184425
29	6	0	-4.977359	-1.014448	0.045812
30	6	0	-4.688377	0.913976	-1.465046
31	6	0	-4.202171	0.075891	-2.469972
32	6	0	-4.099070	-1.356667	-2.240164
33	6	0	-4.467296	-1.888332	-1.000724
34	6	0	-3.637283	-2.898774	-0.376050
35	6	0	-2.487354	-3.357703	-1.016121
36	6	0	-2.120981	-2.829909	-2.317918
37	6	0	-2.907361	-1.838851	-2.913596
38	6	0	-2.269584	-0.701072	-3.558775
39	6	0	-3.061239	0.482860	-3.272288
40	6	0	-2.425823	1.698725	-3.003685
41	6	0	-2.928225	2.566900	-1.957280
42	6	0	-4.050334	2.194255	-1.212418
43	6	0	-1.783898	3.164652	-1.296340
44	6	0	-0.567662	2.641745	-1.890182
45	6	0	-0.976982	1.775552	-2.983390
46	6	0	-0.226328	0.649878	-3.288607
47	6	0	-0.880109	-0.611705	-3.584394
48	6	0	-0.069048	-1.655853	-2.991056
49	6	0	-0.673626	-2.735077	-2.360923
50	6	0	-0.145171	-3.187346	-1.087929
51	6	0	-1.261272	-3.546720	-0.259767
52	6	0	-1.223093	-3.226754	1.098649
53	6	0	1.003484	-2.629742	-0.507251
54	6	0	1.696709	-1.569210	-1.239812
55	6	0	1.094942	-1.052037	-2.386415
56	6	0	0.975337	0.385050	-2.542650
57	6	0	1.409551	1.229000	-1.513461
58	6	0	0.579997	2.366377	-1.115749
59	6	0	2.525915	-0.678716	-0.471581
60	6	0	2.348705	0.674654	-0.571846
61	6	0	2.823143	1.589199	0.543332
62	6	0	3.368724	-1.299723	0.609520
63	6	0	3.970777	-0.238798	1.524389
64	6	0	3.584898	2.798685	-0.026652
65	6	0	3.614957	4.024863	0.642483
66	6	0	4.382524	5.055729	0.106455
67	6	0	5.095788	4.822530	-1.070099
68	6	0	5.012553	3.557655	-1.651678
69	6	0	4.549645	-2.063223	-0.033309
70	6	0	4.887876	-3.379900	0.291810
71	6	0	5.973003	-3.999228	-0.334019
72	6	0	6.733686	-3.309949	-1.277764
73	6	0	6.408190	-1.988453	-1.592484
74	6	0	5.324378	-1.367452	-0.975230
75	7	0	4.275616	2.560695	-1.146657
76	7	0	3.744160	1.008297	1.516797
77	8	0	2.310784	-0.245144	3.667884
78	8	0	2.870271	-2.720149	2.513104
79	1	0	4.647082	-0.628526	2.284190
80	1	0	3.052895	4.159039	1.560640
81	1	0	4.424844	6.023211	0.599099
82	1	0	5.705062	5.597549	-1.524906
83	1	0	5.560116	3.329762	-2.564301
84	1	0	4.321232	-3.925988	1.036601
85	1	0	6.221757	-5.025159	-0.076166
86	1	0	7.576918	-3.795862	-1.761097
87	1	0	6.998644	-1.437843	-2.319881
88	1	0	5.076161	-0.337552	-1.221523

The total electronic energy was calculated to be –3085.7611657 Hartree.

Table S14. Optimized structure of **INT3f** (B3LYP-D3/6-31G(d))



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.066732	2.112507	0.814978
2	6	0	0.826678	1.562463	2.065857
3	6	0	1.325359	0.252795	2.696160
4	6	0	2.298706	-2.043557	0.833932
5	6	0	0.882596	-2.419890	0.536686
6	6	0	-0.119422	-2.600525	1.499679
7	6	0	-0.484936	-1.720777	2.687323
8	6	0	0.025294	-0.475937	3.046287
9	6	0	-0.884378	0.588930	3.395617
10	6	0	-0.430263	1.790418	2.718009
11	6	0	-1.352775	2.695378	2.224796
12	6	0	-1.158868	3.182382	0.878059
13	6	0	-0.045694	2.768387	0.124125
14	6	0	-2.468343	3.366030	0.301015
15	6	0	-3.472013	2.941144	1.263924
16	6	0	-2.772361	2.500866	2.451964
17	6	0	-3.212227	1.369312	3.140968
18	6	0	-2.240824	0.392884	3.604746
19	6	0	-2.772028	-0.924291	3.386548
20	6	0	-1.916895	-1.929605	2.917427
21	6	0	-2.431275	-2.870205	1.955794
22	6	0	-3.734656	-2.784455	1.471866
23	6	0	-4.586518	-1.691593	1.902240
24	6	0	-4.112010	-0.780550	2.844037
25	6	0	-4.375184	0.641832	2.673281
26	6	0	-5.074052	1.088214	1.547300
27	6	0	-4.612094	2.265353	0.828214
28	6	0	-5.565063	0.134123	0.568817
29	6	0	-5.336232	-1.232255	0.748673
30	6	0	-5.418991	0.723354	-0.752582
31	6	0	-5.073970	-0.076390	-1.843621
32	6	0	-4.856141	-1.503259	-1.662216
33	6	0	-4.971953	-2.065935	-0.387529
34	6	0	-3.993276	-3.035023	0.062786
35	6	0	-2.951057	-3.423577	-0.777555
36	6	0	-2.847257	-2.863830	-2.112937
37	6	0	-3.777497	-1.912364	-2.542680
38	6	0	-3.324019	-0.734953	-3.267893
39	6	0	-4.114823	0.400800	-2.825216
40	6	0	-3.506983	1.647468	-2.648912
41	6	0	-3.862715	2.475958	-1.513564
42	6	0	-4.814669	2.034176	-0.590954
43	6	0	-2.652923	3.129267	-1.051851
44	6	0	-1.534533	2.680619	-1.860329
45	6	0	-2.083353	1.803942	-2.881802
46	6	0	-1.339492	0.724629	-3.335604
47	6	0	-1.967126	-0.568769	-3.534022
48	6	0	-1.009727	-1.571194	-3.110831
49	6	0	-1.437115	-2.688517	-2.406620
50	6	0	-0.671053	-3.120445	-1.254127
51	6	0	-1.602720	-3.550144	-0.250549
52	6	0	-1.343155	-3.238945	1.085260
53	6	0	0.528544	-2.502018	-0.873464
54	6	0	1.029685	-1.400295	-1.693181
55	6	0	0.210094	-0.908886	-2.708997
56	6	0	-0.012745	0.520329	-2.818587
57	6	0	0.549225	1.375288	-1.864287
58	6	0	-0.256289	2.459976	-1.303363
59	6	0	1.936362	-0.474429	-1.060614
60	6	0	1.664199	0.863043	-1.110814
61	6	0	2.274362	1.778340	-0.075430
62	6	0	3.013381	-1.075626	-0.174838
63	6	0	3.788580	0.024290	0.599063
64	6	0	2.867122	3.041510	-0.735105
65	6	0	2.915113	4.266959	-0.065454
66	6	0	3.539042	5.342850	-0.692315
67	6	0	4.097020	5.154356	-1.957263
68	6	0	4.009066	3.887137	-2.533610
69	6	0	3.950630	-1.836216	-1.139828
70	6	0	4.002123	-3.230970	-1.216003
71	6	0	4.830651	-3.854284	-2.151587
72	6	0	5.610767	-3.091281	-3.020276
73	6	0	5.552852	-1.697051	-2.954248
74	6	0	4.723820	-1.072530	-2.025004
75	6	0	5.063145	-0.281468	1.322627
76	6	0	5.619378	-1.564093	1.443231
77	6	0	6.822968	-1.760162	2.120302
78	6	0	7.498304	-0.683001	2.690601
79	6	0	6.955668	0.600471	2.580101
80	6	0	5.757450	0.797415	1.904839
81	7	0	3.410026	2.847078	-1.941375
82	7	0	3.388658	1.237163	0.666389
83	8	0	2.432737	-0.107114	3.002943
84	8	0	2.874835	-2.575200	1.760613
85	1	0	2.475082	4.368051	0.920983
86	1	0	3.589911	6.310850	-0.201332
87	1	0	4.591085	5.965032	-2.483973
88	1	0	4.437440	3.693846	-3.515424
89	1	0	3.416380	-3.840492	-0.535500
90	1	0	4.865118	-4.939466	-2.195788
91	1	0	6.257245	-3.578281	-3.745098
92	1	0	6.152049	-1.092494	-3.629650
93	1	0	4.661729	0.012663	-1.991540
94	1	0	5.115884	-2.422736	1.029789
95	1	0	7.228280	-2.765097	2.200856

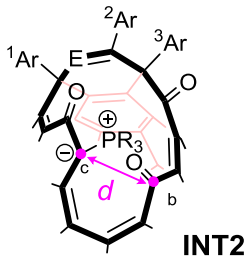
96	1	0	8.436782	-0.839164	3.216429	----------
97	1	0	7.469471	1.450722	3.021152	The total electronic energy was calculated to be –3316.8283768 Hartree.
98	1	0	5.332836	1.789962	1.816701	

6. Stabilization Energies of INT2

The structures of β-oxo-phosphorus ylides **INT2** were optimized at the B3LYP-D3/6-31G(d) level of theory.

Table S15. Stabilization energies and bond distance of **INT2** (B3LYP-D3/6-31G(d))

Addends	$\Delta\Delta G^a$ (kcal/mol)	d[C(b)···C(c)] (Å)
a	0.0	3.35
b	–1.0	3.36
c	+0.1	3.36
d	–1.4	3.34
e	–0.4	3.32
f	–3.3	3.32



INT2

[a]$\Delta\Delta G$ = ΔG(**INT2**) – ΔG(**INT2a**) where ΔG(**INT2**) = G(**INT2**) + G(O=PPh$_3$) – G(**INT1**) – 2G(PPh$_3$).

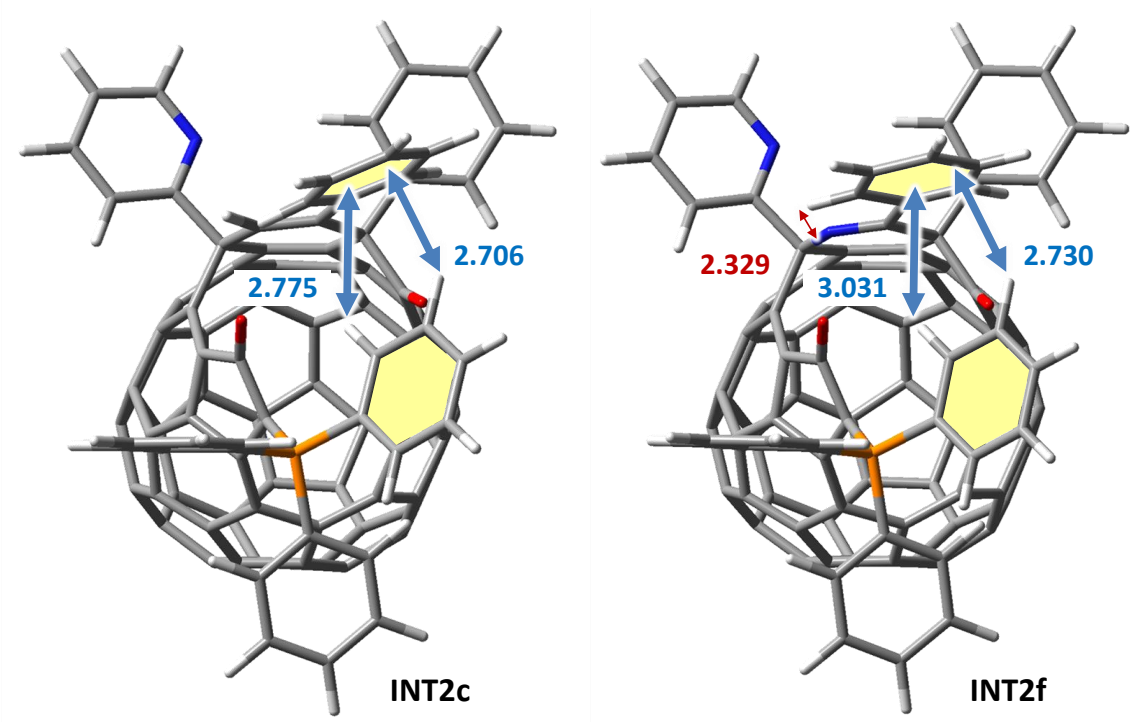
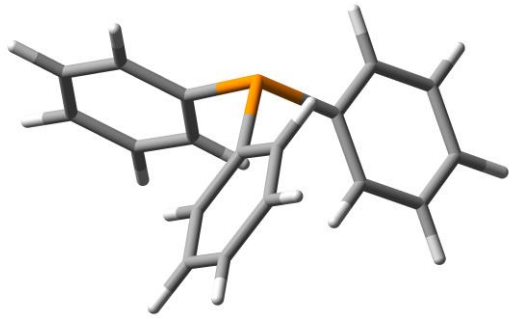


Figure S8. Optimized structure of **INT2c and INT2f** with selected bond lengths (Å), calculated at the B3LYP-D3/6-31G(d) level of theory.

Table S16. Optimized structure of PPh_3 (B3LYP-D3/6-31G(d))

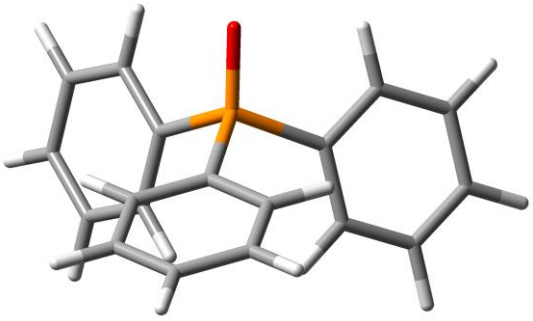


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.000647	0.000582	-1.261843
2	6	0	-0.401543	-1.609211	-0.438332
3	6	0	1.595544	0.457050	-0.437580
4	6	0	-1.193195	1.152592	-0.437740
5	6	0	-1.372277	2.415761	-1.025403
6	6	0	-2.238762	3.350695	-0.459281
7	6	0	-2.953875	3.030571	0.696970
8	6	0	-2.793382	1.773961	1.283593
9	6	0	-1.917509	0.841893	0.723296
10	6	0	-1.411996	-2.390936	-1.022366
11	6	0	-1.790166	-3.608395	-0.456706
12	6	0	-1.150858	-4.072571	0.695171
13	6	0	-0.136958	-3.310275	1.278017
14	6	0	0.233968	-2.085878	0.718278
15	6	0	2.778062	-0.023279	-1.024041
16	6	0	4.021632	0.258617	-0.458873
17	6	0	4.103733	1.041268	0.695014
18	6	0	2.936202	1.534334	1.280445
19	6	0	1.690344	1.242534	0.721325
20	1	0	-0.828904	2.667697	-1.933450
21	1	0	-2.362081	4.324959	-0.925129
22	1	0	-3.635875	3.754621	1.134953
23	1	0	-3.348973	1.517530	2.182140
24	1	0	-1.797069	-0.130313	1.191463
25	1	0	-1.905461	-2.042481	-1.926982
26	1	0	-2.577110	-4.198331	-0.919433
27	1	0	-1.438222	-5.024997	1.132785
28	1	0	0.366239	-3.666803	2.173298
29	1	0	1.019975	-1.498877	1.183468
30	1	0	2.723293	-0.622145	-1.930490
31	1	0	4.926168	-0.124851	-0.923833
32	1	0	5.072258	1.269281	1.132237
33	1	0	2.993182	2.146107	2.177288
34	1	0	0.789099	1.627482	1.188612

The total electronic energy was calculated to be –1036.3294318 Hartree.

Table S17. Optimized structure of $O{=}PPh_3$ (B3LYP-D3/6-31G(d))



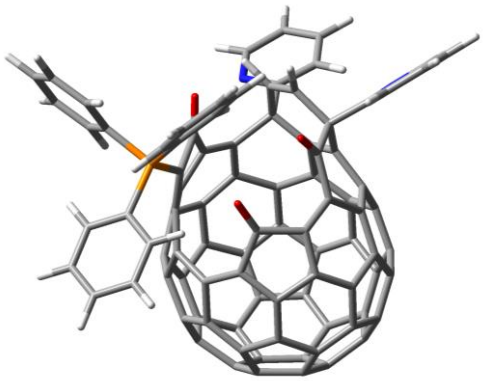
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.007288	0.038031	0.942486
2	8	0	-0.031066	0.194847	2.438172
3	6	0	1.350315	0.995496	0.177474
4	6	0	0.203401	-1.669166	0.322657
5	6	0	-1.549877	0.649296	0.172692
6	6	0	-2.466105	1.295544	1.011851
7	6	0	-3.650944	1.815084	0.486744
8	6	0	-3.925475	1.690924	-0.876103
9	6	0	-3.015671	1.043289	-1.717277
10	6	0	-1.831935	0.523967	-1.195672
11	6	0	1.992643	1.942057	0.986070
12	6	0	3.010502	2.738785	0.459104
13	6	0	3.391916	2.593711	-0.875941
14	6	0	2.758933	1.645986	-1.685267
15	6	0	1.742480	0.848359	-1.161283
16	6	0	1.490313	-2.217965	0.207033
17	6	0	1.658028	-3.549239	-0.172330
18	6	0	0.542441	-4.347132	-0.436446
19	6	0	-0.741667	-3.812057	-0.316538
20	6	0	-0.911559	-2.480516	0.063123
21	1	0	-2.237611	1.377613	2.070410
22	1	0	-4.359427	2.314404	1.142216
23	1	0	-4.848047	2.095117	-1.284451
24	1	0	-3.230685	0.941476	-2.777668
25	1	0	-1.136190	0.010407	-1.853498
26	1	0	1.690108	2.034379	2.025086
27	1	0	3.507116	3.469703	1.091577
28	1	0	4.184872	3.213644	-1.285969
29	1	0	3.061232	1.525488	-2.722174
30	1	0	1.270502	0.098944	-1.790721

31	1	0	2.361528	-1.601064	0.407752	35	1	0	-1.912905	-2.069706	0.151943
32	1	0	2.658599	-3.963328	-0.262766						
33	1	0	0.673913	-5.383978	-0.734406						
34	1	0	-1.611575	-4.430881	-0.519334						

The total electronic energy was calculated to be –1111.585595 Hartree.

Table S18. Optimized structure of **INT2a** (B3LYP-D3/6-31G(d))

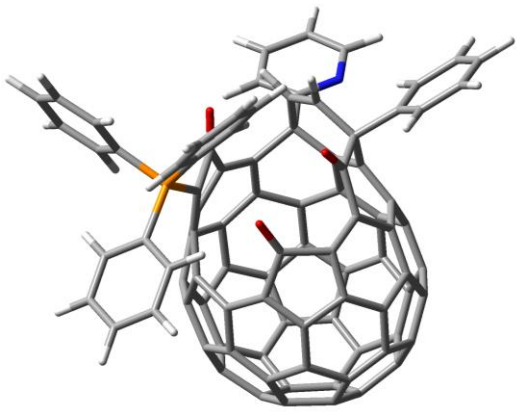


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.100983	-1.492735	1.671510
2	6	0	-4.763022	-0.080101	1.753793
3	6	0	-4.855203	0.710939	0.620616
4	6	0	-5.273720	0.140370	-0.646740
5	6	0	-5.558631	-1.222805	-0.739069
6	6	0	-5.473049	-2.056678	0.446173
7	6	0	-3.645453	0.089413	2.663601
8	6	0	-3.837521	1.699203	0.372279
9	6	0	-4.495882	0.791260	-1.676731
10	6	0	-5.061787	-1.987911	-1.870679
11	6	0	-4.917713	-3.338774	0.050029
12	6	0	-4.223565	-2.205775	2.571459
13	6	0	-4.314902	-1.351745	-2.867024
14	6	0	-4.030429	0.070746	-2.769323
15	6	0	-3.135195	-1.994395	-3.407515
16	6	0	-2.683336	0.312070	-3.239069
17	6	0	-2.619853	1.035599	2.417496
18	6	0	-3.631298	1.770121	-1.057053
19	6	0	-2.142773	-0.964150	-3.636287
20	6	0	-2.368105	2.079986	-1.556356
21	6	0	-2.755433	1.889040	1.240024
22	6	0	-4.649383	-3.290910	-1.377982
23	6	0	-4.040510	-4.012622	0.903802
24	6	0	-1.249084	0.730654	2.846114
25	6	0	-3.702180	-3.450590	2.199322
26	6	0	-3.363599	-1.224916	3.214154
27	6	0	-2.842452	-4.638351	0.369581
28	6	0	-2.316112	-3.774762	2.483624
29	6	0	-2.059039	-1.551616	3.531410
30	6	0	-1.847234	1.295730	-2.674551
31	6	0	-3.498653	-3.901996	-1.890955
32	6	0	-1.586182	2.553039	0.707221
33	6	0	-1.770382	-4.460522	1.330399
34	6	0	-1.514213	-2.855585	3.157577
35	6	0	-1.028474	-0.556736	3.370840
36	6	0	0.152896	-1.262771	2.978036
37	6	0	-0.113049	1.470968	2.282506
38	6	0	-1.421118	2.685664	-0.649696
39	6	0	0.467710	2.195776	-2.217891
40	6	0	-0.147246	-2.646438	2.758481
41	6	0	0.353683	-3.210024	1.577390
42	6	0	1.240773	-2.506646	0.652501
43	6	0	-0.479125	-4.149061	0.874101
44	6	0	-2.724496	-3.234074	-2.916011
45	6	0	2.379546	1.021660	1.244494
46	6	0	-2.567632	-4.569763	-0.993081
47	6	0	-1.218565	-4.272079	-1.446322
48	6	0	1.071637	0.786479	2.019931
49	6	0	-0.406158	1.101527	-2.718395
50	6	0	0.086304	-0.175792	-2.989625
51	6	0	1.068895	-0.634924	2.192529
52	6	0	1.785980	-1.272496	1.091198
53	6	0	-0.195978	-4.006472	-0.528065
54	6	0	0.816682	-2.950150	-0.719285
55	6	0	2.701606	-0.266529	0.620209
56	6	0	-1.317049	-3.482803	-2.637216
57	6	0	-0.798973	-1.211858	-3.385115
58	6	0	1.281022	-0.882339	-2.353711
59	6	0	-0.374176	-2.481443	-2.820516
60	6	0	0.741905	-2.249037	-1.937319
61	6	0	-0.466005	2.855142	1.701434
62	6	0	-0.178604	3.263943	-1.286198
63	6	0	0.846946	3.698622	-0.268580
64	6	0	0.711511	3.524809	1.041788
65	6	0	-0.573677	4.519035	-2.105866
66	6	0	-0.977293	3.829797	2.780009
67	8	0	1.635863	2.290888	-2.556138
68	8	0	3.081944	2.032591	1.224680
69	6	0	-1.662977	4.986115	2.379054
70	6	0	-2.089519	5.875879	3.359115
71	6	0	-1.812566	5.589147	4.698257
72	6	0	-1.109184	4.422027	4.988913
73	7	0	-0.693663	3.553608	4.055693
74	7	0	-1.532796	5.272273	-1.546220
75	6	0	-1.899492	6.395194	-2.170231
76	6	0	-1.337699	6.830381	-3.371782
77	6	0	-0.332395	6.051819	-3.940611
78	6	0	0.062713	4.877849	-3.298862
79	8	0	2.414451	-0.471218	-2.249893
80	15	0	4.343288	-0.589995	0.094948
81	6	0	5.460680	-0.230715	1.506017
82	6	0	5.002107	0.341328	-1.317464
83	6	0	4.502267	-2.373352	-0.251482
84	6	0	4.468301	1.597636	-1.628336
85	6	0	4.991050	2.320073	-2.698663
86	6	0	6.048177	1.805154	-3.450493
87	6	0	6.584998	0.554153	-3.137701
88	6	0	6.060935	-0.182753	-2.075803
89	6	0	6.804200	0.113199	1.302188
90	6	0	7.643737	0.329168	2.394770
91	6	0	7.150017	0.207763	3.694933
92	6	0	5.810923	-0.128259	3.902748
93	6	0	4.967039	-0.345029	2.814374
94	6	0	4.215385	-2.883071	-1.527052
95	6	0	4.255769	-4.258598	-1.749720
96	6	0	4.574213	-5.131934	-0.708343
97	6	0	4.863532	-4.627283	0.560600

98	6	0	4.832442	-3.252721	0.790262	112	1	0	7.402802	0.145583	-3.724881
99	1	0	1.745462	4.152680	-0.672523	113	1	0	6.466742	-1.165044	-1.851349
100	1	0	1.508075	3.827914	1.710725	114	1	0	7.193155	0.227605	0.295819
101	1	0	-1.843577	5.168399	1.322637	115	1	0	8.682362	0.601057	2.228233
102	1	0	-2.629105	6.778647	3.084980	116	1	0	7.805108	0.382381	4.544043
103	1	0	-2.129459	6.253847	5.496381	117	1	0	5.417774	-0.212199	4.911875
104	1	0	-0.864176	4.164948	6.018164	118	1	0	3.923026	-0.590455	2.981876
105	1	0	-2.682344	6.974733	-1.683780	119	1	0	3.942744	-2.207110	-2.327576
106	1	0	-1.678045	7.749492	-3.838772	120	1	0	4.025648	-4.647168	-2.737634
107	1	0	0.141289	6.349627	-4.872218	121	1	0	4.595932	-6.203829	-0.884847
108	1	0	0.850955	4.260412	-3.712365	122	1	0	5.113325	-5.302184	1.374215
109	1	0	3.645258	1.999057	-1.053730	123	1	0	5.059959	-2.869140	1.779369
110	1	0	4.551828	3.280311	-2.951007	---					
111	1	0	6.449517	2.372765	-4.285937	The total electronic energy was calculated to be –4197.3576688 Hartree.					

Table S19. Optimized structure of **INT2b** (B3LYP-D3/6-31G(d))



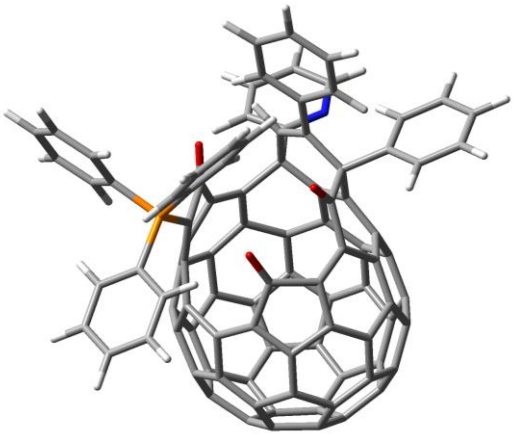
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.081352	-1.532881	1.691268
2	6	0	-4.755345	-0.117011	1.771028
3	6	0	-4.853590	0.670889	0.636129
4	6	0	-5.270222	0.094716	-0.629513
5	6	0	-5.544987	-1.270649	-0.718950
6	6	0	-5.450538	-2.101906	0.467580
7	6	0	-3.636758	0.062978	2.676942
8	6	0	-3.845582	1.668055	0.384570
9	6	0	-4.499875	0.750150	-1.661972
10	6	0	-5.044970	-2.033884	-1.850307
11	6	0	-4.885556	-3.380094	0.072347
12	6	0	-4.196418	-2.237729	2.590162
13	6	0	-4.304938	-1.393362	-2.848940
14	6	0	-4.031620	0.031383	-2.754440
15	6	0	-3.121411	-2.027510	-3.391283
16	6	0	-2.687899	0.282476	-3.228067
17	6	0	-2.620912	1.018758	2.426697
18	6	0	-3.641770	1.736806	-1.045275
19	6	0	-2.137886	-0.989510	-3.625434
20	6	0	-2.380713	2.051930	-1.545737
21	6	0	-2.765206	1.872710	1.250951
22	6	0	-4.621035	-3.332649	-1.356514
23	6	0	-4.001710	-4.046243	0.925201
24	6	0	-1.245865	0.721551	2.851069
25	6	0	-3.665156	-3.478743	2.218745
26	6	0	-3.342173	-1.249048	3.228040
27	6	0	-2.799700	-4.662793	0.389263
28	6	0	-2.276198	-3.791643	2.501085
29	6	0	-2.035465	-1.566028	3.545742
30	6	0	-1.858285	1.272884	-2.666276
31	6	0	-3.466569	-3.935132	-1.871066
32	6	0	-1.602759	2.546977	0.716556
33	6	0	-1.726869	-4.473834	1.347179
34	6	0	-1.480537	-2.866085	3.173114
35	6	0	-1.013390	-0.563376	3.379396
36	6	0	0.172908	-1.260695	2.986511
37	6	0	-0.115314	1.466865	2.280664
38	6	0	-1.433989	2.664423	-0.642171
39	6	0	0.448856	2.198971	-2.219634
40	6	0	-0.115787	-2.647208	2.771457
41	6	0	0.386522	-3.204938	1.588010
42	6	0	1.265974	-2.495123	0.660103
43	6	0	-0.439314	-4.152483	0.887640
44	6	0	-2.700164	-3.263209	-2.899324
45	6	0	2.391671	1.036877	1.261239
46	6	0	-2.528022	-4.593459	-0.973936
47	6	0	-1.182440	-4.285747	-1.430853
48	6	0	1.078269	0.792308	2.027461
49	6	0	-0.416546	1.092758	-2.714782
50	6	0	0.085737	-0.180902	-2.984117
51	6	0	1.085678	-0.627863	2.200950
52	6	0	1.806220	-1.258284	1.097132
53	6	0	-0.159834	-4.010132	-0.515286
54	6	0	0.843029	-2.946197	-0.710876
55	6	0	2.716005	-0.245167	0.628754
56	6	0	-1.289982	-3.499573	-2.622840
57	6	0	-0.791793	-1.225462	-3.376036
58	6	0	1.283608	-0.873283	-2.342129
59	6	0	-0.355727	-2.490692	-2.810181
60	6	0	0.759145	-2.246927	-1.928625
61	6	0	-0.478853	2.852958	1.704932
62	6	0	-0.200601	3.259652	-1.286441
63	6	0	0.826152	3.692706	-0.272549
64	6	0	0.693789	3.528591	1.039185
65	6	0	-0.627237	4.506878	-2.103198
66	6	0	-0.985301	3.825552	2.786986
67	8	0	1.611158	2.305412	-2.571408
68	8	0	3.090141	2.050252	1.260541
69	6	0	-0.565557	3.740675	4.117953
70	6	0	-1.017199	4.697135	5.026110
71	6	0	-1.869398	5.704377	4.576594
72	6	0	-2.223359	5.709620	3.226347
73	7	0	-1.794078	4.800325	2.345895
74	6	0	-1.396911	5.478785	-1.444902
75	6	0	-1.803447	6.628362	-2.117958
76	6	0	-1.447090	6.826397	-3.455109
77	6	0	-0.672495	5.869106	-4.107830

78	6	0	-0.259421	4.714985	-3.435309
79	8	0	2.409360	-0.446354	-2.221618
80	15	0	4.352868	-0.557414	0.078584
81	6	0	5.478075	-0.240450	1.495077
82	6	0	4.997612	0.414328	-1.311252
83	6	0	4.504652	-2.330879	-0.318182
84	6	0	4.422417	1.652660	-1.618358
85	6	0	4.931407	2.403973	-2.675490
86	6	0	6.017007	1.935275	-3.416566
87	6	0	6.595525	0.701564	-3.107982
88	6	0	6.084863	-0.064328	-2.060489
89	6	0	6.816326	0.127303	1.298600
90	6	0	7.659090	0.312032	2.394513
91	6	0	7.174539	0.134959	3.691597
92	6	0	5.840494	-0.224225	3.892901
93	6	0	4.993225	-0.408507	2.801168
94	6	0	4.281375	-2.798486	-1.621957
95	6	0	4.313967	-4.167639	-1.882895
96	6	0	4.559926	-5.075929	-0.851933
97	6	0	4.785368	-4.613186	0.445708
98	6	0	4.762569	-3.245623	0.713488
99	1	0	1.718752	4.153587	-0.681411
100	1	0	1.489916	3.844197	1.703174
101	1	0	0.094189	2.938609	4.431558
102	1	0	-0.709655	4.652871	6.067461
103	1	0	-2.250154	6.467309	5.248685
104	1	0	-2.882679	6.480319	2.830607
105	1	0	-1.668399	5.330327	-0.402105
106	1	0	-2.400122	7.372203	-1.596236
107	1	0	-1.767913	7.722007	-3.980543
108	1	0	-0.383054	6.014990	-5.145316
109	1	0	0.357664	3.990882	-3.955971
110	1	0	3.576792	2.018493	-1.053927
111	1	0	4.457304	3.347612	-2.926520
112	1	0	6.407805	2.524699	-4.241767
113	1	0	7.434993	0.328606	-3.688208
114	1	0	6.522085	-1.034283	-1.840780
115	1	0	7.198872	0.286066	0.296042
116	1	0	8.693282	0.603070	2.233023
117	1	0	7.832404	0.284370	4.543350
118	1	0	5.454297	-0.352185	4.900184
119	1	0	3.952611	-0.670940	2.964542
120	1	0	4.064574	-2.096540	-2.416956
121	1	0	4.134769	-4.523618	-2.893361
122	1	0	4.575179	-6.142466	-1.058827
123	1	0	4.978588	-5.315336	1.251594
124	1	0	4.940434	-2.894185	1.724495

The total electronic energy was calculated to be –4181.3206314 Hartree.

Table S20. Optimized structure of **INT2c** (B3LYP-D3/6-31G(d))

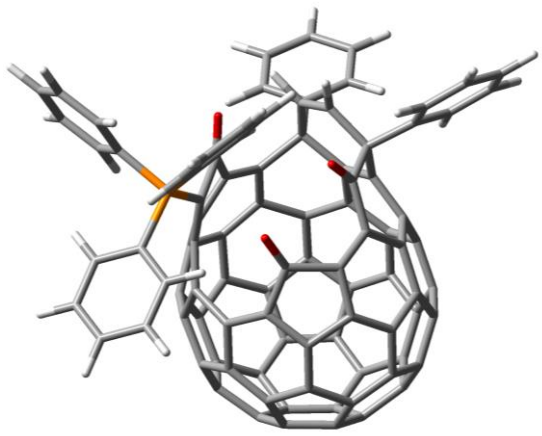


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.620845	0.028676	1.604600
2	6	0	-4.811763	1.222821	1.797667
3	6	0	-4.587166	2.074947	0.728613
4	6	0	-5.143300	1.780965	-0.579917
5	6	0	-5.886303	0.616521	-0.778408
6	6	0	-6.131963	-0.277903	0.338785
7	6	0	-3.730126	0.920826	2.715115
8	6	0	-3.282120	2.658126	0.558823
9	6	0	-4.158843	2.189487	-1.555996
10	6	0	-5.659917	-0.190432	-1.965912
11	6	0	-6.051072	-1.640744	-0.155558
12	6	0	-5.075114	-1.011306	2.446108
13	6	0	-4.711210	0.212901	-2.910520
14	6	0	-3.949331	1.433339	-2.702688
15	6	0	-3.817088	-0.762897	-3.499608
16	6	0	-2.592614	1.218359	-3.153394
17	6	0	-2.431513	1.462048	2.541484
18	6	0	-3.021934	2.751087	-0.860947
19	6	0	-2.520551	-0.133369	-3.649259
20	6	0	-1.718743	2.621032	-1.331368
21	6	0	-2.226178	2.393906	1.438055
22	6	0	-5.744578	-1.587151	-1.575920
23	6	0	-5.491901	-2.641513	0.643319
24	6	0	-1.266890	0.660707	2.939898
25	6	0	-5.013663	-2.329723	1.978519
26	6	0	-3.942055	-0.445656	3.161012
27	6	0	-4.574409	-3.607424	0.061806
28	6	0	-3.837880	-3.140664	2.236942
29	6	0	-2.845876	-1.233153	3.454149
30	6	0	-1.482120	1.798880	-2.512120
31	6	0	-4.867582	-2.524949	-2.134874
32	6	0	-0.883681	2.636820	0.956893
33	6	0	-3.534457	-3.887684	1.033540
34	6	0	-2.784254	-2.615823	2.982158
35	6	0	-1.527306	-0.656459	3.368759
36	6	0	-0.660671	-1.706717	2.928233
37	6	0	0.072968	0.986580	2.428380
38	6	0	-0.636557	2.780620	-0.382270
39	6	0	0.995415	1.819357	-2.005231
40	6	0	-1.420793	-2.875573	2.602333
41	6	0	-1.114389	-3.487408	1.379079
42	6	0	-0.010414	-3.074570	0.511780
43	6	0	-2.203696	-4.018842	0.603825
44	6	0	-3.880676	-2.099570	-3.105127
45	6	0	2.283210	-0.247030	1.416666
46	6	0	-4.254269	-3.540242	-1.291046
47	6	0	-2.874420	-3.703415	-1.719159
48	6	0	0.947052	-0.055563	2.137474
49	6	0	-0.199050	1.123054	-2.569404
50	6	0	-0.175470	-0.223173	-2.934428
51	6	0	0.441656	-1.391881	2.197959
52	6	0	0.924587	-2.152184	1.047178
53	6	0	-1.849188	-3.882665	-0.782797

54	6	0	-0.526349	-3.239091	-0.891137	96	6	0	6.922010	-2.841845	2.468817
55	6	0	2.151024	-1.496301	0.666867	97	6	0	6.366006	-2.952783	3.744432
56	6	0	-2.657239	-2.844999	-2.844260	98	6	0	4.984138	-2.846062	3.912970
57	6	0	-1.355903	-0.852471	-3.411548	99	6	0	4.159687	-2.631389	2.809435
58	6	0	0.675056	-1.342852	-2.344186	100	6	0	2.806226	-4.235693	-1.812703
59	6	0	-1.418614	-2.227357	-2.947614	101	6	0	2.374728	-5.504404	-2.197175
60	6	0	-0.317576	-2.466009	-2.047716	102	6	0	2.260744	-6.526202	-1.253025
61	6	0	0.251365	2.445861	1.947738	103	6	0	2.589831	-6.282017	0.081461
62	6	0	0.743251	2.989390	-0.995656	104	6	0	3.030066	-5.018774	0.472609
63	6	0	1.875863	3.015194	0.044195	105	1	0	2.393978	2.765375	2.059717
64	6	0	1.595656	2.740963	1.330264	106	1	0	0.692592	2.100555	4.684183
65	6	0	0.597374	4.354592	-1.721641	107	1	0	0.533764	3.863977	6.450965
66	6	0	0.110322	3.455283	3.108296	108	1	0	-0.158119	6.187238	5.773336
67	8	0	2.116000	1.502064	-2.354763	109	1	0	-0.626502	6.624409	3.356849
68	8	0	3.303989	0.429580	1.545438	110	1	0	0.488319	5.400453	0.158202
69	6	0	0.405180	3.115543	4.431835	111	1	0	0.189096	7.628886	-0.882823
70	6	0	0.313375	4.101403	5.413668	112	1	0	0.081727	7.847526	-3.361497
71	6	0	-0.068109	5.389356	5.042593	113	1	0	0.287635	5.814650	-4.782599
72	6	0	-0.331049	5.631947	3.693024	114	1	0	0.623585	3.605986	-3.749670
73	7	0	-0.241488	4.696680	2.742869	115	1	0	5.127288	4.850297	-2.815926
74	6	0	0.466075	5.499122	-0.924185	116	1	0	2.844508	4.243933	-2.273003
75	6	0	0.285519	6.748869	-1.513274	117	1	0	4.189017	2.466344	1.405113
76	6	0	0.222795	6.872243	-2.903598	118	1	0	6.472913	3.088525	0.867455
77	6	0	0.337729	5.733048	-3.700049	119	1	0	6.997534	4.298876	-1.253658
78	6	0	0.520368	4.479107	-3.112774	120	1	0	3.809363	0.475872	-0.765511
79	8	0	1.873304	-1.353842	-2.177590	121	1	0	5.199860	1.600759	-2.436051
80	6	0	4.927474	4.342250	-1.875741	122	1	0	6.788656	0.281865	-3.841126
81	6	0	3.613828	3.998515	-1.559021	123	1	0	6.935267	-2.184022	-3.559780
82	6	0	3.285957	3.350917	-0.352772	124	1	0	5.514925	-3.327356	-1.889888
83	6	0	4.362345	3.034258	0.502777	125	1	0	6.545398	-2.526787	0.376401
84	6	0	5.676244	3.367858	0.182797	126	1	0	7.997783	-2.912278	2.334184
85	6	0	5.972616	4.035969	-1.005082	127	1	0	7.008391	-3.113757	4.605882
86	15	0	3.593643	-2.311143	0.084022	128	1	0	4.546618	-2.919464	4.904622
87	6	0	4.713076	-2.529170	1.524076	129	1	0	3.087729	-2.530288	2.948156
88	6	0	4.577536	-1.496379	-1.202065	130	1	0	2.871298	-3.437599	-2.540983
89	6	0	3.134212	-3.986475	-0.471487	131	1	0	2.117475	-5.689432	-3.236155
90	6	0	4.492608	-0.108864	-1.362592	132	1	0	1.916089	-7.511004	-1.556266
91	6	0	5.288253	0.526679	-2.313926	133	1	0	2.505132	-7.073952	0.820039
92	6	0	6.170482	-0.216455	-3.098845	134	1	0	3.288292	-4.838858	1.511012
93	6	0	6.255958	-1.602836	-2.942092	---					
94	6	0	5.458998	-2.247725	-1.997138	The total electronic energy was calculated to be –4412.3872692 Hartree.					
95	6	0	6.101552	-2.629720	1.360873						

Table S21. Optimized structure of **INT2d** (B3LYP-D3/6-31G(d))

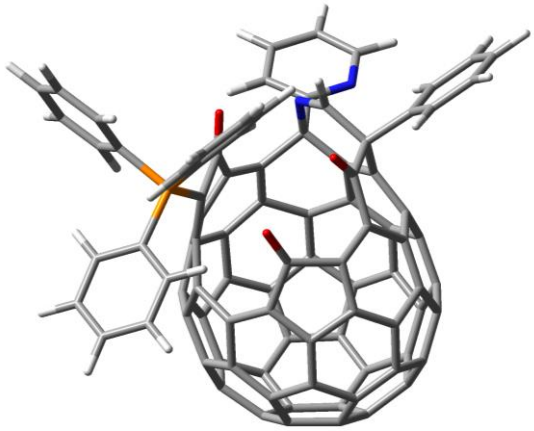


Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	-5.128371	-1.445191	1.663124
2	6	0	-4.777876	-0.036071	1.755423
3	6	0	-4.861921	0.763869	0.627780
4	6	0	-5.283074	0.205190	-0.644119
5	6	0	-5.581214	-1.154381	-0.745976
6	6	0	-5.504838	-1.996990	0.433825
7	6	0	-3.657832	0.116469	2.664933
8	6	0	-3.835839	1.745878	0.388073
9	6	0	-4.496397	0.854348	-1.668278
10	6	0	-5.090998	-1.916952	-1.882152
11	6	0	-4.962569	-3.282104	0.029331
12	6	0	-4.257301	-2.172977	2.557408
13	6	0	-4.335211	-1.282029	-2.872665
14	6	0	-4.034543	0.136105	-2.763514
15	6	0	-3.162356	-1.934084	-3.416635
16	6	0	-2.682959	0.365109	-3.226970
17	6	0	-2.625797	1.056493	2.424880
18	6	0	-3.623435	1.820178	-1.040747
19	6	0	-2.157374	-0.913405	-3.635582

20	6	0	-2.354054	2.115617	-1.532068	74	6	0	-1.653872	5.268312	-1.913318
21	6	0	-2.755785	1.925953	1.259850	75	6	0	-1.936777	6.402230	-2.674274
22	6	0	-4.693659	-3.227872	-1.398305	76	6	0	-1.073260	6.796136	-3.697445
23	6	0	-4.093076	-3.971309	0.878646	77	6	0	0.079052	6.049657	-3.944925
24	6	0	-1.255722	0.730612	2.839977	78	6	0	0.364178	4.915577	-3.182692
25	6	0	-3.748307	-3.420493	2.177273	79	8	0	2.420098	-0.515234	-2.286196
26	6	0	-3.386443	-1.204956	3.204339	80	15	0	4.329984	-0.639458	0.091458
27	6	0	-2.902306	-4.607151	0.340360	81	6	0	5.437478	-0.268691	1.506800
28	6	0	-2.365613	-3.761024	2.459077	82	6	0	5.010986	0.267937	-1.325043
29	6	0	-2.085056	-1.547002	3.518024	83	6	0	4.477358	-2.429100	-0.227634
30	6	0	-1.836246	1.333077	-2.651987	84	6	0	4.524684	1.546171	-1.625005
31	6	0	-3.550138	-3.848724	-1.915372	85	6	0	5.070025	2.253477	-2.694364
32	6	0	-1.580927	2.591742	0.737445	86	6	0	6.101983	1.701783	-3.455031
33	6	0	-1.827945	-4.446610	1.301741	87	6	0	6.592398	0.429732	-3.151068
34	6	0	-1.553327	-2.854253	3.137283	88	6	0	6.046298	-0.292056	-2.090000
35	6	0	-1.045402	-0.561641	3.356896	89	6	0	6.781286	0.075726	1.306359
36	6	0	0.128122	-1.276849	2.958057	90	6	0	7.615561	0.300805	2.401252
37	6	0	-0.114814	1.461905	2.270162	91	6	0	7.116252	0.187362	3.699915
38	6	0	-1.406158	2.719813	-0.622048	92	6	0	5.776832	-0.150128	3.904198
39	6	0	0.491692	2.185816	-2.147820	93	6	0	4.938187	-0.375508	2.813651
40	6	0	-0.184367	-2.657635	2.737797	94	6	0	4.160172	-2.957048	-1.488786
41	6	0	0.310405	-3.221764	1.554296	95	6	0	4.194548	-4.335609	-1.692440
42	6	0	1.205508	-2.525005	0.632280	96	6	0	4.537339	-5.194171	-0.646453
43	6	0	-0.533113	-4.148772	0.846957	97	6	0	4.856655	-4.671493	0.607841
44	6	0	-2.767869	-3.183031	-2.935953	98	6	0	4.831618	-3.293637	0.818597
45	6	0	2.370611	0.994523	1.222328	99	1	0	1.741772	4.212558	-0.627757
46	6	0	-2.626946	-4.533179	-1.021964	100	1	0	1.508340	3.866481	1.747638
47	6	0	-1.274485	-4.250228	-1.474241	101	1	0	-2.059478	5.062764	1.520403
48	6	0	1.061870	0.766345	2.000265	102	1	0	-2.772078	6.653718	3.276263
49	6	0	-0.397556	1.122175	-2.689936	103	1	0	-2.034213	6.324888	5.631787
50	6	0	0.080822	-0.157088	-2.977605	104	1	0	-0.572573	4.392922	6.201818
51	6	0	1.047726	-0.654715	2.171632	105	1	0	0.121115	2.799005	4.444487
52	6	0	1.761758	-1.296280	1.071492	106	1	0	-2.334538	4.974380	-1.120744
53	6	0	-0.248206	-4.003634	-0.554626	107	1	0	-2.834801	6.977471	-2.464789
54	6	0	0.777700	-2.960189	-0.741120	108	1	0	-1.294972	7.677269	-4.293433
55	6	0	2.685496	-0.296852	0.600257	109	1	0	0.762658	6.347106	-4.735829
56	6	0	-1.363805	-3.451067	-2.659444	110	1	0	1.268046	4.350089	-3.381975
57	6	0	-0.817061	-1.178795	-3.386305	111	1	0	3.720953	1.976574	-1.043661
58	6	0	1.273012	-0.891144	-2.365586	112	1	0	4.670435	3.233220	-2.937942
59	6	0	-0.408489	-2.460319	-2.836547	113	1	0	6.520569	2.258094	-4.289566
60	6	0	0.711284	-2.250792	-1.953264	114	1	0	7.391599	-0.006281	-3.744074
61	6	0	-0.456500	2.872355	1.737256	115	1	0	6.417392	-1.288930	-1.870603
62	6	0	-0.159679	3.290789	-1.258663	116	1	0	7.174237	0.182310	0.300616
63	6	0	0.850773	3.737897	-0.231833	117	1	0	8.654463	0.573175	2.237542
64	6	0	0.717591	3.551378	1.077288	118	1	0	7.767280	0.368683	4.550719
65	6	0	-0.504844	4.505877	-2.162723	119	1	0	5.380192	-0.229271	4.912397
66	6	0	-0.937132	3.810095	2.864615	120	1	0	3.894090	-0.623286	2.977709
67	8	0	1.679218	2.225221	-2.419567	121	1	0	3.869219	-2.291871	-2.291925
68	8	0	3.073732	2.003962	1.205748	122	1	0	3.940938	-4.738042	-2.668971
69	6	0	-1.744212	4.910329	2.549143	123	1	0	4.554838	-6.268479	-0.808080
70	6	0	-2.139813	5.809315	3.538030	124	1	0	5.125850	-5.334779	1.424825
71	6	0	-1.724355	5.626441	4.859118	125	1	0	5.083236	-2.896566	1.796398
72	6	0	-0.906242	4.542458	5.178297	---					
73	6	0	-0.513578	3.641454	4.186450	The total electronic energy was calculated to be –4165.2812813 Hartree.					

Table S22. Optimized structure of **INT2e** (B3LYP-D3/6-31G(d))

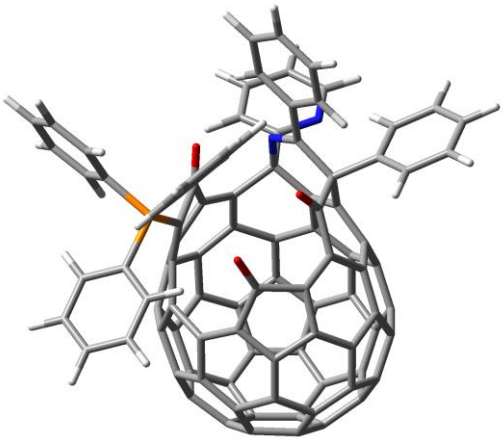


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.135526	-1.423816	1.674627
2	6	0	-4.794812	-0.010358	1.730307
3	6	0	-4.881212	0.758318	0.580679
4	6	0	-5.293114	0.162526	-0.677364
5	6	0	-5.581593	-1.201158	-0.742904
6	6	0	-5.505247	-2.011085	0.459604
7	6	0	-3.677796	0.172439	2.639022
8	6	0	-3.863038	1.742009	0.318384
9	6	0	-4.505185	0.788780	-1.715263
10	6	0	-5.082780	-1.991048	-1.856163
11	6	0	-4.954753	-3.303701	0.091918
12	6	0	-4.263433	-2.122504	2.590982
13	6	0	-4.325295	-1.378714	-2.859641
14	6	0	-4.032527	0.043539	-2.787756
15	6	0	-3.147473	-2.039325	-3.381337
16	6	0	-2.679198	0.266479	-3.250863
17	6	0	-2.651505	1.113023	2.377753
18	6	0	-3.642963	1.778782	-1.111022
19	6	0	-2.146305	-1.019916	-3.622031
20	6	0	-2.372144	2.067119	-1.606854
21	6	0	-2.789688	1.951484	1.192301
22	6	0	-4.680796	-3.286496	-1.335886
23	6	0	-4.085199	-3.965553	0.962553
24	6	0	-1.276455	0.805444	2.799880
25	6	0	-3.746806	-3.377171	2.246524
26	6	0	-3.399117	-1.132732	3.212976
27	6	0	-2.890006	-4.610736	0.445701
28	6	0	-2.363666	-3.703419	2.541863
29	6	0	-2.096207	-1.458410	3.538068
30	6	0	-1.839727	1.253447	-2.696775
31	6	0	-3.532620	-3.915595	-1.831851
32	6	0	-1.619985	2.599560	0.653155
33	6	0	-1.819847	-4.419496	1.406150
34	6	0	-1.557091	-2.773214	3.195760
35	6	0	-1.060711	-0.472673	3.350657
36	6	0	0.116914	-1.192366	2.974197
37	6	0	-0.135127	1.519727	2.210817
38	6	0	-1.433649	2.681543	-0.701808
39	6	0	0.486794	2.129568	-2.200350
40	6	0	-0.188126	-2.582025	2.795692
41	6	0	0.313161	-3.180935	1.632156
42	6	0	1.210250	-2.510482	0.694943
43	6	0	-0.524450	-4.130675	0.947914
44	6	0	-2.749050	-3.273244	-2.866157
45	6	0	2.363298	1.029947	1.165755
46	6	0	-2.609997	-4.572440	-0.917228
47	6	0	-1.257067	-4.296546	-1.372420
48	6	0	1.049300	0.826430	1.957876
49	6	0	-0.398520	1.046999	-2.716474
50	6	0	0.085205	-0.237001	-2.973878
51	6	0	1.037623	-0.588765	2.173112
52	6	0	1.760099	-1.266959	1.098962
53	6	0	-0.234873	-4.022752	-0.456186
54	6	0	0.788249	-2.980957	-0.666817
55	6	0	2.681383	-0.287019	0.597074
56	6	0	-1.344962	-3.528744	-2.578527
57	6	0	-0.805655	-1.272595	-3.361278
58	6	0	1.279363	-0.950873	-2.343575
59	6	0	-0.393120	-2.538419	-2.777478
60	6	0	0.723741	-2.302727	-1.897522
61	6	0	-0.480130	2.901361	1.619373
62	6	0	-0.159427	3.215266	-1.299666
63	6	0	0.840406	3.611574	-0.219723
64	7	0	0.707882	3.508392	1.035299
65	6	0	-0.461185	4.498804	-2.110376
66	6	0	-0.943000	3.908043	2.688153
67	8	0	1.666728	2.196379	-2.501274
68	8	0	3.066224	2.032778	1.090514
69	7	0	-1.806681	4.837446	2.261828
70	6	0	-2.197938	5.776054	3.131632
71	6	0	-1.751483	5.835263	4.451685
72	6	0	-0.840224	4.870586	4.882315
73	6	0	-0.424340	3.889820	3.985077
74	6	0	-1.254286	5.481964	-1.497809
75	6	0	-1.545429	6.667994	-2.168517
76	6	0	-1.049478	6.890034	-3.455737
77	6	0	-0.249480	5.921378	-4.060461
78	6	0	0.050720	4.732372	-3.390430
79	8	0	2.424379	-0.565766	-2.278086
80	15	0	4.328605	-0.639990	0.103113
81	6	0	5.428670	-0.223191	1.510974
82	6	0	5.019977	0.215449	-1.341643
83	6	0	4.476764	-2.438886	-0.158843
84	6	0	4.538185	1.480955	-1.697914
85	6	0	5.093801	2.144783	-2.789634
86	6	0	6.132873	1.562525	-3.517237
87	6	0	6.619466	0.303755	-3.157272
88	6	0	6.062269	-0.374906	-2.073674
89	6	0	6.770736	0.125634	1.306779
90	6	0	7.598555	0.386256	2.398695
91	6	0	7.094673	0.303681	3.697877
92	6	0	5.756915	-0.038169	3.905697
93	6	0	4.924561	-0.298620	2.818216
94	6	0	4.156807	-3.004239	-1.403026
95	6	0	4.191278	-4.388153	-1.565952
96	6	0	4.537201	-5.215082	-0.495764
97	6	0	4.859547	-4.655262	0.741566

98	6	0	4.834212	-3.271687	0.911584	112	1	0	7.424476	-0.155847	-3.724061
99	1	0	1.771454	4.037469	-0.592448	113	1	0	6.430639	-1.362201	-1.810868
100	1	0	-2.902514	6.513596	2.751353	114	1	0	7.167249	0.208035	0.300196
101	1	0	-2.106133	6.616154	5.117529	115	1	0	8.635995	0.662286	2.231908
102	1	0	-0.458865	4.882064	5.899785	116	1	0	7.740733	0.512623	4.546132
103	1	0	0.288400	3.125113	4.274152	117	1	0	5.356546	-0.093114	4.914030
104	1	0	-1.633716	5.317537	-0.491836	118	1	0	3.881432	-0.549082	2.984463
105	1	0	-2.160518	7.420678	-1.682463	119	1	0	3.864770	-2.363302	-2.225441
106	1	0	-1.280854	7.813474	-3.979821	120	1	0	3.935365	-4.819469	-2.529466
107	1	0	0.147870	6.086460	-5.058498	121	1	0	4.554985	-6.293709	-0.625487
108	1	0	0.689483	3.999457	-3.870349	122	1	0	5.131518	-5.293942	1.577041
109	1	0	3.730994	1.935172	-1.140606	123	1	0	5.088542	-2.845593	1.876404
110	1	0	4.696799	3.113996	-3.075654	---					
111	1	0	6.560162	2.084762	-4.369201	The total electronic energy was calculated to be –4197.3569035 Hartree.					

Table S23. Optimized structure of **INT2f** (B3LYP-D3/6-31G(d))



Standard orientation:

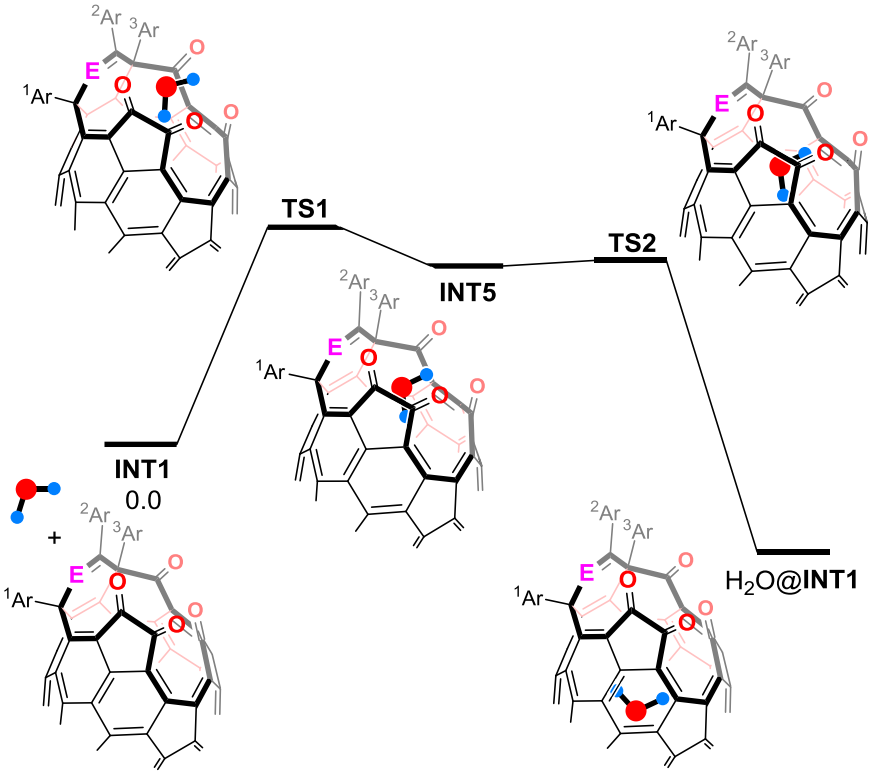
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.619851	0.184859	1.630865
2	6	0	-4.796063	1.375743	1.775816
3	6	0	-4.574967	2.190878	0.676935
4	6	0	-5.143500	1.857100	-0.616434
5	6	0	-5.900697	0.695075	-0.767947
6	6	0	-6.147700	-0.157538	0.381224
7	6	0	-3.708096	1.090278	2.692393
8	6	0	-3.266661	2.756838	0.477188
9	6	0	-4.160355	2.218187	-1.613021
10	6	0	-5.694093	-0.154728	-1.928554
11	6	0	-6.089826	-1.537474	-0.066943
12	6	0	-5.077968	-0.833217	2.501454
13	6	0	-4.746519	0.202467	-2.892971
14	6	0	-3.965110	1.417989	-2.731761
15	6	0	-3.872149	-0.805976	-3.455138
16	6	0	-2.612527	1.165728	-3.179454
17	6	0	-2.406616	1.611888	2.489423
18	6	0	-3.013582	2.793795	-0.947114
19	6	0	-2.566522	-0.202266	-3.630721
20	6	0	-1.713866	2.631305	-1.422271
21	6	0	-2.208595	2.512237	1.360088
22	6	0	-5.795883	-1.536104	-1.490892
23	6	0	-5.536696	-2.518370	0.760360
24	6	0	-1.243544	0.806458	2.889780
25	6	0	-5.038828	-2.167584	2.078875
26	6	0	-3.929386	-0.258877	3.183212
27	6	0	-4.640591	-3.518117	0.203455
28	6	0	-3.871441	-2.985727	2.352323
29	6	0	-2.837952	-1.049459	3.486423
30	6	0	-1.489174	1.749866	-2.562327
31	6	0	-4.939381	-2.505824	-2.025856
32	6	0	-0.872445	2.722812	0.859783
33	6	0	-3.594769	-3.781109	1.173888
34	6	0	-2.799720	-2.448185	3.063312
35	6	0	-1.513432	-0.493296	3.361972
36	6	0	-0.665486	-1.567375	2.944068
37	6	0	0.091254	1.093397	2.344477
38	6	0	-0.632161	2.813648	-0.482588
39	6	0	0.988077	1.695943	-2.004532
40	6	0	-1.444986	-2.739977	2.676584
41	6	0	-1.163841	-3.408398	1.477214
42	6	0	-0.064747	-3.049506	0.583408
43	6	0	-2.271554	-3.951098	0.734902
44	6	0	-3.954697	-2.128537	-3.018091
45	6	0	2.267644	-0.196293	1.300653
46	6	0	-4.334458	-3.502694	-1.154394
47	6	0	-2.962828	-3.705262	-1.591333
48	6	0	0.950674	0.035389	2.061067
49	6	0	-0.220018	1.042044	-2.588359
50	6	0	-0.219272	-0.312078	-2.927268
51	6	0	0.428478	-1.290845	2.183728
52	6	0	0.885812	-2.112045	1.064747
53	6	0	-1.931408	-3.871934	-0.659518
54	6	0	-0.598405	-3.257219	-0.804346
55	6	0	2.108340	-1.493066	0.630226
56	6	0	-2.742621	-2.887742	-2.746674
57	6	0	-1.411986	-0.934021	-3.383850
58	6	0	0.624840	-1.442566	-2.341256
59	6	0	-1.494664	-2.295535	-2.882192
60	6	0	-0.388360	-2.529663	-1.989143
61	6	0	0.282496	2.532760	1.826395
62	6	0	0.761931	2.930015	-1.071474
63	6	0	1.849103	2.956530	0.033782
64	7	0	1.598165	2.740011	1.267721
65	6	0	0.749951	4.259137	-1.862971
66	6	0	0.205296	3.578538	2.960392
67	8	0	2.103493	1.293353	-2.275095
68	8	0	3.289727	0.483162	1.332327
69	6	0	0.578516	3.277959	4.272184
70	6	0	0.544871	4.294819	5.224111
71	6	0	0.145844	5.572424	4.832208
72	6	0	-0.192981	5.773590	3.493730
73	7	0	-0.164558	4.804904	2.571896
74	6	0	0.651845	5.449206	-1.129234
75	6	0	0.597452	6.676564	-1.786813

76	6	0	0.627361	6.731567	-3.182442	106	1	0	0.825584	4.092215	6.254177
77	6	0	0.707548	5.547983	-3.915973	107	1	0	0.100645	6.393991	5.540624
78	6	0	0.766044	4.316427	-3.260185	108	1	0	-0.502121	6.756462	3.142276
79	8	0	1.828818	-1.497370	-2.237785	109	1	0	0.599001	5.407230	-0.043682
80	6	0	5.091518	3.901796	-1.792696	110	1	0	0.526665	7.592263	-1.205934
81	6	0	3.748063	3.596568	-1.573976	111	1	0	0.583610	7.689385	-3.693643
82	6	0	3.281665	3.264736	-0.291918	112	1	0	0.725729	5.577308	-5.002144
83	6	0	4.215725	3.236313	0.761485	113	1	0	0.839279	3.405770	-3.847239
84	6	0	5.557656	3.526352	0.539611	114	1	0	5.419847	4.165737	-2.794901
85	6	0	6.004795	3.867244	-0.739037	115	1	0	3.075927	3.614250	-2.417133
86	15	0	3.532073	-2.368907	0.089962	116	1	0	3.867194	2.955116	1.745546
87	6	0	4.680054	-2.486196	1.517989	117	1	0	6.257976	3.483268	1.369581
88	6	0	4.520245	-1.690321	-1.273968	118	1	0	7.052391	4.100456	-0.912298
89	6	0	3.035855	-4.077941	-0.313360	119	1	0	4.012568	0.364768	-0.830746
90	6	0	4.582911	-0.303438	-1.461165	120	1	0	5.416117	1.291958	-2.615913
91	6	0	5.386127	0.216703	-2.474410	121	1	0	6.753256	-0.222397	-4.082310
92	6	0	6.130369	-0.634340	-3.292483	122	1	0	6.649915	-2.683216	-3.738090
93	6	0	6.074123	-2.016920	-3.101481	123	1	0	5.220935	-3.625094	-1.957956
94	6	0	5.269319	-2.548937	-2.094473	124	1	0	6.474229	-2.625950	0.320871
95	6	0	6.060502	-2.632573	1.323851	125	1	0	7.979107	-2.875821	2.263775
96	6	0	6.909612	-2.768632	2.421990	126	1	0	7.054453	-2.856721	4.571251
97	6	0	6.389810	-2.756046	3.717550	127	1	0	4.607408	-2.583609	4.922035
98	6	0	5.015925	-2.604690	3.915653	128	1	0	3.096898	-2.335740	2.981009
99	6	0	4.162571	-2.467703	2.821759	129	1	0	2.578554	-3.662092	-2.379613
100	6	0	2.587796	-4.413168	-1.600443	130	1	0	1.783956	-5.954398	-2.861594
101	6	0	2.134284	-5.704732	-1.864183	131	1	0	1.753931	-7.668901	-1.060530
102	6	0	2.116017	-6.665883	-0.852167	132	1	0	2.552275	-7.080220	1.220077
103	6	0	2.562653	-6.336434	0.428505	133	1	0	3.373142	-4.804876	1.696858
104	6	0	3.025733	-5.049629	0.698642	---					
105	1	0	0.886529	2.271684	4.534050	The total electronic energy was calculated to be –4428.4291253 Hartree.					

7. Mechanistic Studies on H_2O-Insertion into INT1

The energy profile for H_2O-insertion into **INT1** was calculated at the B3LYP-D3/6-31G(d) level of theory. The transition state **TS1f** was calculated under a fix option (C(7)···H(103) as 6.08077 Å) based on optimized structures of **TS1c** and **TS1e**.

Table S24. Change in Gibbs energies (ΔG, kcal/mol) on a profile for H_2O-insertion into **INT1** (B3LYP-D3/6-31G(d)) at 298 K)



Addends	**TS1**	**INT5**	**TS2**	H_2O@**INT1**
a	+21.6	+17.1	+17.5	–10.0
b	+21.7	+17.2	+17.6	–9.3
c	+21.4	+16.9	+17.2	–8.9
d	+22.0	+17.5	+18.2	–9.7
e	+21.0	+17.3	+17.8	–8.9
f	+21.0	+17.3	+17.8	–10.4

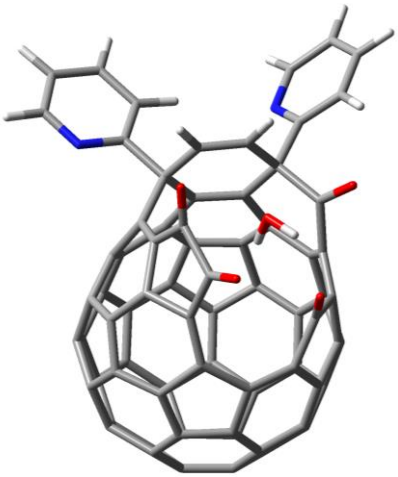
Table S25. Optimized structure of H_2O (B3LYP-D3/6-31G(d))

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.000000	0.000000	0.119774
2	1	0	-0.000000	0.761454	-0.479095
3	1	0	-0.000000	-0.761454	-0.479095

The total electronic energy was calculated to be –76.4089616 Hartree.

Table S26. Optimized structure of **TS1a** (B3LYP-D3/6-31G(d))



Standard orientation:

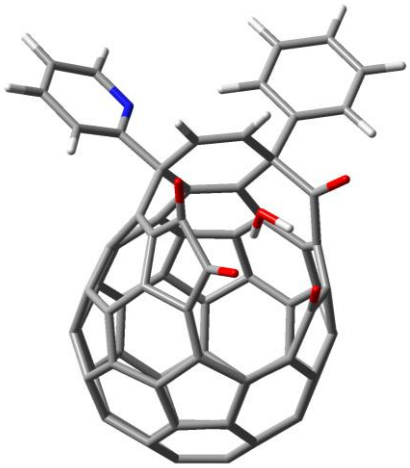
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.657692	1.533494	-3.223125
2	6	0	-1.205515	1.577618	-3.270795
3	6	0	-0.494721	0.413088	-3.505819
4	6	0	-1.188072	-0.849391	-3.695569
5	6	0	-2.578992	-0.903766	-3.609020
6	6	0	-3.329170	0.315672	-3.364677
7	6	0	-0.726954	2.524768	-2.281745
8	6	0	0.716638	0.169128	-2.768361
9	6	0	-0.378634	-1.871124	-3.072128
10	6	0	-3.213326	-1.984234	-2.871087
11	6	0	-4.429280	-0.009405	-2.473135
12	6	0	-3.090260	2.496380	-2.233104
13	6	0	-2.425752	-2.970962	-2.270167
14	6	0	-0.978633	-2.916150	-2.379945
15	6	0	-2.742274	-3.432092	-0.933124
16	6	0	-0.399723	-3.336281	-1.123709
17	6	0	0.438762	2.278070	-1.518689
18	6	0	0.809145	-1.254505	-2.528735
19	6	0	-1.489304	-3.654712	-0.238027
20	6	0	1.431362	-1.713975	-1.373230
21	6	0	1.195461	1.065377	-1.805385
22	6	0	-4.347922	-1.426014	-2.156303
23	6	0	-4.830071	0.905063	-1.496724
24	6	0	0.516803	2.785231	-0.141461
25	6	0	-4.166005	2.193488	-1.386829
26	6	0	-1.906761	3.139778	-1.697701
27	6	0	-5.129310	0.444138	-0.151455
28	6	0	-4.094389	2.544377	0.015277
29	6	0	-1.869970	3.535067	-0.373078
30	6	0	0.784836	-2.780446	-0.610411
31	6	0	-4.645481	-1.868021	-0.861725
32	6	0	2.130498	0.558526	-0.823025
33	6	0	-4.646480	1.439584	0.785007
34	6	0	-2.990917	3.231027	0.507048
35	6	0	-0.644966	3.390755	0.372757
36	6	0	-1.025529	3.100602	1.724193
37	6	0	1.525507	2.267647	0.791047
38	6	0	2.291637	-0.796441	-0.659942
39	6	0	2.448240	-2.483662	1.209607
40	6	0	-2.429697	2.877450	1.790817
41	6	0	-2.871180	1.739660	2.478635
42	6	0	-1.972147	0.838473	3.188206
43	6	0	-4.011925	1.031420	1.962174
44	6	0	-3.821871	-2.883976	-0.242539
45	6	0	1.786299	1.681677	3.447392
46	6	0	-5.020901	-0.907027	0.165791
47	6	0	-4.386431	-1.310436	1.409530
48	6	0	1.189526	2.154026	2.137099
49	6	0	1.004751	-2.755148	0.830070
50	6	0	-0.102999	-2.923139	1.670759
51	6	0	-0.192181	2.349027	2.508570
52	6	0	-0.655795	1.297265	3.384720
53	6	0	-3.835583	-0.361975	2.278144

54	6	0	-2.562892	-0.552958	2.989051
55	6	0	0.564946	1.005855	4.220563
56	6	0	-3.673462	-2.529774	1.160250
57	6	0	-1.354271	-3.316376	1.100970
58	6	0	-2.464858	-2.709689	1.810021
59	6	0	-1.936029	-1.789203	2.785856
60	6	0	2.749182	1.587231	0.127595
61	6	0	3.232570	-1.425323	0.340514
62	6	0	3.891605	-0.379799	1.218026
63	6	0	3.684730	0.931711	1.115849
64	6	0	4.387277	-2.119369	-0.438974
65	6	0	3.584305	2.602294	-0.678031
66	8	0	2.988874	-3.173207	2.048112
67	8	0	2.860309	1.937378	3.928913
68	6	0	4.501125	2.135613	-1.630853
69	6	0	5.272093	3.068075	-2.316989
70	6	0	5.109095	4.425084	-2.027144
71	6	0	4.176920	4.783178	-1.055477
72	7	0	3.424160	3.896240	-0.388643
73	7	0	4.576206	-1.675659	-1.688935
74	6	0	5.592406	-2.181567	-2.397101
75	6	0	6.471187	-3.143464	-1.901587
76	6	0	6.279287	-3.590007	-0.594668
77	6	0	5.225947	-3.070641	0.155542
78	8	0	0.612897	0.522986	5.323524
79	6	0	-0.501315	-2.242775	2.997618
80	8	0	0.129936	-2.099125	4.022963
81	1	0	4.557932	-0.770162	1.979198
82	1	0	4.179299	1.607123	1.806109
83	1	0	4.595455	1.069055	-1.817762
84	1	0	5.989631	2.743171	-3.065739
85	1	0	5.690108	5.186336	-2.538840
86	1	0	4.020956	5.828416	-0.794684
87	1	0	5.704647	-1.794462	-3.408344
88	1	0	7.279493	-3.522946	-2.519082
89	1	0	6.941407	-4.333404	-0.159193
90	1	0	5.049046	-3.393697	1.173219
91	8	0	2.087207	-0.694116	3.032831
92	1	0	1.731877	-1.322911	3.688849
93	1	0	1.388805	-0.630451	2.365926

An imaginary frequency was found at –83.87 cm^{-1}.

The total electronic energy was calculated to be –3312.6077607 Hartree.

Table S27. Optimized structure of **TS1b** (B3LYP-D3/6-31G(d))

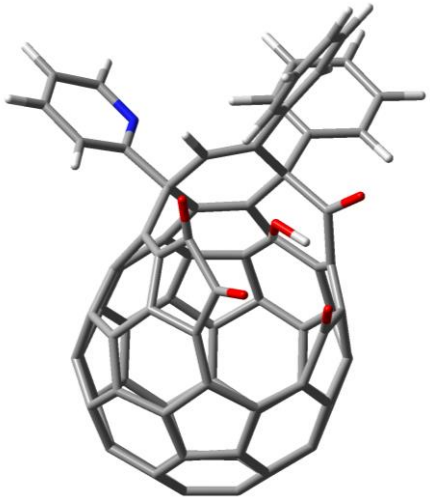


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.584146	1.024346	-3.462966
2	6	0	-1.130657	1.047730	-3.494927
3	6	0	-0.429587	-0.145619	-3.527525
4	6	0	-1.135662	-1.415808	-3.523976
5	6	0	-2.528192	-1.443161	-3.452357
6	6	0	-3.268237	-0.193905	-3.419250
7	6	0	-0.655814	2.134493	-2.660188
8	6	0	0.770181	-0.279001	-2.744721
9	6	0	-0.347886	-2.332079	-2.732458
10	6	0	-3.185358	-2.385477	-2.561854
11	6	0	-4.384885	-0.362101	-2.504796
12	6	0	-3.020237	2.136350	-2.646474
13	6	0	-2.418072	-3.269832	-1.797313
14	6	0	-0.969300	-3.245735	-1.890197
15	6	0	-2.760024	-3.508717	-0.409223
16	6	0	-0.413774	-3.464163	-0.573300
17	6	0	0.497617	2.001435	-1.850509
18	6	0	0.838919	-1.646325	-2.276523
19	6	0	-1.519960	-3.628563	0.333258
20	6	0	1.435523	-1.917500	-1.050900
21	6	0	1.250951	0.756324	-1.933102
22	6	0	-4.324874	-1.710824	-1.964496
23	6	0	-4.789174	0.700119	-1.693835
24	6	0	0.555861	2.715333	-0.566071
25	6	0	-4.112080	1.983123	-1.780671
26	6	0	-1.837123	2.845345	-2.200645
27	6	0	-5.113893	0.463000	-0.297556
28	6	0	-4.057989	2.553433	-0.451651
29	6	0	-1.816665	3.448534	-0.956640
30	6	0	0.768852	-2.842977	-0.136042
31	6	0	-4.646207	-1.937181	-0.620682
32	6	0	2.169631	0.407345	-0.870878
33	6	0	-4.633256	1.590667	0.475780
34	6	0	-2.954824	3.300784	-0.058091
35	6	0	-0.605230	3.410847	-0.176042
36	6	0	-1.011065	3.346262	1.197633
37	6	0	1.538381	2.336580	0.460141
38	6	0	2.295761	-0.905586	-0.479787
39	6	0	2.403716	-2.250610	1.646003
40	6	0	-2.418232	3.152048	1.275242
41	6	0	-2.880723	2.141841	2.128338
42	6	0	-2.004087	1.359400	2.991692
43	6	0	-4.020768	1.369956	1.712827
44	6	0	-3.843413	-2.847882	0.167144
45	6	0	1.755173	2.211203	3.183345
46	6	0	-5.026192	-0.820909	0.233753
47	6	0	-4.414650	-1.025859	1.536413
48	6	0	1.181853	2.457471	1.800549
49	6	0	0.968962	-2.590096	1.285224
50	6	0	-0.154504	-2.613113	2.122713
51	6	0	-0.200754	2.727251	2.110732
52	6	0	-0.688030	1.836810	3.139984
53	6	0	-3.865667	0.044293	2.251231
54	6	0	-2.606909	-0.041909	3.005624
55	6	0	0.516652	1.680941	4.036471
56	6	0	-3.711724	-2.275655	1.497783
57	6	0	-1.401043	-3.082651	1.603949

58	6	0	-2.515408	-2.360481	2.188779	78	8	0	0.539528	1.392123	5.205709
59	6	0	-1.990517	-1.300006	3.013279	79	6	0	-0.561495	-1.722465	3.314500
60	6	0	2.775884	1.563100	-0.069340	80	8	0	0.063291	-1.410229	4.305672
61	6	0	3.218857	-1.387838	0.616586	81	1	0	4.549852	-0.508536	2.133449
62	6	0	3.890518	-0.229743	1.319145	82	1	0	4.197748	1.819794	1.601465
63	6	0	3.696984	1.053542	1.018444	83	1	0	3.242013	4.295906	0.083514
64	6	0	4.320616	-2.248460	-0.069861	84	1	0	4.755804	5.637768	-1.386699
65	6	0	3.634092	2.459894	-0.984434	85	1	0	5.958762	4.467947	-3.263030
66	8	0	2.920208	-2.750738	2.622398	86	1	0	5.595482	2.011495	-3.552162
67	8	0	2.820234	2.558785	3.626543	87	1	0	4.872742	-0.591384	-1.342021
68	6	0	3.779162	3.828705	-0.735508	88	1	0	6.631916	-1.836192	-2.541088
69	6	0	4.624439	4.572671	-1.556583	89	1	0	7.091536	-4.220046	-1.973946
70	6	0	5.293891	3.928011	-2.596067	90	1	0	5.771177	-5.325502	-0.177974
71	6	0	5.089715	2.557189	-2.757665	91	1	0	4.035833	-4.086689	1.034585
72	7	0	4.283624	1.832892	-1.973912	92	8	0	1.999046	-0.142739	3.115001
73	6	0	5.071278	-1.627664	-1.081330	93	1	0	1.665537	-0.686115	3.854022
74	6	0	6.061458	-2.333208	-1.760690	94	1	0	1.336459	-0.255028	2.418894
75	6	0	6.319406	-3.669118	-1.443585						
76	6	0	5.578528	-4.288221	-0.438814	An imaginary frequency was found at –81.56 cm^{-1}.					
77	6	0	4.583980	-3.584479	0.247261	The total electronic energy was calculated to be –3296.5688033 Hartree.					

Table S28. Optimized structure of **TS1c** (B3LYP-D3/6-31G(d))



Standard orientation:

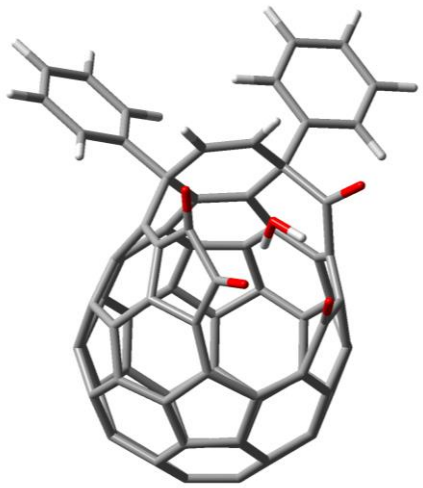
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.778004	0.282465	3.105835
2	6	0	-2.366335	0.312224	3.452433
3	6	0	-1.623821	1.451712	3.193316
4	6	0	-2.243497	2.610318	2.571821
5	6	0	-3.587174	2.570837	2.199369
6	6	0	-4.370736	1.378222	2.471693
7	6	0	-1.787983	-0.992604	3.195495
8	6	0	-0.282534	1.317837	2.691411
9	6	0	-1.259380	3.188322	1.686269
10	6	0	-3.991830	3.095376	0.904848
11	6	0	-5.261628	1.163655	1.343834
12	6	0	-4.095038	-1.064869	2.684305
13	6	0	-3.034496	3.651750	0.050989
14	6	0	-1.641023	3.706978	0.455036
15	6	0	-3.063711	3.343928	-1.365190
16	6	0	-0.811190	3.435219	-0.697138
17	6	0	-0.487418	-1.136456	2.655154
18	6	0	-0.041684	2.416544	1.780745
19	6	0	-1.691308	3.212703	-1.813959
20	6	0	0.810657	2.230260	0.700005
21	6	0	0.297241	0.069770	2.434457
22	6	0	-5.015730	2.214933	0.369832
23	6	0	-5.546111	-0.134582	0.915794
24	6	0	-0.202769	-2.270771	1.764159
25	6	0	-4.973718	-1.274189	1.612315
26	6	0	-2.884949	-1.855368	2.791840
27	6	0	-5.562144	-0.443825	-0.503778
28	6	0	-4.679148	-2.297980	0.632749
29	6	0	-2.640583	-2.877186	1.893091
30	6	0	0.400772	2.730545	-0.607624
31	6	0	-5.036625	1.915030	-0.997783
32	6	0	1.431835	0.026539	1.536784
33	6	0	-4.997613	-1.766543	-0.684419
34	6	0	-3.561308	-3.108962	0.786604
35	6	0	-1.294062	-3.095746	1.426163
36	6	0	-1.406479	-3.564212	0.076706
37	6	0	0.986279	-2.268982	0.898224
38	6	0	1.715480	1.100453	0.733927
39	6	0	2.335923	1.562649	-1.650370
40	6	0	-2.756129	-3.456837	-0.361555
41	6	0	-2.978696	-2.853086	-1.606116
42	6	0	-1.901567	-2.426681	-2.491762
43	6	0	-4.134292	-2.009941	-1.757120
44	6	0	-4.036936	2.486396	-1.874485
45	6	0	1.753011	-3.209711	-1.553306
46	6	0	-5.292641	0.551553	-1.439225
47	6	0	-4.413922	0.271280	-2.562394
48	6	0	0.903468	-2.892695	-0.341624
49	6	0	0.879837	1.966240	-1.750359
50	6	0	-0.039581	1.635337	-2.753213
51	6	0	-0.396202	-3.305820	-0.808934
52	6	0	-0.610867	-2.886712	-2.174444
53	6	0	-3.794873	-0.975487	-2.699723
54	6	0	-2.403500	-1.146028	-3.142002
55	6	0	0.756381	-3.063528	-2.788600
56	6	0	-3.661789	1.461389	-2.836507
57	6	0	-1.337957	2.231008	-2.730288
58	6	0	-0.231210	0.338136	-3.561109
59	6	0	-2.342277	1.310685	-3.228560
60	6	0	-1.718243	0.032491	-3.462721
61	6	0	2.126986	-1.315216	1.344228

62	6	0	2.892056	1.197964	-0.222218
63	6	0	3.714454	-0.104275	-0.275091
64	6	0	3.293816	-1.199019	0.386794
65	6	0	3.722044	2.380311	0.349561
66	6	0	2.746810	-1.791946	2.676653
67	8	0	3.050832	1.637313	-2.626281
68	8	0	2.840343	-3.732636	-1.569454
69	6	0	2.890722	-3.152457	2.966588
70	6	0	3.521121	-3.519873	4.153989
71	6	0	3.983722	-2.520223	5.008925
72	6	0	3.800387	-1.191149	4.625406
73	7	0	3.201003	-0.826915	3.486579
74	6	0	4.235963	2.230393	1.646635
75	6	0	4.970408	3.257169	2.234489
76	6	0	5.190523	4.452229	1.543977
77	6	0	4.667413	4.609308	0.261267
78	6	0	3.934762	3.579645	-0.335496
79	8	0	0.575382	-0.321527	-4.178802
80	8	0	1.027239	-3.266450	-3.944299
81	6	0	7.148153	0.664726	-1.789278
82	6	0	5.956819	0.818130	-1.079954
83	6	0	4.976055	-0.189207	-1.081396
84	6	0	5.242574	-1.357326	-1.821729
85	6	0	6.434232	-1.508464	-2.526214
86	6	0	7.396040	-0.497315	-2.517743
87	1	0	3.885539	-2.105134	0.306751
88	1	0	2.519085	-3.901376	2.274659
89	1	0	3.647425	-4.569232	4.405718
90	1	0	4.477397	-2.759541	5.945627
91	1	0	4.151470	-0.378387	5.258579
92	1	0	4.058039	1.306490	2.191539
93	1	0	5.370488	3.123196	3.236022
94	1	0	5.763976	5.252868	2.003025
95	1	0	4.832942	5.532535	-0.287420
96	1	0	3.567066	3.712699	-1.346272
97	1	0	7.885897	1.462784	-1.763664
98	1	0	5.814923	1.724300	-0.511090
99	1	0	4.497555	-2.139276	-1.875584
100	1	0	6.601419	-2.419350	-3.095182
101	1	0	8.323271	-0.612823	-3.073171
102	8	0	2.396204	-1.122673	-2.508734
103	1	0	2.178581	-0.845621	-3.416483
104	1	0	1.826522	-0.572253	-1.960262

An imaginary frequency was found at –94.30 cm^{-1}.

The total electronic energy was calculated to be –3527.6355484 Hartree.

Table S29. Optimized structure of **TS1d** (B3LYP-D3/6-31G(d))



Standard orientation:

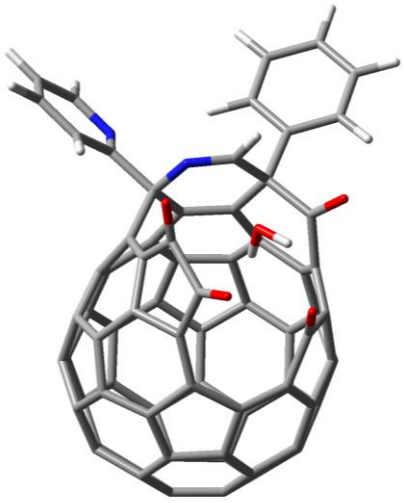
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.565581	0.994379	-3.484027
2	6	0	-1.112066	0.994916	-3.515602
3	6	0	-0.429027	-0.209089	-3.526665
4	6	0	-1.154120	-1.468001	-3.498084
5	6	0	-2.547009	-1.473011	-3.426546
6	6	0	-3.267970	-0.212359	-3.417764
7	6	0	-0.620726	2.090379	-2.701579
8	6	0	0.768568	-0.345180	-2.740505
9	6	0	-0.380704	-2.380109	-2.687845
10	6	0	-3.218660	-2.387761	-2.518213
11	6	0	-4.387769	-0.346188	-2.501395
12	6	0	-2.984527	2.128185	-2.688676
13	6	0	-2.465171	-3.268280	-1.735694
14	6	0	-1.016147	-3.266245	-1.827138
15	6	0	-2.811819	-3.475359	-0.343777
16	6	0	-0.464972	-3.465655	-0.505169
17	6	0	0.530437	1.956236	-1.889977
18	6	0	0.816120	-1.703752	-2.244485
19	6	0	-1.574306	-3.598042	0.402536
20	6	0	1.409112	-1.959593	-1.013679
21	6	0	1.265072	0.698751	-1.949269
22	6	0	-4.348879	-1.685133	-1.935554
23	6	0	-4.775540	0.737297	-1.710795
24	6	0	0.599998	2.690422	-0.618757
25	6	0	-4.078938	2.008084	-1.821063
26	6	0	-1.790903	2.827416	-2.255702
27	6	0	-5.105453	0.531800	-0.310898
28	6	0	-4.016656	2.602213	-0.502867
29	6	0	-1.760962	3.451965	-1.022426
30	6	0	0.726068	-2.853257	-0.078263
31	6	0	-4.674712	-1.880941	-0.587958
32	6	0	2.182101	0.357685	-0.881219
33	6	0	-4.608409	1.666426	0.441700
34	6	0	-2.901629	3.338702	-0.122065
35	6	0	-0.550493	3.408893	-0.240577
36	6	0	-0.957563	3.374411	1.133863
37	6	0	1.575732	2.311501	0.412769
38	6	0	2.290664	-0.951806	-0.467353
39	6	0	2.378167	-2.272573	1.683973
40	6	0	-2.367984	3.205616	1.214177
41	6	0	-2.849310	2.220893	2.086507
42	6	0	-1.986793	1.440263	2.965132
43	6	0	-4.001400	1.459726	1.683788
44	6	0	-3.886516	-2.788528	0.218184
45	6	0	1.788961	2.221359	3.136296
46	6	0	-5.038817	-0.743142	0.244623
47	6	0	-4.432825	-0.932918	1.552108
48	6	0	1.220298	2.457043	1.750782
49	6	0	0.928664	-2.574579	1.339077
50	6	0	-0.196169	-2.567186	2.174232
51	6	0	-0.157809	2.756023	2.056825
52	6	0	-0.661419	1.894409	3.102380
53	6	0	-3.868554	0.142114	2.247412
54	6	0	-2.613030	0.050479	3.005986
55	6	0	0.540999	1.728279	3.998875

56	6	0	-3.748435	-2.193641	1.538094
57	6	0	-1.448816	-3.029595	1.662309
58	6	0	-2.554593	-2.283370	2.232871
59	6	0	-2.016305	-1.216174	3.039316
60	6	0	2.809820	1.520657	-0.104647
61	6	0	3.202505	-1.426713	0.642716
62	6	0	3.878999	-0.265548	1.332828
63	6	0	3.708289	1.013702	1.003287
64	6	0	4.278802	-2.325933	-0.026291
65	6	0	3.676052	2.418047	-1.013792
66	8	0	2.905489	-2.812229	2.631151
67	8	0	2.860953	2.550804	3.576183
68	6	0	4.323383	1.896287	-2.139906
69	6	0	5.161210	2.701657	-2.912414
70	6	0	5.367171	4.037986	-2.565978
71	6	0	4.733561	4.561844	-1.437569
72	6	0	3.895023	3.756530	-0.666815
73	6	0	5.289887	-1.701094	-0.769832
74	6	0	6.240019	-2.455512	-1.456010
75	6	0	6.193553	-3.850244	-1.412577
76	6	0	5.190228	-4.479097	-0.675691
77	6	0	4.237956	-3.724001	0.012105
78	8	0	0.561923	1.454351	5.171724
79	6	0	-0.594824	-1.653974	3.352073
80	8	0	0.028889	-1.338926	4.342961
81	1	0	4.528822	-0.537694	2.156985
82	1	0	4.216314	1.783658	1.574339
83	1	0	4.170768	0.857480	-2.417152
84	1	0	5.651374	2.282513	-3.787128
85	1	0	6.017317	4.665687	-3.169108
86	1	0	4.890151	5.599441	-1.155309
87	1	0	3.408252	4.169484	0.212618
88	1	0	5.333614	-0.616886	-0.804987
89	1	0	7.017867	-1.950706	-2.022767
90	1	0	6.933991	-4.440736	-1.945131
91	1	0	5.145697	-5.563816	-0.628551
92	1	0	3.477381	-4.239363	0.587545
93	8	0	2.011770	-0.170348	3.126216
94	1	0	1.653688	-0.674363	3.881449
95	1	0	1.323930	-0.237883	2.449005

An imaginary frequency was found at –73.25 cm^{-1}.

The total electronic energy was calculated to be –3280.5291721 Hartree.

Table S30. Optimized structure of **TS1e** (B3LYP-D3/6-31G(d))



Standard orientation:

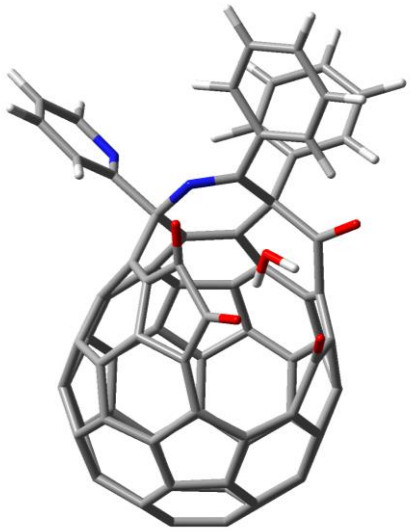
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.682643	0.995813	-3.435213
2	6	0	-1.230813	0.985274	-3.510451
3	6	0	-0.557855	-0.224124	-3.545819
4	6	0	-1.291617	-1.477655	-3.499158
5	6	0	-2.681645	-1.471777	-3.384545
6	6	0	-3.392244	-0.205622	-3.350742
7	6	0	-0.707808	2.074098	-2.706784
8	6	0	0.662171	-0.372480	-2.797589
9	6	0	-0.500453	-2.399326	-2.716852
10	6	0	-3.331904	-2.383265	-2.457458
11	6	0	-4.484171	-0.332933	-2.400411
12	6	0	-3.069360	2.130880	-2.625290
13	6	0	-2.561747	-3.272304	-1.701327
14	6	0	-1.116215	-3.283914	-1.839570
15	6	0	-2.865503	-3.477962	-0.299070
16	6	0	-0.525224	-3.493334	-0.536228
17	6	0	0.464086	1.926417	-1.927817
18	6	0	0.715686	-1.733875	-2.309729
19	6	0	-1.606221	-3.612581	0.406922
20	6	0	1.346046	-2.003106	-1.099687
21	6	0	1.187078	0.665859	-2.017606
22	6	0	-4.437322	-1.673018	-1.838091
23	6	0	-4.840865	0.751727	-1.597041
24	6	0	0.576526	2.654185	-0.654550
25	6	0	-4.138680	2.017606	-1.726046
26	6	0	-1.858260	2.819376	-2.225800
27	6	0	-5.129450	0.546154	-0.187894
28	6	0	-4.033607	2.609920	-0.409855
29	6	0	-1.786842	3.442129	-0.993422
30	6	0	0.684622	-2.892779	-0.147641
31	6	0	-4.722525	-1.868721	-0.481286
32	6	0	2.123468	0.311255	-0.977115
33	6	0	-4.603349	1.676703	0.550878
34	6	0	-2.902714	3.338496	-0.061202
35	6	0	-0.554998	3.388215	-0.246049
36	6	0	-0.923758	3.361913	1.138894
37	6	0	1.571528	2.266834	0.355267
38	6	0	2.233143	-0.994885	-0.569708
39	6	0	2.376734	-2.291741	1.577247
40	6	0	-2.332658	3.202765	1.259359
41	6	0	-2.794432	2.219939	2.144441
42	6	0	-1.910839	1.433577	2.996490
43	6	0	-3.961106	1.464750	1.774279
44	6	0	-3.915365	-2.782595	0.298343
45	6	0	1.865739	2.230930	3.082261
46	6	0	-5.053101	-0.729942	0.363559
47	6	0	-4.407598	-0.925425	1.651192
48	6	0	1.264339	2.431671	1.701977
49	6	0	0.931295	-2.612520	1.260690
50	6	0	-0.164688	-2.593644	2.132138
51	6	0	-0.102619	2.742684	2.041936
52	6	0	-0.581614	1.883494	3.101532
53	6	0	-3.817201	0.145087	2.331085
54	6	0	-2.537745	0.045950	3.048338
55	6	0	0.640554	1.720661	3.971202
56	6	0	-3.730479	-2.189420	1.613589
57	6	0	-1.435943	-3.045160	1.662653

58	6	0	-2.514209	-2.286271	2.267804
59	6	0	-1.941233	-1.221543	3.054081
60	6	0	2.771833	1.438505	-0.174520
61	6	0	3.162008	-1.432993	0.532312
62	6	0	3.793296	-0.214902	1.216534
63	7	0	3.636674	1.008470	0.918955
64	6	0	4.339527	-2.221686	-0.108799
65	6	0	3.677263	2.323372	-1.054808
66	8	0	2.911769	-2.784648	2.548470
67	8	0	2.922732	2.620044	3.501649
68	6	0	4.166465	3.527721	-0.535431
69	6	0	5.012601	4.293506	-1.329964
70	6	0	5.344993	3.828331	-2.605236
71	6	0	4.821998	2.605535	-3.018962
72	7	0	4.002851	1.859045	-2.262797
73	6	0	5.001400	-1.615452	-1.189734
74	6	0	6.069943	-2.254534	-1.814584
75	6	0	6.495931	-3.508843	-1.373341
76	6	0	5.846168	-4.111557	-0.297504
77	6	0	4.776969	-3.473336	0.337027
78	8	0	0.684831	1.445503	5.143172
79	6	0	-0.508101	-1.662779	3.312359
80	8	0	0.162573	-1.338382	4.268161
81	1	0	4.470949	-0.457474	2.032077
82	1	0	3.898964	3.827084	0.472812
83	1	0	5.410995	5.234640	-0.961247
84	1	0	6.000591	4.394697	-3.259609
85	1	0	5.067288	2.198086	-3.997831
86	1	0	4.678765	-0.643380	-1.552580
87	1	0	6.568333	-1.768246	-2.648882
88	1	0	7.327933	-4.008927	-1.861613
89	1	0	6.169963	-5.085287	0.060109
90	1	0	4.303242	-3.955714	1.182129
91	8	0	2.213662	-0.164018	3.166932
92	1	0	1.923335	-0.682761	3.939088
93	1	0	1.478313	-0.273263	2.548611

An imaginary frequency was found at –77.56 cm^{-1}.

The total electronic energy was calculated to be –3312.6065075 Hartree.

Table S31. Optimized structure of **TS1f** (B3LYP-D3/6-31G(d))



Standard orientation:

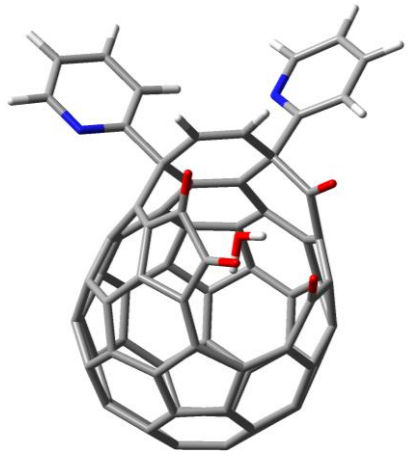
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.722091	2.575897	-1.908903
2	6	0	-2.302557	2.791854	-2.136838
3	6	0	-1.603936	1.922893	-2.959356
4	6	0	-2.276712	0.799039	-3.587709
5	6	0	-3.630059	0.567133	-3.341491
6	6	0	-4.367226	1.475126	-2.480051
7	6	0	-1.693810	3.262759	-0.906927
8	6	0	-0.275957	1.514548	-2.586709
9	6	0	-1.338314	-0.300443	-3.601151
10	6	0	-4.093253	-0.785739	-3.078568
11	6	0	-5.286970	0.683049	-1.681273
12	6	0	-4.009453	2.962824	-0.544091
13	6	0	-3.182627	-1.846387	-3.093047
14	6	0	-1.778337	-1.598074	-3.367989
15	6	0	-3.250423	-2.869574	-2.068691
16	6	0	-0.980599	-2.455477	-2.521910
17	6	0	-0.408268	2.826904	-0.504057
18	6	0	-0.093923	0.143361	-3.013674
19	6	0	-1.890363	-3.237420	-1.725966
20	6	0	0.731013	-0.703159	-2.277698
21	6	0	0.328050	1.950513	-1.403857
22	6	0	-5.107281	-0.714138	-2.041123
23	6	0	-5.545537	1.037841	-0.355803
24	6	0	-0.114369	2.679895	0.929622
25	6	0	-4.914121	2.213357	0.220687
26	6	0	-2.773822	3.430996	0.050723
27	6	0	-5.596544	0.012116	0.672229
28	6	0	-4.616645	1.928994	1.608265
29	6	0	-2.523830	3.214518	1.394206
30	6	0	0.252175	-2.049580	-1.984415
31	6	0	-5.164882	-1.700863	-1.049368
32	6	0	1.428048	1.168882	-0.888674
33	6	0	-4.993682	0.548882	1.876166
34	6	0	-3.467888	2.446111	2.195292
35	6	0	-1.186293	2.884954	1.819412
36	6	0	-1.320886	2.003587	2.942977
37	6	0	1.044964	1.902386	1.386585
38	6	0	1.662019	-0.102874	-1.343097
39	6	0	2.192280	-2.387619	-0.475137
40	6	0	-2.685931	1.631704	3.097596
41	6	0	-2.968054	0.269769	3.264554
42	6	0	-1.933956	-0.751688	3.370816
43	6	0	-4.156004	-0.259920	2.649804
44	6	0	-4.214091	-2.791681	-1.064991
45	6	0	1.788957	0.274728	3.448905
46	6	0	-5.391170	-1.323885	0.338793
47	6	0	-4.542143	-2.157308	1.173633
48	6	0	0.958602	1.199922	2.582844
49	6	0	0.708323	-2.603526	-0.721105
50	6	0	-0.226253	-3.244669	0.098362
51	6	0	-0.343158	1.077527	3.193756
52	6	0	-0.618117	-0.292263	3.568352
53	6	0	-3.883893	-1.626453	2.288151
54	6	0	-2.504228	-1.972587	2.658019
55	6	0	0.737145	-0.798565	3.991824
56	6	0	-3.840308	-3.066135	0.313604
57	6	0	-1.539920	-3.494852	-0.408379
58	6	0	-2.532815	-3.380975	0.642801
59	6	0	-1.876815	-2.923057	1.843321

60	6	0	2.159487	1.700380	0.333338
61	6	0	2.800833	-0.981101	-0.847558
62	6	0	3.563700	-0.268292	0.320237
63	7	0	3.236746	0.862637	0.814404
64	6	0	3.827474	-1.088426	-2.015108
65	6	0	2.860529	3.044218	0.030476
66	8	0	2.848521	-3.371130	-0.200667
67	8	0	2.908521	0.419780	3.860360
68	6	0	3.354053	3.816936	1.087924
69	6	0	4.034175	4.991912	0.786458
70	6	0	4.204534	5.348042	-0.554307
71	6	0	3.693131	4.498678	-1.532512
72	7	0	3.033296	3.364585	-1.253421
73	6	0	4.208844	0.109521	-2.642963
74	6	0	5.154950	0.105538	-3.665338
75	6	0	5.735110	-1.093072	-4.084085
76	6	0	5.364023	-2.283095	-3.460988
77	6	0	4.421249	-2.284720	-2.429936
78	8	0	0.995397	-1.721513	4.722426
79	6	0	-0.407097	-3.253163	1.626724
80	8	0	0.396174	-3.485273	2.505183
81	6	0	4.899359	-0.781270	0.767124
82	6	0	5.951491	0.150240	0.761041
83	6	0	7.236051	-0.219740	1.149775
84	6	0	7.489190	-1.527254	1.568281
85	6	0	6.447382	-2.454774	1.590965
86	6	0	5.162491	-2.090478	1.188132
87	1	0	3.219998	3.479104	2.110226
88	1	0	4.430199	5.617724	1.581402
89	1	0	4.728396	6.256570	-0.835159
90	1	0	3.815914	4.728867	-2.589059
91	1	0	3.771620	1.054134	-2.332005
92	1	0	5.437011	1.044726	-4.133846
93	1	0	6.472105	-1.097726	-4.882606
94	1	0	5.813087	-3.223720	-3.768536
95	1	0	4.172786	-3.218916	-1.945299
96	1	0	5.746994	1.167664	0.444659
97	1	0	8.037656	0.513928	1.128754
98	1	0	8.489371	-1.819467	1.877712
99	1	0	6.630266	-3.471496	1.928470
100	1	0	4.370612	-2.822349	1.210807
101	8	0	2.143872	-1.628227	1.922569
102	1	0	2.025170	-2.498752	2.345308
103	1	0	1.258517	-1.429386	1.591744

An imaginary frequency was found at –34.29 cm^{-1}.

The total electronic energy was calculated to be –3543.6715816 Hartree.

Table S32. Optimized structure of **INT5a** (B3LYP-D3/6-31G(d))



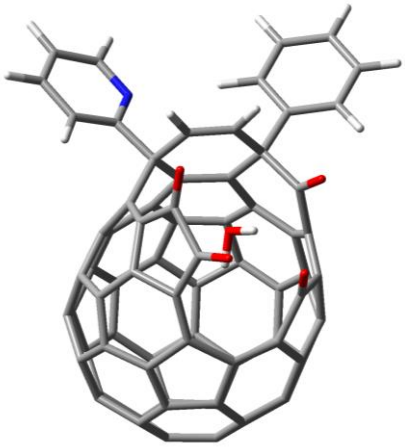
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.677278	1.640922	-3.132513
2	6	0	-1.225932	1.697508	-3.187866
3	6	0	-0.510579	0.545695	-3.463464
4	6	0	-1.195120	-0.712968	-3.698759
5	6	0	-2.585435	-0.780217	-3.607875
6	6	0	-3.341494	0.424136	-3.312692
7	6	0	-0.745984	2.616682	-2.172721
8	6	0	0.703397	0.283416	-2.737023
9	6	0	-0.374981	-1.751298	-3.118080
10	6	0	-3.206027	-1.891969	-2.907126
11	6	0	-4.429600	0.058637	-2.421640
12	6	0	-3.108668	2.567223	-2.108076
13	6	0	-2.407618	-2.898470	-2.355263
14	6	0	-0.961784	-2.831776	-2.472364
15	6	0	-2.707529	-3.418842	-1.037075
16	6	0	-0.366838	-3.315653	-1.245391
17	6	0	0.427738	2.359700	-1.426304
18	6	0	0.807268	-1.144308	-2.549532
19	6	0	-1.449039	-3.685906	-0.368791
20	6	0	1.442832	-1.647779	-1.417020
21	6	0	1.185753	1.153669	-1.749951
22	6	0	-4.334684	-1.368374	-2.157924
23	6	0	-4.825146	0.934947	-1.408910
24	6	0	0.520643	2.849799	-0.040415
25	6	0	-4.173119	2.225836	-1.262240
26	6	0	-1.926495	3.206015	-1.563496
27	6	0	-5.095137	0.422579	-0.076368
28	6	0	-4.085732	2.529451	0.150426
29	6	0	-1.881625	3.568119	-0.229943
30	6	0	0.825626	-2.780349	-0.715313
31	6	0	-4.608850	-1.860148	-0.875486
32	6	0	2.123985	0.619389	-0.791888
33	6	0	-4.605808	1.388072	0.886612
34	6	0	-2.988105	3.218731	0.651106
35	6	0	-0.646226	3.430623	0.500587
36	6	0	-1.006972	3.107618	1.850606
37	6	0	1.547005	2.338936	0.869232
38	6	0	2.292265	-0.743851	-0.674817
39	6	0	2.379904	-2.388319	1.226798
40	6	0	-2.404331	2.835756	1.916378
41	6	0	-2.809167	1.658117	2.558667
42	6	0	-1.878780	0.751630	3.220636
43	6	0	-3.937553	0.944517	2.031748
44	6	0	-3.774201	-2.897202	-0.307742
45	6	0	1.857017	1.557765	3.416099
46	6	0	-4.967092	-0.936793	0.191221
47	6	0	-4.297906	-1.376941	1.404158
48	6	0	1.238642	2.233184	2.225860
49	6	0	1.053744	-2.866967	0.713787
50	6	0	-0.042796	-3.102713	1.557096
51	6	0	-0.143730	2.379148	2.626616
52	6	0	-0.589807	1.265807	3.448101
53	6	0	-3.726469	-0.456168	2.288424
54	6	0	-2.435122	-0.661858	2.964968
55	6	0	0.651696	0.858923	4.176395

56	6	0	-3.595819	-2.588429	1.104602	76	6	0	6.001099	-3.870935	-0.582180
57	6	0	-1.301590	-3.433314	0.990772	77	6	0	4.970308	-3.272122	0.141572
58	6	0	-2.382311	-2.802460	1.732677	78	8	0	0.768362	0.215550	5.189680
59	6	0	-1.815443	-1.905370	2.718331	79	6	0	-0.375555	-2.416625	2.896143
60	6	0	2.749073	1.627036	0.182102	80	8	0	0.331051	-2.249357	3.863464
61	6	0	3.201338	-1.392390	0.339713	81	1	0	4.586816	-0.779967	1.947526
62	6	0	3.891716	-0.373255	1.219874	82	1	0	4.238114	1.603658	1.807036
63	6	0	3.696995	0.941934	1.140727	83	1	0	4.609074	1.098702	-1.748132
64	6	0	4.319540	-2.163255	-0.411600	84	1	0	6.015404	2.764164	-2.994274
65	6	0	3.597850	2.639331	-0.617744	85	1	0	5.723373	5.210095	-2.475757
66	8	0	2.822554	-2.792469	2.286483	86	1	0	4.052170	5.863332	-0.737863
67	8	0	2.985056	1.560643	3.844053	87	1	0	5.903099	-1.774641	-3.240273
68	6	0	4.517558	2.166369	-1.565218	88	1	0	7.148291	-3.782560	-2.420830
69	6	0	5.295766	3.094020	-2.249682	89	1	0	6.519270	-4.735852	-0.177159
70	6	0	5.137346	4.452551	-1.964211	90	1	0	4.683731	-3.651255	1.115083
71	6	0	4.203879	4.816825	-0.996284	91	8	0	1.109402	-0.384733	1.873507
72	7	0	3.444605	3.934695	-0.330168	92	1	0	1.257302	-0.900944	2.682745
73	7	0	4.666062	-1.643438	-1.599111	93	1	0	0.149916	-0.356378	1.752377
74	6	0	5.656811	-2.227026	-2.281179						
75	6	0	6.353908	-3.345605	-1.823698						

The total electronic energy was calculated to be –3312.614949 Hartree.

Table S33. Optimized structure of **INT5b** (B3LYP-D3/6-31G(d))



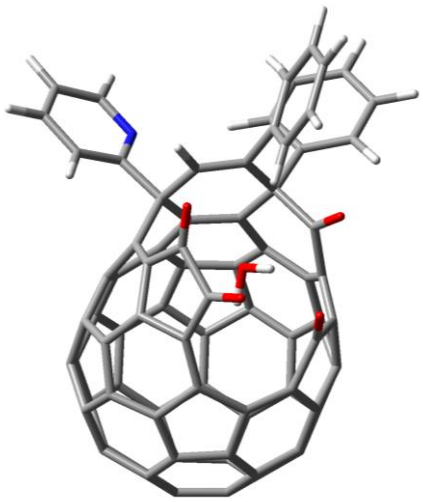
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.635009	1.444936	-3.261999
2	6	0	-1.182325	1.487784	-3.307488
3	6	0	-0.473357	0.314439	-3.493490
4	6	0	-1.165688	-0.952878	-3.648456
5	6	0	-2.557117	-1.004139	-3.567765
6	6	0	-3.306946	0.223185	-3.363726
7	6	0	-0.704881	2.469506	-2.351852
8	6	0	0.733172	0.094578	-2.741173
9	6	0	-0.359168	-1.954246	-2.989863
10	6	0	-3.192892	-2.060954	-2.798928
11	6	0	-4.405766	-0.072749	-2.460425
12	6	0	-3.069153	2.440929	-2.306866
13	6	0	-2.407254	-3.032145	-2.170290
14	6	0	-0.960004	-2.983465	-2.276749
15	6	0	-2.724154	-3.458198	-0.822384
16	6	0	-0.381051	-3.383852	-1.012831
17	6	0	0.461423	2.254985	-1.579670
18	6	0	0.822327	-1.317468	-2.453177
19	6	0	-1.474025	-3.686485	-0.124115
20	6	0	1.440191	-1.743678	-1.280362
21	6	0	1.217614	1.027981	-1.814348
22	6	0	-4.324273	-1.479057	-2.098644
23	6	0	-4.806117	0.873676	-1.514795
24	6	0	0.540310	2.833168	-0.226642
25	6	0	-4.143827	2.165501	-1.450000
26	6	0	-1.886868	3.105652	-1.794332
27	6	0	-5.093201	0.455975	-0.152666
28	6	0	-4.068736	2.565294	-0.060784
29	6	0	-1.853298	3.559233	-0.488833
30	6	0	0.809053	-2.820826	-0.508345
31	6	0	-4.614612	-1.879193	-0.788558
32	6	0	2.145695	0.556186	-0.814782
33	6	0	-4.606070	1.481626	0.747078
34	6	0	-2.971244	3.279783	0.402695
35	6	0	-0.626787	3.460055	0.262194
36	6	0	-1.003648	3.234333	1.627554
37	6	0	1.549876	2.372257	0.729084
38	6	0	2.289000	-0.797402	-0.591522
39	6	0	2.353060	-2.304178	1.415373
40	6	0	-2.404236	2.980876	1.697628
41	6	0	-2.824088	1.853037	2.415353
42	6	0	-1.907637	0.987001	3.148578
43	6	0	-3.953405	1.113192	1.927756
44	6	0	-3.794442	-2.880704	-0.142021
45	6	0	1.831091	1.778992	3.330586
46	6	0	-4.976718	-0.882387	0.208477
47	6	0	-4.323916	-1.243213	1.455991
48	6	0	1.227546	2.368604	2.087162
49	6	0	1.025138	-2.809388	0.925043
50	6	0	-0.081801	-2.979246	1.771146
51	6	0	-0.155567	2.555371	2.462908
52	6	0	-0.617846	1.505916	3.357060
53	6	0	-3.755358	-0.268087	2.281757
54	6	0	-2.472875	-0.436476	2.984554
55	6	0	0.613995	1.139046	4.123188
56	6	0	-3.627904	-2.477024	1.247501
57	6	0	-1.337711	-3.340490	1.215628
58	6	0	-2.422170	-2.655688	1.901527
59	6	0	-1.859658	-1.697404	2.830243
60	6	0	2.762995	1.619296	0.103188
61	6	0	3.191884	-1.388695	0.465537
62	6	0	3.882067	-0.319401	1.278803
63	6	0	3.699417	0.989456	1.113210

64	6	0	4.283866	-2.228654	-0.250567
65	6	0	3.632362	2.582450	-0.735037
66	8	0	2.778689	-2.632358	2.506868
67	8	0	2.953873	1.822369	3.768975
68	6	0	3.775980	3.930302	-0.390869
69	6	0	4.632008	4.728733	-1.147906
70	6	0	5.314386	4.156896	-2.220422
71	6	0	5.111009	2.800467	-2.478925
72	7	0	4.295329	2.024785	-1.757788
73	6	0	4.999374	-1.613218	-1.290207
74	6	0	5.996095	-2.310915	-1.968181
75	6	0	6.295972	-3.630649	-1.619426
76	6	0	5.596191	-4.241063	-0.580271
77	6	0	4.596646	-3.544229	0.105362
78	8	0	0.716293	0.568710	5.180266
79	6	0	-0.424114	-2.204398	3.057824
80	8	0	0.271785	-1.975746	4.020131
81	1	0	4.571667	-0.684030	2.033075
82	1	0	4.246868	1.687537	1.736245
83	1	0	3.227006	4.341564	0.449902
84	1	0	4.761242	5.779439	-0.903067
85	1	0	5.988354	4.740442	-2.839854
86	1	0	5.626967	2.310644	-3.302798
87	1	0	4.775763	-0.583843	-1.560118
88	1	0	6.541564	-1.821124	-2.770733
89	1	0	7.072443	-4.174854	-2.150380
90	1	0	5.825841	-5.263701	-0.292969
91	1	0	4.080805	-4.032963	0.924090
92	8	0	1.090062	-0.249663	1.923986
93	1	0	1.238896	-0.734665	2.752424
94	1	0	0.132698	-0.255159	1.785140

The total electronic energy was calculated to be –3296.5760824 Hartree.

Table S34. Optimized structure of **INT5c** (B3LYP-D3/6-31G(d))

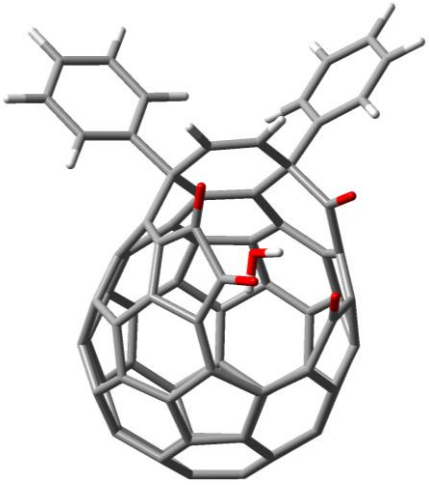


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.806083	2.180534	-2.181869
2	6	0	-2.397837	2.446209	-2.426228
3	6	0	-1.644499	1.525026	-3.132604
4	6	0	-2.248824	0.303387	-3.633970
5	6	0	-3.590499	0.026863	-3.369951
6	6	0	-4.384257	0.985880	-2.621513
7	6	0	-1.827163	3.095193	-1.261618
8	6	0	-0.302702	1.235303	-2.702726
9	6	0	-1.252406	-0.736194	-3.517926
10	6	0	-3.979360	-1.310284	-2.954502
11	6	0	-5.261653	0.240503	-1.734732
12	6	0	-4.127828	2.711798	-0.875312
13	6	0	-3.011961	-2.314373	-2.850428
14	6	0	-1.621289	-2.023912	-3.150194
15	6	0	-3.028091	-3.220546	-1.720182
16	6	0	-0.780020	-2.747148	-2.223233
17	6	0	-0.522009	2.794344	-0.804517
18	6	0	-0.044269	-0.160744	-2.969931
19	6	0	-1.652437	-3.491427	-1.350476
20	6	0	0.818855	-0.871480	-2.141345
21	6	0	0.269347	1.844418	-1.579064
22	6	0	-4.999119	-1.176770	-1.929016
23	6	0	-5.545943	0.733241	-0.459534
24	6	0	-0.230660	2.875844	0.636070
25	6	0	-4.991732	2.005226	-0.027421
26	6	0	-2.927348	3.323157	-0.339363
27	6	0	-5.531622	-0.165737	0.681809
28	6	0	-4.683990	1.907035	1.383622
29	6	0	-2.680000	3.297067	1.020692
30	6	0	0.433875	-2.225323	-1.734243
31	6	0	-4.999120	-2.042593	-0.827972
32	6	0	1.406396	1.192691	-0.969695
33	6	0	-4.964947	0.544916	1.810109
34	6	0	-3.579858	2.568796	1.905963
35	6	0	-1.327938	3.122703	1.489772
36	6	0	-1.417361	2.387669	2.718675
37	6	0	0.977760	2.260669	1.193368
38	6	0	1.706885	-0.113469	-1.282138
39	6	0	2.294286	-2.201558	-0.034699
40	6	0	-2.751774	1.924854	2.899984
41	6	0	-2.929983	0.569854	3.209475
42	6	0	-1.821538	-0.354023	3.427198
43	6	0	-4.068553	-0.110118	2.660123
44	6	0	-3.991233	-3.075953	-0.723428
45	6	0	1.801750	0.883841	3.334195
46	6	0	-5.241404	-1.515130	0.507024
47	6	0	-4.333792	-2.186163	1.422971
48	6	0	0.921827	1.753564	2.490115
49	6	0	0.918929	-2.663572	-0.442954
50	6	0	0.015716	-3.272502	0.440302
51	6	0	-0.373309	1.592209	3.109769
52	6	0	-0.560716	0.241812	3.614481
53	6	0	-3.696514	-1.484504	2.451230
54	6	0	-2.294121	-1.698162	2.842789
55	6	0	0.826941	-0.174131	4.001395
56	6	0	-3.593261	-3.157465	0.675219
57	6	0	-1.288917	-3.607476	-0.014066
58	6	0	-0.136638	-3.059104	1.956285
59	6	0	-2.273770	-3.373430	1.029379
60	6	0	-1.623514	-2.726199	2.149964
61	6	0	2.104823	1.947444	0.161988
62	6	0	2.865372	-0.895613	-0.694960
63	6	0	3.662675	-0.070593	0.324620
64	6	0	3.285305	1.160318	0.693129
65	6	0	3.799442	-1.274097	-1.875530
66	6	0	2.712021	3.257389	-0.390423
67	8	0	2.948551	-2.881861	0.730806

68	8	0	2.976835	0.965223	3.596177	88	1	0	2.489564	4.385224	1.437033
69	6	0	2.856978	4.390719	0.415987	89	1	0	3.605950	6.412112	0.486676
70	6	0	3.480069	5.517654	-0.117220	90	1	0	4.424125	6.330011	-1.892512
71	6	0	3.935789	5.475699	-1.434107	91	1	0	4.094231	4.216589	-3.185225
72	6	0	3.750327	4.295530	-2.155473	92	1	0	3.744266	0.741058	-2.651758
73	7	0	3.157752	3.207316	-1.653091	93	1	0	5.276459	0.269112	-4.532019
74	6	0	4.142857	-0.261551	-2.786097	94	1	0	6.237237	-2.011399	-4.823225
75	6	0	5.015912	-0.526499	-3.838791	95	1	0	5.648806	-3.804679	-3.201500
76	6	0	5.557278	-1.804889	-4.001058	96	1	0	4.139089	-3.332596	-1.318805
77	6	0	5.224468	-2.809998	-3.094861	97	1	0	8.198846	-1.185871	0.160985
78	6	0	4.354115	-2.547210	-2.033349	98	1	0	6.126542	-0.284886	-0.837018
79	8	0	0.710986	-3.082567	2.820560	99	1	0	4.008516	-1.112037	2.811054
80	8	0	1.187330	-1.058031	4.738169	100	1	0	6.073816	-2.007753	3.811983
81	6	0	7.280959	-1.177422	0.743413	101	1	0	8.185382	-2.060459	2.492061
82	6	0	6.110943	-0.670378	0.176857	102	8	0	1.149365	-0.687034	1.493797
83	6	0	4.915234	-0.647458	0.910054	103	1	0	1.434551	-1.448702	2.027908
84	6	0	4.920267	-1.131522	2.226101	104	1	0	0.184369	-0.743964	1.452211
85	6	0	6.090575	-1.635957	2.791079	---					
86	6	0	7.273912	-1.664935	2.050960	The total electronic energy was calculated to be –3527.6430779 Hartree.					
87	1	0	3.899274	1.690699	1.413036						

Table S35. Optimized structure of **INT5d** (B3LYP-D3/6-31G(d))



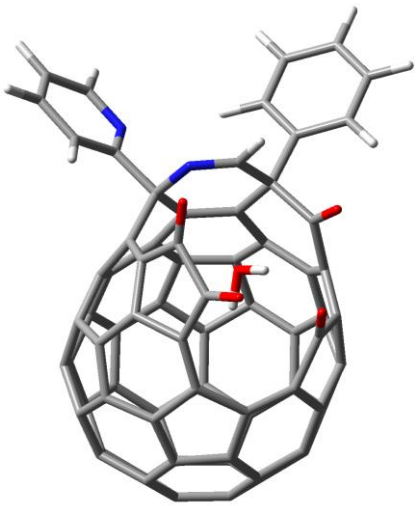
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.717367	1.624395	-3.124038
2	6	0	-1.266793	1.694219	-3.188610
3	6	0	-0.542529	0.548956	-3.467465
4	6	0	-1.217050	-0.716159	-3.697489
5	6	0	-2.606179	-0.796155	-3.598608
6	6	0	-3.371275	0.401447	-3.299241
7	6	0	-0.788699	2.616906	-2.176032
8	6	0	0.678517	0.298809	-2.747915
9	6	0	-0.384699	-1.746457	-3.120659
10	6	0	-3.212590	-1.913108	-2.893870
11	6	0	-4.450852	0.026356	-2.401697
12	6	0	-3.150774	2.546296	-2.096705
13	6	0	-2.401911	-2.911833	-2.345787
14	6	0	-0.957668	-2.831350	-2.470566
15	6	0	-2.689435	-3.434892	-1.025848
16	6	0	-0.351339	-3.309100	-1.246734
17	6	0	0.393042	2.370760	-1.439001
18	6	0	0.794065	-1.127811	-2.557607
19	6	0	-1.424727	-3.690953	-0.364629
20	6	0	1.437652	-1.622546	-1.425951
21	6	0	1.164048	1.175300	-1.768177
22	6	0	-4.341749	-1.399721	-2.138428
23	6	0	-4.848632	0.899285	-1.386991
24	6	0	0.486377	2.856395	-0.051934
25	6	0	-4.206862	2.195611	-1.244280
26	6	0	-1.970901	3.194765	-1.558648
27	6	0	-5.106451	0.384727	-0.052879
28	6	0	-4.114191	2.500243	0.167972
29	6	0	-1.922173	3.557809	-0.225565
30	6	0	0.838707	-2.763307	-0.722844
31	6	0	-4.603925	-1.893729	-0.854435
32	6	0	2.119126	0.653616	-0.817593
33	6	0	-4.619910	1.354394	0.907191
34	6	0	-3.020244	3.199644	0.662402
35	6	0	-0.681592	3.428335	0.497317
36	6	0	-1.030711	3.102570	1.849549
37	6	0	1.522160	2.350946	0.851102
38	6	0	2.291041	-0.712112	-0.692137
39	6	0	2.393525	-2.341637	1.215535
40	6	0	-2.425949	2.821703	1.924393
41	6	0	-2.816480	1.640659	2.569101
42	6	0	-1.874470	0.741941	3.226209
43	6	0	-3.941718	0.917087	2.048917
44	6	0	-3.757146	-2.923529	-0.291022
45	6	0	1.855756	1.577605	3.398762
46	6	0	-4.964256	-0.973383	0.214087
47	6	0	-4.284755	-1.407658	1.423436
48	6	0	1.223179	2.245834	2.210715
49	6	0	1.077861	-2.849978	0.703524
50	6	0	-0.011998	-3.095884	1.553339
51	6	0	-0.156857	2.382044	2.621290
52	6	0	-0.588686	1.265861	3.447153
53	6	0	-3.717042	-0.481627	2.304578
54	6	0	-2.420437	-0.676066	2.973582
55	6	0	0.661210	0.866715	4.165676
56	6	0	-3.573446	-2.612841	1.120107
57	6	0	-1.271429	-3.437353	0.994167
58	6	0	-2.354295	-2.816096	1.741395
59	6	0	-1.790227	-1.912973	2.722439
60	6	0	2.740970	1.671279	0.154619
61	6	0	3.215775	-1.358164	0.310245
62	6	0	3.901262	-0.328693	1.181408
63	6	0	3.692928	0.984909	1.108940

64	6	0	4.321635	-2.180740	-0.411699
65	6	0	3.580529	2.704062	-0.634851
66	8	0	2.820164	-2.703209	2.296301
67	8	0	2.985051	1.599539	3.821409
68	6	0	4.477296	2.245208	-1.609653
69	6	0	5.286154	3.138413	-2.308351
70	6	0	5.218946	4.507476	-2.036050
71	6	0	4.343784	4.969733	-1.054050
72	6	0	3.531402	4.072750	-0.355803
73	6	0	4.628858	-1.949984	-1.759880
74	6	0	5.667735	-2.641391	-2.384131
75	6	0	6.419693	-3.575046	-1.670945
76	6	0	6.127533	-3.803969	-0.325710
77	6	0	5.090725	-3.111894	0.300884
78	8	0	0.790508	0.227941	5.179788
79	6	0	-0.342895	-2.408791	2.892753
80	8	0	0.365910	-2.226795	3.854931
81	1	0	4.612717	-0.724796	1.898340
82	1	0	4.241417	1.647976	1.767687
83	1	0	4.548751	1.179840	-1.810408
84	1	0	5.972265	2.764790	-3.063793
85	1	0	5.848332	5.205394	-2.581343
86	1	0	4.289291	6.030893	-0.826102
87	1	0	2.856621	4.445779	0.408291
88	1	0	4.055260	-1.228926	-2.332425
89	1	0	5.886472	-2.446771	-3.430749
90	1	0	7.226950	-4.115924	-2.157110
91	1	0	6.707801	-4.524815	0.243991
92	1	0	4.879461	-3.296638	1.348430
93	8	0	1.063168	-0.347074	1.810121
94	1	0	1.246051	-0.857836	2.615071
95	1	0	0.101123	-0.350975	1.710048

The total electronic energy was calculated to be –3280.5360922 Hartree.

Table S36. Optimized structure of **INT5e** (B3LYP-D3/6-31G(d))



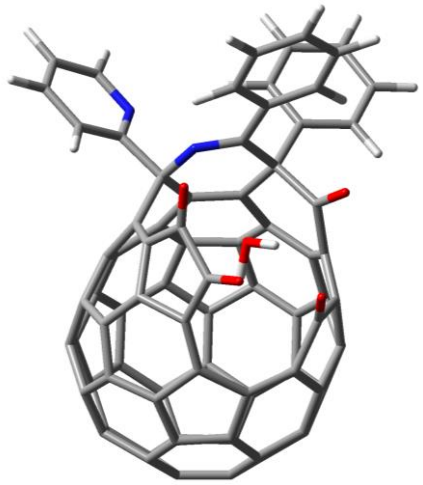
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.704477	1.514530	-3.207273
2	6	0	-1.252976	1.533905	-3.287938
3	6	0	-0.568538	0.351884	-3.509778
4	6	0	-1.285735	-0.901618	-3.662994
5	6	0	-2.675317	-0.930866	-3.547487
6	6	0	-3.399179	0.305578	-3.308956
7	6	0	-0.736874	2.494987	-2.330599
8	6	0	0.652698	0.102022	-2.791292
9	6	0	-0.480110	-1.925012	-3.037750
10	6	0	-3.309278	-1.987247	-2.776838
11	6	0	-4.481061	0.015645	-2.383451
12	6	0	-3.098782	2.504801	-2.228951
13	6	0	-2.524780	-2.979317	-2.180272
14	6	0	-1.080007	-2.952808	-2.321697
15	6	0	-2.816114	-3.418204	-0.830893
16	6	0	-0.477152	-3.379780	-1.077156
17	6	0	0.442902	2.250237	-1.589576
18	6	0	0.725829	-1.315792	-2.523886
19	6	0	-1.553340	-3.675899	-0.166314
20	6	0	1.366167	-1.771021	-1.373149
21	6	0	1.171505	1.016783	-1.864260
22	6	0	-4.414098	-1.396584	-2.042081
23	6	0	-4.842155	0.955731	-1.416004
24	6	0	0.565880	2.804639	-0.228851
25	6	0	-4.157268	2.235854	-1.350385
26	6	0	-1.893765	3.142899	-1.736273
27	6	0	-5.103366	0.524678	-0.052934
28	6	0	-4.041846	2.615609	0.041657
29	6	0	-1.819996	3.577426	-0.425986
30	6	0	0.734833	-2.843492	-0.595032
31	6	0	-4.679198	-1.809361	-0.730522
32	6	0	2.109203	0.513897	-0.894104
33	6	0	-4.577950	1.530302	0.847984
34	6	0	-2.921328	3.305209	0.487975
35	6	0	-0.577674	3.447854	0.294884
36	6	0	-0.926196	3.212357	1.665808
37	6	0	1.583800	2.312569	0.701052
38	6	0	2.236688	-0.841640	-0.693697
39	6	0	2.323478	-2.356891	1.304959
40	6	0	-2.328952	2.980571	1.765092
41	6	0	-2.751659	1.851233	2.478487
42	6	0	-1.832823	0.961639	3.179220
43	6	0	-3.903590	1.135794	2.007686
44	6	0	-3.859932	-2.832452	-0.117307
45	6	0	1.924152	1.699109	3.301102
46	6	0	-5.000359	-0.820142	0.287861
47	6	0	-4.323438	-1.207985	1.514137
48	6	0	1.302450	2.305335	2.068659
49	6	0	0.983605	-2.848659	0.833369
50	6	0	-0.105064	-3.016361	1.703615
51	6	0	-0.069530	2.512320	2.475527
52	6	0	-0.530957	1.458296	3.365966
53	6	0	-3.719328	-0.253146	2.338355
54	6	0	-2.423825	-0.451185	3.008510
55	6	0	0.709777	1.059688	4.101354
56	6	0	-3.653106	-2.450058	1.272874
57	6	0	-1.379134	-3.351177	1.174528
58	6	0	-2.435540	-2.657215	1.895368
59	6	0	-1.835708	-1.720324	2.822712
60	6	0	2.761678	1.524597	0.052073
61	6	0	3.138439	-1.417552	0.362278
62	6	0	3.766477	-0.307624	1.203946
63	7	0	3.625082	0.946119	1.076280
64	6	0	4.306513	-2.181245	-0.311063
65	6	0	3.687279	2.478771	-0.732632
66	8	0	2.770895	-2.698598	2.384065
67	8	0	3.045894	1.737697	3.734138

68	6	0	4.078877	3.698580	-0.172205
69	6	0	4.963025	4.503204	-0.884685
70	6	0	5.427536	4.060327	-2.124706
71	6	0	4.990209	2.820646	-2.587758
72	7	0	4.138813	2.038370	-1.910690
73	6	0	4.947968	-1.570289	-1.401095
74	6	0	6.019490	-2.199508	-2.031348
75	6	0	6.468845	-3.444201	-1.584565
76	6	0	5.844226	-4.047314	-0.493821
77	6	0	4.772419	-3.419369	0.145832
78	8	0	0.819378	0.464795	5.144463
79	6	0	-0.405346	-2.255138	3.009482
80	8	0	0.316888	-2.054588	3.958761
81	1	0	4.417891	-0.659649	2.004810
82	1	0	3.704842	3.990931	0.803099
83	1	0	5.287047	5.457479	-0.478720
84	1	0	6.116393	4.655831	-2.715933
85	1	0	5.336039	2.431118	-3.543375
86	1	0	4.613942	-0.597041	-1.751579
87	1	0	6.505071	-1.712819	-2.873051
88	1	0	7.302577	-3.935573	-2.078761
89	1	0	6.189908	-5.011300	-0.130359
90	1	0	4.316535	-3.898189	1.004352
91	8	0	1.078212	-0.307685	1.850585
92	1	0	1.194933	-0.785817	2.687698
93	1	0	0.122823	-0.257566	1.707874

The total electronic energy was calculated to be –3312.6124243 Hartree.

Table S37. Optimized structure of **INT5f** (B3LYP-D3/6-31G(d))



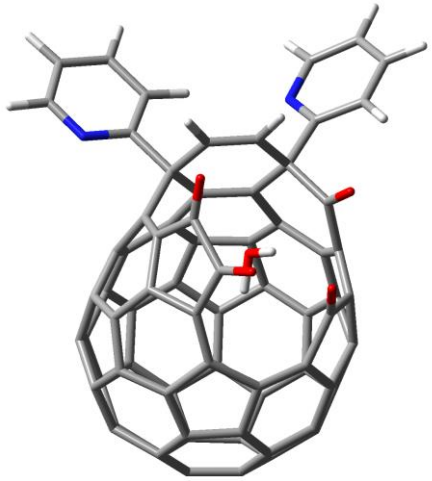
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.755687	1.239232	-2.877015
2	6	0	-2.343401	1.320600	-3.211687
3	6	0	-1.641978	0.159855	-3.490648
4	6	0	-2.303480	-1.132474	-3.448976
5	6	0	-3.649012	-1.218581	-3.090846
6	6	0	-4.388847	-0.004530	-2.793601
7	6	0	-1.724663	2.358004	-2.408108
8	6	0	-0.303303	0.010432	-2.987791
9	6	0	-1.346334	-2.078003	-2.921709
10	6	0	-4.082590	-2.254149	-2.167620
11	6	0	-5.278552	-0.287469	-1.680204
12	6	0	-4.030249	2.267293	-1.896519
13	6	0	-3.153338	-3.170290	-1.665350
14	6	0	-1.758049	-3.086087	-2.059031
15	6	0	-3.184183	-3.537142	-0.263930
16	6	0	-0.929373	-3.402331	-0.916907
17	6	0	-0.424227	2.207456	-1.870687
18	6	0	-0.104796	-1.384072	-2.661355
19	6	0	-1.813390	-3.687973	0.183623
20	6	0	0.743701	-1.733838	-1.615015
21	6	0	0.312328	0.997259	-2.208822
22	6	0	-5.077223	-1.671929	-1.283610
23	6	0	-5.519472	0.691448	-0.714162
24	6	0	-0.101116	2.835831	-0.578721
25	6	0	-4.906200	2.003740	-0.834570
26	6	0	-2.795497	2.987503	-1.654498
27	6	0	-5.522514	0.331867	0.693171
28	6	0	-4.575872	2.470432	0.495042
29	6	0	-2.521153	3.498782	-0.399401
30	6	0	0.310796	-2.776372	-0.684446
31	6	0	-5.093076	-2.017099	0.073854
32	6	0	1.428282	0.596682	-1.389367
33	6	0	-4.907546	1.412415	1.436924
34	6	0	-3.434324	3.233750	0.705018
35	6	0	-1.168585	3.461322	0.100461
36	6	0	-1.266441	3.290563	1.520953
37	6	0	1.085896	2.433689	0.186581
38	6	0	1.671760	-0.729060	-1.139066
39	6	0	2.217745	-2.153916	0.846609
40	6	0	-2.616585	3.009410	1.875149
41	6	0	-2.850072	1.908620	2.709545
42	6	0	-1.780450	1.102854	3.286998
43	6	0	-4.027378	1.118488	2.482287
44	6	0	-4.124151	-2.961198	0.588311
45	6	0	1.900373	2.041636	2.723978
46	6	0	-5.292504	-0.984814	1.080901
47	6	0	-4.399368	-1.267389	2.192301
48	6	0	1.040791	2.502391	1.576829
49	6	0	0.800561	-2.653831	0.673186
50	6	0	-0.109094	-2.816240	1.727478
51	6	0	-0.251387	2.672182	2.201644
52	6	0	-0.489502	1.657806	3.213661
53	6	0	-3.719134	-0.238002	2.851324
54	6	0	-2.321480	-0.336010	3.300204
55	6	0	0.883882	1.394845	3.761586
56	6	0	-3.708650	-2.488598	1.901511
57	6	0	-1.431425	-3.263145	1.449989
58	6	0	-0.234902	-2.015598	3.036072
59	6	0	-2.392307	-2.596218	2.313234
60	6	0	-1.703015	-1.581713	3.081613
61	6	0	2.179625	1.680311	-0.628917
62	6	0	2.816749	-1.226609	-0.279197
63	6	0	3.618467	-0.028977	0.321388
64	7	0	3.274321	1.197361	0.180943
65	6	0	3.703015	-2.042099	-1.253396
66	6	0	2.870475	2.651987	-1.616847
67	8	0	2.873559	-2.565074	1.782021
68	8	0	3.067106	2.219480	2.959959
69	6	0	3.179665	3.960739	-1.234753
70	6	0	3.867557	4.770654	-2.134076
71	6	0	4.225565	4.245658	-3.376943
72	6	0	3.884016	2.923048	-3.655566
73	7	0	3.221988	2.135519	-2.798018

74	6	0	4.368225	-1.343775	-2.270756
75	6	0	5.140666	-2.028571	-3.206641
76	6	0	5.249149	-3.419921	-3.149639
77	6	0	4.575114	-4.120464	-2.149526
78	6	0	3.803908	-3.436983	-1.207129
79	8	0	0.621206	-1.732131	3.845023
80	8	0	1.198880	0.901010	4.814954
81	6	0	6.712580	-1.634438	1.921452
82	6	0	5.513651	-1.507495	1.221399
83	6	0	4.883909	-0.258806	1.089973
84	6	0	5.503663	0.859180	1.684763
85	6	0	6.693557	0.727693	2.390776
86	6	0	7.308490	-0.521084	2.511382
87	1	0	2.893659	4.322812	-0.252979
88	1	0	4.122334	5.793108	-1.869045
89	1	0	4.760522	4.841643	-4.109939
90	1	0	4.152119	2.469097	-4.607810
91	1	0	4.261668	-0.264509	-2.341288
92	1	0	5.655210	-1.471761	-3.985144
93	1	0	5.851347	-3.953223	-3.880021
94	1	0	4.648990	-5.203243	-2.095086
95	1	0	3.305447	-3.999906	-0.424658
96	1	0	7.176764	-2.613368	2.005160
97	1	0	5.079100	-2.392943	0.787104
98	1	0	5.023375	1.823652	1.596112
99	1	0	7.141047	1.604472	2.851181
100	1	0	8.240603	-0.624212	3.061165
101	8	0	1.324562	-0.138128	1.760940
102	1	0	1.542515	-0.637723	2.569453
103	1	0	0.358924	-0.135467	1.707425

The total electronic energy was calculated to be –3543.6798064 Hartree.

Table S38. Optimized structure of **TS2a** (B3LYP-D3/6-31G(d))



Standard orientation:

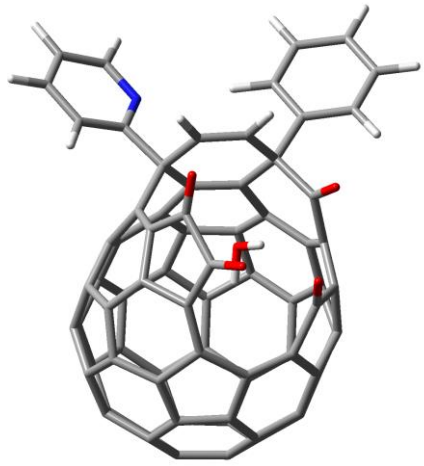
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.679954	1.674156	-3.109342
2	6	0	-1.228714	1.728357	-3.169697
3	6	0	-0.516922	0.577835	-3.458908
4	6	0	-1.204987	-0.676888	-3.703389
5	6	0	-2.595127	-0.742118	-3.608561
6	6	0	-3.347696	0.460878	-3.299410
7	6	0	-0.742849	2.636529	-2.147071
8	6	0	0.699908	0.306396	-2.740415
9	6	0	-0.384945	-1.721818	-3.134252
10	6	0	-3.215723	-1.859122	-2.916499
11	6	0	-4.433709	0.089114	-2.408162
12	6	0	-3.105611	2.591046	-2.074107
13	6	0	-2.417494	-2.872267	-2.376775
14	6	0	-0.971937	-2.806983	-2.497116
15	6	0	-2.714294	-3.405160	-1.063017
16	6	0	-0.374149	-3.304221	-1.276746
17	6	0	0.434323	2.372223	-1.409339
18	6	0	0.800593	-1.122340	-2.564287
19	6	0	-1.454519	-3.683081	-0.401499
20	6	0	1.440791	-1.637818	-1.438367
21	6	0	1.191180	1.168448	-1.749687
22	6	0	-4.341038	-1.340706	-2.158747
23	6	0	-4.823915	0.956220	-1.385607
24	6	0	0.532010	2.849910	-0.018423
25	6	0	-4.168221	2.243979	-1.228210
26	6	0	-1.920286	3.221593	-1.527279
27	6	0	-5.090701	0.431281	-0.057246
28	6	0	-4.075613	2.533536	0.187126
29	6	0	-1.870622	3.570917	-0.190386
30	6	0	0.822080	-2.776923	-0.745105
31	6	0	-4.612138	-1.844685	-0.880379
32	6	0	2.134273	0.624731	-0.804447
33	6	0	-4.596234	1.386318	0.913549
34	6	0	-2.974520	3.215144	0.691047
35	6	0	-0.633150	3.423821	0.534092
36	6	0	-0.988718	3.087317	1.882335
37	6	0	1.560623	2.331848	0.880773
38	6	0	2.296126	-0.741527	-0.695698
39	6	0	2.359856	-2.390055	1.209663
40	6	0	-2.387088	2.818475	1.950526
41	6	0	-2.794230	1.636316	2.583038
42	6	0	-1.864028	0.720502	3.232338
43	6	0	-3.925941	0.930357	2.052584
44	6	0	-3.778031	-2.889287	-0.325377
45	6	0	1.874790	1.512028	3.418434
46	6	0	-4.964890	-0.930984	0.196460
47	6	0	-4.292728	-1.384566	1.402794
48	6	0	1.257050	2.204235	2.238149
49	6	0	1.050730	-2.885183	0.681418
50	6	0	-0.042430	-3.131685	1.526878
51	6	0	-0.123800	2.347576	2.646627
52	6	0	-0.572102	1.227219	3.457937
53	6	0	-3.717295	-0.473383	2.294430
54	6	0	-2.423618	-0.688346	2.962945
55	6	0	0.669590	0.808401	4.175873
56	6	0	-3.594409	-2.594893	1.089619
57	6	0	-1.303436	-3.449911	0.961891
58	6	0	-0.360830	-2.433235	2.862656
59	6	0	-2.379626	-2.819396	1.712151
60	6	0	-1.806028	-1.929974	2.700387
61	6	0	2.756634	1.623009	0.182199
62	6	0	3.188935	-1.396900	0.329506
63	6	0	3.869454	-0.387371	1.226148
64	6	0	3.689592	0.929242	1.145319
65	6	0	4.314174	-2.171446	-0.407193
66	6	0	3.612093	2.638567	-0.605572
67	8	0	2.782473	-2.762935	2.288483
68	8	0	3.001557	1.508553	3.851375
69	6	0	4.539070	2.168558	-1.547466

70	6	0	5.322090	3.098306	-2.223517
71	6	0	5.160593	4.456024	-1.935930
72	6	0	4.219744	4.817327	-0.974059
73	7	0	3.456128	3.933133	-0.315615
74	6	0	4.944091	-3.291341	0.147760
75	6	0	5.981969	-3.894033	-0.562601
76	6	0	6.362026	-3.361461	-1.792855
77	6	0	5.684266	-2.231961	-2.252727
78	7	0	4.687097	-1.644627	-1.583493
79	8	0	0.361240	-2.238370	3.812535
80	8	0	0.789914	0.167052	5.189931
81	1	0	4.547134	-0.801847	1.965457
82	1	0	4.226809	1.584307	1.821230
83	1	0	4.631792	1.101423	-1.733006
84	1	0	6.047460	2.770731	-2.963542
85	1	0	5.749828	5.215215	-2.441315
86	1	0	4.065491	5.863116	-0.714251
87	1	0	4.637576	-3.676410	1.112916
88	1	0	6.484453	-4.767411	-0.156001
89	1	0	7.162689	-3.801039	-2.379581
90	1	0	5.952379	-1.773580	-3.203056
91	8	0	0.907664	-0.358763	1.642534
92	1	0	-0.054982	-0.341770	1.549068
93	1	0	1.077848	-0.796599	2.489864

An imaginary frequency was found at –51.89 cm^{-1}.

The total electronic energy was calculated to be –3312.6148006 Hartree.

Table S39. Optimized structure of **TS2b** (B3LYP-D3/6-31G(d))



Standard orientation:

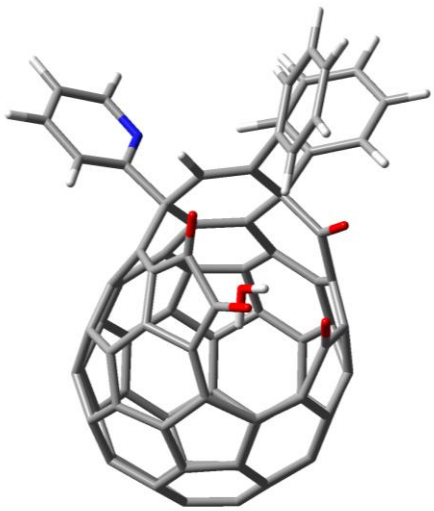
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.640577	1.494582	-3.232149
2	6	0	-1.188066	1.535375	-3.283489
3	6	0	-0.482418	0.363549	-3.489604
4	6	0	-1.177889	-0.899877	-3.659524
5	6	0	-2.569029	-0.949634	-3.574036
6	6	0	-3.315587	0.276031	-3.349314
7	6	0	-0.704277	2.502305	-2.315469
8	6	0	0.727558	0.130698	-2.746540
9	6	0	-0.370609	-1.911375	-3.017218
10	6	0	-3.203933	-2.016167	-2.818190
11	6	0	-4.411534	-0.030813	-2.446033
12	6	0	-3.068709	2.477240	-2.260557
13	6	0	-2.417651	-2.997500	-2.206521
14	6	0	-0.970794	-2.949488	-2.317003
15	6	0	-2.730343	-3.443246	-0.864095
16	6	0	-0.387948	-3.369922	-1.061259
17	6	0	0.466258	2.276631	-1.553614
18	6	0	0.814206	-1.284265	-2.476385
19	6	0	-1.478384	-3.686197	-0.173906
20	6	0	1.437830	-1.728405	-1.311788
21	6	0	1.221621	1.052085	-1.811741
22	6	0	-4.331572	-1.442535	-2.105250
23	6	0	-4.806451	0.902456	-1.485264
24	6	0	0.550909	2.836751	-0.192131
25	6	0	-4.140821	2.191661	-1.403695
26	6	0	-1.883099	3.131584	-1.742855
27	6	0	-5.089074	0.465188	-0.128257
28	6	0	-4.059521	2.570698	-0.008929
29	6	0	-1.843881	3.566323	-0.430983
30	6	0	0.806198	-2.817056	-0.552811
31	6	0	-4.617797	-1.861561	-0.800198
32	6	0	2.155578	0.565540	-0.827654
33	6	0	-4.596448	1.476554	0.784643
34	6	0	-2.958430	3.275718	0.460930
35	6	0	-0.614669	3.454233	0.313054
36	6	0	-0.984967	3.207646	1.676777
37	6	0	1.563754	2.364253	0.750055
38	6	0	2.292870	-0.792685	-0.618793
39	6	0	2.331797	-2.310277	1.386717
40	6	0	-2.386528	2.956567	1.748938
41	6	0	-2.808151	1.820251	2.452155
42	6	0	-1.891146	0.940658	3.168206
43	6	0	-3.941009	1.089926	1.957934
44	6	0	-3.797403	-2.874432	-0.171477
45	6	0	1.850779	1.714058	3.340776
46	6	0	-4.973938	-0.878609	0.212613
47	6	0	-4.317034	-1.259144	1.452130
48	6	0	1.247331	2.330222	2.110727
49	6	0	1.023622	-2.835713	0.879282
50	6	0	-0.079163	-3.021205	1.728756
51	6	0	-0.134010	2.512566	2.496773
52	6	0	-0.597943	1.450018	3.375211
53	6	0	-3.744571	-0.297060	2.290427
54	6	0	-2.459102	-0.478213	2.983911
55	6	0	0.633865	1.067114	4.129327
56	6	0	-3.624546	-2.491442	1.223371
57	6	0	-1.337660	-3.366631	1.172867
58	6	0	-0.405278	-2.236772	3.013876
59	6	0	-2.416924	-2.683874	1.870586
60	6	0	-1.847251	-1.737380	2.806386
61	6	0	2.769751	1.616407	0.107954
62	6	0	3.178604	-1.393616	0.447728
63	6	0	3.857931	-0.336099	1.282924
64	6	0	3.689962	0.974538	1.120977
65	6	0	4.279670	-2.233146	-0.254329
66	6	0	3.646822	2.585942	-0.714453
67	8	0	2.733795	-2.604030	2.496563
68	8	0	2.972225	1.747579	3.785212
69	6	0	3.782471	3.933286	-0.365325
70	6	0	4.645073	4.736167	-1.110260
71	6	0	5.342118	4.169027	-2.175693
72	6	0	5.146224	2.812485	-2.439599
73	7	0	4.324115	2.032731	-1.730393
74	6	0	5.006778	-1.619817	-1.286950
75	6	0	6.012852	-2.318415	-1.950100

76	6	0	6.310437	-3.636445	-1.592963
77	6	0	5.599433	-4.244366	-0.559930
78	6	0	4.590629	-3.546558	0.110895
79	8	0	0.308826	-1.980465	3.954787
80	8	0	0.740626	0.496357	5.185668
81	1	0	4.529510	-0.710413	2.048298
82	1	0	4.232799	1.664158	1.757226
83	1	0	3.222127	4.341074	0.469566
84	1	0	4.767926	5.786731	-0.861543
85	1	0	6.021558	4.756145	-2.785703
86	1	0	5.673937	2.326090	-3.258042
87	1	0	4.785493	-0.591326	-1.562137
88	1	0	6.567492	-1.830652	-2.747569
89	1	0	7.094072	-4.181291	-2.112599
90	1	0	5.827469	-5.265493	-0.266093
91	1	0	4.065534	-4.032874	0.925424
92	8	0	0.861586	-0.239629	1.655041
93	1	0	-0.099004	-0.280748	1.549745
94	1	0	1.045054	-0.647354	2.514546

An imaginary frequency was found at –56.60 cm^{-1}.

The total electronic energy was calculated to be –3296.5758637 Hartree.

Table S40. Optimized structure of **TS2c** (B3LYP-D3/6-31G(d))

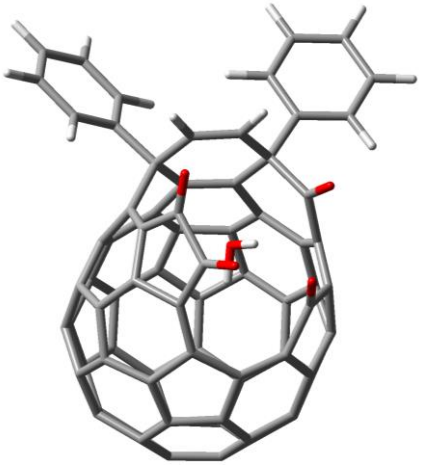


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.807896	2.183996	-2.170089
2	6	0	-2.400922	2.444020	-2.427426
3	6	0	-1.657077	1.517407	-3.136099
4	6	0	-2.269549	0.296462	-3.627614
5	6	0	-3.610261	0.026037	-3.352708
6	6	0	-4.394630	0.990581	-2.601392
7	6	0	-1.817656	3.095846	-1.269811
8	6	0	-0.312036	1.225071	-2.717331
9	6	0	-1.275455	-0.745928	-3.513357
10	6	0	-4.001046	-1.308056	-2.930108
11	6	0	-5.267573	0.251354	-1.704776
12	6	0	-4.116427	2.720307	-0.862419
13	6	0	-3.036489	-2.315258	-2.830397
14	6	0	-1.646803	-2.030933	-3.140176
15	6	0	-3.047342	-3.218911	-1.698306
16	6	0	-0.801254	-2.756330	-2.218649
17	6	0	-0.508525	2.797422	-0.824623
18	6	0	-0.061079	-0.172516	-2.976313
19	6	0	-1.670215	-3.499100	-1.340654
20	6	0	0.809092	-0.883755	-2.151373
21	6	0	0.276137	1.842714	-1.605351
22	6	0	-5.011962	-1.167643	-1.896872
23	6	0	-5.539540	0.749204	-0.428942
24	6	0	-0.206873	2.887790	0.615303
25	6	0	-4.976174	2.019850	-0.005160
26	6	0	-2.909737	3.329074	-0.338360
27	6	0	-5.518376	-0.146546	0.715202
28	6	0	-4.657156	1.924895	1.403736
29	6	0	-2.652569	3.308036	1.020236
30	6	0	0.420519	-2.238877	-1.740309
31	6	0	-5.005899	-2.030267	-0.793370
32	6	0	1.416874	1.193373	-1.008852
33	6	0	-4.939756	0.565478	1.836556
34	6	0	-3.546310	2.584436	1.914968
35	6	0	-1.297670	3.133104	1.478862
36	6	0	-1.375992	2.400254	2.710212
37	6	0	1.002779	2.279590	1.163591
38	6	0	1.706337	-0.121085	-1.309174
39	6	0	2.244008	-2.193491	-0.001397
40	6	0	-2.711252	1.941438	2.903976
41	6	0	-2.894032	0.588468	3.220271
42	6	0	-1.787123	-0.338818	3.430506
43	6	0	-4.039001	-0.089783	2.681956
44	6	0	-4.001857	-3.068086	-0.694178
45	6	0	1.839080	0.876183	3.285679
46	6	0	-5.234263	-1.497264	0.541896
47	6	0	-4.320735	-2.168639	1.451759
48	6	0	0.960050	1.761255	2.459006
49	6	0	0.908185	-2.693200	-0.458425
50	6	0	0.014055	-3.307477	0.432174
51	6	0	-0.329380	1.602324	3.093113
52	6	0	-0.522834	0.252948	3.602207
53	6	0	-3.672978	-1.465925	2.472847
54	6	0	-2.267128	-1.682389	2.850210
55	6	0	0.863432	-0.174342	3.965708
56	6	0	-3.591645	-3.146625	0.701739
57	6	0	-1.296703	-3.626476	-0.006413
58	6	0	-0.115088	-3.036560	1.941087
59	6	0	-2.270136	-3.370910	1.044813
60	6	0	-1.605168	-2.713447	2.150444
61	6	0	2.113190	1.949324	0.125026
62	6	0	2.838217	-0.912338	-0.679756
63	6	0	3.628851	-0.090155	0.344261
64	6	0	3.269921	1.153931	0.681319
65	6	0	3.796505	-1.337640	-1.824028
66	6	0	2.742752	3.244499	-0.437672
67	8	0	2.849666	-2.804170	0.856915
68	8	0	3.016544	0.937273	3.546490
69	6	0	2.874363	4.395917	0.344868
70	6	0	3.518576	5.506102	-0.198699
71	6	0	4.008646	5.429620	-1.501468
72	6	0	3.834019	4.233508	-2.199121
73	7	0	3.221121	3.161493	-1.686865
74	6	0	4.152209	-0.369119	-2.776010
75	6	0	5.051392	-0.678800	-3.794187
76	6	0	5.606923	-1.958494	-3.878824
77	6	0	5.263876	-2.919113	-2.929037

78	6	0	4.367650	-2.610900	-1.902175	93	1	0	5.321243	0.083159	-4.520824
79	8	0	0.747696	-2.986382	2.786899	94	1	0	6.306899	-2.200203	-4.674129
80	8	0	1.233690	-1.048742	4.709081	95	1	0	5.700298	-3.913208	-2.974586
81	6	0	7.283085	-1.045884	0.774164	96	1	0	4.144200	-3.360427	-1.151914
82	6	0	6.094013	-0.574284	0.216581	97	1	0	8.206522	-0.980137	0.204316
83	6	0	4.890097	-0.650298	0.932224	98	1	0	6.098174	-0.143449	-0.779478
84	6	0	4.903470	-1.195029	2.223783	99	1	0	3.983682	-1.258333	2.791879
85	6	0	6.093314	-1.661431	2.780848	100	1	0	6.084445	-2.080419	3.783414
86	6	0	7.285852	-1.592890	2.057804	101	1	0	8.211589	-1.959785	2.493982
87	1	0	3.887159	1.687583	1.395884	102	8	0	0.630163	-0.529135	1.151541
88	1	0	2.479986	4.417638	1.355487	103	1	0	0.970293	-1.154420	1.807289
89	1	0	3.634321	6.414158	0.386659	104	1	0	-0.329872	-0.647168	1.160313
90	1	0	4.514739	6.269630	-1.967010	---					
91	1	0	4.204541	4.127604	-3.217169	An imaginary frequency was found at –79.41 cm^{-1}.					
92	1	0	3.744482	0.635728	-2.698656	The total electronic energy was calculated to be –3527.6421041 Hartree.					

Table S41. Optimized structure of **TS2d** (B3LYP-D3/6-31G(d))



Standard orientation:

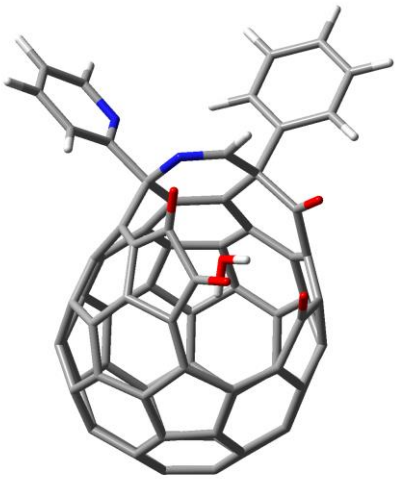
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.621638	1.426670	-3.276615
2	6	0	-1.168764	1.438899	-3.332672
3	6	0	-0.485158	0.248612	-3.502601
4	6	0	-1.203755	-1.006815	-3.627850
5	6	0	-2.595380	-1.028420	-3.537053
6	6	0	-3.319034	0.217312	-3.351392
7	6	0	-0.664557	2.428407	-2.398186
8	6	0	0.723035	0.019037	-2.755016
9	6	0	-0.413234	-2.010998	-2.954177
10	6	0	-3.246671	-2.057382	-2.744079
11	6	0	-4.417541	-0.039366	-2.435641
12	6	0	-3.028397	2.448647	-2.336892
13	6	0	-2.476826	-3.032352	-2.102034
14	6	0	-1.029698	-3.013072	-2.216937
15	6	0	-2.793570	-3.427547	-0.744762
16	6	0	-0.450699	-3.400832	-0.949041
17	6	0	0.503233	2.207188	-1.631832
18	6	0	0.784437	-1.387809	-2.437092
19	6	0	-1.544111	-3.669245	-0.049623
20	6	0	1.405154	-1.804313	-1.261149
21	6	0	1.235377	0.961582	-1.851766
22	6	0	-4.361980	-1.440113	-2.048157
23	6	0	-4.791733	0.932325	-1.505211
24	6	0	0.603593	2.808797	-0.290341
25	6	0	-4.102706	2.211228	-1.468336
26	6	0	-1.829585	3.098446	-1.844577
27	6	0	-5.078011	0.545690	-0.133704
28	6	0	-4.010295	2.634984	-0.087255
29	6	0	-1.777722	3.574760	-0.547657
30	6	0	0.754578	-2.852958	-0.462123
31	6	0	-4.651330	-1.810014	-0.729045
32	6	0	2.168844	0.493246	-0.855569
33	6	0	-4.564851	1.577973	0.743732
34	6	0	-2.894672	3.334343	0.356043
35	6	0	-0.548276	3.464843	0.196676
36	6	0	-0.919249	3.271721	1.568984
37	6	0	1.609519	2.345619	0.663542
38	6	0	2.283986	-0.862484	-0.604961
39	6	0	2.297440	-2.316337	1.455020
40	6	0	-2.324656	3.047971	1.652581
41	6	0	-2.765039	1.943916	2.394410
42	6	0	-1.862095	1.072113	3.136926
43	6	0	-3.912513	1.218494	1.927318
44	6	0	-3.847819	-2.816230	-0.068738
45	6	0	1.894664	1.780298	3.272218
46	6	0	-4.986971	-0.787906	0.251439
47	6	0	-4.333512	-1.138895	1.501385
48	6	0	1.298227	2.366372	2.025043
49	6	0	0.974736	-2.827374	0.969730
50	6	0	-0.128322	-2.966488	1.826714
51	6	0	-0.078518	2.587873	2.408605
52	6	0	-0.558855	1.564084	3.323159
53	6	0	-3.740531	-0.159968	2.305185
54	6	0	-2.456678	-0.341402	3.001699
55	6	0	0.668623	1.184506	4.086610
56	6	0	-3.664359	-2.390729	1.312408
57	6	0	-1.394123	-3.307933	1.285542
58	6	0	-0.436408	-2.135086	3.086655
59	6	0	-2.458822	-2.583586	1.963239
60	6	0	-1.869184	-1.617094	2.866065
61	6	0	2.808518	1.565696	0.039495
62	6	0	3.159477	-1.447637	0.481009
63	6	0	3.859899	-0.374939	1.277992
64	6	0	3.714563	0.932832	1.072216
65	6	0	4.226231	-2.344554	-0.199339
66	6	0	3.688035	2.535129	-0.784733
67	8	0	2.704803	-2.589638	2.566859
68	8	0	3.019403	1.802404	3.709039
69	6	0	3.960143	3.817449	-0.292093
70	6	0	4.813675	4.678597	-0.981634
71	6	0	5.410746	4.268226	-2.175032
72	6	0	5.150266	2.989407	-2.669343
73	6	0	4.296941	2.128599	-1.977711

74	6	0	5.159361	-1.729320	-1.046166
75	6	0	6.122284	-2.483846	-1.711935
76	6	0	6.169227	-3.869848	-1.540797
77	6	0	5.250146	-4.487846	-0.694343
78	6	0	4.284533	-3.730804	-0.025433
79	8	0	0.286103	-1.862525	4.016519
80	8	0	0.767870	0.646849	5.160906
81	1	0	4.528153	-0.735081	2.053063
82	1	0	4.273020	1.631332	1.684223
83	1	0	3.500171	4.143291	0.636923
84	1	0	5.010550	5.671108	-0.585359
85	1	0	6.073498	4.939245	-2.714425
86	1	0	5.609603	2.658317	-3.596944
87	1	0	4.097466	1.137880	-2.374014
88	1	0	5.133663	-0.650782	-1.170223
89	1	0	6.838535	-1.988451	-2.362028
90	1	0	6.920041	-4.460554	-2.058329
91	1	0	5.282338	-5.563699	-0.545017
92	1	0	3.592395	-4.234153	0.641130
93	8	0	0.887613	-0.214908	1.673055
94	1	0	-0.073776	-0.229878	1.567380
95	1	0	1.058112	-0.598123	2.546616

An imaginary frequency was found at –57.51 cm^{-1}.

The total electronic energy was calculated to be –3280.5357607 Hartree.

Table S42. Optimized structure of **TS2e** (B3LYP-D3/6-31G(d))



Standard orientation:

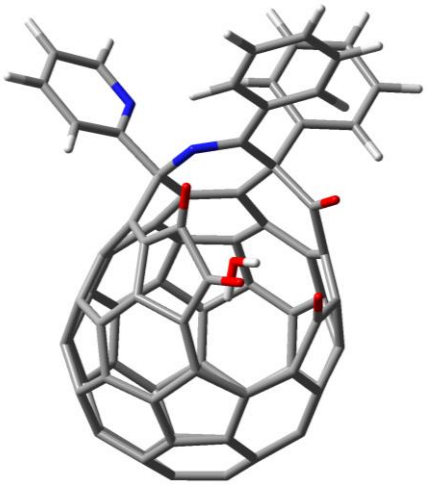
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.710870	1.540745	-3.189112
2	6	0	-1.259634	1.559162	-3.274384
3	6	0	-0.577301	0.378135	-3.507202
4	6	0	-1.296411	-0.873217	-3.667400
5	6	0	-2.685671	-0.901828	-3.548013
6	6	0	-3.407405	0.333539	-3.297981
7	6	0	-0.739179	2.512654	-2.311557
8	6	0	0.646290	0.121624	-2.794841
9	6	0	-0.490000	-1.901779	-3.051612
10	6	0	-3.318558	-1.963291	-2.783607
11	6	0	-4.486864	0.037846	-2.371353
12	6	0	-3.100876	2.523979	-2.201974
13	6	0	-2.533353	-2.960633	-2.196954
14	6	0	-1.088988	-2.934375	-2.341983
15	6	0	-2.821254	-3.410100	-0.850370
16	6	0	-0.483040	-3.372201	-1.102659
17	6	0	0.443467	2.262450	-1.577364
18	6	0	0.718113	-1.297584	-2.536829
19	6	0	-1.557074	-3.675892	-0.191610
20	6	0	1.362328	-1.762318	-1.391194
21	6	0	1.171089	1.030120	-1.864363
22	6	0	-4.420543	-1.377111	-2.041040
23	6	0	-4.843751	0.970911	-1.395644
24	6	0	0.570992	2.808516	-0.213061
25	6	0	-4.157058	2.249666	-1.322233
26	6	0	-1.893700	3.156948	-1.708232
27	6	0	-5.101036	0.529623	-0.035063
28	6	0	-4.036786	2.618558	0.072379
29	6	0	-1.815691	3.581996	-0.394988
30	6	0	0.731570	-2.841309	-0.619683
31	6	0	-4.682055	-1.799812	-0.731895
32	6	0	2.112392	0.519358	-0.903205
33	6	0	-4.571523	1.527712	0.871875
34	6	0	-2.914074	3.303554	0.520504
35	6	0	-0.571210	3.446599	0.320671
36	6	0	-0.914635	3.200178	1.691136
37	6	0	1.591235	2.311088	0.708362
38	6	0	2.236844	-0.838631	-0.710526
39	6	0	2.311301	-2.359657	1.288108
40	6	0	-2.317600	2.968616	1.793128
41	6	0	-2.739890	1.834478	2.499214
42	6	0	-1.819675	0.937953	3.189265
43	6	0	-3.894018	1.123755	2.026481
44	6	0	-3.862290	-2.828848	-0.129087
45	6	0	1.938537	1.665724	3.300183
46	6	0	-4.998516	-0.817898	0.295003
47	6	0	-4.317883	-1.215968	1.515963
48	6	0	1.314796	2.288096	2.077454
49	6	0	0.982418	-2.863693	0.807507
50	6	0	-0.103121	-3.040281	1.680483
51	6	0	-0.055391	2.492208	2.491952
52	6	0	-0.516310	1.430364	3.373866
53	6	0	-3.710100	-0.268006	2.345444
54	6	0	-2.412179	-0.472615	3.008556
55	6	0	0.725707	1.020429	4.098565
56	6	0	-3.650281	-2.457247	1.263434
57	6	0	-1.379134	-3.365719	1.152712
58	6	0	-0.392207	-2.273280	2.985263
59	6	0	-2.431236	-2.671886	1.880829
60	6	0	-1.825759	-1.741007	2.810351
61	6	0	2.763658	1.522970	0.052193
62	6	0	3.129805	-1.419734	0.350363
63	6	0	3.751529	-0.317337	1.204088
64	7	0	3.616046	0.937114	1.079814
65	6	0	4.302986	-2.183165	-0.314104
66	6	0	3.696753	2.477591	-0.722992
67	8	0	2.746952	-2.681232	2.377982
68	8	0	3.060155	1.699102	3.734950
69	6	0	4.088814	3.694215	-0.155888
70	6	0	4.979246	4.498906	-0.860409
71	6	0	5.449432	4.059178	-2.099413
72	6	0	5.011120	2.822484	-2.569456
73	7	0	4.153659	2.040179	-1.900112
74	6	0	4.949500	-1.575259	-1.402739
75	6	0	6.026438	-2.204709	-2.023519

76	6	0	6.476118	-3.446223	-1.568303
77	6	0	5.846552	-4.045992	-0.478514
78	6	0	4.769297	-3.417818	0.151622
79	8	0	0.341355	-2.058597	3.922174
80	8	0	0.839657	0.421554	5.138918
81	1	0	4.392217	-0.674684	2.011013
82	1	0	3.709905	3.984307	0.818196
83	1	0	5.303693	5.450787	-0.449199
84	1	0	6.143276	4.654899	-2.684563
85	1	0	5.361098	2.435497	-3.524591
86	1	0	4.615676	-0.603998	-1.758850
87	1	0	6.516143	-1.720575	-2.864304
88	1	0	7.314124	-3.937676	-2.055122
89	1	0	6.192609	-5.007331	-0.108481
90	1	0	4.309324	-3.893704	1.009729
91	8	0	0.951903	-0.296851	1.699162
92	1	0	-0.004362	-0.264416	1.556698
93	1	0	1.073023	-0.728981	2.558498

An imaginary frequency was found at –44.44 cm^{-1}.

The total electronic energy was calculated to be –3312.6123696 Hartree.

Table S43. Optimized structure of **TS2f** (B3LYP-D3/6-31G(d))



Standard orientation:

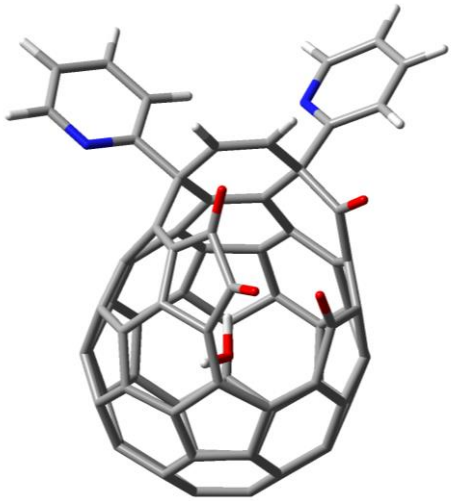
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.759361	1.372523	-2.809895
2	6	0	-2.348622	1.465392	-3.148636
3	6	0	-1.651903	0.316414	-3.480241
4	6	0	-2.315899	-0.974618	-3.491892
5	6	0	-3.659800	-1.073476	-3.131565
6	6	0	-4.395593	0.128010	-2.777839
7	6	0	-1.722555	2.466534	-2.304402
8	6	0	-0.310095	0.142600	-2.992555
9	6	0	-1.357767	-1.943150	-3.009300
10	6	0	-4.090338	-2.147519	-2.252744
11	6	0	-5.279391	-0.201572	-1.672256
12	6	0	-4.025650	2.356928	-1.783409
13	6	0	-3.160437	-3.087136	-1.796680
14	6	0	-1.766692	-2.988559	-2.191725
15	6	0	-3.184594	-3.517209	-0.413642
16	6	0	-0.932031	-3.361356	-1.070278
17	6	0	-0.417781	2.296414	-1.786143
18	6	0	-0.114531	-1.262425	-2.723081
19	6	0	-1.812518	-3.699861	0.018734
20	6	0	0.743312	-1.661262	-1.698465
21	6	0	0.318051	1.099074	-2.182577
22	6	0	-5.078597	-1.602914	-1.338293
23	6	0	-5.512596	0.734479	-0.662959
24	6	0	-0.086970	2.878467	-0.471497
25	6	0	-4.896370	2.049112	-0.728961
26	6	0	-2.788561	3.063917	-1.517163
27	6	0	-5.506270	0.312986	0.727513
28	6	0	-4.556763	2.456557	0.617974
29	6	0	-2.507606	3.522293	-0.243031
30	6	0	0.314460	-2.752062	-0.815065
31	6	0	-5.086414	-2.007777	0.002515
32	6	0	1.437055	0.661281	-1.394324
33	6	0	-4.884293	1.358893	1.513790
34	6	0	-3.413092	3.209376	0.854387
35	6	0	-1.152444	3.466972	0.246173
36	6	0	-1.237794	3.233718	1.659080
37	6	0	1.101190	2.453200	0.264009
38	6	0	1.675812	-0.677945	-1.196947
39	6	0	2.157300	-2.120325	0.798655
40	6	0	-2.587170	2.934583	2.008171
41	6	0	-2.818740	1.798138	2.794092
42	6	0	-1.745506	0.966380	3.326900
43	6	0	-3.996831	1.018415	2.538813
44	6	0	-4.117941	-2.977163	0.468954
45	6	0	1.930984	1.887492	2.757291
46	6	0	-5.275389	-1.019595	1.054722
47	6	0	-4.373695	-1.352364	2.145187
48	6	0	1.069966	2.446404	1.659206
49	6	0	0.805734	-2.720888	0.544859
50	6	0	-0.095828	-2.940119	1.598941
51	6	0	-0.215501	2.587142	2.306072
52	6	0	-0.456261	1.525129	3.271135
53	6	0	-3.686854	-0.353664	2.843391
54	6	0	-2.284995	-0.474271	3.273207
55	6	0	0.916665	1.206581	3.776555
56	6	0	-3.690870	-2.562862	1.798771
57	6	0	-1.422486	-3.350776	1.308266
58	6	0	-0.197874	-2.139207	2.911993
59	6	0	-2.372882	-2.698542	2.198220
60	6	0	-1.671227	-1.711812	2.990555
61	6	0	2.177952	1.709548	-0.572933
62	6	0	2.789260	-1.204787	-0.312058
63	6	0	3.587541	-0.040655	0.342843
64	7	0	3.239202	1.188401	0.252313
65	6	0	3.693667	-2.027900	-1.260738
66	6	0	2.912972	2.697496	-1.513718
67	8	0	2.733331	-2.360168	1.840023
68	8	0	3.106181	2.006112	2.993398
69	6	0	3.175664	4.012833	-1.121023
70	6	0	3.905587	4.830810	-1.979967
71	6	0	4.349993	4.306987	-3.194468
72	6	0	4.048566	2.977065	-3.486591
73	7	0	3.347790	2.182549	-2.668366
74	6	0	4.397652	-1.335508	-2.255499
75	6	0	5.197229	-2.028242	-3.162317
76	6	0	5.295058	-3.420210	-3.097652
77	6	0	4.582790	-4.114381	-2.119901
78	6	0	3.783888	-3.422760	-1.207000
79	8	0	0.672218	-1.821806	3.688756

80	8	0	1.245910	0.672697	4.805706
81	6	0	6.654758	-1.708969	1.934831
82	6	0	5.442875	-1.560898	1.262851
83	6	0	4.862255	-0.293628	1.090949
84	6	0	5.545586	0.820934	1.617431
85	6	0	6.749173	0.670030	2.296334
86	6	0	7.314245	-0.597180	2.456956
87	1	0	2.820766	4.376569	-0.162820
88	1	0	4.125303	5.858714	-1.704785
89	1	0	4.919934	4.908651	-3.895753
90	1	0	4.383629	2.523704	-4.417698
91	1	0	4.300982	-0.255212	-2.328982
92	1	0	5.742396	-1.477464	-3.924110
93	1	0	5.919081	-3.959025	-3.805300
94	1	0	4.648134	-5.197400	-2.060228
95	1	0	3.251491	-3.981052	-0.442781
96	1	0	7.078715	-2.702586	2.051917
97	1	0	4.958067	-2.445955	0.883848
98	1	0	5.104102	1.800511	1.496328
99	1	0	7.247364	1.546417	2.702204
100	1	0	8.257275	-0.716076	2.984413
101	8	0	0.625791	-0.136161	1.253828
102	1	0	0.923509	-0.460551	2.115769
103	1	0	-0.340317	-0.134633	1.301263

An imaginary frequency was found at –78.31 cm^{-1}.

The total electronic energy was calculated to be –3543.6782559 Hartree.

Table S44. Optimized structure of H_2O@**INT1a** (B3LYP-D3/6-31G(d))



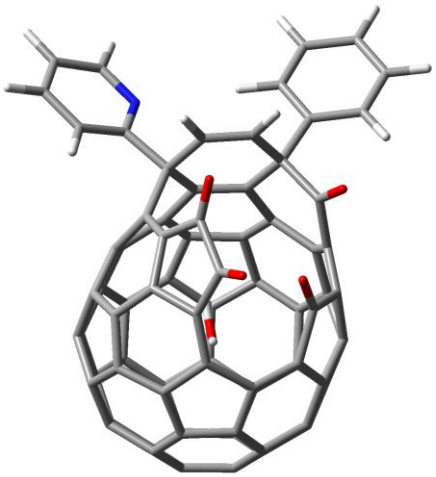
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.968808	-0.258305	1.300184
2	6	0	3.768395	1.041698	1.112069
3	6	0	2.814963	1.624141	0.101477
4	6	0	1.573071	2.267903	0.754100
5	6	0	1.227957	2.137870	2.100510
6	6	0	1.814450	1.536179	3.359281
7	6	0	0.575150	1.093571	4.238676
8	6	0	-0.633616	1.397570	3.410146
9	6	0	-1.943380	0.939157	3.223377
10	6	0	-2.497791	-0.456437	3.061902
11	6	0	-1.807019	-1.660632	2.875843
12	6	0	-0.311155	-1.905949	2.958929
13	6	0	0.012517	-2.833951	1.797284
14	6	0	1.120755	-2.697584	0.963364
15	6	0	2.434292	-2.205953	1.466416
16	6	0	3.290571	-1.340738	0.495864
17	7	0	4.786435	-1.804155	-1.373158
18	8	0	2.949982	1.486805	3.764088
19	8	0	2.847036	-2.507905	2.569498
20	7	0	3.415518	3.941631	-0.474546
21	6	0	2.402348	-0.790326	-0.594189
22	6	0	1.286326	1.012866	-1.816594
23	8	0	0.635578	0.827506	5.411919
24	6	0	1.559830	-1.750951	-1.274037
25	6	0	0.570341	2.762199	-0.192815
26	8	0	0.480377	-1.334162	3.674882
27	6	0	-0.665369	2.420169	-2.325062
28	6	0	4.143039	4.832396	-1.163993
29	6	0	-1.852747	3.038763	-1.760310
30	6	0	3.616632	2.645974	-0.728143
31	6	0	0.506889	2.220399	-1.560290
32	6	0	0.810781	0.070927	-2.738772
33	6	0	2.228575	0.553879	-0.819838
34	6	0	-1.822930	3.479593	-0.449598
35	6	0	-0.408259	0.271144	-3.477096
36	6	0	-0.977279	3.118066	1.666344
37	6	0	-1.132938	1.433638	-3.280723
38	6	0	0.924040	-1.341876	-2.443464
39	6	0	0.925878	-2.797365	-0.469607
40	6	0	-0.599973	3.362823	0.304974
41	6	0	5.026910	-3.256968	0.527524
42	6	0	4.408526	-2.200070	-0.149226
43	6	0	-4.040721	2.488512	-0.032607
44	6	0	-0.260316	-3.382915	-0.951459
45	6	0	-0.260804	-1.993664	-2.957056
46	6	0	6.064206	-3.937667	-0.108954
47	6	0	-0.145199	2.387874	2.477500
48	6	0	-2.583538	1.373931	-3.229709
49	6	0	5.090702	4.475994	-2.121380
50	6	0	-4.592143	1.411063	0.775959
51	6	0	-3.238368	0.144191	-3.323460
52	6	0	-2.388574	2.909011	1.738507
53	6	0	6.452656	-3.541683	-1.387470
54	6	0	4.555163	2.180921	-1.660146
55	6	0	-2.841209	1.805286	2.470897
56	6	0	5.782987	-2.465832	-1.970956
57	6	0	-1.084689	-1.005946	-3.615264
58	6	0	-5.051229	0.371807	-0.123531
59	6	0	-4.287852	-1.308826	1.507809
60	6	0	-2.945445	3.205981	0.437461
61	6	0	-1.347950	-3.679381	-0.052755
62	6	0	-3.027714	2.365328	-2.274538
63	6	0	-4.334581	-0.161053	-2.421557
64	6	0	-3.970048	1.060658	1.978027
65	6	0	5.300424	3.117203	-2.369434
66	6	0	-1.223857	-3.287842	1.275368
67	6	0	-3.774956	-0.318855	2.350636
68	6	0	-4.750262	0.784094	-1.483455
69	6	0	-4.100861	2.081929	-1.420391
70	6	0	-2.330472	-2.650322	1.963875
71	6	0	-2.473332	-1.073227	-3.522007
72	6	0	-3.092634	-2.130923	-2.742983
73	6	0	-0.847850	-3.014722	-2.220672

74	6	0	-4.523671	-1.956776	-0.739677
75	6	0	-2.293210	-3.082112	-2.105719
76	6	0	-2.601971	-3.494829	-0.751991
77	6	0	-3.545237	-2.521013	1.310782
78	6	0	-4.919662	-0.963613	0.246550
79	6	0	-3.684630	-2.932304	-0.078965
80	6	0	-4.233709	-1.562109	-2.049949
81	1	0	4.634814	-0.605786	2.082622
82	1	0	4.275862	1.762871	1.741634
83	1	0	3.953579	5.879252	-0.933800
84	1	0	4.710594	-3.532079	1.526466
85	1	0	6.559930	-4.765262	0.390985
86	1	0	5.649525	5.240314	-2.652769
87	1	0	7.253707	-4.045984	-1.919025
88	1	0	4.688665	1.112527	-1.809662
89	1	0	6.056887	-2.115312	-2.964485
90	1	0	6.033998	2.794038	-3.103126
91	8	0	-1.616614	-0.205894	-0.291033
92	1	0	-1.775212	0.546655	0.297531
93	1	0	-0.675083	-0.136278	-0.508060

The total electronic energy was calculated to be –3312.6523731 Hartree.

Table S45. Optimized structure of H_2O@**INT1b** (B3LYP-D3/6-31G(d))



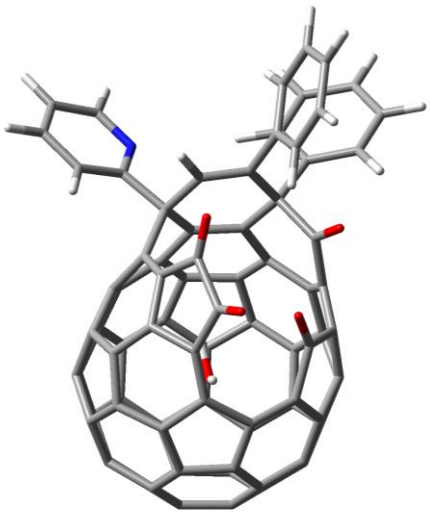
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.539403	1.244603	-3.312877
2	6	0	-1.087422	1.294378	-3.351576
3	6	0	-0.367351	0.119430	-3.484469
4	6	0	-1.050130	-1.159569	-3.571861
5	6	0	-2.440475	-1.214326	-3.491832
6	6	0	-3.200529	0.015374	-3.357784
7	6	0	-0.624507	2.319561	-2.435078
8	6	0	0.843319	-0.053496	-2.725183
9	6	0	-0.239995	-2.120315	-2.858885
10	6	0	-3.075096	-2.232096	-2.672925
11	6	0	-4.308432	-0.242274	-2.455204
12	6	0	-2.987660	2.279486	-2.407501
13	6	0	-2.288180	-3.157126	-1.983116
14	6	0	-0.841452	-3.103237	-2.083503
15	6	0	-2.615097	-3.505943	-0.615887
16	6	0	-0.271119	-3.415741	-0.791881
17	6	0	0.540223	2.148123	-1.651423
18	6	0	0.942500	-1.451563	-2.361561
19	6	0	-1.370207	-3.666504	0.106117
20	6	0	1.558005	-1.806693	-1.164558
21	6	0	1.318486	0.928359	-1.844708
22	6	0	-4.220594	-1.625891	-2.019909
23	6	0	-4.728676	0.746474	-1.565692
24	6	0	0.587284	2.746184	-0.305913
25	6	0	-4.070880	2.040874	-1.553183
26	6	0	-1.814638	2.967626	-1.910189
27	6	0	-5.046592	0.397650	-0.192373
28	6	0	-4.024276	2.509577	-0.185198
29	6	0	-1.798123	3.467530	-0.621293
30	6	0	0.911352	-2.813673	-0.322178
31	6	0	-4.528357	-1.959544	-0.696965
32	6	0	2.248986	0.512557	-0.819077
33	6	0	-4.591120	1.473463	0.664426
34	6	0	-2.931300	3.241347	0.264210
35	6	0	-0.585445	3.374718	0.151391
36	6	0	-0.979512	3.193804	1.517451
37	6	0	1.573649	2.284873	0.675638
38	6	0	2.396664	-0.820103	-0.517327
39	6	0	2.406104	-2.139536	1.599889
40	6	0	-2.392296	3.000264	1.583370
41	6	0	-2.859980	1.934911	2.360380
42	6	0	-1.976720	1.099244	3.163873
43	6	0	-3.988048	1.175812	1.889288
44	6	0	-3.703079	-2.908848	0.017172
45	6	0	1.784618	1.686183	3.318902
46	6	0	-4.929328	-0.920334	0.238649
47	6	0	-4.313859	-1.211287	1.521421
48	6	0	1.213574	2.224207	2.023995
49	6	0	1.093454	-2.651316	1.106110
50	6	0	-0.024593	-2.747112	1.933506
51	6	0	-0.161272	2.498737	2.372627
52	6	0	-0.665032	1.556032	3.345668
53	6	0	-3.806836	-0.186732	2.326397
54	6	0	-2.538689	-0.300418	3.059242
55	6	0	0.532932	1.284693	4.201850
56	6	0	-3.576226	-2.435387	1.388325
57	6	0	-1.258213	-3.218140	1.417327
58	6	0	-2.370121	-2.543718	2.062002
59	6	0	-1.851494	-1.516584	2.934816
60	6	0	2.826767	1.617243	0.065630
61	6	0	3.278525	-1.331484	0.599653
62	6	0	3.953095	-0.219436	1.360585
63	6	0	3.767745	1.072498	1.111253
64	6	0	4.379139	-2.229287	-0.022732
65	6	0	3.645051	2.601984	-0.792610
66	8	0	2.800907	-2.389439	2.721416
67	8	0	2.914714	1.669935	3.740010
68	6	0	3.707350	3.966853	-0.496903
69	6	0	4.525061	4.784002	-1.276361
70	6	0	5.250330	4.212071	-2.320260
71	6	0	5.127488	2.837418	-2.529707
72	7	0	4.349206	2.043704	-1.787052
73	6	0	5.124533	-1.695378	-1.085439
74	6	0	6.135868	-2.445373	-1.681124
75	6	0	6.419215	-3.735319	-1.223610
76	6	0	5.688793	-4.262996	-0.160196
77	6	0	4.673964	-3.513695	0.442371
78	8	0	0.579174	1.072083	5.386228
79	6	0	-0.356265	-1.768753	3.049477

80	8	0	0.426271	-1.167464	3.750863
81	1	0	4.612480	-0.538538	2.160213
82	1	0	4.281363	1.815718	1.709904
83	1	0	3.125572	4.377581	0.321844
84	1	0	4.591469	5.848886	-1.071082
85	1	0	5.896541	4.809815	-2.955501
86	1	0	5.679452	2.348076	-3.330097
87	1	0	4.913160	-0.687896	-1.436691
88	1	0	6.705464	-2.020184	-2.503342
89	1	0	7.207305	-4.320652	-1.689592
90	1	0	5.906462	-5.261115	0.210414
91	1	0	4.131764	-3.934354	1.281808
92	8	0	-1.653603	-0.183729	-0.328078
93	1	0	-0.757276	-0.035928	-0.663798
94	1	0	-1.610615	0.108090	0.593980

The total electronic energy was calculated to be –3296.6130923 Hartree.

Table S46. Optimized structure of H_2O@**INT1c** (B3LYP-D3/6-31G(d))

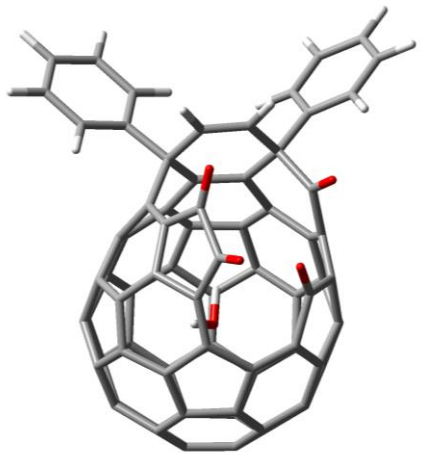


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.696698	1.777303	-2.530784
2	6	0	-2.285818	1.997626	-2.798832
3	6	0	-1.527541	0.976631	-3.346160
4	6	0	-2.127338	-0.312601	-3.641490
5	6	0	-3.470205	-0.540913	-3.345172
6	6	0	-4.270970	0.528228	-2.776344
7	6	0	-1.726700	2.819409	-1.742145
8	6	0	-0.186005	0.764148	-2.870979
9	6	0	-1.133080	-1.318467	-3.345675
10	6	0	-3.867346	-1.789182	-2.717765
11	6	0	-5.165441	-0.060059	-1.795001
12	6	0	-4.033027	2.510841	-1.330370
13	6	0	-2.902618	-2.757209	-2.430256
14	6	0	-1.509125	-2.519922	-2.758970
15	6	0	-2.936036	-3.454726	-1.161085
16	6	0	-0.681355	-3.066377	-1.707317
17	6	0	-0.426656	2.593699	-1.232601
18	6	0	0.076523	-0.659527	-2.902442
19	6	0	-1.567160	-3.641806	-0.726677
20	6	0	0.933739	-1.219228	-1.960166
21	6	0	0.377882	1.548539	-1.856483
22	6	0	-4.903631	-1.488382	-1.747356
23	6	0	-5.473341	0.635281	-0.625797
24	6	0	-0.163403	2.857939	0.192317
25	6	0	-4.914802	1.955322	-0.395488
26	6	0	-2.835258	3.187004	-0.877829
27	6	0	-5.499155	-0.062961	0.647154
28	6	0	-4.640009	2.088072	1.018728
29	6	0	-2.607235	3.366363	0.473849
30	6	0	0.527498	-2.464226	-1.310956
31	6	0	-4.928753	-2.159148	-0.520037
32	6	0	1.512179	1.004609	-1.141777
33	6	0	-4.961999	0.822694	1.660031
34	6	0	-3.534221	2.811346	1.449816
35	6	0	-1.266252	3.229835	0.983935
36	6	0	-1.381709	2.692074	2.307656
37	6	0	1.018197	2.286376	0.845048
38	6	0	1.815685	-0.330448	-1.227251
39	6	0	2.319658	-2.102307	0.435677
40	6	0	-2.739819	2.328569	2.556275
41	6	0	-2.976480	1.063397	3.104306
42	6	0	-1.900270	0.167602	3.509267
43	6	0	-4.117298	0.313633	2.649987
44	6	0	-3.918420	-3.150689	-0.221465
45	6	0	1.767716	1.123144	3.170446
46	6	0	-5.211547	-1.423701	0.702695
47	6	0	-4.341468	-1.938004	1.745554
48	6	0	0.925126	1.880758	2.176335
49	6	0	0.967782	-2.615532	0.057881
50	6	0	0.041079	-3.026086	1.014248
51	6	0	-0.370875	1.913803	2.812914
52	6	0	-0.613469	0.715408	3.584524
53	6	0	-3.761547	-1.083521	2.687925
54	6	0	-2.371004	-1.220736	3.142031
55	6	0	0.743584	0.380240	4.122790
56	6	0	-3.560463	-3.002577	1.182330
57	6	0	-1.233695	-3.502066	0.615772
58	6	0	-0.133679	-2.372591	2.374449
59	6	0	-2.242019	-3.127615	1.590173
60	6	0	-1.635719	-2.281722	2.592216
61	6	0	2.171697	1.916755	-0.114107
62	6	0	2.947912	-0.997526	-0.466970
63	6	0	3.745370	-0.014049	0.393695
64	6	0	3.355286	1.254446	0.547761
65	6	0	3.898342	-1.639176	-1.510228
66	6	0	2.743078	3.166104	-0.818424
67	8	0	2.913744	-2.592851	1.373996
68	8	0	2.957920	1.143850	3.370167
69	6	0	2.812185	4.405828	-0.176070
70	6	0	3.410320	5.472961	-0.844319
71	6	0	3.917564	5.265689	-2.126136
72	6	0	3.806205	3.988656	-2.678489
73	7	0	3.237576	2.956928	-2.045962
74	6	0	4.252544	-0.873074	-2.631581
75	6	0	5.146788	-1.375888	-3.574252
76	6	0	5.698879	-2.649283	-3.411052
77	6	0	5.357558	-3.407318	-2.292141
78	6	0	4.464994	-2.904861	-1.341860
79	8	0	0.727781	-1.849740	3.047434
80	8	0	1.036477	-0.108555	5.183888
81	6	0	7.438199	-0.762115	0.854597

82	6	0	6.221272	-0.394715	0.279572	95	1	0	5.791582	-4.392797	-2.146723
83	6	0	5.032588	-0.457819	1.021576	96	1	0	4.239525	-3.494343	-0.460721
84	6	0	5.086291	-0.883141	2.355688	97	1	0	8.349578	-0.709704	0.264382
85	6	0	6.304799	-1.244636	2.929772	98	1	0	6.188586	-0.060745	-0.752821
86	6	0	7.482787	-1.189951	2.182138	99	1	0	4.176194	-0.931217	2.939167
87	1	0	3.954000	1.906898	1.173584	100	1	0	6.330234	-1.570387	3.966209
88	1	0	2.405021	4.529118	0.822313	101	1	0	8.430034	-1.475407	2.632839
89	1	0	3.477283	6.448467	-0.370585	102	8	0	-2.175153	-0.218219	-0.203132
90	1	0	4.389155	6.067835	-2.685225	103	1	0	-1.968492	-0.209557	0.742624
91	1	0	4.191695	3.781394	-3.675089	104	1	0	-1.384031	0.152716	-0.621087
92	1	0	3.846212	0.128670	-2.748291	---					
93	1	0	5.415254	-0.769803	-4.435579	The total electronic energy was calculated to be –3527.6793144 Hartree.					
94	1	0	6.395111	-3.042205	-4.147053						

Table S47. Optimized structure of H_2O@**INT1d** (B3LYP-D3/6-31G(d))

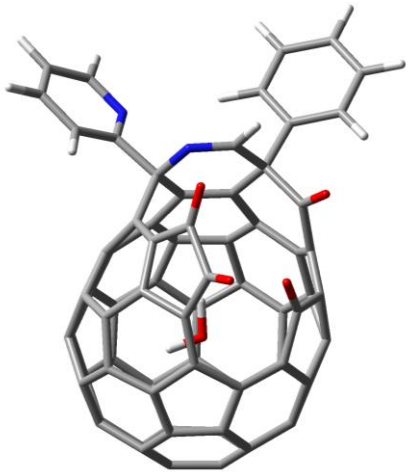


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.611629	1.456865	-3.182634
2	6	0	-1.161774	1.525895	-3.245625
3	6	0	-0.432352	0.372958	-3.479632
4	6	0	-1.104058	-0.904048	-3.643729
5	6	0	-2.491832	-0.980879	-3.540444
6	6	0	-3.261352	0.226986	-3.304113
7	6	0	-0.690544	2.487539	-2.266695
8	6	0	0.795249	0.161030	-2.757828
9	6	0	-0.270695	-1.903548	-3.015765
10	6	0	-3.100237	-2.061737	-2.784891
11	6	0	-4.349803	-0.107926	-2.403154
12	6	0	-3.052167	2.418728	-2.196377
13	6	0	-2.291175	-3.024312	-2.177196
14	6	0	-0.846963	-2.943955	-2.298238
15	6	0	-2.589767	-3.474841	-0.833259
16	6	0	-0.249773	-3.337885	-1.040712
17	6	0	0.490921	2.272718	-1.520972
18	6	0	0.913930	-1.258286	-2.493940
19	6	0	-1.330251	-3.667809	-0.145572
20	6	0	1.555480	-1.688692	-1.335029
21	6	0	1.279144	1.082593	-1.820080
22	6	0	-4.240654	-1.517965	-2.070502
23	6	0	-4.762300	0.809134	-1.436414
24	6	0	0.559464	2.765190	-0.135977
25	6	0	-4.116620	2.106570	-1.341892
26	6	0	-1.875964	3.082079	-1.672614
27	6	0	-5.053130	0.358681	-0.086722
28	6	0	-4.047297	2.474142	0.056089
29	6	0	-1.837605	3.484817	-0.349965
30	6	0	0.933322	-2.754661	-0.548836
31	6	0	-4.520910	-1.949541	-0.770000
32	6	0	2.240979	0.607848	-0.847752
33	6	0	-4.590500	1.373584	0.838035
34	6	0	-2.951563	3.181942	0.538143
35	6	0	-0.608627	3.345535	0.390357
36	6	0	-0.973431	3.057973	1.746824
37	6	0	1.570795	2.240221	0.787428
38	6	0	2.410605	-0.743699	-0.645668
39	6	0	2.435749	-2.164395	1.399663
40	6	0	-2.383913	2.848146	1.825508
41	6	0	-2.829412	1.724373	2.531293
42	6	0	-1.925412	0.839756	3.254958
43	6	0	-3.961464	0.992339	2.026578
44	6	0	-3.673716	-2.939131	-0.140837
45	6	0	1.838566	1.432108	3.366064
46	6	0	-4.915367	-0.985901	0.245643
47	6	0	-4.277241	-1.364181	1.493921
48	6	0	1.236396	2.068271	2.131759
49	6	0	1.136045	-2.685739	0.885751
50	6	0	0.034110	-2.861904	1.721999
51	6	0	-0.133452	2.304257	2.528365
52	6	0	-0.612059	1.290642	3.440938
53	6	0	-3.763459	-0.396012	2.361321
54	6	0	-2.484784	-0.551121	3.064521
55	6	0	0.608163	0.970330	4.249654
56	6	0	-3.530860	-2.567467	1.259035
57	6	0	-1.201667	-3.313883	1.191921
58	6	0	-2.313123	-2.710996	1.903839
59	6	0	-1.794263	-1.748062	2.843967
60	6	0	2.828960	1.659389	0.098583
61	6	0	3.311724	-1.324645	0.418378
62	6	0	4.019369	-0.256544	1.215230
63	6	0	3.806511	1.047470	1.071004
64	6	0	4.382983	-2.254607	-0.214522
65	6	0	3.595394	2.745064	-0.686166
66	8	0	2.821229	-2.419140	2.523443
67	8	0	2.979726	1.374474	3.751451
68	6	0	4.418337	2.368683	-1.754913
69	6	0	5.174774	3.319502	-2.437661
70	6	0	5.126761	4.661731	-2.053880
71	6	0	4.323049	5.041449	-0.978824
72	6	0	3.563805	4.087948	-0.297512
73	6	0	4.773387	-2.080715	-1.549183
74	6	0	5.782330	-2.867310	-2.104797
75	6	0	6.421607	-3.838710	-1.333487
76	6	0	6.048012	-4.008777	0.000007
77	6	0	5.039098	-3.222231	0.557888

78	8	0	0.682401	0.686029	5.417370	88	1	0	4.288742	-1.327320	-2.162123
79	6	0	-0.299247	-1.995764	2.930400	89	1	0	6.068156	-2.717158	-3.142504
80	8	0	0.472640	-1.471669	3.700307	90	1	0	7.205749	-4.453705	-1.766367
81	1	0	4.718452	-0.617695	1.961241	91	1	0	6.541259	-4.757212	0.614290
82	1	0	4.338159	1.752416	1.699117	92	1	0	4.766171	-3.360534	1.598330
83	1	0	4.471631	1.323391	-2.047018	93	8	0	-1.659422	-0.176485	-0.281295
84	1	0	5.804134	3.011109	-3.268149	94	1	0	-0.755812	-0.232241	-0.625504
85	1	0	5.714972	5.404048	-2.586235	95	1	0	-1.616393	0.533670	0.375825
86	1	0	4.283785	6.081487	-0.666469	---					
87	1	0	2.942744	4.394471	0.539016	The total electronic energy was calculated to be –3280.5737969 Hartree.					

Table S48. Optimized structure of H_2O@**INT1e** (B3LYP-D3/6-31G(d))



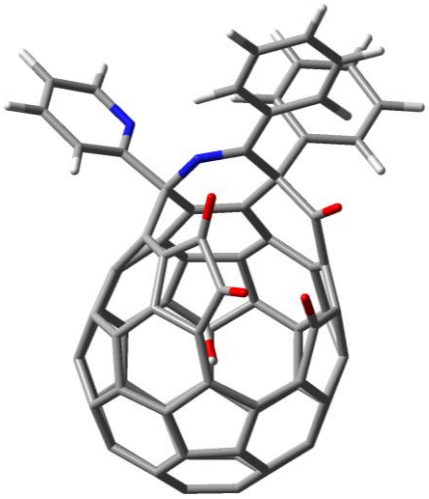
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.590487	1.287511	-3.284149
2	6	0	-1.138880	1.318407	-3.347137
3	6	0	-0.438296	0.134547	-3.502021
4	6	0	-1.138690	-1.134161	-3.586989
5	6	0	-2.527125	-1.171910	-3.482356
6	6	0	-3.268333	0.066556	-3.326164
7	6	0	-0.647322	2.330733	-2.430044
8	6	0	0.783181	-0.059964	-2.768149
9	6	0	-0.328719	-2.110874	-2.896026
10	6	0	-3.160205	-2.187188	-2.659578
11	6	0	-4.364134	-0.183330	-2.406463
12	6	0	-3.011148	2.322152	-2.363748
13	6	0	-2.373687	-3.126370	-1.989240
14	6	0	-0.928352	-3.090235	-2.115135
15	6	0	-2.681673	-3.480603	-0.618928
16	6	0	-0.339998	-3.419246	-0.834805
17	6	0	0.526048	2.135078	-1.665346
18	6	0	0.871293	-1.461573	-2.417228
19	6	0	-1.426823	-3.660439	0.080481
20	6	0	1.505057	-1.837929	-1.235775
21	6	0	1.283256	0.909985	-1.889899
22	6	0	-4.286197	-1.571279	-1.982502
23	6	0	-4.759144	0.804555	-1.503185
24	6	0	0.604714	2.715201	-0.311526
25	6	0	-4.085449	2.092023	-1.492845
26	6	0	-1.819535	2.990063	-1.878920
27	6	0	-5.061050	0.449994	-0.126874
28	6	0	-4.010272	2.549798	-0.120686
29	6	0	-1.773881	3.477559	-0.584526
30	6	0	0.858674	-2.835635	-0.382941
31	6	0	-4.575410	-1.909532	-0.656455
32	6	0	2.219534	0.471911	-0.884790
33	6	0	-4.579590	1.514389	0.730458
34	6	0	-2.897385	3.261780	0.317437
35	6	0	-0.549956	3.360569	0.169952
36	6	0	-0.925510	3.177753	1.540918
37	6	0	1.591798	2.224890	0.656056
38	6	0	2.357777	-0.861769	-0.597573
39	6	0	2.386579	-2.172894	1.523528
40	6	0	-2.341185	3.004503	1.626912
41	6	0	-2.813523	1.939344	2.400404
42	6	0	-1.932703	1.087794	3.185730
43	6	0	-3.957863	1.198152	1.941715
44	6	0	-3.750263	-2.873693	0.037644
45	6	0	1.833872	1.583286	3.299646
46	6	0	-4.949827	-0.872874	0.292953
47	6	0	-4.318776	-1.181210	1.564020
48	6	0	1.257713	2.159297	2.011997
49	6	0	1.064334	-2.674510	1.043361
50	6	0	-0.041926	-2.761272	1.887199
51	6	0	-0.106010	2.464004	2.380413
52	6	0	-0.616767	1.528375	3.357442
53	6	0	-3.786576	-0.169060	2.366657
54	6	0	-2.509922	-0.301816	3.078194
55	6	0	0.581452	1.227156	4.198436
56	6	0	-3.596874	-2.412347	1.409795
57	6	0	-1.288196	-3.218484	1.391799
58	6	0	-2.380638	-2.536437	2.060704
59	6	0	-1.837638	-1.521439	2.932649
60	6	0	2.822184	1.536716	0.027735
61	6	0	3.236002	-1.345658	0.524476
62	6	0	3.858129	-0.185698	1.291800
63	7	0	3.707466	1.053677	1.076268
64	6	0	4.407746	-2.175584	-0.055523
65	6	0	3.681194	2.520627	-0.788914
66	8	0	2.804272	-2.435356	2.634393
67	8	0	2.964482	1.496919	3.701852
68	6	0	3.896212	3.828824	-0.347876
69	6	0	4.738142	4.650597	-1.092764
70	6	0	5.337278	4.135327	-2.243053
71	6	0	5.070530	2.811115	-2.589132
72	7	0	4.261049	2.012984	-1.881602
73	6	0	5.113448	-1.630150	-1.139746
74	6	0	6.188632	-2.319973	-1.696157
75	6	0	6.574660	-3.558696	-1.178539
76	6	0	5.883904	-4.095427	-0.092747
77	6	0	4.807750	-3.406741	0.472926
78	8	0	0.632031	1.016230	5.383432
79	6	0	-0.344645	-1.780068	3.009146
80	8	0	0.463584	-1.183018	3.685469
81	1	0	4.501254	-0.479668	2.120805
82	1	0	3.419991	4.182628	0.560309
83	1	0	4.925699	5.673853	-0.779551

84	1	0	5.999037	4.740326	-2.855145	90	1	0	4.297285	-3.830863	1.329653
85	1	0	5.524450	2.366048	-3.472459	91	8	0	-1.557578	-0.246700	-0.262609
86	1	0	4.824715	-0.661830	-1.541899	92	1	0	-0.600751	-0.098813	-0.218054
87	1	0	6.726717	-1.886099	-2.534701	93	1	0	-1.928255	0.647206	-0.298720
88	1	0	7.411716	-4.097280	-1.614352						
89	1	0	6.181145	-5.053761	0.324374						

The total electronic energy was calculated to be –3312.6503141 Hartree.

Table S49. Optimized structure of H_2O@**INT1f** (B3LYP-D3/6-31G(d))



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.650105	1.136255	-2.918439
2	6	0	-2.236982	1.214616	-3.247417
3	6	0	-1.529680	0.050340	-3.499733
4	6	0	-2.184081	-1.243898	-3.418435
5	6	0	-3.529097	-1.324007	-3.061909
6	6	0	-4.277962	-0.106270	-2.807581
7	6	0	-1.627478	2.270775	-2.459889
8	6	0	-0.187848	-0.078398	-2.997174
9	6	0	-1.224738	-2.167428	-2.855993
10	6	0	-3.963999	-2.331312	-2.110415
11	6	0	-5.180080	-0.362414	-1.698733
12	6	0	-3.936599	2.185321	-1.964587
13	6	0	-3.033560	-3.220403	-1.568070
14	6	0	-1.636563	-3.138753	-1.952658
15	6	0	-3.077744	-3.538714	-0.155719
16	6	0	-0.816822	-3.399827	-0.789791
17	6	0	-0.327378	2.139335	-1.919064
18	6	0	0.016518	-1.462715	-2.622050
19	6	0	-1.711545	-3.648068	0.311711
20	6	0	0.862719	-1.771173	-1.559891
21	6	0	0.425179	0.935593	-2.249626
22	6	0	-4.975265	-1.732009	-1.259318
23	6	0	-5.441371	0.640449	-0.765247
24	6	0	-0.028584	2.758689	-0.614740
25	6	0	-4.825085	1.947371	-0.909261
26	6	0	-2.704500	2.906317	-1.720954
27	6	0	-5.478430	0.321466	0.650697
28	6	0	-4.521805	2.451018	0.412821
29	6	0	-2.444307	3.434941	-0.470100
30	6	0	0.415194	-2.753666	-0.576613
31	6	0	-5.010588	-2.037070	0.105195
32	6	0	1.543060	0.561434	-1.420020
33	6	0	-4.890408	1.427432	1.378788
34	6	0	-3.377349	3.211298	0.624828
35	6	0	-1.101489	3.378874	0.051908
36	6	0	-1.216727	3.224431	1.472144
37	6	0	1.133038	2.326078	0.169423
38	6	0	1.786502	-0.749067	-1.116804
39	6	0	2.227667	-1.952497	1.011532
40	6	0	-2.586204	3.013090	1.817895
41	6	0	-2.874542	1.963648	2.696988
42	6	0	-1.835527	1.165920	3.334861
43	6	0	-4.056250	1.173293	2.470502
44	6	0	-4.037877	-2.950253	0.664379
45	6	0	1.875258	1.774987	2.724986
46	6	0	-5.248586	-0.982953	1.079106
47	6	0	-4.389945	-1.228845	2.223907
48	6	0	1.050649	2.291688	1.561641
49	6	0	0.864773	-2.526552	0.781602
50	6	0	-0.063598	-2.637906	1.816704
51	6	0	-0.233351	2.563581	2.166679
52	6	0	-0.522223	1.644511	3.244125
53	6	0	-3.763701	-0.173953	2.894799
54	6	0	-2.377438	-0.244374	3.373907
55	6	0	0.826258	1.410151	3.854140
56	6	0	-3.660795	-2.440342	1.974767
57	6	0	-1.358080	-3.161364	1.564451
58	6	0	-0.203873	-1.663238	2.977689
59	6	0	-2.344623	-2.504712	2.402993
60	6	0	-1.698098	-1.447658	3.142027
61	6	0	2.254792	1.662590	-0.654054
62	6	0	2.895554	-1.191370	-0.179770
63	6	0	3.708884	0.016520	0.357734
64	7	0	3.355032	1.231744	0.169627
65	6	0	3.785440	-2.122750	-1.035943
66	6	0	2.908391	2.660819	-1.636396
67	8	0	2.791240	-2.121302	2.072387
68	8	0	3.064674	1.748440	2.908424
69	6	0	3.066681	4.010457	-1.313140
70	6	0	3.736915	4.835059	-2.213872
71	6	0	4.226902	4.282563	-3.397495
72	6	0	4.028638	2.919789	-3.619824
73	7	0	3.385785	2.118740	-2.761853
74	6	0	4.494732	-1.543665	-2.096958
75	6	0	5.277611	-2.336750	-2.933382
76	6	0	5.352419	-3.716722	-2.729259
77	6	0	4.636025	-4.297731	-1.682936
78	6	0	3.853479	-3.505422	-0.840496
79	8	0	0.676828	-1.052211	3.538931
80	8	0	1.103991	1.250693	5.015028
81	6	0	6.761506	-1.527958	2.088821
82	6	0	5.544842	-1.430749	1.415808
83	6	0	4.987587	-0.178719	1.110930
84	6	0	5.692319	0.973231	1.512717
85	6	0	6.902834	0.874784	2.187917
86	6	0	7.447992	-0.378675	2.477375
87	1	0	2.678526	4.397655	-0.377129
88	1	0	3.875570	5.890070	-1.994211
89	1	0	4.753195	4.888053	-4.128915

90	1	0	4.401787	2.445473	-4.525583	98	1	0	5.260151	1.941097	1.296513
91	1	0	4.416625	-0.473548	-2.274588	99	1	0	7.421215	1.779851	2.493037
92	1	0	5.827818	-1.874718	-3.748571	100	1	0	8.395631	-0.457541	3.004020
93	1	0	5.962738	-4.334160	-3.382472	101	8	0	-2.160655	-0.191133	-0.112650
94	1	0	4.684869	-5.370230	-1.515534	102	1	0	-1.942426	0.189823	0.750342
95	1	0	3.316599	-3.972853	-0.020527	103	1	0	-1.375724	-0.015977	-0.652388
96	1	0	7.167866	-2.510660	2.312017	---					
97	1	0	5.036367	-2.341816	1.144166	The total electronic energy was calculated to be –3543.7164107 Hartree.					

8. References

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(2) Sheldrick, G. M. *SHELX-97*; University of Göttingen: Göttingen, Germany, 1997.