Reductive coupling and protonation leading to diboron corroles with a B-H-B bridge

Amelia M. Albrett, Peter D. W. Boyd, George R. Clark, Emmanuel Gonzalez, Abhik Ghosh, and Penelope J. Brothers.

Supplementary information

Contents

References

[1] B. Koszarna, D. T. Gryko, *J. Org. Chem.* **2006**, *71*, 3707.

[2] (*a*) The OPTX exchange functional: N. C. Handy and A. J. Cohen, *Mol. Phys.*, 2001, **99**, 403–412; (*b*) The LYP correlation functional: C. Lee, W. Yang and R. G. Parr, *Phys. Rev.*, 1988, **B37**, 785–789.

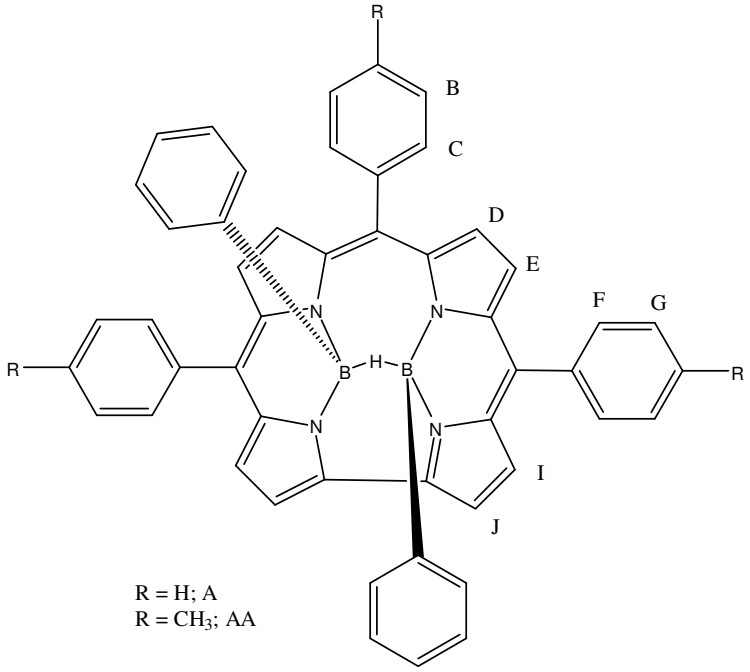
[3] The ADF program system was obtained from Scientific Computing and Modeling, Amsterdam (http://www.scm.com/). For a description of the methods used in ADF, see: G. T. Velde, F. M. Bickelhaupt, E. J. Baerends, C. F. Guerra, S. J. A. Van Gisbergen, J. G. Snijders and T. Ziegler, *J. Comput. Chem.*, 2001, **22**, 931–967.

1. Synthesis and characterisation of new compounds

Corrole ligands 5,10,15-triphenylcorrole (TPC), 5,10,15-tris(4-methylphenyl)corrole (T(4-Me-P)C) and 5,10,15-tris(4- 5,10,15-tris[(4-trifluoromethyl)phenyl]corrole (T(4-CF_3-P)C) were prepared as described in the literature.[1]

B. Koszarna, D. T. Gryko, *J. Org. Chem.* **2006**, *71*, 3707.

Assignments used for NMR spectra:



1.1 Experimental data for B_2Ph_2H(T(4-CF_3-P)C)

Procedure: BCl_2Ph (0.267 mL, 2.05 mmol) was added dropwise via syringe to a solution of H_3T(4-CF_3-P)C) (125 mg, 0.17 mmol) in dry CH_2Cl_2 (15 mL), under nitrogen. $NEt(^iPr)_2$ (0.477 mL, 2.74 mmol) was added dropwise and the bright green solution stirred at room temperature for 15 min. The solvent was removed in vacuo and the crude solid purified by column chromatography (SiO_2, CH_2Cl_2/hexanes, 1:2), then recrystallised from CH_2Cl_2/hexanes, 1:1. Yield: 109 mg, 70.9 %

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = -6.51 (br s, 1H, B*H*B), 2.20 – 2.22 (d, 4H, J = 7.6 Hz, BPh_o), 5.42 – 5.46 (t, 4H, J = 7.6 Hz, BPh_m), 5.79 – 5.83 (t, 2H, J = 7.4 Hz, BPh_p), 7.99 – 8.01 (d, 4H, J = 8.04 Hz, 5, 15 – $C_6H_4CF_3$), 8.11 – 8.13 (d, 2H, J = 8.1 Hz, 10 – $C_6H_4CF_3$), 8.21 – 8.23 (d, 4H, J = 8.0 Hz, 5,15 – $C_6H_4CF_3$), 8.27 – 8.28 (d, 2H, J = 4.8 Hz, *βH*), 8.31 – 8.32 (d, 2H, J = 4.5 Hz, *βH*), 8.51 – 8.53 (d, 2H, J = 7.8 Hz, 10 – $C_6H_4CF_3$), 8.84 – 8.85 (d, 2H, J = 4.4 Hz, *βH*), 9.56 – 9.57 (d, 2H, J = 4.3 Hz, *βH*).

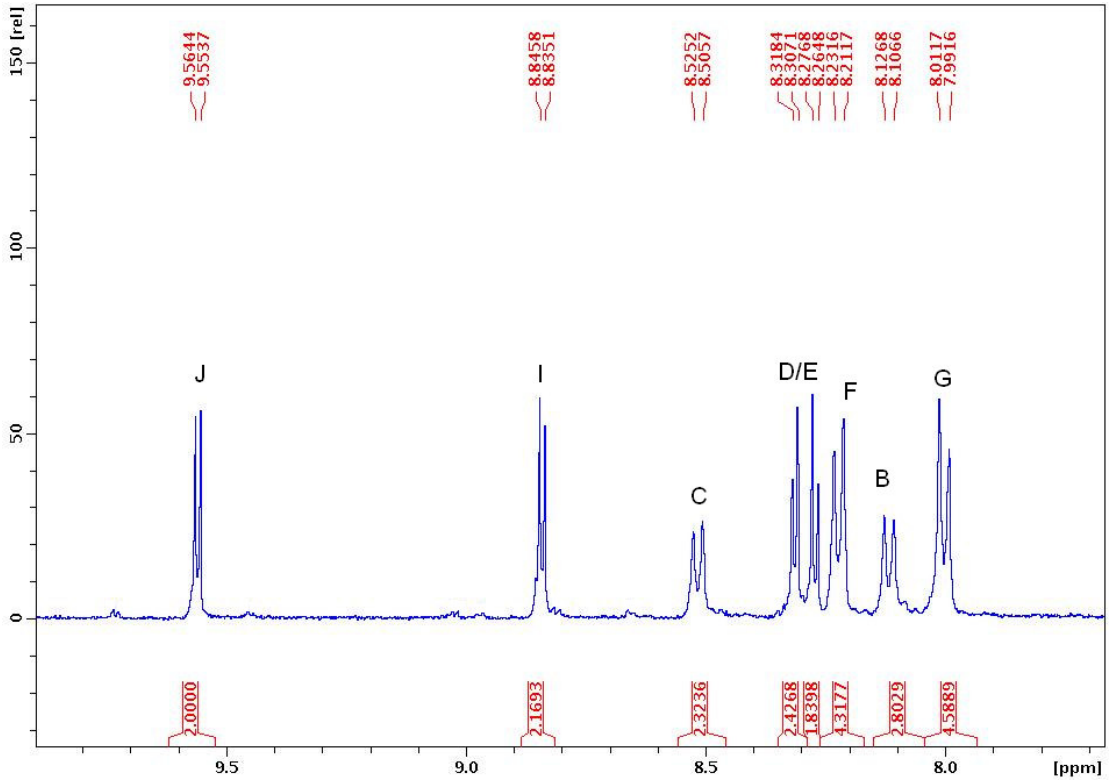
^{13}C (100 MHz, $CDCl_3$): 112.10, 118.82, 119.84, 120.06, 120.32, 121.04, 123.57, 124.15, 124.78, 125.27, 125.79, 125.85, 128.13, 128.47, 129.79, 130.11, 131.19, 133.89, 134.31, 135.35, 136.01, 137.09, 141.47, 142.54

UV-vis (λ_{max}/nm (ε/M^{-1} cm^{-1}) in CH_2Cl_2): 427 (3968612), 445 (2540153), 543 (236825), 580 (320017), 625 (955394)

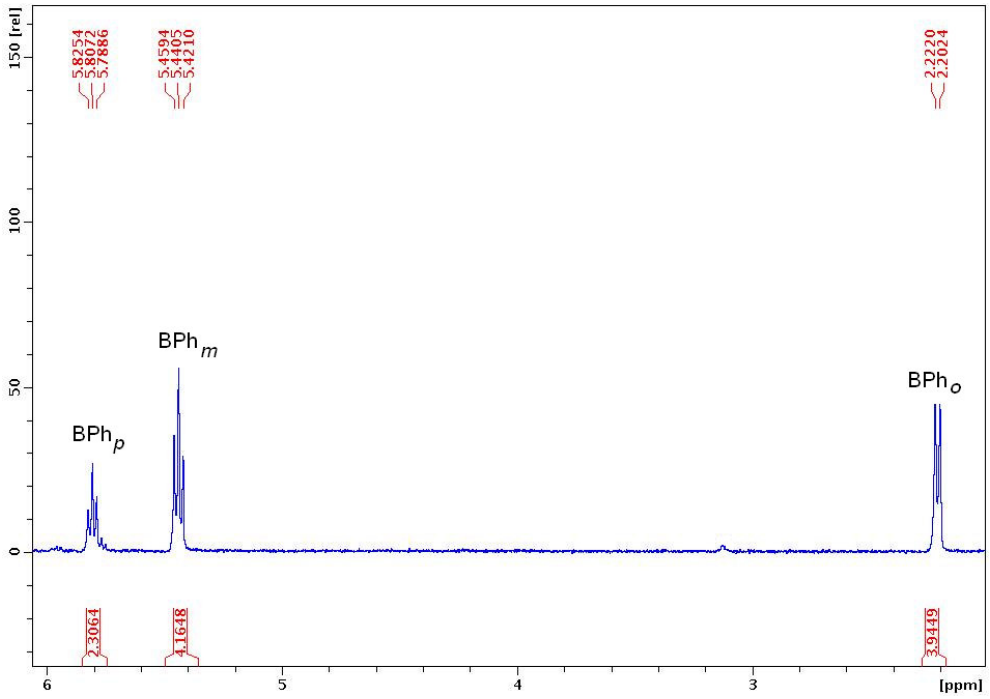
IR: 3047 (w), 2500 (w), 1932 (w), 1615 (m), 1573 (w), 1445 (w), 1406 (w), 1319 (s), 1259 (w), 1157 (m), 1105 (s), 1067 (s), 1017 (s), 899 (m), 839 (m), 814 (m), 784 (m), 770 (m), 742 (m), 714 (m), 696 (m)

HRMS (FAB+): Calculated for $C_{52}H_{31}{}^{10}B^{11}BF_9N_4$: 903.26274, found: 903.26142. Calculated for $C_{52}H_{31}{}^{11}B_2F_9N_4$: 904.25911, found: 904.25749

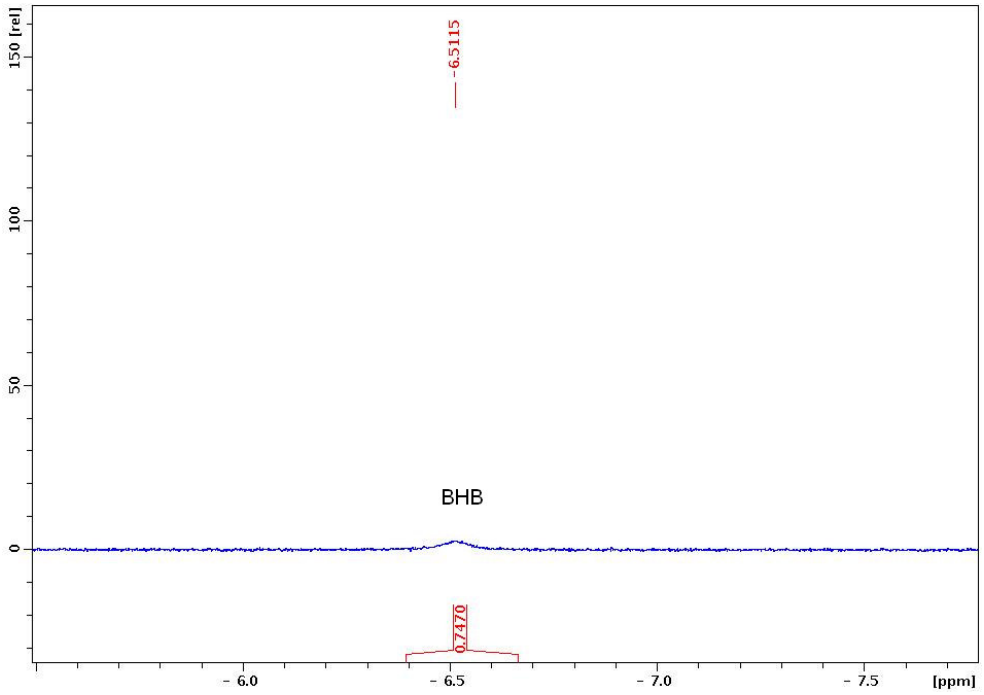
^{1}H NMR spectrum, aromatic region:



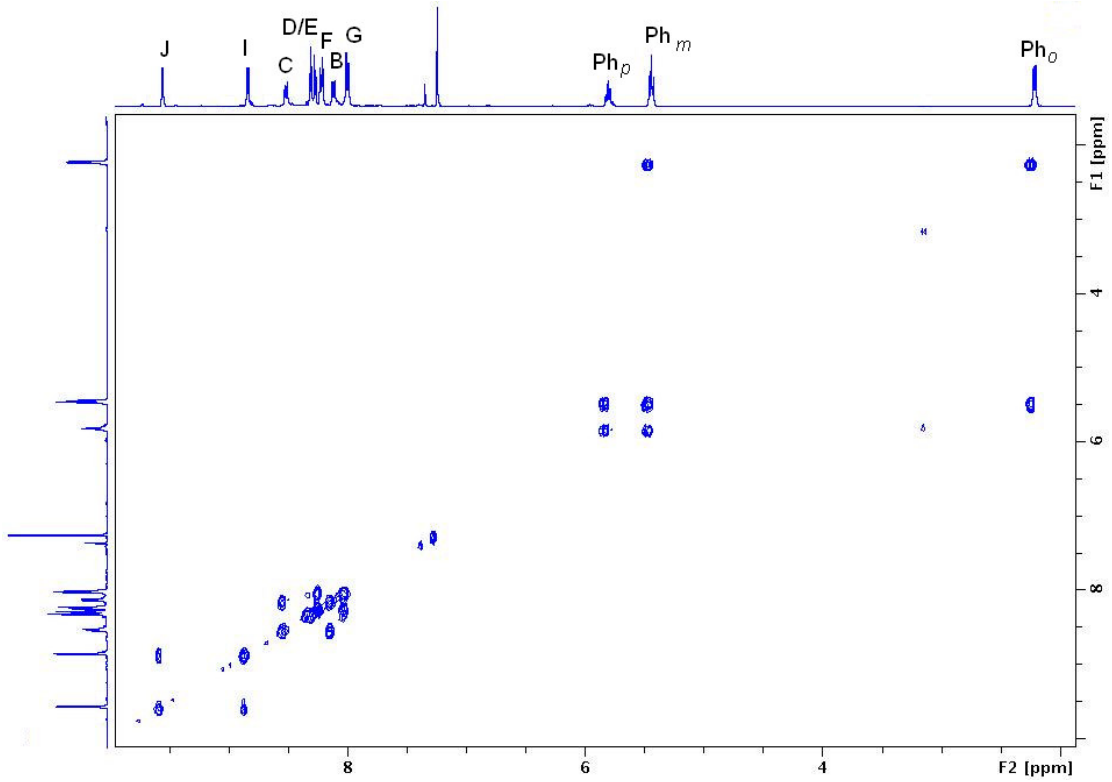
^{1}H NMR spectrum, BPh region:



^{1}H NMR spectrum, BHB region:

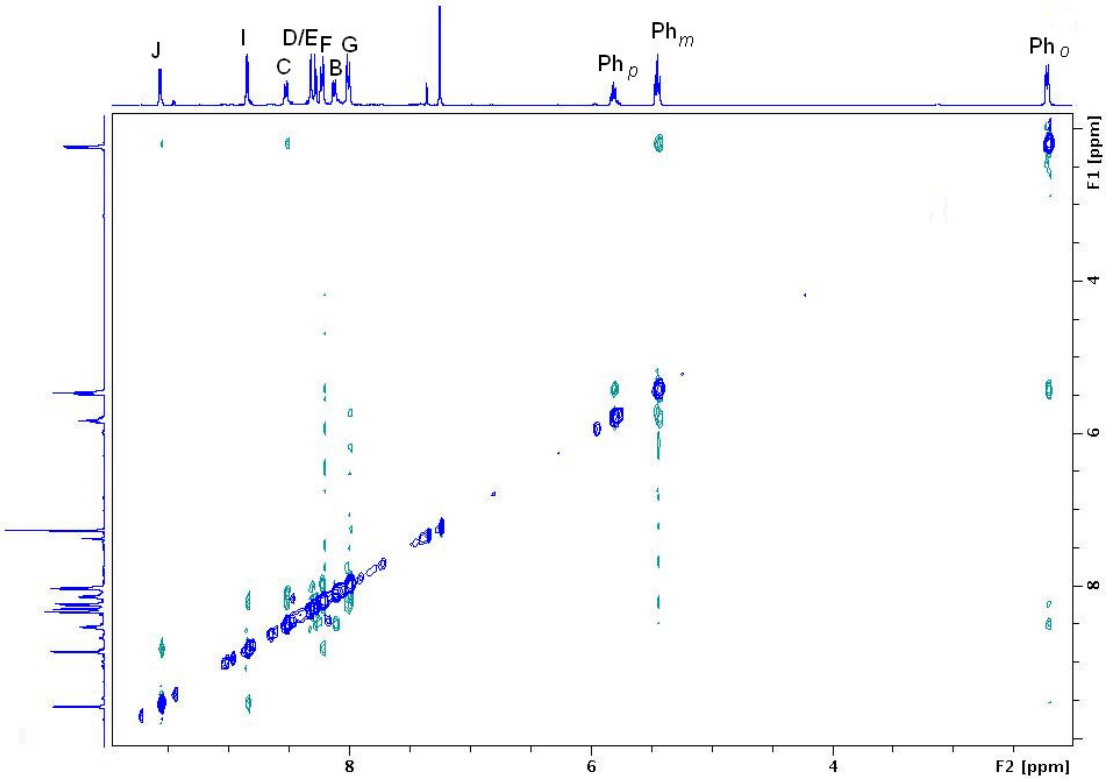


Example COSY spectrum:



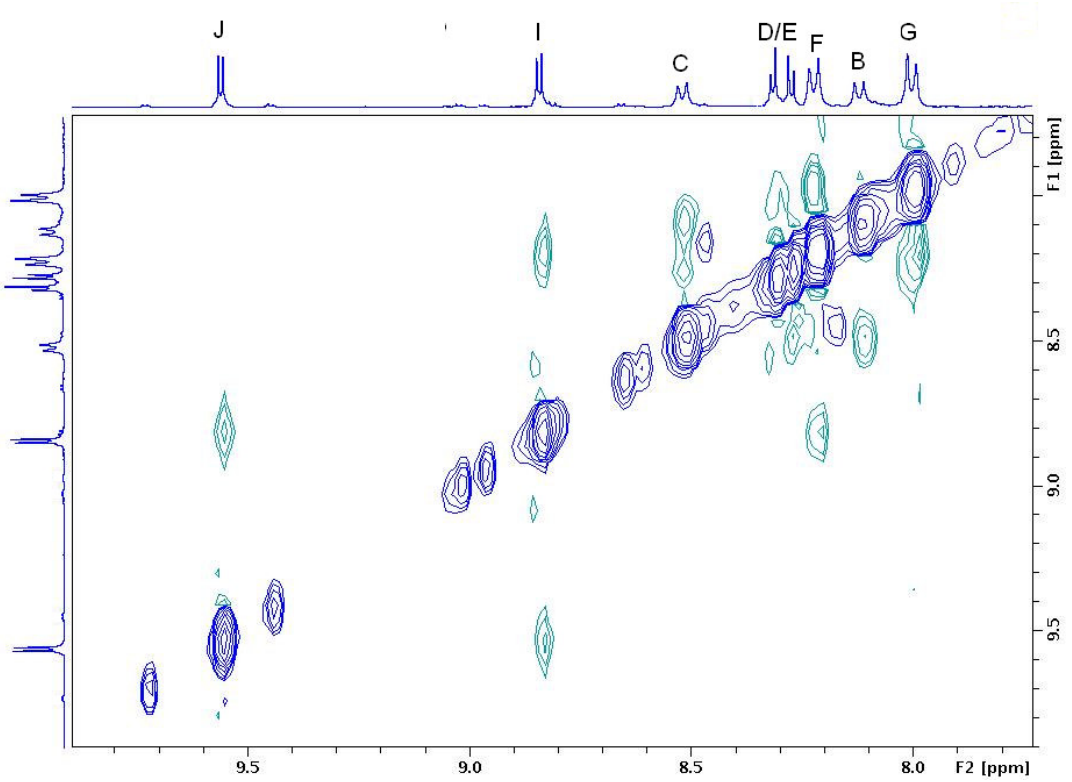
Cosy couplings:
J – I
C – B
F – G
D – E
Ph_p – Ph_m
Ph_m – Ph_o

Example NOESY spectrum:



NOE's:

J – I	C – B	Ph_m – Ph_o	Ph_p – Ph_m
F – G	I –F	C – Ph_o	



1.2 Experimental data for $B_2Ph_2H(T(4\text{-}Me\text{-}P)C)$

Procedure: as described for $B_2Ph_2H(T(4\text{-}CF_3\text{-}P)C)$ using $H_3(T(4\text{-}CH_3\text{-}P)C$ (273 mg, 0.480 mmol), BCl_2Ph (0.748 mL, 5.76 mmol) and $NEt(^iPr)_2$ (0.690 mL, 3.96 mmol).
Yield: 215 mg, 60.3 %.

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = -6.34 (1H, br s, B*H*), 2.27 – 2.29 (2H, d, J = 7.60 Hz, BPh_o), 2.60 (6H, s, $C_6H_4CH_3$), 2.73 (3H, s, $C_6H_4CH_3$), 5.41 – 5.45 (2H, t, J = 7.60 Hz, BPh_m), 5.76 – 5.79 (1H, t, J = 7.20 Hz, BPh_p), 7.52 – 7.54 (4H, d, J = 7.60 Hz, *5,15 - meta*), 7.61 – 7.63 (2H, d, J = 7.60 Hz, *10 – meta*), 8.00 – 8.02 (4H, d, J = 8.00 Hz, *5,15 – ortho*), 8.25 – 8.29 (8H, m, *8,12-β/7,13-β/10-ortho*), 8.82 – 8.83 (2H, d, J = 4.00 Hz, *3,17-β*), 9.44 – 9.45 (2H, d, J = 4.40, *2,18-β*)

^{13}C (100 MHz, $CDCl_3$): 21.38, 21.53, 113.11, 119.07, 119.33, 120.17, 120.96, 124.58, 125.43, 127.45, 127.80, 128.36, 128.81, 129.09, 130.63, 133.67, 135.20, 135.27, 135.87, 137.23, 137.31, 137.41, 142.85, 143.36,

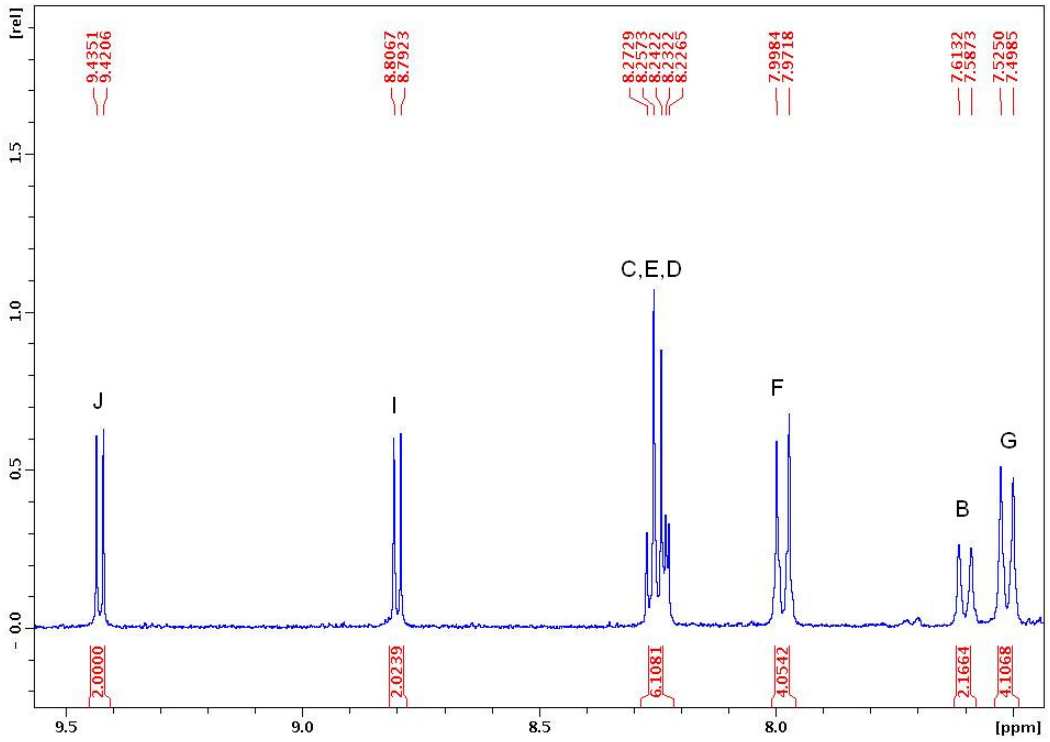
UV-vis (λ_{max}/nm (ε/M^{-1} cm^{-1}) in CH_2Cl_2): 424 (127779), 448 (80907), 539 (8899), 586 (14357), 630 (36631)

IR [cm^{-1}] $\tilde{\nu}$: 3019 (w), 2918 (w), 2483 (w), 2161 (w), 1569 (w), 1507 (m), 1443 (m), 1404 (m), 1365 (m), 1307 (s), 1254 (m), 1197 (m), 1181 (s), 1153 (s), 1113 (s), 1067 (m), 1042 (s), 1020 (s), 965 (m), 898 (w), 872 (w), 818 (s), 781 (s), 721 (s)

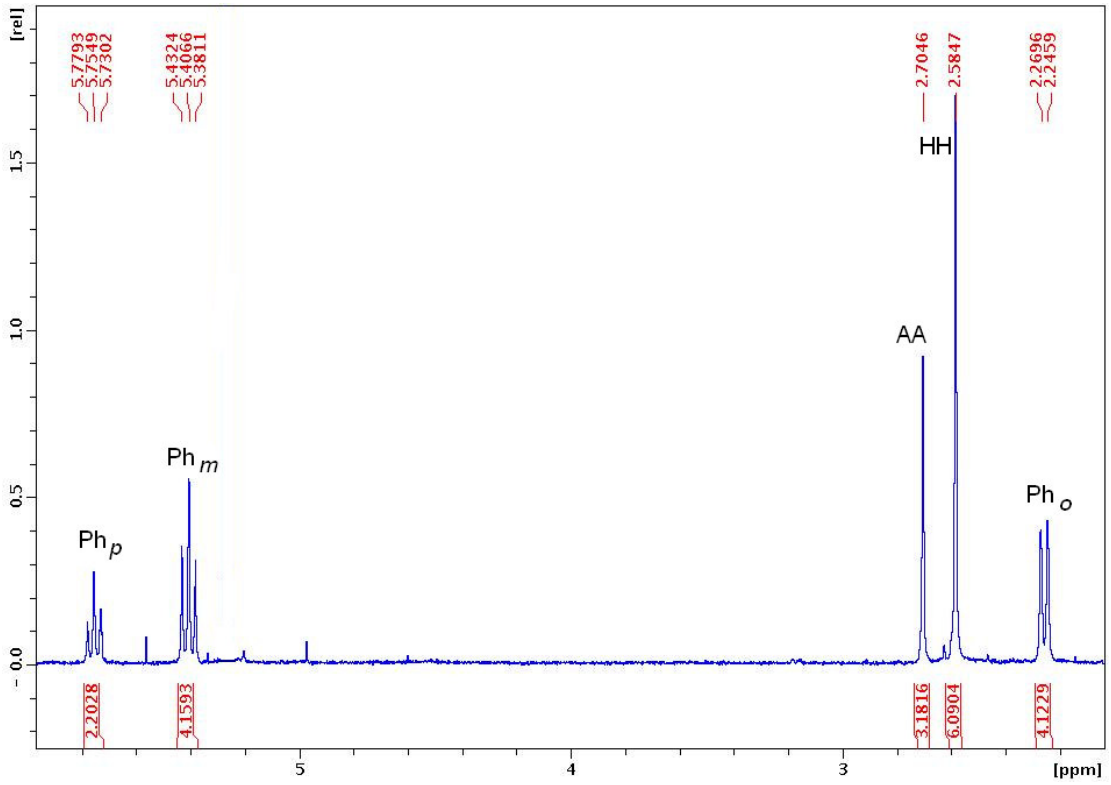
Mass spec (FAB+): Calculated for $C_{52}H_{40}{}^{10}B^{11}BN_4$: 741.34754, found: 741.34884.
Calculated for $C_{52}H_{40}{}^{11}B_2N_4$: 742.34391, found: 742.34524

Anal, calculated for $C_{52}H_{40}B_2N_4.2H_2O$: C, 80.22; H, 5.70; N, 7.20. Found: C, 80.01; H, 5.34; N, 7.76

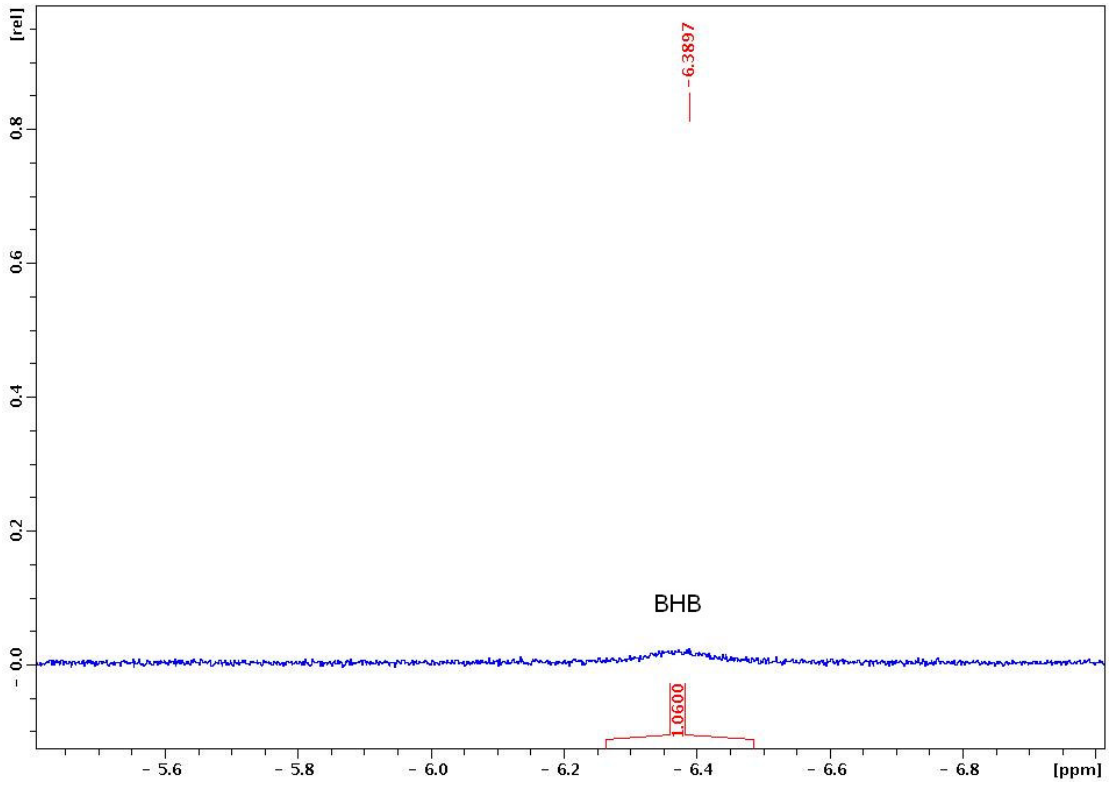
^{1}H NMR spectrum, aromatic region:



^{1}H NMR spectrum, BPh region:



^{1}H NMR spectrum, BHB region:



1.3 Experimental data for B_2Ph_2H(TPC)

Procedure: As described for B_2Ph_2H(T(4-CF_3-P)C) using H_3(TPC) (111 mg, 0.198 mmol), BCl_2Ph (0.308 mL, 2.38 mmol) and $NEt(^iPr)_2$ (0.690 mL, 3.96 mmol). Yield: 104 mg, 75.0 %

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = -6.35 (1H, br s, B*H*), 2.29 – 2.31 (4H, d, J = 7.88 Hz, BPh_o), 5.44 – 5.48 (4H, t, J = 7.80 Hz, BPh_m), 5.78 – 5.83 (2H, t, J = 7.32 Hz, BPh_p), 7.63 – 7.67 (t, 2H, J = 7.56 Hz, *5,15-para*), 7.72 – 7.75 (4H, t, J = 7.72 Hz, *5,15 – meta*), 7.80 – 7.84 (m, 3H, *10 – meta/para*), 8.12 – 8.14 (4H, d, J = 7.16 Hz, *5,15 – ortho*), 8.27 – 8.28 (2H, d, J = 4.56 Hz, *βH*), 8.32 – 8.33 (2H, d, J = 4.6 Hz, *βH*), 8.40 – 8.42 (2H, d, J = 7.8 Hz, *10-ortho*), 8.85 – 8.86 (d, 2H, J = 4.36 Hz, *βH*), 9.49 – 9.50 (d, 2H, J = 4.24 Hz, *βH*).

^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) = 77.21, 113.27, 119.33, 119.51, 120.22, 121.04, 124.64, 125.53, 127.08, 127.64, 128.31, 128.42, 130.78, 133.82, 135.36, 135.94, 137.21, 138.07, 143.20, 145.47

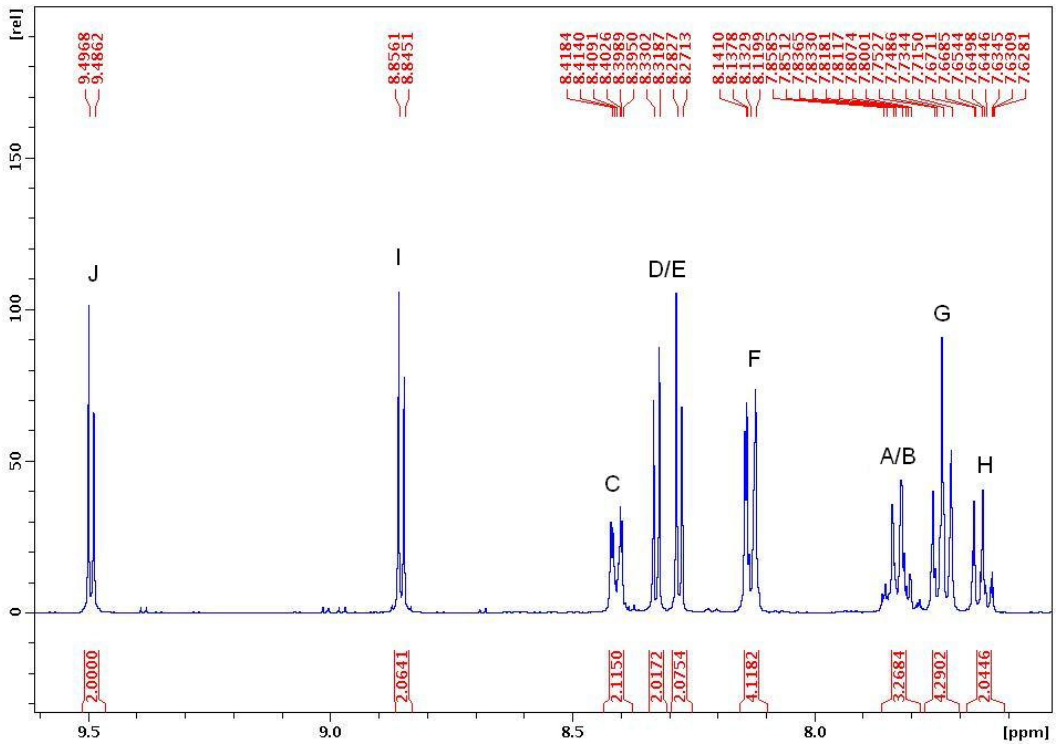
^{11}B NMR (128 MHz, $CDCl_3$): δ (ppm) = -8.90

UV-vis (λ_{max}/nm (ε/M^{-1} cm^{-1}) in CH_2Cl_2): 424 (108041), 446 (68509), 539 (5855), 580 (8614), 628 (29600)

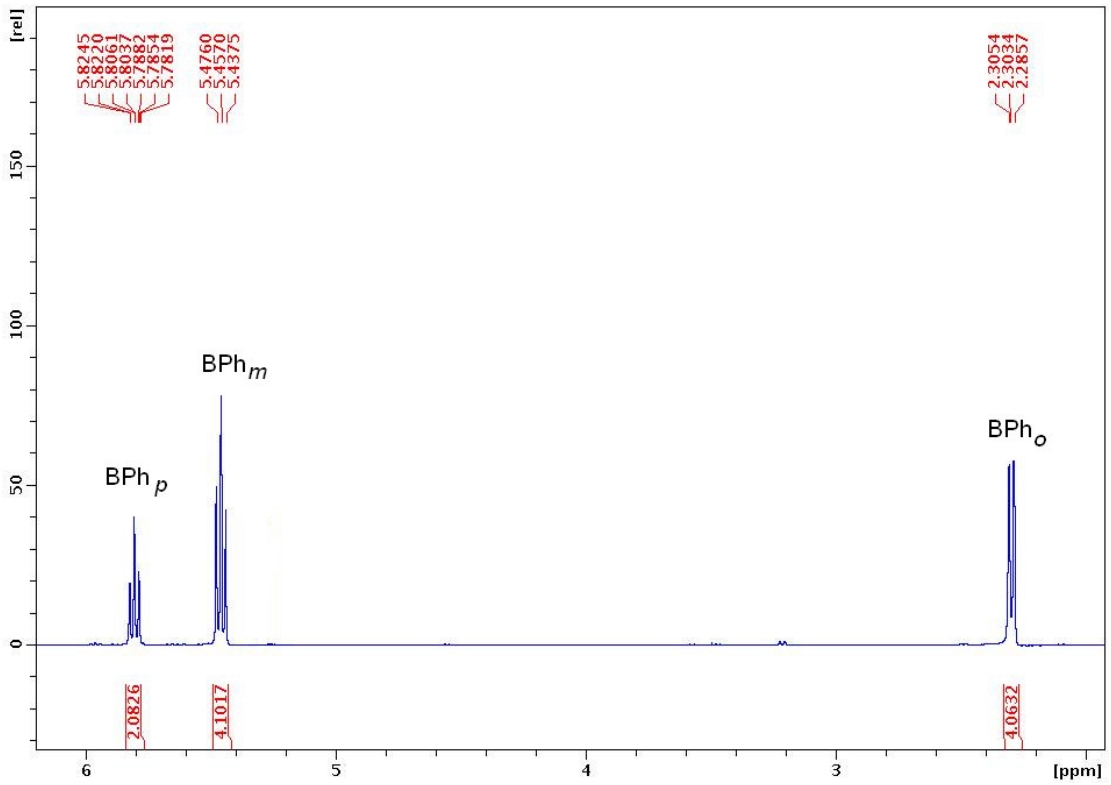
IR: 3045 (w), 2541 (w), 1975 (w), 1594 (w), 1489 (w), 1445 (m), 1405 (m), 1365 (m), 1334 (w), 1302 (m), 1252 (m), 1200 (m), 1176 (m), 1153 (m), 1113 (m), 1078 (m), 1065 (m), 1050 (m), 1027 (m), 999 (w), 957 (w), 911 (w), 857 (w), 837 (w), 821 (m), 789 (m), 754 (m)

Anal, calculated for $C_{50}H_{38}B_2N_4.0.6H_2O$: C, 82.74; H, 4.99; N, 7.88
Found: C, 82.83: 82.64; H, 5.18:5.34; N, 8.15

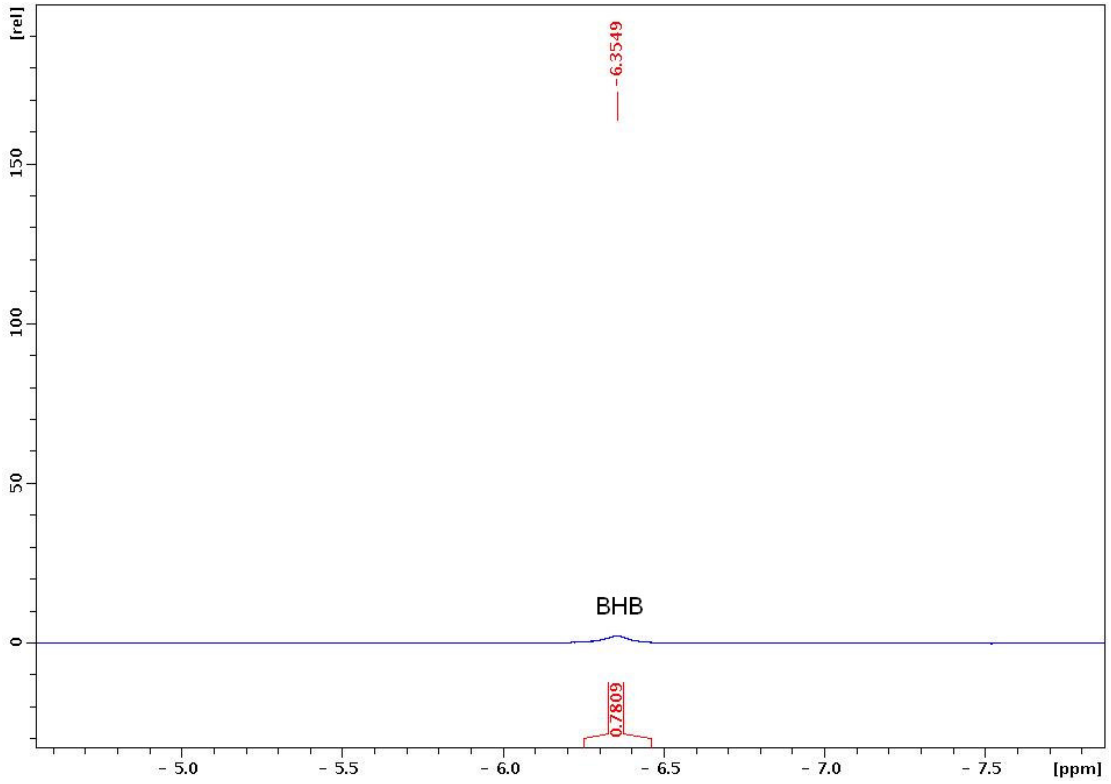
^{1}H NMR spectrum, aromatic region:



^{1}H NMR spectrum, BPh region:



^{1}H NMR spectrum, BHB region:



1.4 Experimental data for PhBFBPh(T(4-Me-P)C)

Procedure: BF_2Ph (0.133 mL, 1.06 mmol) was added to a solution of $H_3T(4\text{-Me-P})C$ (50 mg, 0.088 mmol) in dry CH_2Cl_2 under nitrogen. $NEt(^iPr)_2$ (0.307 mL, 1.76 mmol) was added dropwise via syringe and the bright green solution was stirred for 10 minutes then the solvent removed *in vacuo*. The crude solid was subject to purification by chromatography with CH_2Cl_2/n-hexane 1:1 as eluent. The bright green first band was collected and recrystallized from CH_2Cl_2/n-hexane. Yield: 48.8 mg, 73 %

^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm) = 2.00 - 2.02 (d, 2H, J = 7.2 Hz, $FBPh_o$), 2.54 (s, 3H, $C_6H_4CH_3$), 2.66 (s, 3H, $C_6H_4CH_3$), 2.75 (s, 3H, $C_6H_4CH_3$), 4.40 - 4.42 (d, 2H, J = 6.9 Hz, BPh_o), 5.24 - 5.30 (t, 2H, J = 7.5 Hz, $FBPh_m$), 5.74 - 5.79 (t, 1H, J = 7.2 Hz, $FBPh_p$), 6.23 - 6.28 (t, 2H, J = 7.8 Hz, BPh_m), 6.37 – 6.42 (t, 1H, J = 7.2 Hz, BPh_p), 7.34 - 7.42 (q, 4H, J = 8.1 Hz, Ar), 7.54 - 7.56 (d, 1H, J = 4.2 Hz, βH), 7.61 – **7**.64 (d, 3H, J = 7.5 Hz, Ar), 7.73 - 7.75 (d, 1H, J = 6.6 Hz, Ar), 7.85 - 7.87 (d, 1H, J = 4.2 Hz, βH), 8.05 - 8.08 (dd, 1H, J = 7.8 Hz, Ar), 8.15 - 8.17 (d, 2H, J = 7.8 Hz, Ar), 8.47 - 8.48 (d, 1H, J = 4.2 Hz, βH), 8.65 - 8.68 (dd, 1H, J = 7.5 Hz, Ar), 8.71 - 8.73 (d, 1H, J = 4.8 Hz, βH), 8.81 - 8.83 (d, 1H, J = 4.5 Hz, βH), 8.87 - 8.88 (d, 1H, J = 4.5 Hz, βH), 9.31 - 9.33 (d, 1H, J = 4.5 Hz, βH), 9.54 - 9.55 (d, 1H, J = 3.9 Hz, βH).

^{13}C NMR (100 MHz, $CDCl_3$): 21.31, 21.43, 21.50, 114.77, 115.08, 116.55, 118.48, 118.69, 118.93, 121.02, 121.29, 123.85, 124.97, 125.39, 125.78, 126.62, 127.5, 127.91, 128.00, 128.27, 128.31, 128.52, 129.11, 129.32, 130.42, 131.37, 132.73, 133.33, 134.55, 134.73, 135.48, 136.50, 137.50, 137.58, 137.78, 140.06, 141.07, 142.83, 143.16, 144.83, 146.51, 148.74

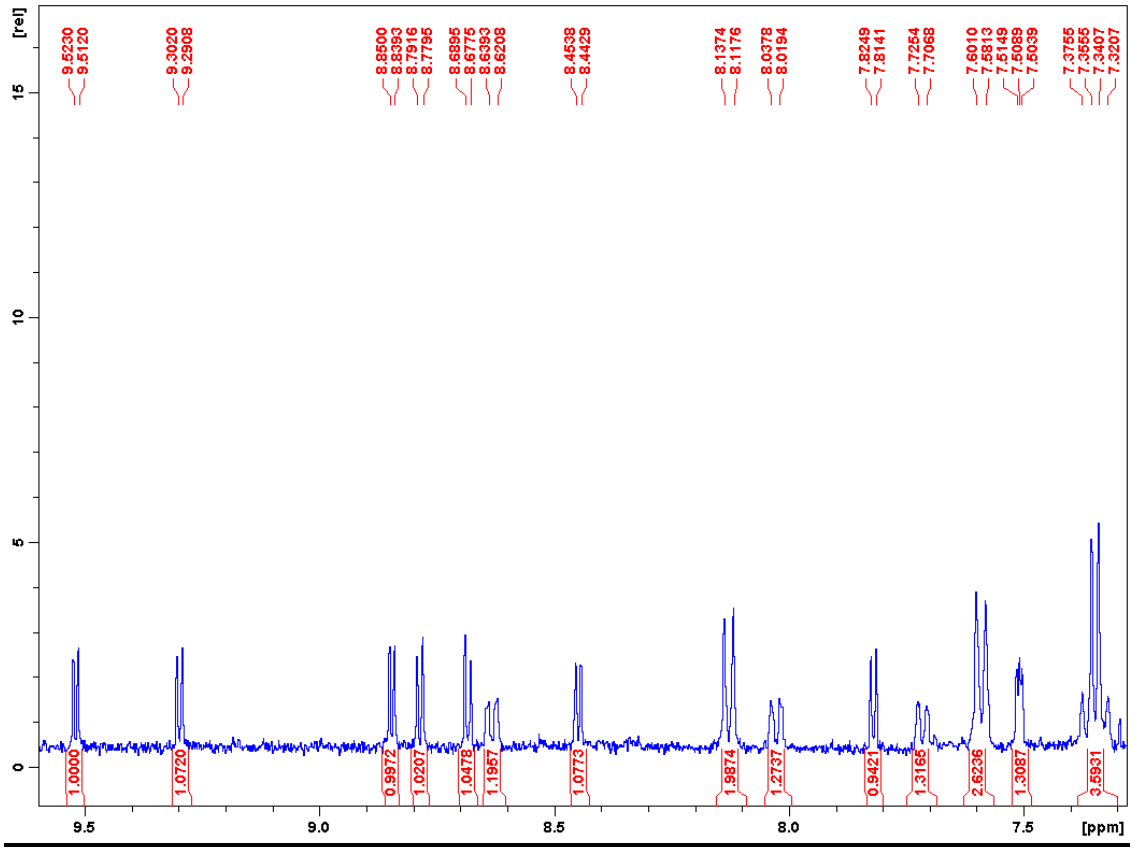
^{11}B NMR (128 MHz, $CDCl_3$): δ 29.39, -5.89 ppm

HRMS (FAB+): Calculated for $C_{52}H_{39}{}^{10}B^{11}BFN_4$: 759.33812, found: 759.33627.
Calculated for $C_{52}H_{39}{}^{11}B_2FN_4$: 760.33449, found: 760.33535.

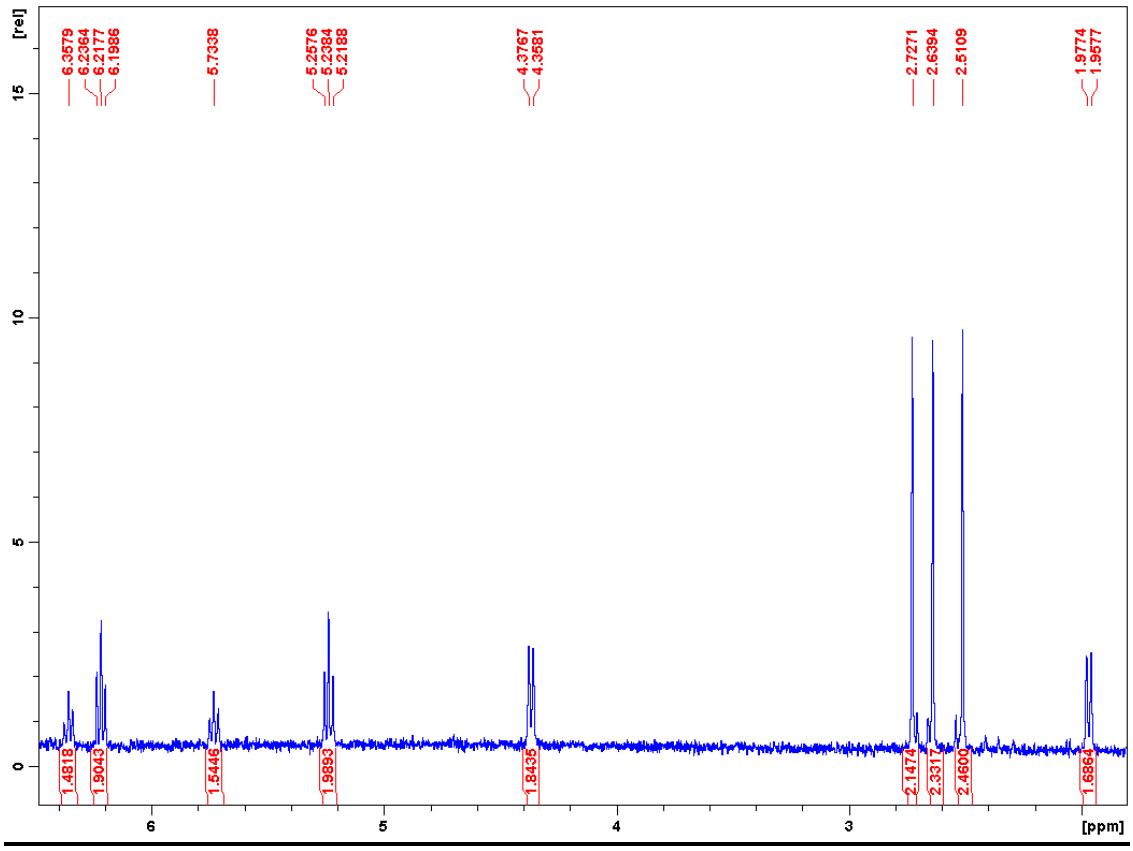
UV-vis (λ_{max}/nm (ε/M^{-1} cm^{-1}) in CH_2Cl_2): 413 (63431), 434 (75117), 455 (85434), 543 (7188), 582 (8540), 666 (30783)

Anal, calculated for $C_{52}H_{39}B_2FN_4$: C, 82.12; H, 5.17; N, 7.37
Found: C, 81.00-81.25; H, 5.29 – 5.32; N, 7.28 – 7.36

^{1}H NMR spectrum, aromatic region:



^{1}H NMR spectrum, BPh region:



2. Computational details and DFT Optimised coordinates

2.1 Computational details

All DFT calculations were carried out using the OLYP[2] generalized gradient approximation, triple-ξ plus double polarization Slater-type orbital basis sets, and a fine mesh for numerical integration of matrix elements, all as implemented in the ADF 2006 program system.[3]

2.2 *Cisoid* PhBHBPh corrole (peripheral Ph groups omitted): -390.22738927 eV

C	3.317113000	1.361003000	2.435549000
C	2.562022000	0.924744000	1.291554000
H	4.385755000	1.531249000	2.429454000
N	1.243250000	0.877654000	1.687659000
C	3.108963000	0.822876000	-0.000849000
H	4.193083000	0.891663000	-0.000988000
C	2.444189000	1.636735000	3.460081000
N	-1.168231000	1.013832000	-1.446408000
C	-1.283689000	1.541287000	-2.718953000
H	2.680758000	2.052067000	-4.432471000
H	2.681900000	2.048464000	4.431949000
H	4.385031000	1.533497000	-2.430770000
C	-3.191197000	1.996036000	-1.593637000
C	1.127930000	1.364657000	2.983587000
H	-2.977911000	2.603135000	-3.706971000
C	-2.583838000	2.104835000	2.830692000
C	-1.283057000	1.539325000	2.718992000
H	-4.152778000	2.399754000	-1.309550000
N	-1.167889000	1.012913000	1.445968000
C	1.127153000	1.366609000	-2.984399000
C	-3.190903000	1.994777000	1.594532000
C	-0.136270000	1.620247000	3.527681000
H	-0.213574000	2.022012000	4.531229000
H	-2.977178000	2.599979000	3.708367000
H	-4.152663000	2.398521000	1.311088000
C	-2.277609000	1.347416000	0.709595000
C	-0.137136000	1.622742000	-3.527949000
H	-0.214634000	2.025455000	-4.531109000
C	-2.277759000	1.347909000	-0.709479000
C	3.316446000	1.362964000	-2.436824000
C	2.561684000	0.925595000	-1.293036000
C	-2.584438000	2.107102000	-2.829846000
N	1.242818000	0.878525000	-1.688869000
C	2.443279000	1.639367000	-3.460939000
B	0.022491000	0.086536000	-1.240547000
B	0.022824000	0.085804000	1.239450000
H	0.190382000	-0.218512000	-0.000636000
C	-0.135592000	-1.391887000	1.854549000
C	-1.398597000	-1.988151000	2.017786000
C	0.982339000	-2.145933000	2.253927000
C	-1.542904000	-3.261822000	2.567815000
C	0.848239000	-3.419075000	2.807453000
C	-0.417948000	-3.982365000	2.969958000

H	-2.294497000	-1.449723000	1.720279000
H	1.981688000	-1.734113000	2.143472000
H	-2.535900000	-3.690935000	2.685292000
H	1.734138000	-3.970630000	3.115701000
H	-0.526562000	-4.973626000	3.405374000
C	-0.135801000	-1.391245000	-1.855307000
C	0.982787000	-2.147146000	-2.249382000
C	-1.398806000	-1.986436000	-2.022156000
C	0.849528000	-3.421115000	-2.801055000
C	-1.542245000	-3.260956000	-2.570535000
C	-0.416621000	-3.983444000	-2.967173000
H	1.982162000	-1.736219000	-2.135751000
H	-2.295324000	-1.446635000	-1.728879000
H	1.736046000	-3.974144000	-3.104879000
H	-2.535270000	-3.689266000	-2.690873000
H	-0.524735000	-4.975427000	-3.401028000

2.3 *Transoid* PhBHBPh corrole (peripheral Ph groups omitted): -390.04983163 eV

C	-1.269147000	-2.205919000	-3.153201000
C	-0.812605000	-1.042692000	-2.431036000
H	-1.071776000	-2.391718000	-4.200837000
N	-1.279128000	-1.214199000	-1.147052000
C	0.001164000	0.000815000	-2.956217000
H	0.000699000	0.000998000	-4.044203000
C	-1.889975000	-3.061869000	-2.272420000
N	1.055107000	0.988863000	1.281532000
C	1.669929000	2.206521000	1.456110000
H	2.282620000	4.048968000	-2.490238000
H	-2.278914000	-4.047932000	-2.488867000
H	1.074121000	2.393032000	-4.201502000
C	0.784207000	1.526494000	3.436472000
C	-1.857031000	-2.450606000	-0.975699000
H	1.886517000	3.438935000	3.306521000
C	-1.527356000	-2.528527000	2.837863000
C	-1.665844000	-2.204255000	1.457058000
H	0.438959000	1.508121000	4.461470000
N	-1.051223000	-0.986526000	1.281848000
C	1.861238000	2.451886000	-0.976741000
C	-0.781149000	-1.522505000	3.437297000
C	-2.133729000	-2.907642000	0.322437000
H	-2.610876000	-3.871629000	0.456954000
H	-1.882677000	-3.435387000	3.308337000
H	-0.436348000	-1.503126000	4.462430000
C	-0.443699000	-0.564826000	2.439796000
C	2.138020000	2.909315000	0.321133000
H	2.615128000	3.873346000	0.455356000
C	0.446758000	0.568236000	2.439650000
C	1.272100000	2.207182000	-3.154007000
C	0.815745000	1.044043000	-2.431625000
C	1.531085000	2.531824000	2.836635000
N	1.283216000	1.215383000	-1.147866000
C	1.893602000	3.062985000	-2.273570000

B	1.204251000	0.236262000	-0.012390000
B	-1.202987000	-0.234292000	-0.011979000
H	-0.001472000	0.006923000	-0.293802000
C	2.164535000	-1.047972000	-0.033428000
C	2.666659000	-1.587196000	-1.234082000
C	2.650055000	-1.622836000	1.156881000
C	3.582237000	-2.638924000	-1.248852000
C	3.567648000	-2.673792000	1.153911000
C	4.037930000	-3.191779000	-0.051951000
H	2.353328000	-1.174705000	-2.186446000
H	2.327711000	-1.236940000	2.117659000
H	3.946526000	-3.021955000	-2.200057000
H	3.921113000	-3.081644000	2.098774000
H	4.756984000	-4.008461000	-0.059092000
C	-2.168747000	1.046206000	-0.032316000
C	-2.658165000	1.617124000	1.158239000
C	-2.669421000	1.586871000	-1.232919000
C	-3.578796000	2.665478000	1.155593000
C	-3.587925000	2.636060000	-1.247359000
C	-4.047872000	3.184815000	-0.050176000
H	-2.336381000	1.230203000	2.118831000
H	-2.352582000	1.177525000	-2.185488000
H	-3.935435000	3.070281000	2.100535000
H	-3.950902000	3.020455000	-2.198472000
H	-4.769140000	3.999576000	-0.057080000

2.4 *Cisoid* PhBHBPh corrole (peripheral Ph groups included): -587.49912570 eV

C	2.955734000	2.508217000	2.647397000
C	2.385098000	1.622014000	1.667137000
H	4.006009000	2.748631000	2.721895000
N	1.020214000	1.627459000	1.896188000
C	3.123314000	1.061395000	0.590702000
C	1.946735000	3.061337000	3.388300000
N	-1.006836000	0.232753000	-1.136140000
C	-1.035613000	0.205276000	-2.516639000
H	3.050959000	0.390041000	-3.993891000
H	2.053342000	3.795778000	4.173999000
H	4.580584000	0.800667000	-1.867652000
C	-3.108007000	0.728223000	-1.771138000
C	0.715702000	2.537354000	2.905626000
H	-2.740151000	0.485996000	-3.931197000
C	-3.015099000	2.644564000	2.255100000
C	-1.657798000	2.263039000	2.465507000
H	-4.142328000	1.038556000	-1.728159000
N	-1.347822000	1.305482000	1.522585000
C	1.393767000	0.227050000	-2.509915000
C	-3.463332000	1.969178000	1.134808000
C	-0.624797000	2.828712000	3.251131000
H	-3.551127000	3.389221000	2.820977000
H	-4.421755000	2.095583000	0.651118000
C	-2.395302000	1.165718000	0.646330000
C	0.183613000	0.103715000	-3.229339000

C	-2.230917000	0.627780000	-0.656408000
C	3.521388000	0.592650000	-1.859992000
C	2.688267000	0.613634000	-0.685166000
C	-2.380234000	0.455402000	-2.916231000
N	1.407525000	0.325622000	-1.122310000
C	2.734190000	0.383554000	-2.959688000
B	0.222501000	-0.391401000	-0.496535000
B	-0.049585000	0.553435000	1.761132000
H	0.265700000	-0.198296000	0.770559000
C	-0.105905000	-0.578947000	2.904842000
C	-1.305403000	-1.241765000	3.215022000
C	1.039674000	-0.965319000	3.624711000
C	-1.367130000	-2.228565000	4.201720000
C	0.987878000	-1.948426000	4.613943000
C	-0.217758000	-2.583717000	4.907574000
H	-2.219005000	-0.986094000	2.685173000
H	1.993276000	-0.486729000	3.424179000
H	-2.313778000	-2.718239000	4.417203000
H	1.892095000	-2.214642000	5.157962000
H	-0.262082000	-3.349778000	5.679815000
C	0.266464000	-2.001932000	-0.493789000
C	1.483702000	-2.704733000	-0.427296000
C	-0.909466000	-2.769147000	-0.545094000
C	1.526383000	-4.100014000	-0.431217000
C	-0.877434000	-4.165371000	-0.548298000
C	0.344232000	-4.836567000	-0.494146000
H	2.422633000	-2.161090000	-0.380648000
H	-1.877069000	-2.277121000	-0.593258000
H	2.486503000	-4.610339000	-0.387073000
H	-1.807508000	-4.726728000	-0.596117000
H	0.373562000	-5.924847000	-0.500635000
C	-0.954540000	3.796756000	4.324493000
C	-1.802434000	3.421341000	5.376970000
C	-0.451414000	5.110152000	4.316690000
C	-2.126646000	4.319767000	6.394920000
C	-0.774580000	6.006301000	5.334607000
C	-1.610243000	5.615524000	6.378645000
H	-2.194212000	2.409326000	5.407015000
H	0.179905000	5.433910000	3.496430000
H	-2.777305000	4.000282000	7.203881000
H	-0.375813000	7.018049000	5.303115000
H	-1.860771000	6.315066000	7.173532000
C	4.618126000	1.124030000	0.774397000
C	5.273377000	0.115467000	1.494282000
C	5.387246000	2.180898000	0.267975000
C	6.652492000	0.159153000	1.700369000
C	6.767303000	2.224482000	0.467085000
C	7.405931000	1.213514000	1.185759000
H	4.693909000	-0.709493000	1.900958000
H	4.896818000	2.977929000	-0.283757000
H	7.136734000	-0.632966000	2.266645000
H	7.343135000	3.053553000	0.062700000
H	8.481002000	1.249122000	1.345136000

C	0.210162000	-0.001401000	-4.710407000
C	0.836422000	-1.093366000	-5.334186000
C	-0.370527000	0.982133000	-5.525868000
C	0.875668000	-1.197530000	-6.724295000
C	-0.333893000	0.875076000	-6.916699000
C	0.289467000	-0.216161000	-7.521396000
H	1.281291000	-1.869899000	-4.720636000
H	-0.835386000	1.849411000	-5.067834000
H	1.363011000	-2.054883000	-7.182681000
H	-0.785586000	1.653387000	-7.526248000
H	0.319711000	-0.298477000	-8.605843000

2.5 *Transoid* PhBHBPh corrole (peripheral Ph groups included): -587.45796257 eV

C	-2.469265000	0.149067000	-3.017120000
C	-1.269750000	0.361031000	-2.248480000
H	-2.491235000	-0.052560000	-4.077327000
N	-1.710212000	0.557189000	-0.947884000
C	0.068914000	0.317583000	-2.756890000
C	-3.552060000	0.148969000	-2.173197000
N	1.260046000	-0.464771000	1.534911000
C	2.602381000	-0.339769000	1.811609000
H	4.633708000	0.803277000	-1.888455000
H	-4.578379000	-0.052789000	-2.442138000
H	2.709004000	1.053842000	-3.696450000
C	1.434665000	-0.303176000	3.762011000
C	-3.072785000	0.364031000	-0.843410000
H	3.635267000	-0.189687000	3.789723000
C	-3.162545000	-0.296669000	2.926831000
C	-2.899154000	0.092036000	1.581714000
H	1.169630000	-0.195640000	4.805049000
N	-1.530895000	0.205676000	1.475672000
C	3.015694000	-0.019431000	-0.580509000
C	-1.943676000	-0.487249000	3.563065000
C	-3.703498000	0.228788000	0.415083000
H	-4.138869000	-0.461583000	3.355750000
H	-1.795646000	-0.848883000	4.571810000
C	-0.911523000	-0.209061000	2.631257000
C	3.519538000	-0.170132000	0.734661000
C	0.512753000	-0.374962000	2.683190000
C	2.604847000	0.627427000	-2.710105000
C	1.355768000	0.209138000	-2.124914000
C	2.716205000	-0.285034000	3.232023000
N	1.682143000	-0.227659000	-0.856691000
C	3.603410000	0.498574000	-1.776491000
B	0.815178000	-0.908833000	0.158725000
B	-0.860809000	0.785302000	0.262694000
H	-0.258383000	-0.353184000	-0.069946000
C	0.490767000	-2.477288000	-0.047334000
C	0.610155000	-3.092379000	-1.306892000
C	0.085738000	-3.303146000	1.017338000
C	0.340000000	-4.447283000	-1.498515000
C	-0.186184000	-4.660091000	0.837840000

C	-0.063912000	-5.240592000	-0.424472000
H	0.930906000	-2.507899000	-2.162387000
H	-0.012462000	-2.891815000	2.016504000
H	0.446535000	-4.884733000	-2.489356000
H	-0.491562000	-5.265181000	1.689070000
H	-0.276175000	-6.298026000	-0.568526000
C	-0.136920000	2.210586000	0.398512000
C	0.248887000	2.753130000	1.641053000
C	-0.007880000	3.071465000	-0.710211000
C	0.762548000	4.044078000	1.765154000
C	0.507273000	4.362567000	-0.600265000
C	0.905380000	4.855922000	0.641076000
H	0.134835000	2.172578000	2.547970000
H	-0.327058000	2.739372000	-1.689641000
H	1.044815000	4.416148000	2.747510000
H	0.592951000	4.984661000	-1.488384000
H	1.309270000	5.862602000	0.732684000
C	0.148131000	0.444838000	-4.253730000
C	-0.235686000	1.628458000	-4.901915000
C	0.613098000	-0.616116000	-5.044943000
C	-0.151855000	1.751137000	-6.288453000
C	0.685712000	-0.502657000	-6.432788000
C	0.306653000	0.683842000	-7.061502000
H	-0.594501000	2.467102000	-4.311884000
H	0.909619000	-1.545836000	-4.568149000
H	-0.444038000	2.683861000	-6.764723000
H	1.037859000	-1.344717000	-7.023564000
H	0.367790000	0.775853000	-8.142993000
C	4.974335000	-0.017985000	0.981004000
C	5.471045000	0.951763000	1.868167000
C	5.900707000	-0.830500000	0.306573000
C	6.840607000	1.096836000	2.078559000
C	7.270775000	-0.684486000	0.516277000
C	7.748318000	0.278657000	1.405035000
H	4.777612000	1.616509000	2.372871000
H	5.538034000	-1.592359000	-0.376678000
H	7.199896000	1.861606000	2.762694000
H	7.966247000	-1.329959000	-0.014107000
H	8.816971000	0.393749000	1.568483000
C	-5.178802000	0.085093000	0.479801000
C	-6.018944000	1.072910000	-0.059352000
C	-5.777550000	-1.050133000	1.051293000
C	-7.405454000	0.933456000	-0.023698000
C	-7.163395000	-1.187880000	1.088640000
C	-7.985291000	-0.196672000	0.552048000
H	-5.577551000	1.962363000	-0.498577000
H	-5.149043000	-1.843610000	1.442408000
H	-8.034102000	1.714626000	-0.444624000
H	-7.601205000	-2.081478000	1.527789000
H	-9.066624000	-0.306373000	0.578742000

2.6 *Transoid* PhBFBPh corrole: -391.67426151 eV

C	-2.467175000	0.394348000	-3.005090000
C	-1.277163000	0.569105000	-2.226176000
H	-2.471040000	0.248846000	-4.076981000
N	-1.696321000	0.704679000	-0.902509000
C	0.025410000	0.477082000	-2.728504000
C	-3.546702000	0.313692000	-2.160567000
N	1.250267000	-0.463908000	1.494246000
C	2.567026000	-0.159246000	1.770063000
H	4.521072000	1.148212000	-1.866771000
H	-4.576264000	0.118137000	-2.428527000
H	2.565892000	1.299245000	-3.699896000
C	1.423727000	-0.075813000	3.719774000
C	-3.066910000	0.438156000	-0.825341000
H	3.600489000	0.299405000	3.698486000
C	-3.138224000	-0.426529000	2.849619000
C	-2.889431000	0.087780000	1.554677000
H	1.134942000	0.116924000	4.744507000
N	-1.525166000	0.341381000	1.470300000
C	2.938775000	0.203126000	-0.603188000
C	-1.915335000	-0.571755000	3.493244000
C	-3.682126000	0.236693000	0.405564000
H	-4.108054000	-0.726912000	3.222380000
H	-1.744218000	-1.038601000	4.453486000
C	-0.899688000	-0.147721000	2.609637000
C	3.440294000	0.089898000	0.699996000
C	0.517094000	-0.314987000	2.642959000
C	2.509298000	0.845449000	-2.718869000
C	1.299630000	0.338038000	-2.126154000
C	2.689683000	0.034686000	3.177721000
N	1.621338000	-0.125370000	-0.874117000
C	3.508159000	0.778397000	-1.778635000
B	1.022220000	-1.227962000	0.101712000
B	-1.017488000	1.127039000	0.329138000
C	1.868128000	-2.622473000	0.035064000
C	2.390787000	-3.100982000	-1.179086000
C	1.995683000	-3.467891000	1.150727000
C	3.027890000	-4.339956000	-1.274381000
C	2.631102000	-4.709244000	1.069391000
C	3.157493000	-5.149830000	-0.145536000
H	2.303672000	-2.498251000	-2.080454000
H	1.592474000	-3.159049000	2.112981000
H	3.425767000	-4.671479000	-2.232126000
H	2.716999000	-5.332974000	1.957708000
H	3.659579000	-6.113263000	-0.212717000
C	-0.198459000	2.445142000	0.456285000
C	0.224872000	2.944974000	1.707242000
C	-0.032586000	3.303303000	-0.653783000
C	0.810737000	4.200672000	1.837015000
C	0.551934000	4.560189000	-0.530582000
C	0.985785000	5.012251000	0.715879000
H	0.082438000	2.353297000	2.602772000

H	-0.378985000	2.993914000	-1.632313000
H	1.126050000	4.548998000	2.817757000
H	0.663326000	5.191253000	-1.409228000
H	1.444750000	5.993791000	0.814619000
F	-0.310447000	-1.494465000	-0.149060000
H	4.476773000	0.340128000	0.896930000
H	0.068816000	0.582145000	-3.810254000
H	-4.750175000	0.063898000	0.454528000

2.7 *Cisoid* PhBFBPh corrole: -391.55089649 eV

C	-2.457474000	1.528578000	0.060728000
C	-1.465548000	0.496550000	0.212768000
H	-2.301087000	2.441823000	-0.498341000
N	-2.025808000	-0.463000000	1.031538000
C	-0.126397000	0.681155000	-0.187501000
C	-3.536785000	1.225155000	0.855499000
N	0.948237000	-2.439057000	2.869318000
C	2.178345000	-2.204342000	3.461968000
H	4.194226000	1.024006000	1.358400000
H	-4.413633000	1.833896000	1.031187000
H	2.360747000	1.991374000	-0.336403000
C	0.854692000	-3.219910000	4.982810000
C	-3.254033000	-0.013487000	1.500754000
H	2.947005000	-2.730877000	5.488059000
C	-3.395286000	-2.276460000	4.526888000
C	-3.220118000	-1.723073000	3.228298000
H	0.460366000	-3.609387000	5.910402000
N	-2.002562000	-2.171462000	2.742148000
C	2.672526000	-0.563393000	1.738980000
C	-2.235808000	-2.952484000	4.845132000
C	-3.895363000	-0.702023000	2.538338000
H	-4.247395000	-2.104768000	5.170654000
H	-2.000084000	-3.404948000	5.797663000
C	-1.330920000	-2.835664000	3.743788000
C	3.086253000	-1.337030000	2.830182000
C	0.084775000	-2.962666000	3.806041000
C	2.297734000	1.075090000	0.235837000
C	1.119149000	0.250910000	0.311929000
C	2.138382000	-2.760650000	4.770176000
N	1.422585000	-0.783608000	1.173390000
C	3.234500000	0.588330000	1.114656000
B	0.960065000	-2.231025000	1.351354000
B	-1.851138000	-1.967149000	1.228962000
C	-4.314223000	-4.639689000	-1.324750000
C	-3.863909000	-5.073043000	-0.077059000
C	-3.996794000	-3.351783000	-1.757591000
C	-3.108789000	-4.220390000	0.728354000
C	-3.240509000	-2.506981000	-0.944338000
C	-2.782070000	-2.915888000	0.319435000
H	-4.102099000	-6.076148000	0.270696000
H	-4.340073000	-3.002539000	-2.729322000

H	-2.770836000	-4.585497000	1.695151000
H	-3.008168000	-1.509413000	-1.308216000
F	-0.446686000	-2.344519000	0.785961000
H	4.052861000	-1.150203000	3.283242000
H	-0.019581000	1.538041000	-0.847156000
H	-4.846591000	-0.341051000	2.911576000
H	-4.907109000	-5.300054000	-1.954199000
C	1.774054000	-3.334242000	0.505528000
C	2.157618000	-4.571038000	1.049263000
C	2.074111000	-3.109927000	-0.850298000
C	2.821343000	-5.532852000	0.285464000
C	2.729079000	-4.067080000	-1.624041000
C	3.110764000	-5.283774000	-1.055918000
H	1.941480000	-4.795818000	2.090481000
H	1.788718000	-2.171551000	-1.319813000
H	3.112991000	-6.477325000	0.740404000
H	2.943338000	-3.862856000	-2.671042000
H	3.628409000	-6.030507000	-1.654419000