Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Oxidation of a triple carbo[5]helicene with hypervalent iodine

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Section S1: General materials and methods

S1.1. Synthesis

Unless otherwise noted, reagents and solvents (reagent grade), including anhydrous dichloromethane, were obtained from Aldrich and used as received. Reactions were generally carried out in tubular oven-dried glassware. All reagents were weighed and handled in air at room temperature unless otherwise mentioned, and solvents were introduced via syringes. Reactions were monitored by thin layer chromatography (TLC) on Merck Kieselgel 60 F254 0.2 mm plates. Visualization was accomplished using ultraviolet light (254 and/or 365 nm) and/or using an acidic p-anisaldehyde ethanolic stain. Purifications were routinely performed using flash chromatography columns packed with 40-63 μm silica gel generally eluted with pentane, dichloromethane, toluene, ethyl acetate, diethyl ether and methanol. *C*$_2$-**HBTP** and *D*$_3$-**HBTP** were synthesized according to literature procedures from commercially available 9-phenanthrol.[1-3]

S1.2. Characterization

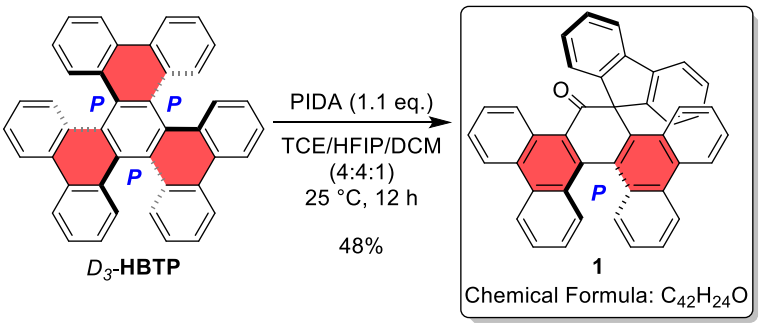
Melting points were recorded using a Büchi Melting Point B-540 apparatus and are reported without any corrections. NMR data were generally recorded in deuterated chloroform at 298 ± 3 K at 300 MHz, 400 MHz, or 500 MHz using the residual non-deuterated solvent as an internal standard for ^{1}H NMR (δ = 7.26 ppm) and the deuterated solvent signal for ^{13}C NMR (δ = 77.16 ppm). Chemical shifts (δ) are in ppm, coupling constants (J) are in Hertz (Hz) and the classical abbreviations are used to describe the signal multiplicities. DEPT135 experiments were used to support assignments. High resolution mass spectra (HRMS) were recorded in triplicate at the Spectropole (http://fr-chimie.univ-amu.fr/spectropole/) on a Waters Synapt G2 HRMS apparatus using a positive electrospray (ESI) ionization source.
Single crystals were obtained by slow evaporation of a diluted dichloromethane or acetonitrile solution at room temperature. Suitable crystals were selected and mounted on a SuperNova, Dual, Cu at home/near, AtlasS2 diffractometer. Crystals were kept at 295 K during data collection. Using Olex2, the structure was solved with the SHELXT structure solution program using Intrinsic Phasing and refined with the SHELXL refinement package using Least Squares minimization. Fluorescence was measured using the Jasco FP-8600 Fluorescence Spectrometer. Quartz Fluorescence cuvettes (10 x 10 mm) were used with a PTFE stopper to prevent solution evaporation. An auto zero of the spectrometer was realized. Mode Emission, Ex bandwidth = 1 nm, Em bandwidth = 10 nm, Response = 0.2 sec, Sensitivity = Medium, Measurement range = 365 - 700 nm, Data interval = 1 nm, Ex wavelength = 355.0 nm, Scan speed = 500 nm/min. Diphenyl Anthracene (DPA) was used as reference; λ_{FL}(max) = 409 nm, Φf = 0.97 ± 0.03 at 355 nm (cyclohexane)[4]. Absorbance was measured using the Shimadzu UV-2401PC UV-VIS Spectrometer. Quartz UV cuvettes (10 x 10 mm) were used with a PTFE stopper to prevent solution evaporation. An auto zero and baseline measurement for each solvent was realized. Mode Absorbance, Slit width = 0,5 nm, Measurement range = 200 - 700 nm, Data interval = 1 nm, Scan speed = Medium.

S1.3 Computational methods

Geometries of all stationary points were optimized without symmetry constraint with the *Gaussian* 16 program[5] using the DFT ωB97XD hybrid exchange-correlation functional.[6] The def2-SVP basis set was employed for all atoms.[7,8] The electronic energy was improved by performing single-point energy calculations with the def2-TZVP basis set and the same density functional. Analytical Hessians were computed to determine the nature of stationary points (one and zero imaginary frequencies for transition states and minima, respectively) and to calculate unscaled zero-point energies (ZPEs) as well as thermal corrections and entropy effects using the standard statistical-mechanics relationships for an ideal gas.[9] These two latter terms were computed at 298.15 K and 1 atm to provide the reported relative Gibbs energies. As a summary, the reported Gibbs energies contain electronic energies calculated at the ωB97XD/def2-TZVP//ωB97XD/def2-SVP level together with gas phase thermal and entropic contributions computed at 298.15 K and 1 atm with the ωB97XD/def2-SVP method. Input geometries for transition state calculations in conformational analyses were obtained using the CHAIN algorithm[10] as implemented in the AMPAC software (http://www.semichem.com/ampac/default.php). EDDB(*r*) surfaces were computed at the B3LYP-GIAO/6-311++G(d,p)//B3LYP-D3BJ/def2-SVP level of theory using NBO 6.0 software first to obtain the natural atomic orbitals and then running the EDDB program available at http://aromaticity.eu.[11] The EDDB(*r*) isosurfaces were generated using the *Formchk* and *Cubegen* tools implemented in the Gaussian 16 package. Molecular graphics and analyses were performed with UCSF Chimera[12] All computational data concerning reaction mechanisms and conformational analyses was uploaded to the ioChem-BD repository and is available through the following link: https://iochem.udg.edu:8443/browse/handle/100/4771

Section S2: Synthesis

S2.1. Representative synthesis of 1

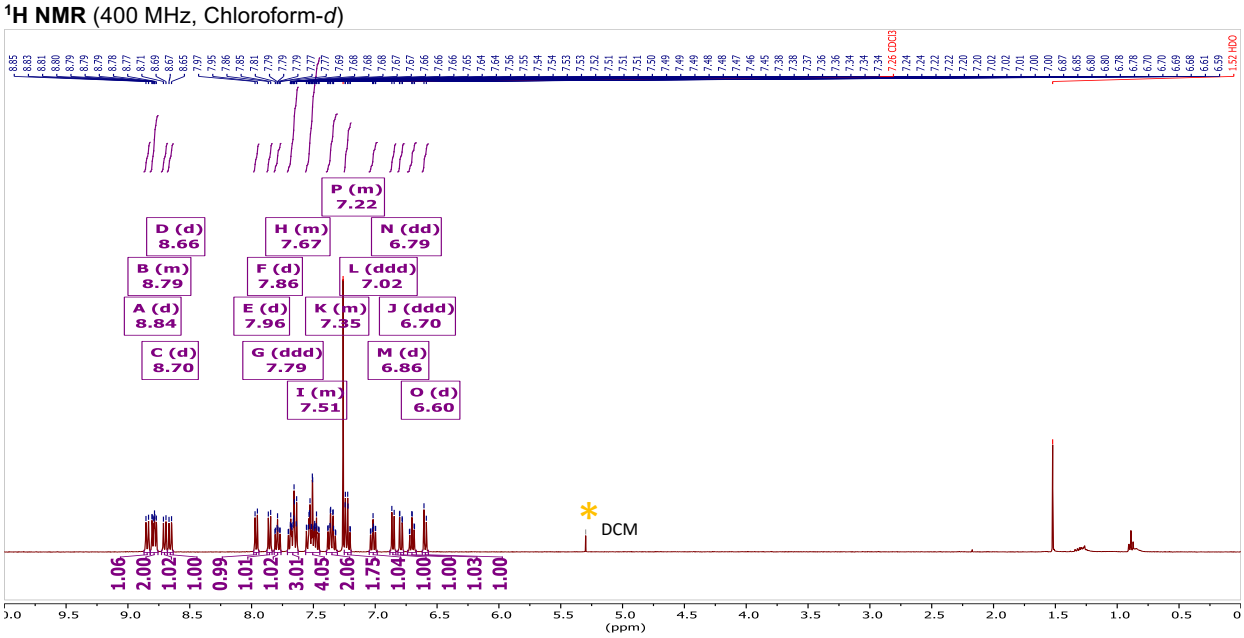


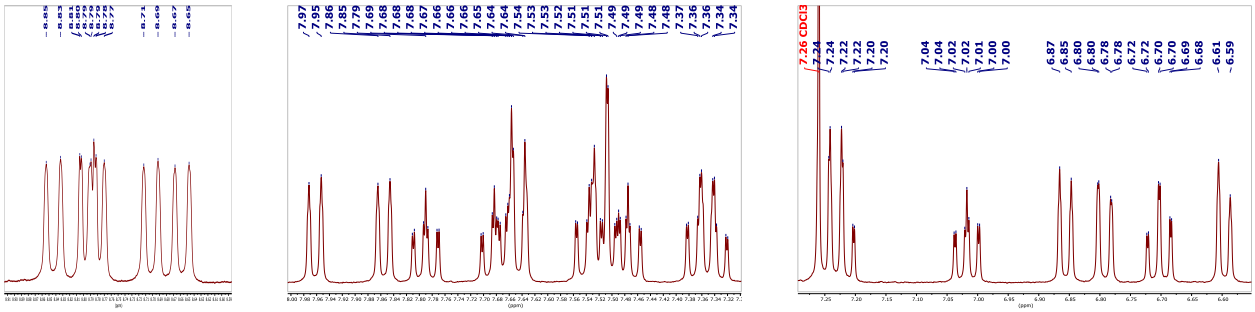
A sealable oven-dried tubular flask was charged with *D*$_3$-**HBTP** (20 mg, 0.038 mmol), 1,1,2,2-tetrachloroethane (0.8 mL) and dichloromethane (0.2 mL) and was stirred for 5 min at room temperature. Diacetoxyiodobenzene (13.5 mg, 0.042 mmol) and hexafluoroisopropanol (0.8 mL) were then added and the biphasic medium was vigorously stirred for 12 h. The resulting dark mixture was filtered on a silica plug (rinsed with dichloromethane) and evaporated to dryness under vacuum. The crude product thus obtained was purified by column flash chromatography to afford the title compound (9.5 mg, yield: 48%) as a yellow solid. Analytical samples of monocrystalline material suitable for X-ray diffraction analysis were obtained by slow evaporation of a diluted dichloromethane solution at room temperature.

S2.2. Spectroscopic data for 1

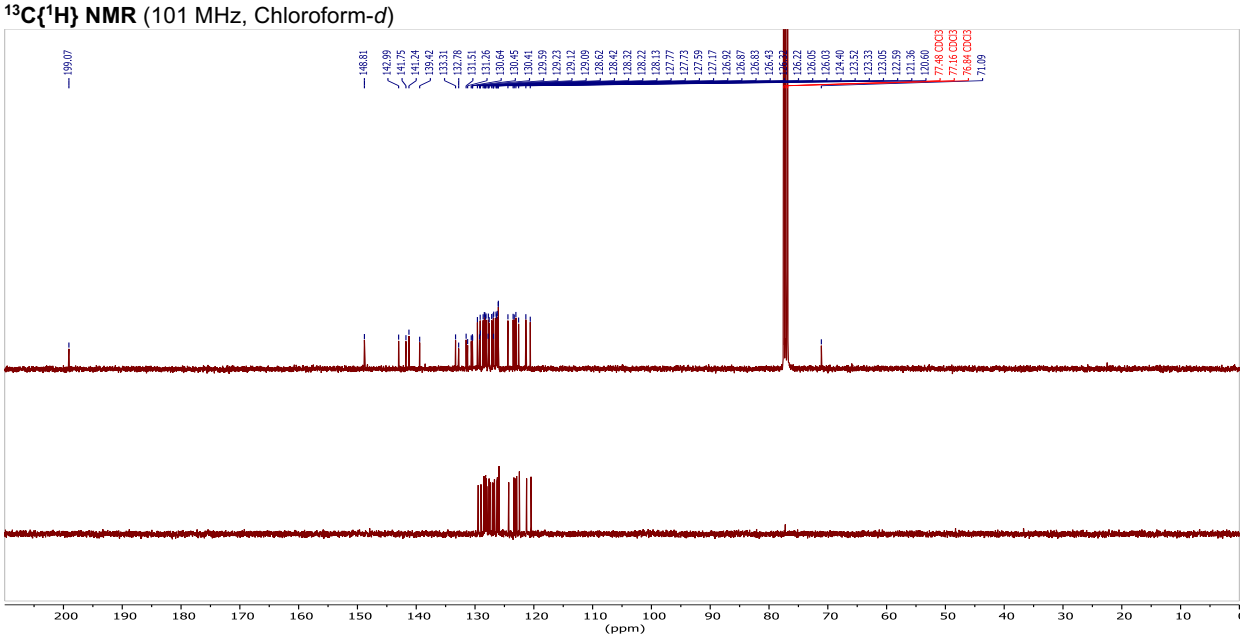
MW ($C_{42}H_{24}O$): 544.7 g/mol; ***Rf***: 0.32 (ethyl acetate/pentane 1:9); **m.p. (ºC)** > 350 (amorphous, decomposition); **^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm):** 8.84 (d, *J* = 8.3 Hz, 1H), 8.82 – 8.76 (m, 2H), 8.70 (d, *J* = 8.2 Hz, 1H), 8.66 (d, *J* = 8.1 Hz, 1H), 7.96 (d, *J* = 7.6 Hz, 1H), 7.86 (d, *J* = 7.5 Hz, 1H), 7.79 (ddd, *J* = 8.3, 7.0, 1.3 Hz, 1H), 7.71 – 7.62 (m, 3H), 7.56 – 7.45 (m, 4H), 7.39 – 7.31 (m, 2H), 7.25 – 7.20 (m, 2H), 7.02 (ddd, *J* = 8.3, 7.0, 1.2 Hz, 1H), 6.86 (d, *J* = 7.6 Hz, 1H), 6.79 (dd, *J* = 8.2, 0.7 Hz, 1H), 6.70 (ddd, *J* = 7.6, 7.6 1.1 Hz, 1H), 6.60 (d, *J* = 7.6 Hz, 1H); **^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm):** 199.1 (C), 148.8 (C), 143.0 (C), 141.7 (C), 141.2 (C), 139.4 (C), 133.3 (C), 132.8 (C), 131.5 (C), 131.3 (C), 130.6 (C), 130.4 (C), 130.4 (C), 129.6 (C-H), 129.2 (C), 129.1 (C-H), 129.1 (C), 128.6 (C-H), 128.4 (C-H), 128.3 (C-H), 128.2 (C-H), 128.1 (C-H), 127.8 (C), 127.7 (C-H), 127.6 (C-H), 127.2 (C-H), 126.9 (C-H), 126.9 (C), 126.8 (C-H), 126.4 (C-H), 126.3 (C-H), 126.2 (C-H), 126.0 (C-H), 126.0 (C-H), 124.4 (C-H), 123.5 (C-H), 123.3 (C-H), 123.1 (C-H), 122.6 (C-H), 121.4 (C-H), 120.6 (C-H), 71.1 (C); the structure of **1** was ascertained by single-crystal X-ray diffraction analysis.

^{1}H NMR (400 MHz, Chloroform-*d*)





$^{13}C\{^{1}H\}$ NMR (101 MHz, Chloroform-*d*)



S2.3. X-Ray crystallographic analysis of 1

Suitable crystals were selected and mounted on a Rigaku Oxford Diffraction SuperNova diffractometer. Crystals were kept at 295 K during data collection. Using Olex2,[13] the structure was solved with the SHELXT[14] structure solution program using Intrinsic Phasing and refined with the SHELXL[15] refinement package using Least Squares minimization. All H-atoms were found experimentally and refined as riding atoms with their Uiso parameters constrained to 1.2 Ueq (parent atoms). CCDC 2285158 contains the supplementary crystallographic data for **1**. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

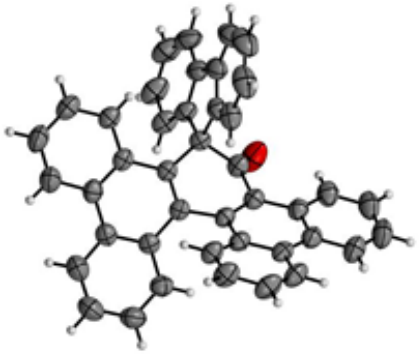
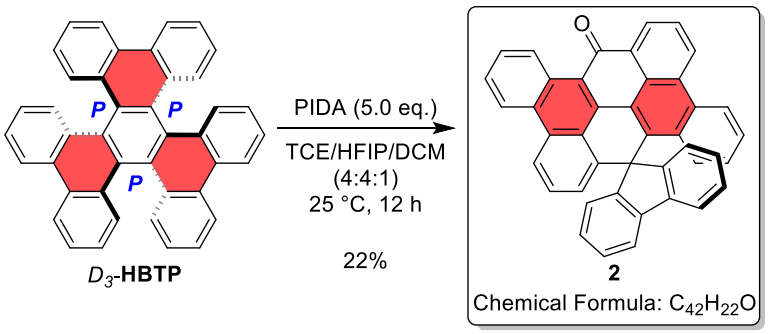


Figure S1. Solid-state molecular structure of **1**. Ellipsoids are draw at the 50% probability level and H atoms are drawn as 0.15 Å radius spheres.

Table S1. Crystal data and structure refinement for **1**

Crystal data and structure refinement for 1	
Identification code	CCDC 2285158
Empirical formula	$C_{42}H_{24}O$
Formula weight	544.61
Temperature/K	295.00
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	10.0228(2)
b/Å	13.5614(3)
c/Å	20.8656(5)
β/°	100.979(2)
Volume/Å^3	2784.21(11)
Z	4
ρcalcg/cm^3	1.299
μ/mm-1	0.588
F(000)	1136.0
Crystal size/mm	0.15 × 0.1 × 0.03
Radiation	Cu Kα (λ = 1.54184 Å)
2Θ range for data collection/°	7.818 to 152.258
Index ranges	-11 ≤ h ≤ 12, -15 ≤ k ≤ 17, -26 ≤ l ≤ 26
Reflections collected	24607
Independent reflections	5797 [Rint = 0.0321, Rsigma = 0.0211]
Data/restraints/parameters	5797/0/388
Goodness-of-fit on F2	1.027
Final R indexes [I>=2σ (I)]	R1 = 0.0451, wR2 = 0.1173
Final R indexes [all data]	R1 = 0.0636, wR2 = 0.1308
Largest diff. peak/hole / e Å-3	0.39/-0.19

S2.4. Representative synthesis of 2



D$_3$-**HBTP**

2

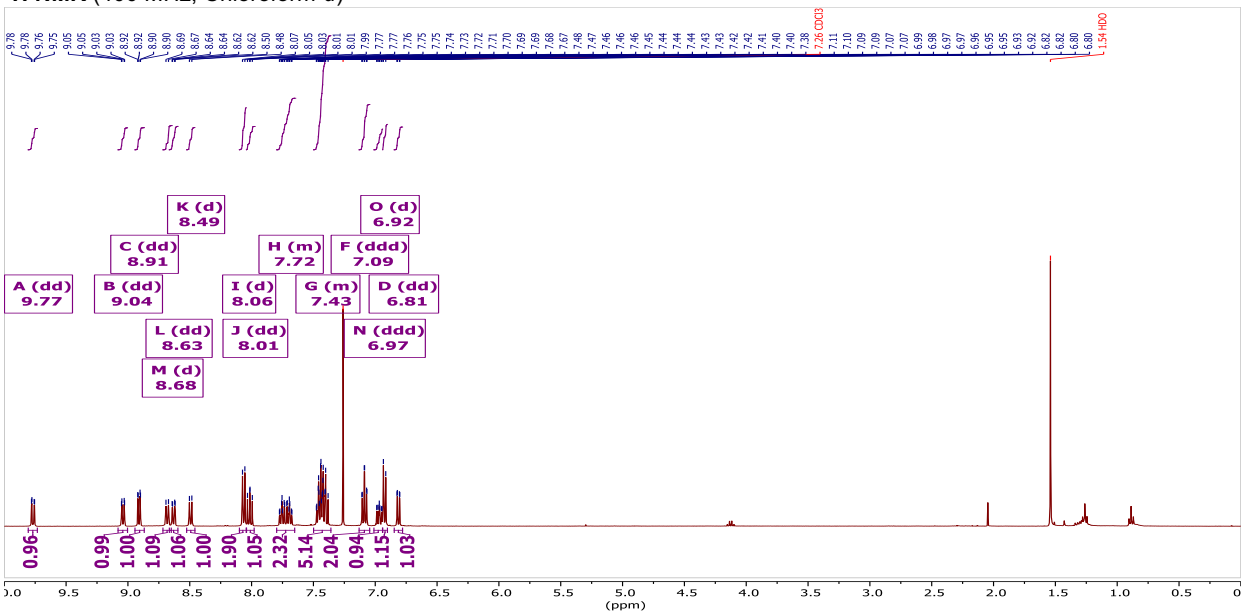
Chemical Formula: $C_{42}H_{22}O$

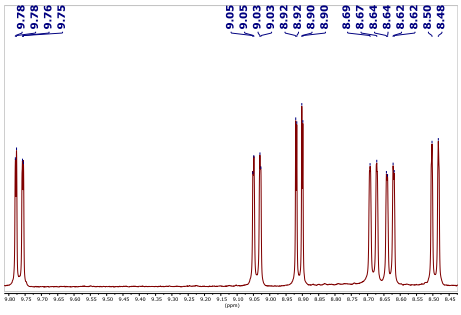
A sealable oven-dried tubular flask was charged with ***D*$_3$-HBTP** (20 mg, 0.038 mmol), 1,1,2,2-tetrachloroethane (0.8 mL) and dichloromethane (0.2 mL), and was stirred for 5 min at room temperature. Diacetoxyiodobenzene (60 mg, 0.186 mmol) and hexafluoroisopropanol (0.8 mL) were then added and the biphasic medium was vigorously stirred for 12 h. The resulting dark mixture was filtered on a silica plug (rinsed with dichloromethane) and evaporated to dryness under vacuum. The crude product was purified by column flash chromatography to afford the title compound (4.3 mg, Yield: 22%) as an orange solid. Analytical samples of monocrystalline material suitable for X-ray diffraction analysis were obtained by slow evaporation of a diluted acetonitrile solution at room temperature.

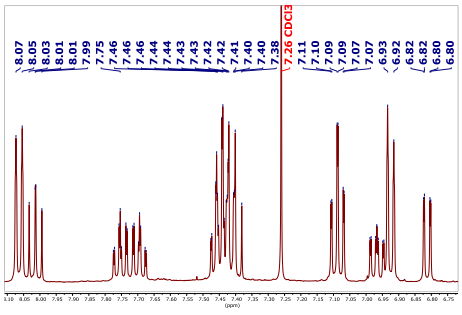
S2.5. Spectroscopic data for 2

MW ($C_{42}H_{22}O$): 542.6 g/mol; ***Rf*:** 0.25 (ethyl acetate/pentane 1:9); **m.p. (ºC)** > 350 (amorphous, decomposition); **^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm):** 9.77 (dd, *J* = 8.6, 1.3 Hz, 1H), 9.04 (dd, *J* = 8.7, 1.2 Hz, 1H), 8.91 (dd, *J* = 7.5, 1.3 Hz, 1H), 8.68 (d, *J* = 8.2 Hz, 1H), 8.63 (dd, *J* = 8.2, 1.4 Hz, 1H), 8.49 (d, *J* = 7.8 Hz, 1H), 8.06 (d, *J* = 7.6 Hz, 2H), 8.01 (dd, *J* = 8.1, 7.5 Hz, 1H), 7.80 – 7.65 (m, 2H), 7.50 – 7.36 (m, 5H), 7.09 (ddd, *J* = 7.5, 7.5, 1.1 Hz, 2H), 6.97 (ddd, *J* = 8.7, 6.9, 1.4 Hz, 1H), 6.92 (d, *J* = 7.6 Hz, 1H), 6.81 (dd, *J* = 7.8, 1.1 Hz, 1H); **^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm):** 186.7 (C), 157.0 (2C), 140.6 (2C), 140.5 (C), 139.6 (C), 133.3 (C), 132.5 (C), 132.1 (C), 131.4 (C), 131.2 (C), 129.9 (C), 129.8 (C), 129.5 (C), 129.3 (C-H), 129.2 (C-H), 129.1 (2C-H), 128.8 (C-H), 128.7 (C-H), 128.1 (2C-H), 128.1 (C-H), 128.1 (C-H), 127.8 (C-H), 127.8 (C-H), 127.8 (C-H), 126.9 (C-H), 126.7 (C-H), 125.9 (C), 125.0 (C), 124.8 (2C-H), 124.4 (C), 123.7 (C), 122.9 (C-H), 122.7 (C-H), 121.4 (2C-H), 121.0 (C-H), 60.3 (C); the structure of **2** was ascertained by single-crystal X-ray diffraction analysis.

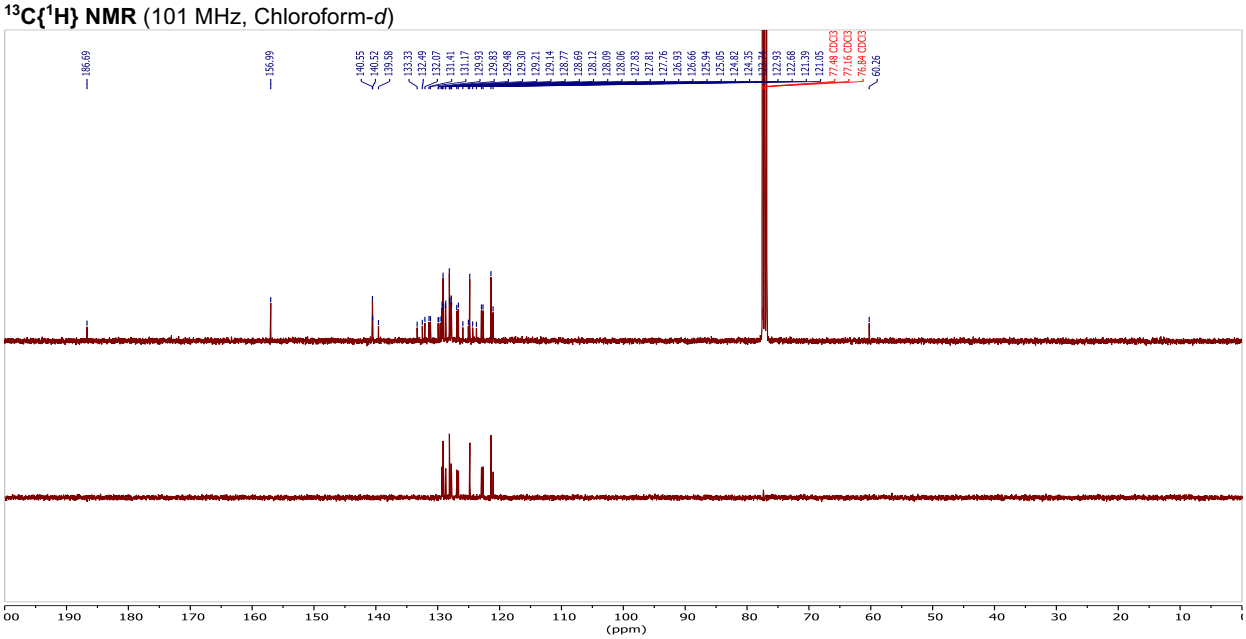
^{1}H NMR (400 MHz, Chloroform-*d*)







$^{13}C\{^{1}H\}$ NMR (101 MHz, Chloroform-*d*)



S2.6. X-Ray crystallographic analysis of 2

Suitable crystals were selected and mounted on a Rigaku Oxford Diffraction SuperNova diffractometer. Crystals were kept at 295 K during data collection. Using Olex2,[13] the structure was solved with the SHELXT[14] structure solution program using Intrinsic Phasing and refined with the SHELXL[15] refinement package using Least Squares minimization. All H-atoms were found experimentally and refined as riding atoms with their Uiso parameters constrained to 1.2 Ueq (parent atoms). CCDC 2285157 contains the supplementary crystallographic data for **2**. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

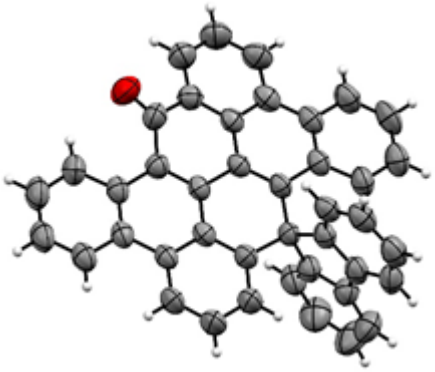
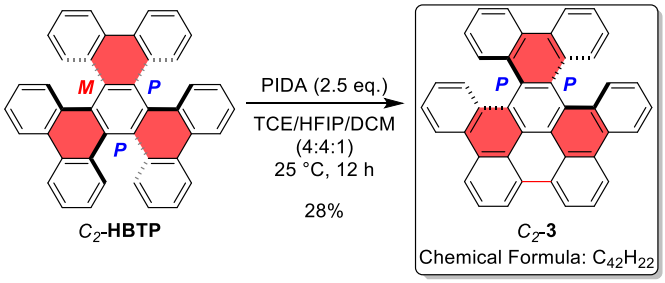


Figure S2. Solid-state molecular structure of **2.** Ellipsoids are draw at the 50% probability level and H atoms are drawn as 0.15 Å radius spheres.

Table S2. Crystal data and structure refinement for **2**

Crystal data and structure refinement for 2	
Identification code	CCDC 2285157
Empirical formula	$C_{42}H_{22}O$
Formula weight	542.59
Temperature/K	295
Crystal system	triclinic
Space group	P-1
a/Å	8.5907(8)
b/Å	10.8197(13)
c/Å	15.6611(15)
α/°	78.459(9)
β/°	81.575(8)
γ/°	67.199(10)
Volume/Å^3	1311.0(3)
Z	2
ρcalcg/cm^3	1.375
μ/mm-1	0.625
F(000)	564.0
Crystal size/mm	0.16 × 0.05 × 0.03
Radiation	Cu Kα (λ = 1.54184 Å)
2Θ range for data collection/°	5.776 to 152.382
Index ranges	-10 ≤ h ≤ 10, -13 ≤ k ≤ 13, -11 ≤ l ≤ 19
Reflections collected	11307
Independent reflections	5398 [Rint = 0.0532, Rsigma = 0.0892]
Data/restraints/parameters	5398/0/388
Goodness-of-fit on F2	0.984
Final R indexes [I>=2σ (I)]	R1 = 0.0644, wR2 = 0.1509
Final R indexes [all data]	R1 = 0.1433, wR2 = 0.1996
Largest diff. peak/hole / e Å-3	0.22/-0.14

S2.7. Representative synthesis of C_2-3

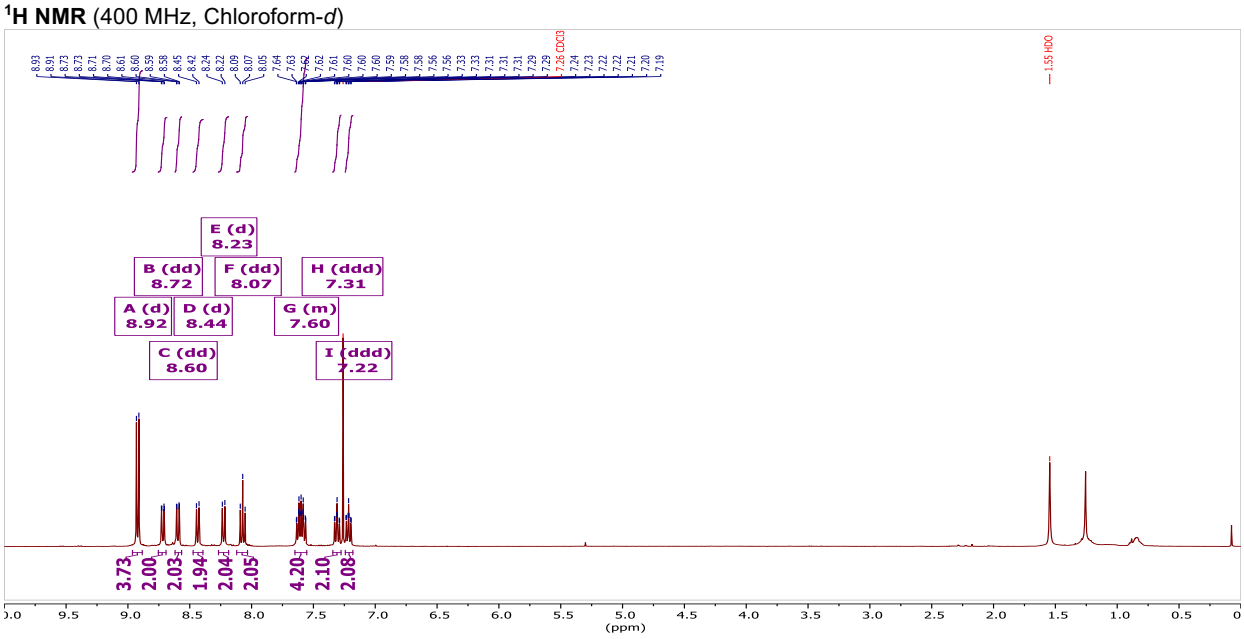


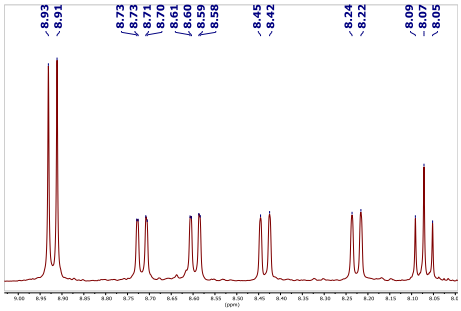
A sealable oven-dried tubular flask was charged with ***C*$_2$-HBTP** (20 mg, 0.038 mmol), 1,1,2,2-tetrachloroethane (0.8 mL) and dichloromethane (0.2 mL), and was stirred for 5 min at room temperature. Diacetoxyiodobenzene (30 mg, 0.093 mmol) and hexafluoroisopropanol (0.8 mL) were then added and the biphasic medium was vigorously stirred for 12 h. The resulting dark mixture was filtered on a silica plug (rinsed with dichloromethane) and evaporated to dryness under vacuum. The crude product was purified by column flash chromatography to afford the title compound (5.6 mg, Yield: 28%) as a yellow solid.

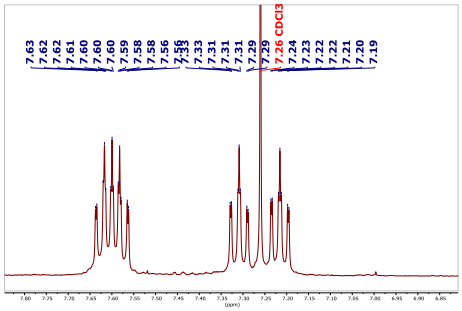
S2.8. Spectroscopic data for C_2-3

MW ($C_{42}H_{22}$): 526.6 g/mol; ***Rf*:** 0.39 (ethyl acetate/pentane 1:9; green fluorescence under 366 nm UV light); **m.p. (ºC)** > 350 (amorphous, decomposition); **^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm):** 8.92 (d, *J* = 7.9 Hz, 4H), 8.72 (dd, *J* = 8.3, 1.3 Hz, 2H), 8.60 (dd, *J* = 8.0, 1.3 Hz, 2H), 8.44 (d, *J* = 8.3 Hz, 2H), 8.23 (d, *J* = 8.1 Hz, 2H), 8.07 (dd, *J* = 7.9, 7.9 Hz, 2H), 7.65 – 7.55 (m, 4H), 7.31 (ddd, *J* = 8.2, 7.1, 1.2 Hz, 2H), 7.22 (ddd, *J* = 8.2, 6.9, 1.2 Hz, 2H); **^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm):** 132.5 (2C), 132.0 (2C-H), 130.9 (2C-H), 130.8 (2C), 130.6 (2C), 130.5 (2C), 130.3 (2C), 129.7 (2C), 128.7 (2C), 127.4 (2C-H), 127.2 (2C-H), 127.0 (2C-H), 126.0 (2C-H), 125.5 (2C-H), 125.0 (2C), 123.9 (2C-H), 123.9 (2C), 123.6 (2C-H), 123.6 (2C), 122.7 (2C-H), 121.5 (2C-H); **ESI-HRMS(m/z):** $[M+Ag]^+$ calcd for $C_{42}H_{22}Ag^+$ = 635.0771, found 635.0776.

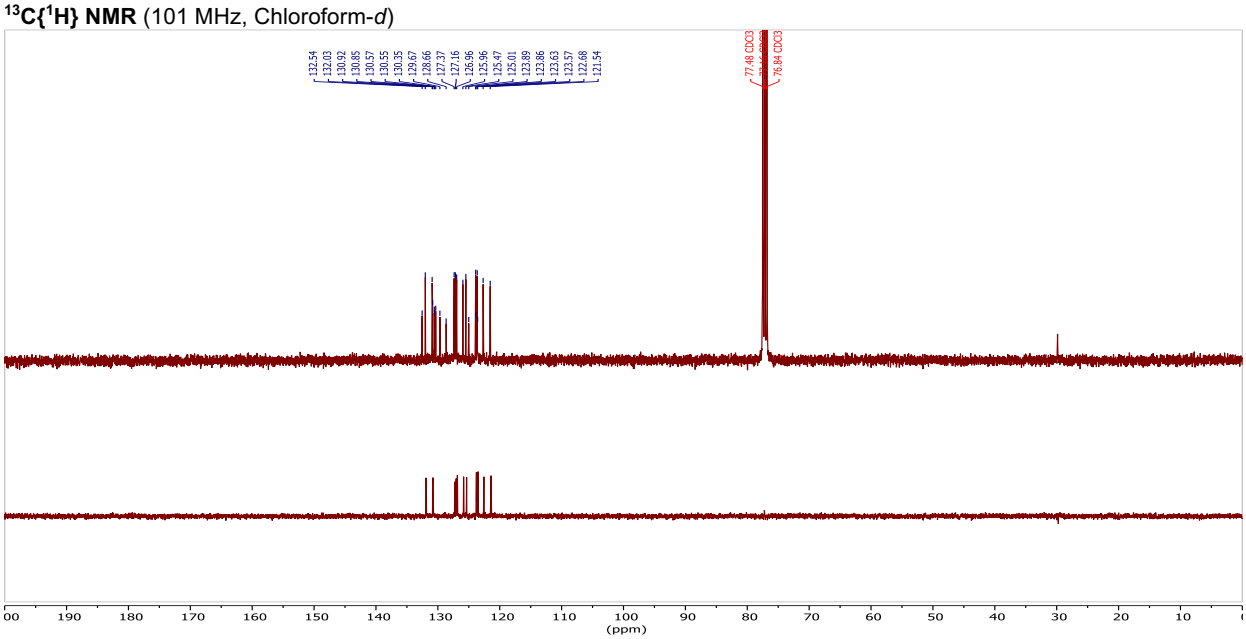
^{1}H NMR (400 MHz, Chloroform-*d*)



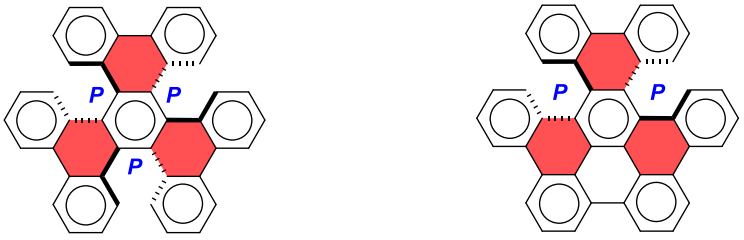




$^{13}C\{^{1}H\}$ NMR (101 MHz, Chloroform-*d*)



Section S3: Aromaticity



D_3-**HBTP** C_2-**3**

Figure S3. Clar structure for D_3-**HBTP** and C_2-**3** proposed based on EDDB(*r*) analyses and 3D IMS maps.

The 3D IMS maps of D_3-**HBTP** (as ESI of reference 16) and C_2-**3** (as ESI of the present article) are available as vtk files, to be viewed, and possibly modified, using the Paraview software as described earlier.[16]

Section S4: Cartesian coordinates

hbtp_ox_p_spe
Energy (POTENTIAL) = -1690.2052404 Eh

	Atom	X	Y	Z
1	O	-0.1459	-2.1104	-2.0934
2	C	0.0567	-1.3357	-1.1932
3	C	1.3982	-0.8067	-0.8174
4	C	2.6042	-1.6002	-0.9521
5	C	2.6157	-2.8442	-1.6288
6	H	1.6884	-3.2201	-2.0549
7	C	3.7862	-3.5571	-1.7817
8	H	3.7733	-4.5108	-2.3132
9	C	4.9911	-3.0517	-1.2694
10	H	5.9217	-3.6073	-1.4026
11	C	4.9998	-1.8484	-0.5954
12	H	5.9472	-1.4753	-0.2074
13	C	3.8155	-1.1010	-0.4075
14	C	3.7960	0.1343	0.3677
15	C	4.9280	0.5792	1.0896
16	H	5.8606	0.0189	1.0353
17	C	4.8773	1.6956	1.8973
18	H	5.7664	2.0078	2.4490
19	C	3.6754	2.4084	2.0331
20	H	3.6169	3.2689	2.7022
21	C	2.5626	2.0128	1.3238
22	H	1.6317	2.5640	1.4481
23	C	2.6009	0.8931	0.4556
24	C	1.4163	0.4438	-0.2575
25	C	0.1708	1.2577	-0.2746
26	C	0.1969	2.6796	-0.5800
27	C	1.3267	3.2784	-1.1880
28	H	2.2111	2.6725	-1.3865
29	C	1.3210	4.6075	-1.5537
30	H	2.2004	5.0441	-2.0310
31	C	0.1777	5.3903	-1.3251
32	H	0.1659	6.4428	-1.6158
33	C	-0.9424	4.8213	-0.7553
34	H	-1.8322	5.4363	-0.6208
35	C	-0.9664	3.4593	-0.3779
36	C	-2.1482	2.8293	0.1952
37	C	-3.2595	3.5846	0.6303
38	H	-3.2378	4.6717	0.5543
39	C	-4.3704	2.9797	1.1808
40	H	-5.2125	3.5881	1.5168
41	C	-4.4030	1.5845	1.3263
42	H	-5.2666	1.0985	1.7843
43	C	-3.3354	0.8219	0.9026
44	H	-3.3718	-0.2545	1.0499
45	C	-2.1899	1.4162	0.3196
46	C	-1.0280	0.6297	-0.0556
47	C	-1.0931	-0.8835	-0.2386
48	C	-2.3884	-1.4218	-0.8224
49	C	-3.0623	-1.0012	-1.9590
50	H	-2.6945	-0.1554	-2.5437
51	C	-4.2260	-1.6738	-2.3349
52	H	-4.7749	-1.3507	-3.2219
53	C	-4.6956	-2.7575	-1.5875
54	H	-5.6073	-3.2728	-1.8971
55	C	-4.0117	-3.1858	-0.4498
56	H	-4.3814	-4.0318	0.1339
57	C	-2.8535	-2.5099	-0.0719
58	C	-1.9691	-2.6905	1.0885
59	C	-2.0311	-3.5883	2.1516
60	H	-2.8160	-4.3465	2.1955
61	C	-1.0766	-3.4977	3.1656
62	H	-1.1123	-4.1945	4.0058
63	C	-0.0814	-2.5190	3.1214
64	H	0.6526	-2.4549	3.9272
65	C	-0.0141	-1.6184	2.0554
66	H	0.7643	-0.8535	2.0278
67	C	-0.9584	-1.7154	1.0414

hbtp_ox_p_m_ts_spe
Energy (POTENTIAL) = -1690.1551053 Eh

	Atom	X	Y	Z
1	O	0.8558	-2.2149	1.9150
2	C	0.4596	-1.3667	1.1539
3	C	-0.9294	-1.3368	0.6638
4	C	-1.5230	-2.5206	0.0764
5	C	-0.7707	-3.6940	-0.1562
6	H	0.2155	-3.7960	0.2955
7	C	-1.2674	-4.6941	-0.9691
8	H	-0.6712	-5.5905	-1.1507
9	C	-2.5249	-4.5503	-1.5751
10	H	-2.9056	-5.3302	-2.2379
11	C	-3.2894	-3.4248	-1.3272
12	H	-4.2686	-3.3334	-1.7989
13	C	-2.8178	-2.4050	-0.4784
14	C	-3.6403	-1.2923	-0.0116
15	C	-5.0466	-1.3492	-0.1120
16	H	-5.5082	-2.1299	-0.7171
17	C	-5.8592	-0.5011	0.6139
18	H	-6.9452	-0.5780	0.5332
19	C	-5.2728	0.3739	1.5353
20	H	-5.8928	0.9462	2.2282
21	C	-3.8967	0.4844	1.5945
22	H	-3.4636	1.0720	2.3975
23	C	-3.0428	-0.2403	0.7363
24	C	-1.5686	-0.1191	0.7314
25	C	-0.7386	1.1358	0.5145
26	C	-1.3392	2.4568	0.2330
27	C	-2.4533	2.9792	0.9209
28	H	-2.8120	2.4745	1.8021
29	C	-3.0675	4.1640	0.5670
30	H	-3.9244	4.5205	1.1422
31	C	-2.5734	4.9060	-0.5103
32	H	-3.0606	5.8316	-0.8230
33	C	-1.4106	4.4901	-1.1239
34	H	-0.9742	5.1253	-1.8935
35	C	-0.7455	3.3051	-0.7386
36	C	0.6021	3.0230	-1.2087
37	C	1.2426	3.8154	-2.1855
38	H	0.6826	4.5857	-2.7144
39	C	2.5786	3.6470	-2.4846
40	H	3.0524	4.2728	-3.2437
41	C	3.3247	2.6858	-1.7891
42	H	4.3921	2.5670	-1.9842
43	C	2.7081	1.8746	-0.8599
44	H	3.3169	1.1432	-0.3395
45	C	1.3247	1.9855	-0.5758
46	C	0.6083	0.9951	0.2224
47	C	1.3630	-0.2743	0.5757
48	C	2.5594	-0.1249	1.4991
49	C	2.6474	0.5785	2.6894
50	H	1.8034	1.1714	3.0490
51	C	3.8410	0.5183	3.4129
52	H	3.9349	1.0728	4.3490
53	C	4.9163	-0.2441	2.9501
54	H	5.8408	-0.2809	3.5303
55	C	4.8237	-0.9550	1.7526
56	H	5.6684	-1.5468	1.3932
57	C	3.6377	-0.8904	1.0259
58	C	3.2694	-1.4656	-0.2764
59	C	3.9868	-2.2571	-1.1692
60	H	4.9990	-2.5909	-0.9308
61	C	3.3904	-2.6151	-2.3804
62	H	3.9419	-3.2355	-3.0901
63	C	2.1001	-2.1854	-2.6983
64	H	1.6525	-2.4712	-3.6522
65	C	1.3748	-1.3931	-1.8046
66	H	0.3634	-1.0576	-2.0459
67	C	1.9716	-1.0398	-0.6036

hbtp_scholl_pm_spe
Energy (POTENTIAL) = -1613.8044769 Eh

	Atom	X	Y	Z
1	C	-1.1802	-0.7101	-0.0468
2	C	0.0207	-1.3998	0.1681
3	C	1.2446	-0.7050	-0.1044
4	C	1.2446	0.7050	-0.1044
5	C	0.0207	1.3998	0.1681
6	C	-1.1802	0.7101	-0.0468
7	C	-2.4153	-1.4331	-0.2504
8	C	-3.5799	-0.7364	-0.6630
9	C	-4.7058	-1.4813	-1.0291
10	C	-4.6968	-2.8708	-0.9681
11	C	-3.5792	-3.5469	-0.4980
12	C	-2.4325	-2.8434	-0.1113
13	C	-1.2801	-3.4920	0.5215
14	C	-1.3668	-4.7961	1.0519
15	C	-0.3324	-5.3443	1.7864
16	C	0.8165	-4.5833	2.0434
17	C	0.9310	-3.3132	1.5140
18	C	-0.0852	-2.7607	0.7044
19	C	2.4875	-1.4153	-0.4435
20	C	2.4886	-2.7573	-0.8842
21	C	3.6642	-3.4528	-1.0855
22	C	4.8928	-2.8184	-0.8597
23	C	4.9156	-1.4739	-0.5433
24	C	3.7243	-0.7331	-0.3875
25	C	3.7244	0.7330	-0.3875
26	C	4.9157	1.4738	-0.5433
27	C	4.8929	2.8183	-0.8596
28	C	3.6643	3.4527	-1.0855
29	C	2.4886	2.7573	-0.8842
30	C	2.4875	1.4152	-0.4435
31	C	-0.0851	2.7607	0.7044
32	C	0.9310	3.3132	1.5140
33	C	0.8166	4.5832	2.0434
34	C	-0.3323	5.3444	1.7864
35	C	-1.3667	4.7962	1.0519
36	C	-1.2800	3.4920	0.5215
37	C	-2.4325	2.8434	-0.1113
38	C	-3.5791	3.5470	-0.4980
39	C	-4.6968	2.8709	-0.9681
40	C	-4.7058	1.4815	-1.0291
41	C	-3.5799	0.7365	-0.6630
42	C	-2.4153	1.4332	-0.2504
43	H	-5.6114	-0.9806	-1.3705
44	H	-5.5817	-3.4315	-1.2758
45	H	-3.6033	-4.6352	-0.4370
46	H	-2.2830	-5.3730	0.9223
47	H	-0.4297	-6.3512	2.1975
48	H	1.6150	-4.9849	2.6703
49	H	1.8197	-2.7205	1.7309
50	H	1.5416	-3.2607	-1.0701
51	H	3.6306	-4.4915	-1.4199
52	H	5.8294	-3.3661	-0.9827
53	H	5.8808	-0.9761	-0.4546
54	H	5.8809	0.9759	-0.4545
55	H	5.8295	3.3659	-0.9826
56	H	3.6307	4.4914	-1.4198
57	H	1.5417	3.2607	-1.0701
58	H	1.8198	2.7205	1.7308
59	H	1.6152	4.9848	2.6703
60	H	-0.4296	6.3512	2.1975
61	H	-2.2829	5.3730	0.9223
62	H	-3.6032	4.6353	-0.4370
63	H	-5.5816	3.4316	-1.2758
64	H	-5.6113	0.9808	-1.3704

hbtp_scholl_pp_spe
Energy (POTENTIAL) = -1613.8086974 Eh

	Atom	X	Y	Z
1	C	1.2137	0.7133	0.0433
2	C	-0.0023	1.4197	0.0446
3	C	-1.2190	0.6926	-0.1162
4	C	-1.2190	-0.6927	0.1162
5	C	-0.0023	-1.4197	-0.0446
6	C	1.2138	-0.7133	-0.0433
7	C	2.4699	1.4382	0.0083
8	C	3.6961	0.7310	-0.0677
9	C	4.8797	1.4418	-0.2892
10	C	4.8700	2.8262	-0.4074
11	C	3.6825	3.5275	-0.2633
12	C	2.4749	2.8566	-0.0309
13	C	1.2320	3.5755	0.2572
14	C	1.2317	4.9564	0.5488
15	C	0.0905	5.6024	0.9821
16	C	-1.0855	4.8674	1.1805
17	C	-1.1103	3.5198	0.8827
18	C	0.0220	2.8557	0.3589
19	C	-2.4742	1.2645	-0.6391
20	C	-2.4528	2.3665	-1.5192
21	C	-3.6114	2.8359	-2.1103
22	C	-4.8343	2.2046	-1.8509
23	C	-4.8695	1.0945	-1.0258
24	C	-3.6995	0.5997	-0.4198
25	C	-3.6994	-0.5999	0.4198
26	C	-4.8695	-1.0948	1.0258
27	C	-4.8342	-2.2049	1.8510
28	C	-3.6113	-2.8361	2.1103
29	C	-2.4527	-2.3667	1.5192
30	C	-2.4741	-1.2646	0.6391
31	C	0.0221	-2.8557	-0.3590
32	C	-1.1101	-3.5199	-0.8827
33	C	-1.0853	-4.8675	-1.1806
34	C	0.0908	-5.6024	-0.9822
35	C	1.2320	-4.9563	-0.5488
36	C	1.2322	-3.5755	-0.2572
37	C	2.4751	-2.8565	0.0309
38	C	3.6826	-3.5273	0.2633
39	C	4.8701	-2.8259	0.4074
40	C	4.8798	-1.4416	0.2892
41	C	3.6962	-0.7308	0.0677
42	C	2.4700	-1.4381	-0.0083
43	H	5.8244	0.9109	-0.4038
44	H	5.7996	3.3623	-0.6080
45	H	3.6996	4.6141	-0.3430
46	H	2.1569	5.5272	0.4735
47	H	0.1206	6.6699	1.2098
48	H	-1.9774	5.3501	1.5850
49	H	-2.0226	2.9569	1.0716
50	H	-1.5023	2.8465	-1.7526
51	H	-3.5646	3.6865	-2.7932
52	H	-5.7516	2.5660	-2.3203
53	H	-5.8169	0.5759	-0.8714
54	H	-5.8168	-0.5762	0.8714
55	H	-5.7515	-2.5663	2.3203
56	H	-3.5643	-3.6867	2.7932
57	H	-1.5022	-2.8466	1.7526
58	H	-2.0224	-2.9570	-1.0716
59	H	-1.9771	-5.3502	-1.5851
60	H	0.1210	-6.6699	-1.2099
61	H	2.1572	-5.5271	-0.4736
62	H	3.6999	-4.6139	0.3430
63	H	5.7998	-3.3620	0.6081
64	H	5.8245	-0.9106	0.4038

hbtp_scholl_pm_pp_ts_spe
Energy (POTENTIAL) = -1613.7742081 Eh

	Atom	X	Y	Z
1	C	1.3199	0.3475	-0.2842
2	C	0.9987	-1.0046	-0.3871
3	C	-0.3457	-1.3656	-0.0677
4	C	-1.3830	-0.4683	-0.4094
5	C	-1.0488	0.9398	-0.5133
6	C	0.2753	1.3077	-0.1845
7	C	2.7059	0.7505	-0.1986
8	C	3.0245	2.0588	0.2420
9	C	4.3675	2.4383	0.3117
10	C	5.3788	1.5382	-0.0075
11	C	5.0684	0.2405	-0.3879
12	C	3.7350	-0.1795	-0.4906
13	C	3.3716	-1.5399	-0.8995
14	C	4.3265	-2.4519	-1.3962
15	C	3.9670	-3.7220	-1.8049
16	C	2.6232	-4.1187	-1.7513
17	C	1.6701	-3.2424	-1.2731
18	C	2.0228	-1.9537	-0.8146
19	C	-0.6223	-2.4858	0.8501
20	C	0.4162	-3.1040	1.5834
21	C	0.1494	-3.9978	2.6031
22	C	-1.1749	-4.2863	2.9523
23	C	-2.2070	-3.6737	2.2664
24	C	-1.9538	-2.7809	1.2077
25	C	-3.0255	-2.1798	0.4152
26	C	-4.3156	-2.7411	0.4209
27	C	-5.2982	-2.3205	-0.4570
28	C	-4.9706	-1.3656	-1.4185
29	C	-3.7113	-0.7879	-1.4155
30	C	-2.7316	-1.0968	-0.4541
31	C	-1.9783	2.0795	-0.6928
32	C	-3.0043	2.1333	-1.6550
33	C	-3.9297	3.1621	-1.7031
34	C	-3.8432	4.2116	-0.7870
35	C	-2.7454	4.2729	0.0521
36	C	-1.7675	3.2601	0.0686
37	C	-0.4568	3.5026	0.6785
38	C	-0.1696	4.6401	1.4417
39	C	1.1368	4.9360	1.8063
40	C	2.1822	4.1175	1.3942
41	C	1.9357	2.9542	0.6581
42	C	0.5948	2.6165	0.3446
43	H	4.6379	3.4494	0.6167
44	H	6.4229	1.8510	0.0542
45	H	5.8819	-0.4530	-0.5998
46	H	5.3707	-2.1517	-1.4828
47	H	4.7270	-4.4049	-2.1900
48	H	2.3262	-5.1090	-2.1019
49	H	0.6217	-3.5427	-1.2578
50	H	1.4539	-2.8513	1.3739
51	H	0.9766	-4.4517	3.1525
52	H	-1.3940	-4.9720	3.7733
53	H	-3.2345	-3.8763	2.5693
54	H	-4.5361	-3.5670	1.0971
55	H	-6.2886	-2.7794	-0.4372
56	H	-5.6869	-1.0892	-2.1949
57	H	-3.4593	-0.1422	-2.2412
58	H	-3.0222	1.3977	-2.4473
59	H	-4.7053	3.1567	-2.4715
60	H	-4.5817	5.0157	-0.7861
61	H	-2.6102	5.1616	0.6682
62	H	-0.9685	5.3136	1.7514
63	H	1.3459	5.8222	2.4087
64	H	3.2002	4.3772	1.6846

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