Electronic Supplementary Material (ESI) for ChemComm.

Supplementary Information

for

Synthesis, Structure and Properties of C_3-Symmetric Heterosuperbenzene with Three BN Units

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1. Experimental Section

General. All commercially available chemicals were used without further purification unless otherwise noted. Column chromatography was performed with silica gel. Analytical thin-layer chromatography (TLC) was performed on 0.2 mm silica gel-coated glass sheets with F254 indicator. All yields given referred to isolated yields. Nuclear Magnetic Resonance (NMR) spectra were recorded on 400 MHz or 500 MHz Bruker AVANCE III spectrometers. Chemical shifts were reported in ppm. Coupling constants (*J* values) were reported in Hertz. ^{1}H NMR chemical shifts were referenced to TMS (0 ppm). ^{13}C NMR chemical shifts were referenced to $CDCl_3$ (77.00 ppm). ^{11}B NMR chemical shifts were referenced to the external standard boron signal of $BF_3{\cdot}Et_2O$ (0 ppm). ESI-HRMS spectra were recorded on a Bruker Apex IV Fourier Transform Ion Cyclotron Resonance Mass Spectrometer.

Absorption spectra were recorded on PerkinElmer Lambda 750 UV-*vis* Spectrometer. Photoluminescence spectra were recorded on an Edinburgh Photonics FLS980 spectrometer. The fluorescence quantum yield was measured with the integrating sphere system on an Edinburgh Photonics FLS920 spectrometer. Cyclic voltammetry was performed on BASi Epsilon workstation and measurements were carried out in dichloromethane containing 0.1 M *n*-Bu_4NPF_6 as supporting electrolyte (scan rate: 100 mV s^{-1}.). Glassy carbon electrode was used as working electrode, a platinum sheet as counter electrode and Ag/AgCl as reference electrode. Thermogravimetric analysis (TGA) was carried out on a TA Instrument Q600 analyzer under N_2 (10 °C min^{-1}). Photoelectron spectroscopy (PES) was performed on AC-2 photoelectron spectrometer (Riken-Keiki Co.).

Synthetic Procedure.

3,4,7,8,11,12-Hexamethoxy-2,6,10-triphenyl-1,5,9-triaza-2,6,10-triboracoronene (1): To a solution of compound **3** (453 mg, 1.0 mmol) in *o*-dichlorobenzene (30 mL) under nitrogen was added dichlorophenylborane (632 mg, 4.0 mmol) and triethylamine (607 mg, 6.0 mmol). The reaction mixture was heated at 180 °C for 12 h. After removal of the solvent under reduced pressure, the residue was purified by

column chromatography over silica gel (eluent: petroleum ether/CH_2Cl_2 = 2 : 3) and recrystallization from $CHCl_3$/MeOH to afford 249 mg (35%) of compound **1** as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$, 298 K, ppm) δ 9.02 (s, 3H), 7.93 (d, J = 6.5 Hz, 6H), 7.52 (m, 9H), 4.16 (s, 9H), 3.60 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$, 298 K, ppm) δ 156.8, 138.1, 136.0, 132.6, 131.4, 127.5, 127.1, 114.2, 61.1, 61.0; ^{11}B NMR (160 MHz, $CDCl_3$, 298 K, ppm): δ 37.2; HRMS (ESI) *m/z*: Calcd for $C_{42}H_{37}B_3N_3O_6$: 712.2975; Found: 712.2980 $[M + H]^+$.

2. Thermogravimetric Analysis (TGA)

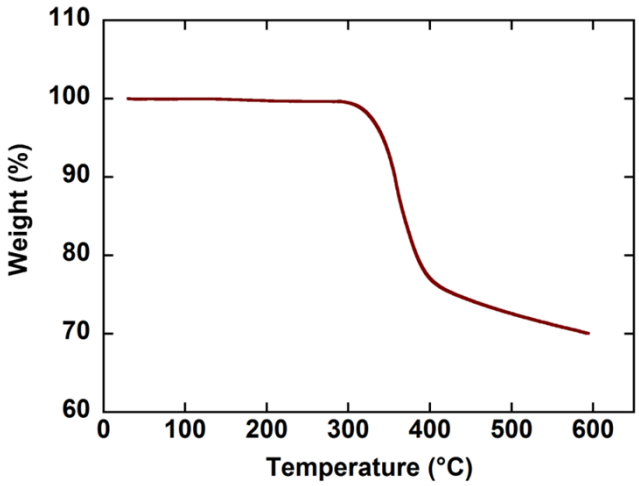

Figure S1. TGA curve of compound **1** (5% weight loss: 341 °C).

3. Absorption Spectra

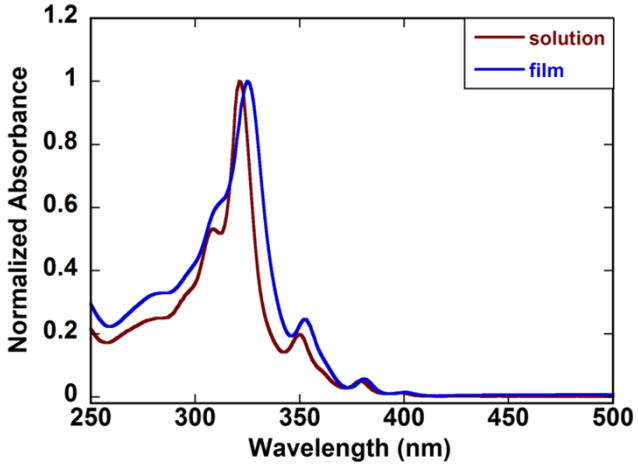

Figure S2. Comparison of the absorption spectra of compound **1** in solution and in thin film, showing a slight redshift of absorption maximum from 321 nm to 325 nm.

4. Cyclic Voltammogram

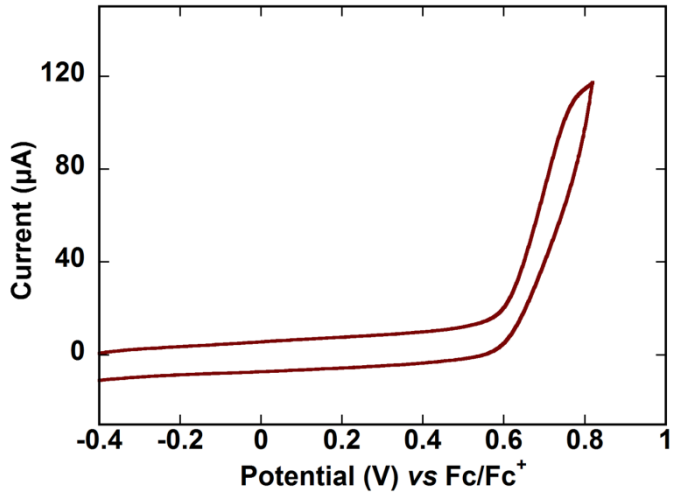

Figure S3. Cyclic voltammogram of compound **1** in CH_2Cl_2 (1 mM) with 0.1 M *n*-Bu_4PF_6 as supporting electrolyte and ferrocene as an external standard. The HOMO energy level is estimated from the equation HOMO = −4.80 − E_{ox} based on the oxidation onset.

5. Photoelectron Spectroscopy (PES)

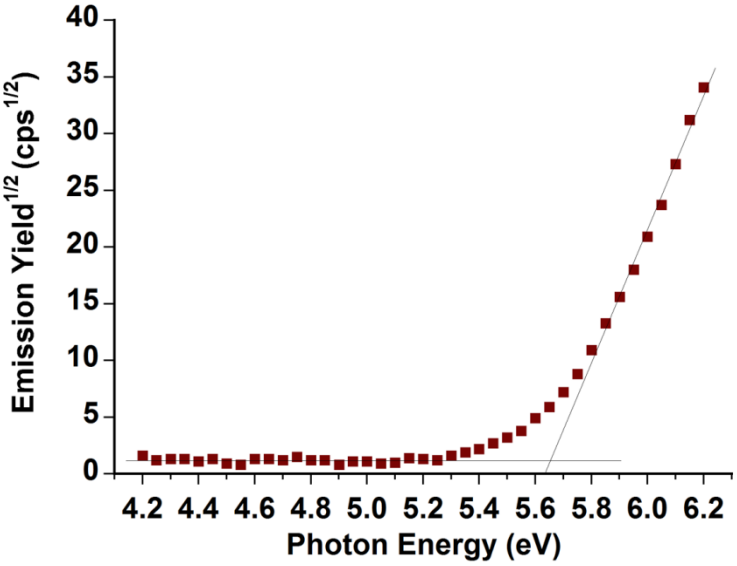

Figure S4. PES spectrum of compound **1** in thin film (work function: –5.65 eV).

6. Single Crystal Data

Table S1. Crystal data and structure refinement for compound **1** (CCDC 1039514).

Empirical formula	$C_{42}H_{36}N_3O_6B_3$
Formula weight	711.17
Temperature/K	100.01(10)
Crystal system	triclinic
Space group	*P*1
a/Å	7.3418(2)
b/Å	15.7880(5)
c/Å	31.0079(8)
α/°	83.135(2)
β/°	87.475(2)
γ/°	89.797(2)
Volume/Å^3	3564.96(17)
Z	4
ρ_{calc}/mg mm^{-3}	1.325
Absorption coefficient/mm^{-1}	0.703
F(000)	1488.0
Crystal size/mm^3	0.7 × 0.1 × 0.05
Radiation	CuKα (λ = 1.54184)
2θ range for data collection	6.628 to 151.864°
Index ranges	$-8 \le h \le 9$, $-15 \le k \le 19$, $-32 \le l \le 38$
Reflections collected	25470
Independent reflections	16692 [R_{int} = 0.0600, R_{sigma} = 0.0687]
Data/restraints/parameters	16692/3/1969
Goodness-of-fit on F^2	1.106
Final R indexes [I>=2σ (I)]	R_1 = 0.0636, wR_2 = 0.1801
Final R indexes [all data]	R_1 = 0.0740, wR_2 = 0.1871
Largest diff. peak/hole / e Å^{-3}	0.50/–0.32

7. Computational Studies

Calculations were performed using the Gaussian 09 software package.[1] The geometries were optimized at the B3LYP/6-311G(d,p) level, and energies were calculated at the same level. Nucleus independent chemical shifts (NICS) were calculated using the gauge invariant atomic orbital (GIAO) approach at the GIAO-

B3LYP/6-311+G(2d,p) level of theory.[2] The NICS(1) values were averaged by the two positions (above and below the plane) of all the equivalent rings.

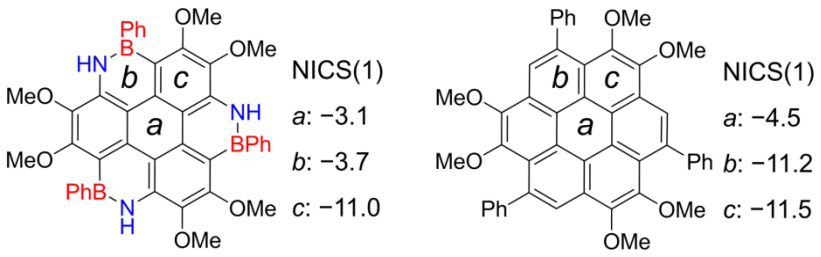

Figure S5. DFT-Calculated NICS(1) values (ppm) of compound **1** and its corresponding carbon analogue.

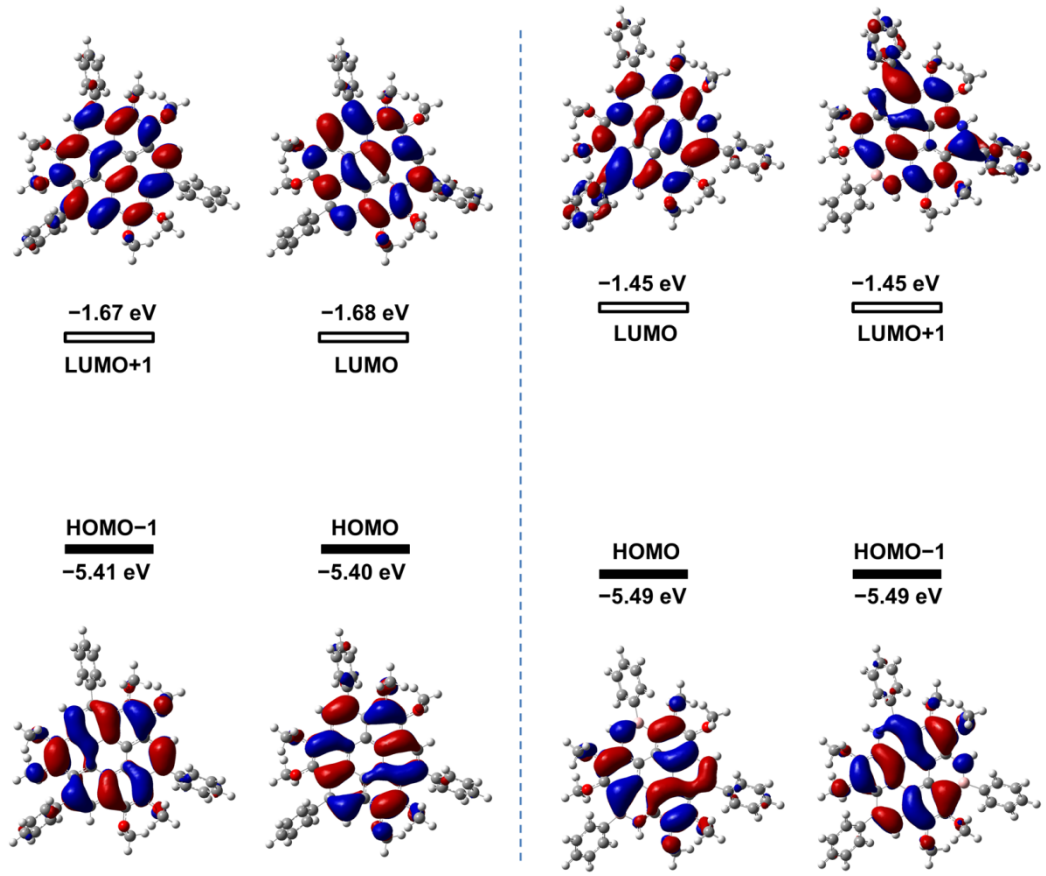

Figure S6. Degenerate HOMO and LUMO levels and their molecular orbitals of BN heterocoronene **1** (right) and its corresponding carbon analogue (left).

Appendix: Cartesian coordinates

Optimized geometry of compound 1

Tag	Symbol	X	Y	Z
1	O	2.357573	3.068288	23.46810
2	O	0.380242	3.356501	21.54443
3	O	6.669092	8.425572	25.04961
4	O	-0.47267	9.617464	18.40153
5	O	6.301183	10.87286	23.79646
6	O	1.145985	11.77006	19.06196
7	N	3.998938	5.119528	24.08034
8	H	3.985787	4.183896	24.46744
9	N	-0.13765	7.219490	19.59148
10	H	-0.78478	7.473011	18.85491
11	N	4.340976	11.21230	21.97449
12	H	4.988749	11.90002	22.33914
13	C	1.720293	8.041926	20.90397
14	C	0.523727	9.504645	19.35009
15	C	-3.11248	3.303701	18.21627
16	H	-3.86140	2.684809	17.73411
17	C	2.181825	4.256687	22.78827
18	C	5.506307	9.784460	23.49803
19	C	1.182632	4.433284	21.8417
20	C	0.698954	8.248111	19.95351
21	C	1.008197	5.660372	21.16688
22	C	5.655087	8.558067	24.13037
23	C	4.482299	9.974529	22.55522
24	C	4.828035	7.457857	23.81931
25	C	3.793324	7.656227	22.85127
26	C	2.560190	9.139937	21.24843
27	C	3.607122	8.920396	22.22104
28	C	5.966323	5.550664	25.60239
29	C	1.364934	10.55922	19.67553
30	C	1.875721	6.742303	21.51768
31	C	-1.77834	2.897158	18.24668
32	H	-1.48716	1.961173	17.78166
33	C	2.842052	1.971708	22.67182
34	H	2.125323	1.716709	21.89012
35	H	2.962816	1.132728	23.35665
36	H	3.809339	2.220197	22.22313
37	C	2.897441	6.578376	22.49708
38	C	7.673404	10.76237	23.37941
39	H	7.735751	10.61309	22.29642
40	H	8.168368	9.938168	23.89487
41	H	8.146410	11.70740	23.64536
42	C	7.363215	5.601680	25.45679
43	H	7.790223	6.104028	24.59757
44	C	3.031877	5.323284	23.12569
45	C	3.388870	13.08506	20.57231
46	C	2.387485	10.42228	20.6384
47	C	-3.47458	4.509162	18.81012
48	H	-4.50975	4.833577	18.79732
49	C	-1.15421	4.910181	19.47579
50	C	4.606750	13.63480	20.13397
51	H	5.480134	12.99510	20.04321
52	C	5.464233	4.899222	26.74334
53	H	4.390307	4.838818	26.89577
54	C	8.212952	5.025997	26.39657
55	H	9.287171	5.070766	26.2509
56	C	2.290743	13.95657	20.66911
57	H	1.332246	13.56962	20.99274
58	C	-0.65938	3.096559	22.49682
59	H	-1.20845	2.234794	22.11928
60	H	-1.33751	3.952575	22.56622
61	H	-0.23938	2.870438	23.48066
62	C	4.723084	14.98171	19.79142
63	H	5.67291	15.37152	19.44091
64	C	6.398232	9.003450	26.33426
65	H	6.237365	10.08157	26.25086
66	H	7.275604	8.803794	26.94824
67	H	5.524505	8.527817	26.78987
68	C	-2.50312	5.303807	19.41811
69	H	-2.80565	6.243732	19.87116
70	C	3.621139	15.82405	19.90562
71	H	3.706688	16.87437	19.64887
72	C	2.405088	15.30673	20.35245
73	H	1.542742	15.95802	20.44883
74	C	-0.81896	3.684061	18.87652
75	H	0.207632	3.340151	18.90799
76	C	-1.58086	10.45692	18.77134
77	H	-2.28997	10.40107	17.94573
78	H	-1.25361	11.48762	18.91437
79	H	-2.05470	10.08807	19.68701

80	C	7.689633	4.39792	27.52689
81	H	8.352843	3.958314	28.26402
82	C	6.310052	4.340756	27.70139
83	H	5.891146	3.859170	28.57859
84	C	1.644458	11.86967	17.72120
85	H	1.161707	11.13610	17.06989
86	H	2.729516	11.72914	17.70444
87	H	1.409599	12.87884	17.38496
88	B	3.336862	11.57738	21.03540
89	B	4.961730	6.076739	24.50441
90	B	-0.08489	5.890631	20.09636

Optimized geometry of the carbon analogue

Tag	Symbol	X	Y	Z
1	C	-1.06948	-0.96789	-0.08108
2	C	-1.33717	0.434260	-0.13341
3	C	-0.27558	1.387402	-0.07588
4	C	1.069836	0.920418	0.033029
5	C	1.363585	-0.47676	0.054812
6	C	0.284411	-1.41178	0.012768
7	C	2.716980	-0.93623	0.144309
8	C	2.938481	-2.34896	0.232172
9	C	1.893565	-3.24546	0.156045
10	C	0.549593	-2.79990	0.045174
11	C	-0.55459	2.791579	-0.10143
12	C	0.548079	3.695220	0.040452
13	C	1.846337	3.236636	0.114556
14	C	2.135442	1.845957	0.109814
15	C	-2.14444	-1.91242	-0.13415
16	C	-3.47533	-1.40346	-0.28258
17	C	-3.72750	-0.04784	-0.29506
18	C	-2.66973	0.897284	-0.22403
19	O	0.324893	5.049638	0.076113
20	O	2.897112	4.112958	0.253263
21	O	4.213180	-2.84040	0.371485
22	O	2.118360	-4.59861	0.253272
23	O	-4.53551	-2.27033	-0.38103
24	O	-5.00974	0.427630	-0.44056
25	C	2.776337	-5.19699	-0.87414
26	C	4.550225	-3.28286	1.694052
27	C	3.190734	4.910760	-0.90483
28	C	0.446551	5.652654	1.372250
29	C	-5.86922	0.234210	0.693474
30	C	-5.08862	-2.40657	-1.69813
31	C	-2.85980	-4.41499	-0.02167
32	C	-2.97469	-5.30346	-1.09531
33	C	-3.85437	-6.38482	-1.03758
34	C	-4.62128	-6.60047	0.103030
35	C	-4.50233	-5.72808	1.185757
36	C	-3.63143	-4.64669	1.123557
37	C	5.242281	-0.29224	0.162438
38	C	6.043554	0.048839	1.256937
39	C	7.422254	-0.16285	1.227217
40	C	8.020926	-0.70612	0.095032
41	C	7.232000	-1.03636	-1.00788
42	C	5.857734	-0.83271	-0.97367
43	C	-2.35271	4.652961	-0.39435
44	C	-3.13970	5.257042	0.591269
45	C	-3.62884	6.552477	0.421261
46	C	-3.34842	7.256758	-0.74530
47	C	-2.57557	6.657418	-1.74089
48	C	-2.08193	5.370122	-1.56634
49	H	2.843350	-6.26190	-0.65281
50	H	3.776259	-4.78090	-1.00979
51	H	2.185245	-5.05155	-1.78440
52	H	5.581239	-3.63041	1.641388
53	H	3.894934	-4.09822	2.009969
54	H	4.486631	-2.45310	2.404554
55	H	4.058287	5.515242	-0.64132
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57	H	3.439442	4.270451	-1.75741
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59	H	1.463447	5.545257	1.757404
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62	H	-6.00379	-0.82812	0.905302
63	H	-5.46146	0.741520	1.574055
64	H	-5.89646	-3.13202	-1.61124
65	H	-5.47828	-1.45107	-2.05720
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69	H	-5.30189	-7.44304	0.153335
70	H	-5.08976	-5.89353	2.082351
71	H	-3.54604	-3.97156	1.967177
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73	H	8.025308	0.102032	2.088915

74	H	9.092851	-0.86716	0.067163
75	H	7.691201	-1.45279	-1.89785
76	H	5.250791	-1.09475	-1.83254
77	H	-3.36567	4.708776	1.499469
78	H	-4.23199	7.006165	1.200211
79	H	-3.73132	8.261846	-0.88284
80	H	-2.35908	7.195948	-2.65709
81	H	-1.47961	4.911744	-2.34212
82	C	-1.91911	3.227443	-0.24027
83	C	-2.92195	2.286982	-0.28306
84	H	-3.94679	2.610542	-0.40559
85	C	3.46528	1.372649	0.177908
86	H	4.261521	2.103775	0.213918
87	C	3.78033	0.033566	0.172917
88	C	-0.52656	-3.71603	0.011952
89	H	-0.29587	-4.77022	0.085759
90	C	-1.84058	-3.31713	-0.062130

NICS calculations for compound 1

Tag	Symbol	X	Y	Z
1	O	2.357573	3.068288	23.46811
2	O	0.380242	3.356501	21.54443
3	O	6.669092	8.425572	25.04961
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16	H	-3.86141	2.684809	17.73411
17	C	2.181825	4.256687	22.78827
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27	C	3.607122	8.920396	22.22104
28	C	5.966323	5.550664	25.60239
29	C	1.364934	10.55922	19.67553
30	C	1.875721	6.742303	21.51768
31	C	-1.77834	2.897158	18.24668
32	H	-1.48716	1.961173	17.78167
33	C	2.842052	1.971708	22.67182
34	H	2.125323	1.716708	21.89012
35	H	2.962815	1.132728	23.35665
36	H	3.809339	2.220197	22.22313
37	C	2.897441	6.578376	22.49708
38	C	7.673404	10.76237	23.37941
39	H	7.735751	10.61309	22.29642
40	H	8.168368	9.938168	23.89487
41	H	8.146410	11.70740	23.64536
42	C	7.363215	5.601679	25.4568
43	H	7.790223	6.104028	24.59757
44	C	3.031877	5.323284	23.12569
45	C	3.38887	13.08507	20.57231
46	C	2.387485	10.42228	20.6384
47	C	-3.47458	4.509161	18.81012
48	H	-4.50976	4.833577	18.79732
49	C	-1.15421	4.910181	19.47579
50	C	4.606750	13.63480	20.13397
51	H	5.480134	12.99510	20.04321
52	C	5.464233	4.899222	26.74334
53	H	4.390307	4.838817	26.89577
54	C	8.212952	5.025997	26.39657
55	H	9.287170	5.070766	26.25090
56	C	2.290743	13.95657	20.66911
57	H	1.332246	13.56962	20.99274
58	C	-0.65938	3.096559	22.49682
59	H	-1.20845	2.234794	22.11928
60	H	-1.33751	3.952575	22.56622
61	H	-0.23938	2.870438	23.48066
62	C	4.723084	14.98171	19.79142
63	H	5.672910	15.37152	19.44091
64	C	6.398232	9.003450	26.33426
65	H	6.237365	10.08157	26.25086
66	H	7.275604	8.803794	26.94824
67	H	5.524505	8.527816	26.78987

68	C	-2.50312	5.303807	19.41811
69	H	-2.80565	6.243732	19.87116
70	C	3.621139	15.82405	19.90562
71	H	3.706688	16.87437	19.64888
72	C	2.405088	15.30673	20.35245
73	H	1.542742	15.95802	20.44883
74	C	-0.81896	3.684061	18.87652
75	H	0.207632	3.340151	18.90799
76	C	-1.58086	10.45692	18.77134
77	H	-2.28997	10.40107	17.94573
78	H	-1.25361	11.48763	18.91437
79	H	-2.05470	10.08807	19.68701
80	C	7.689633	4.397920	27.52689
81	H	8.352843	3.958314	28.26402
82	C	6.310052	4.340756	27.70139
83	H	5.891146	3.859169	28.57859
84	C	1.644458	11.86967	17.72120
85	H	1.161707	11.13610	17.06989
86	H	2.729516	11.72914	17.70444
87	H	1.409599	12.87884	17.38496
88	B	3.336862	11.57738	21.03540
89	B	4.961730	6.076739	24.50441
90	B	-0.08489	5.890631	20.09636
91	Bq	2.742167	7.846333	21.87317
92	Bq	2.110069	8.108725	22.60228
93	Bq	3.374264	7.583942	21.14406
94	Bq	0.846667	6.967000	20.53833
95	Bq	0.214173	7.236245	21.26460
96	Bq	1.479160	6.697755	19.81207
97	Bq	2.029667	5.498833	22.15633
98	Bq	1.388901	5.785519	22.86854
99	Bq	2.670432	5.212147	21.44413
100	Bq	3.918500	6.368667	23.4795
101	Bq	3.290005	6.671496	24.19594
102	Bq	4.546995	6.065838	22.76306
103	Bq	4.645167	8.725167	23.17900
104	Bq	4.024766	9.007011	23.91089
105	Bq	5.265567	8.443323	22.44711
106	Bq	3.452333	10.20767	21.61183
107	Bq	2.836230	10.48444	22.34927
108	Bq	4.068437	9.930892	20.87440
109	Bq	1.542500	9.319333	20.29500
110	Bq	0.910244	9.578141	21.02525
111	Bq	2.174756	9.060526	19.56475

NICS calculations for the carbon analogue

Tag	Symbol	X	Y	Z
1	C	-1.06948	-0.96789	-0.08108
2	C	-1.33717	0.434260	-0.13341
3	C	-0.27558	1.387402	-0.07588
4	C	1.069836	0.920418	0.033029
5	C	1.363584	-0.47676	0.054812
6	C	0.284411	-1.41179	0.012768
7	C	2.716980	-0.93623	0.144309
8	C	2.938481	-2.34896	0.232172
9	C	1.893565	-3.24546	0.156045
10	C	0.549593	-2.7999	0.045174
11	C	-0.55459	2.791579	-0.10143
12	C	0.548079	3.69522	0.040452
13	C	1.846337	3.236636	0.114556
14	C	2.135442	1.845957	0.109813
15	C	-2.14444	-1.91242	-0.13415
16	C	-3.47533	-1.40346	-0.28258
17	C	-3.72750	-0.04784	-0.29506
18	C	-2.66974	0.897284	-0.22403
19	O	0.324893	5.049638	0.076113
20	O	2.897112	4.112958	0.253263
21	O	4.213180	-2.84041	0.371485
22	O	2.118360	-4.59861	0.253272
23	O	-4.53551	-2.27033	-0.38103
24	O	-5.00974	0.427630	-0.44056
25	C	2.776337	-5.19699	-0.87414
26	C	4.550225	-3.28286	1.694052
27	C	3.190734	4.91076	-0.90483
28	C	0.446551	5.652654	1.372249
29	C	-5.86922	0.23421	0.693474
30	C	-5.08862	-2.40657	-1.69813
31	C	-2.85980	-4.41499	-0.02167
32	C	-2.97469	-5.30347	-1.09531
33	C	-3.85437	-6.38482	-1.03758
34	C	-4.62128	-6.60047	0.103030
35	C	-4.50233	-5.72808	1.185757
36	C	-3.63143	-4.64670	1.123557
37	C	5.242281	-0.29224	0.162438
38	C	6.043554	0.048839	1.256937
39	C	7.422254	-0.16285	1.227217
40	C	8.020926	-0.70612	0.095032
41	C	7.232000	-1.03636	-1.00788
42	C	5.857734	-0.83271	-0.97367

43	C	-2.35271	4.652961	-0.39435	78	H	-4.23199	7.006165	1.200211
44	C	-3.13970	5.257042	0.591269	79	H	-3.73132	8.261846	-0.88284
45	C	-3.62884	6.552477	0.421261	80	H	-2.35908	7.195948	-2.65709
46	C	-3.34842	7.256757	-0.74530	81	H	-1.47961	4.911744	-2.34212
47	C	-2.57557	6.657418	-1.74089	82	C	-1.91911	3.227443	-0.24027
48	C	-2.08193	5.370122	-1.56634	83	C	-2.92195	2.286982	-0.28306
49	H	2.843350	-6.26190	-0.65281	84	H	-3.94679	2.610542	-0.40559
50	H	3.776259	-4.78090	-1.00979	85	C	3.465280	1.372649	0.177908
51	H	2.185245	-5.05155	-1.78440	86	H	4.261521	2.103775	0.213918
52	H	5.581239	-3.63041	1.641388	87	C	3.780330	0.033566	0.172917
53	H	3.894934	-4.09822	2.009969	88	C	-0.52656	-3.71603	0.011952
54	H	4.486631	-2.4531	2.404554	89	H	-0.29587	-4.77022	0.085759
55	H	4.058287	5.515242	-0.64132	90	C	-1.84058	-3.31713	-0.06213
56	H	2.348666	5.557313	-1.15833	91	Bq	0.006000	-0.01933	-0.03150
57	H	3.439442	4.270451	-1.75741	92	Bq	-0.05340	-0.00145	0.966574
58	H	0.205901	6.706289	1.236547	93	Bq	0.065399	-0.03722	-1.02957
59	H	1.463447	5.545257	1.757404	94	Bq	-2.40367	-0.50000	-0.19167
60	H	-0.26727	5.208166	2.072637	95	Bq	-2.48804	-0.49603	0.804760
61	H	-6.82521	0.684421	0.427086	96	Bq	-2.31929	-0.50397	-1.18809
62	H	-6.00379	-0.82812	0.905302	97	Bq	-0.79117	-2.35417	-0.03450
63	H	-5.46146	0.74152	1.574055	98	Bq	-0.84115	-2.32967	0.963950
64	H	-5.89646	-3.13202	-1.61124	99	Bq	-0.74119	-2.37867	-1.03295
65	H	-5.47828	-1.45108	-2.05720	100	Bq	1.624500	-1.86983	0.1075
66	H	-4.33498	-2.78947	-2.39300	101	Bq	1.541822	-1.84515	1.103771
67	H	-2.37269	-5.14320	-1.98327	102	Bq	1.707178	-1.89452	-0.88877
68	H	-3.93369	-7.05929	-1.88330	103	Bq	2.421833	0.460000	0.115500
69	H	-5.30189	-7.44304	0.153335	104	Bq	2.483244	0.454803	-0.88260
70	H	-5.08976	-5.89353	2.082351	105	Bq	2.360423	0.465197	1.113599
71	H	-3.54604	-3.97156	1.967177	106	Bq	0.794667	2.312833	0.020167
72	H	5.581694	0.479536	2.138738	107	Bq	0.722372	2.28853	1.017254
73	H	8.025308	0.102032	2.088915	108	Bq	0.866962	2.337136	-0.97692
74	H	9.092851	-0.86716	0.067163	109	Bq	-1.61317	1.837333	-0.17617
75	H	7.691201	-1.45279	-1.89785	110	Bq	-1.54787	1.829219	-1.17400
76	H	5.250791	-1.09475	-1.83254	111	Bq	-1.67847	1.845448	0.821666
77	H	-3.36567	4.708776	1.499469					

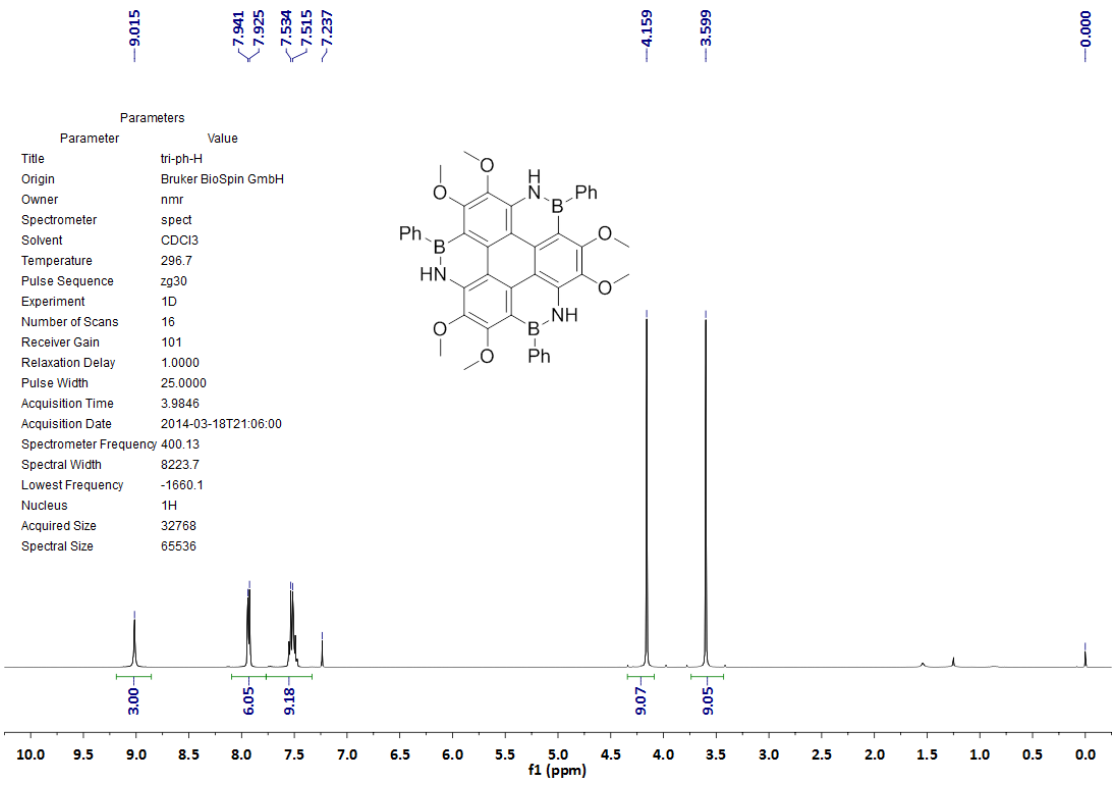
Reference:

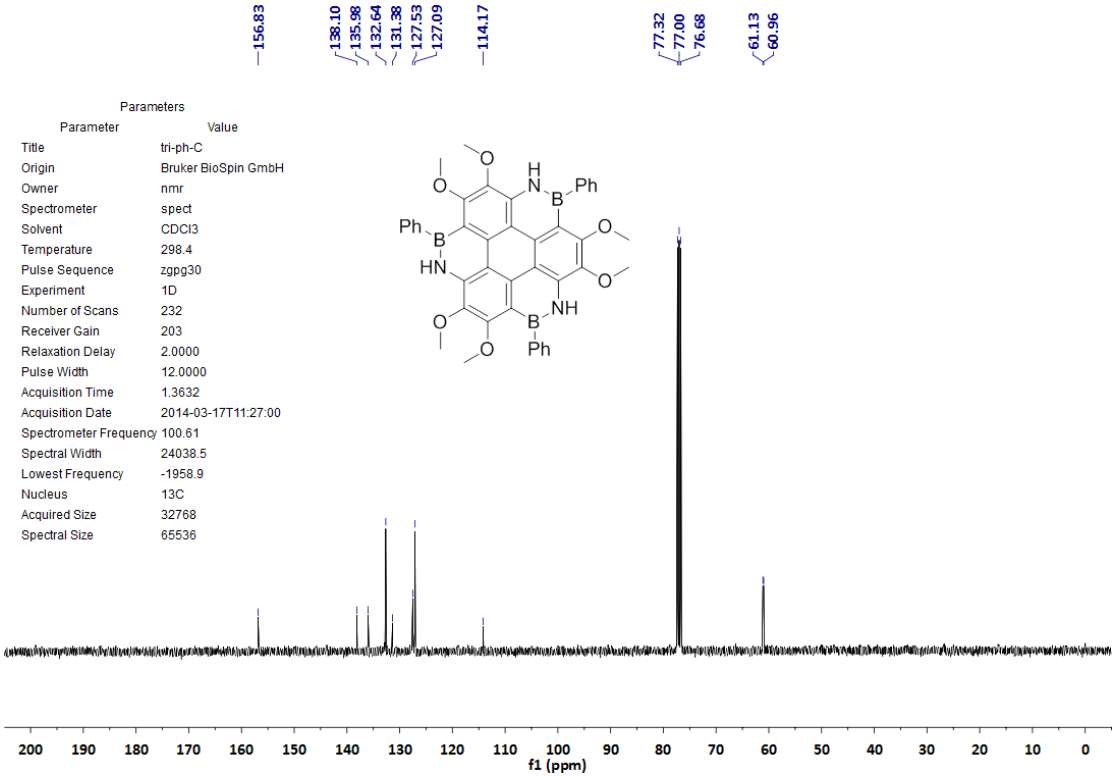
(1) Gaussian 09, Revision B.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.;Rega, N.;

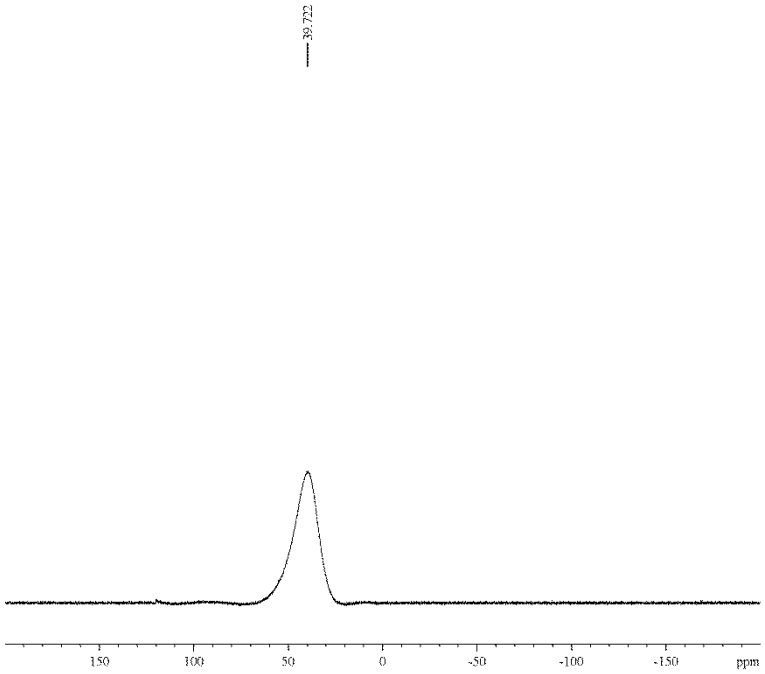
Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2010.

(2) (a) Chen, Z.; Wannere, C. S.; Corminboeuf, C.; Puchta, R.; Schleyer, P. R. *Chem. Rev.* **2005,** *105*, 3842. (b) Schleyer, P. R.; Maerker, C.; Dransfeld, A.; Jiao, H.; Hommes, N. J. R. E. *J. Am. Chem. Soc.* **1996**, *118*, 6317. (c) Wolinski, K.; Hinton, J. F.; Pulay, P. *J. Am. Chem. Soc.* **1990**, *112,* 8251.

8. NMR Spectra







Current Data Parameters
NAME BNMR14120670
EXPNO 1
PROCNO 2

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SOLVENT CDCl3
NS 128
DS 4
SWH 64102.563 Hz
FIDRES 0.978127 Hz
AQ 0.5111808 sec
RG 198.55
DW 7.800 usec
DE 6.50 usec
TE 303.1 K
D1 1.00000000 sec
TD0 2

======== CHANNEL f1 ========
SFO1 160.4615792 MHz
NUC1 11B
P1 9.90 usec
PLW1 100.00000000 W

F2 - Processing parameters
SI 32768
SF 160.4615714 MHz
WDW EM
SSB 0
LB 5.00 Hz
GB 0
PC 1.40