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Supporting Information

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Subpyriporphyrin – A [14]triphyrin(1.1.1) Homologue with An Embedded Pyridine Moiety.

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Materials. Selenium dioxide, trifluoroacetic acid (TFA), phenylboron dichloride, 2,3-dichloro-5,6-dicyano-*p*-benzoquinone (DDQ), 2,6-pyridinedimethanol, mesyl chloride, solutions of *n*-buthyllithium, ethylmagnesiumbromide, mesitylmagnesiumbromide and tetrafluoroboric acid were used as received. Chloroform (stabilized with amylene) was received from AppliChem and before synthesis was passed throw by grade I basic alumina (45 mL/40g). Basic alumina was deactivated by water before chromatography (100g, 3 mL). Silica gel **60** 0.063-0.2 mm was used as received. Pyrrole, triethylamine (TEA), and benzoyl chloride were distillated (under N_2) before use. All NMR data was collected at Bruker Avance 500 (^{1}H NMR 500.13MHz, ^{13}C NMR 125.7 MHz). UV-Vis spectra was collected at HP 8453 spectrophotomether.

2,6-pyridinedicarboxaldehyde was obtain as described in literature (N.W. Alcock, R.G. Kingston, P. Moore and C. Pierpoint, *Dalton Trans.* **1984**, 1937-1943).

2,6-bis[hydroxy-(mesityl)-methyl]pyridine 6: 2,6-pyridinedicarboxaldehyde (1485 mg, 11 mmol) were dissolved in dry THF (under N_2) and 22 mL of 1 M mesitylmagnesium bromide (in Et_2O) was added dropwise. After 3h of stirring the solution of NH_4Cl was added and mixture was evaporated. 20 mL of CH_2Cl_2 and 20% H_2SO_4 were added to the residue. The white precipitate was separated by filtration. The volume was reduced and procedure was repeated 4-6 times. (Last portion of **6** sulfate contains only one stereoisomer.) The combined precipitates were washed with small portion of CH_2Cl_2 and 20% H_2SO_4, dissolved in CH_2Cl_2/CH_3OH 1:1, alkalized by K_2CO_3 and evaporated. The residue were dissolved in CH_2Cl_2, washed 3 times with water and dried over Na_2SO_4. Yield of **3** 1586 mg (38.4%) (after evaporation and vacuum drying).

4-M. **^{1}H NMR** ($CDCl_3$, 298 K, one stereoisomer): *d* = 7.47 (1H, 4-pyridine), 6.86 (2H, 3/5-pyridine), 6.82 (4H, 3/5-Mes), 6.25, (2H, C*H*OH), 4.58 (2H, CHO*H*), 2.26 (6H, 4-Me), 2.20

ppm (12H, 2/6-Me). **^{13}C NMR** ($CDCl_3$, 298 K, one stereoisomer): *d* = 160.1, 138.0, 137.8, 137.6, 135.0, 130.2, 70.9, 21.1, 20.6 ppm. **MS** (ESI, *m*/*z*): 390.

2,6-bis[mesityl-(2-pyrrolyl)-methyl]pyridine 7. Mesyl chloride (483 μl, 2.1 eq.) in 1 mL of $CHCl_3$) was added dropwise (2 hr) to the solution of **6** (1110 mg, 2.96 mmol) and triethylamine (870 μl, 2.1 eq.) in $CHCl_3$ (25 mL) under nitrogen at 0 ^oC. Subsequently the reaction mixture was refrigerated for 3 days. After that time the solvent was removed under vacuum (RT). The residue was dissolved in 5 mL of pyrrole and the reaction mixture, protected form light, was stirred under nitrogen for 3 days The reaction was quenched by addition of CH_2Cl_2 (50 mL). The resulting solution was washed with 10% H_2SO_4 (10 mL, six times), water, diluted K_2CO_3 (10 mL, tree times) and dried with $MgSO_4$, filtered, and the solvent was removed with a vacuum rotary evaporator and vacuum line. The black residue was dissolved in CH_2Cl_2 and *n*-hexane was added. The volume was reduced. The yellow solution of **7** was decanted. The procedure was repeated 7-9 times. The solutions were combined and the solvent was removed with a vacuum rotary evaporator. Yield 1307 mg (93%).

^{1}H NMR ($CDCl_3$, 298 K, mixture of stereoisomers): *d* = 9.42/9.30 (2H, NH), 7.44-7.36 (1H, 4-pyridine), 6.90/6.89 (4H, *m*-Mes), 6.88/6.85 (2H, 3/5-pyridine), pyrroles: 6.58/6.50 (2H), 6.09/6.08 (2H), 5.69/5.65 (2H), 5.93 (2H, methine), 2.31/2.30 (6-H, 4-Me), 2.01 ppm (12-H, 2/6-Me). **^{13}C NMR** ($CDCl_3$, 298 K, mixture of stereoisomers): *d* = 161.7/161.4, 137.7/137.6, 137.4/137.3, 136.6/136.58, 136.3/136.1, 131.3/131.1, 130.3/130.2, 120.2/119.9, 116,7/116.4, 107.9/07.8, 107.24/107.17, 45.55/45.47, 21.14, 21.06 ppm. **MS** (ESI, *m*/*z*): 474.

2-[4-benzoylpyrrol-2-yl-(mesityl)-methyl]-6-[mesityl-(2-pyrrolyl)-methyl]pyridine 8: The solution of **7** (1061 mg, 2.24 mmol) in dry THF (5 mL) was added dropwise to 5.5 mL 1M EtMgBr (in THF, 2,4eq) under N_2. After 40 min. the solution of benzoyl chloride (5.5mmol, 640μl) in THF (2 mL) was added and the mixture was stirred for 6h. The reaction was quenched by addition of CH_2Cl_2 (10 mL) and diluted ammonia. The mixture were filtrated, the solid residue was washed by CH_2Cl_2 and water and separated. The organic layer was dried with Na_2SO_4, evaporated and left overnight under vacuum. The black foam was chromatographed on silica gel/CH_2Cl_2 (150 g, 1500 mL). The pale yellow fraction of **8** was evaporated. Yield 539 mg (41.6%).

^{1}H NMR ($CDCl_3$, 298 K, mixture of stereoisomers): *d* = 10.03/10.22 (2H, 5”), 9.85/9.77 (2H, 5’), 7.86 (2H, *o*-Ph), 7.53 (1H, *p*-Ph), 7.45 (2H, *m*-Ph), 7.44 (1H, 4-pyridine), 7.04/7.03 (1H, 3-pyridine), 6.95/6.94 (2H, “2”-3/5-Mes), 6.87-6.85 (2H+1H, “6”-3/5-Me+3’-pyrrole),

6.74/6.73 (1H, 5-pyridine); pyrrole 4", 3", 2": 6.34/6.61 (2H), 5.95-5.93 (2H), 5.40 (2H), 6.13 (1H, "2"-methine), 6.08 (1H, 2'-pyrrole), 5.84 (1H, "6"-methine), 2.34/2.33 (3H, "2"-4-Me), 2.28/2.27 (3H, "6"-4-Me), 2.08 (6H, "2"-2/6-Me), 1.99 ppm (6H, "6"-2/6-Me). **^{13}C NMR** ($CDCl_3$, 298 K, mixture of stereoisomers): *d* = 184.4/184.3, 162.5, 159.6, 159.1, 140.1, 139.7, 138.70/138.67, 137.7, 137.59, 137.56, 137.4/137.3, 136.5/136.44, 136.40/ 136.2, 131.9, 131.82/131.79, 130.7, 130.62/130.58, 130.0, 129.04/129.3, 128.5, 120.56/120.55, 120.5, 120.4, 120.0, 115.9/115.8, 111.32/111.31, 107.3/107.2, 106.5/10.64, 51.0, 46.98/46.95, 44.6, 21.4, 21.06, 20.99 ppm. **MS** (ESI, *m*/*z*): 474.

6,16-dimesityl-11-phenyl-subpyriporphyrin 5: $NaBH_4$ (155 mg, 40 eq) was added in several portion to the solution of **8** (57.5 mg, 0.1 mmol) in THF/EtOH under N_2. The mixture was stirred for 3 h and CH_2Cl_2 (10 mL) was added. The organic layer was washed 3 times with diluted NaOH and water, dried with Na_2SO_4, evaporated and dried in vacuum for 1 h. The residue was dissolved in 250 mL of dry CH_3CN (under N_2), TFA (200 µl, 2.6 mmol) or $Et_2O{:}BF_3$ (25.5 µl, 0.2mmol) was added and the solution was stirred for 4 h protected of light. The condensation was quenched by addition of TEA in excess. Subsequently DDQ (113.5 mg, 5eq) was added and the reaction mixture was stirred for 1h. The solvent was evaporated to dryness. The residue was dissolved in dichloromethane and chromatographed on basic alumina. The first green fraction containing **5** was eluted with dichloromethane. Recrystallization from CH_2Cl_2/CH_3OH produced 3.3 mg of 5 (yield 6 %).

^{1}H NMR ($CDCl_3$, 213 K): *d* = 17.82 (s, 1H, 18), 8.00, 7.76 (AB_2, (1+2)H, $^{3}J_{(H,H)}$ = 7.95 Hz, 3+2/4), 7.73, 7.53, 7.39 (A_2M_2X, (2+2+1)H, Ph), 7.41 (**A**B, 2H, $^{3}J_{(H,H)}$ = 4.62, 9/13), 7.18 (A**B**, 2H, $^{3}J_{(H,H)}$ = 4.62, 8/14), 7.05 (bs, 4H, *m*-Mes), 2.41 (s, 6H, 4-Me), 1.99 ppm (s, 12H, 2/6-Me). **^{13}C NMR** ($CDCl_3$, 213 K): *d* = 157.9, 149.8, 149.3, 139.3, 137.9, 137.7, 135.3, 133.7, 131.2, 130.7, 130.0, 128.7, 127.9, 126.1, 125.8, 123.2, 111.7, 108.2, 22.0, 21.5 ppm. **UV-Vis** (CH_2Cl_2) l_{max} (log ε) = 346 (4.40), 730 nm (very broad, 3.71). **HRMS** (ESI, *m*/*z*): 558.29054 (558.29038 for $[C_{40}H_{35}N_3+H]^+$).

[6,16-dimesityl-11-phenyl-subpyriporphyrin-phenylboron] tertafluoroborate 9. Phenylboron dichloride (8 µl, 10eq) was added to the solution of **5** (3.3 mg, 0.006 mmol) in dry toluene (under N_2). The mixture was stirred for 1.5 h. $AgBF_4$ (excess) was added and the solvent was removed under vacuum. The green solid was dissolved in CH_2Cl_2, filtrated and purified by recrystallization form CH_2Cl_2/*n*-hexane to give 4.2 mg of **9** (95%).

^{1}H NMR ($CDCl_3$, 298 K): *d* = 9.33, 9.08 (AB_2: (2+1)H, $^{3}J_{(H,H)}$ = 8.08 Hz, 3+2/4), 8.07, 7.85 (AB, (2+2)H, $^{3}J_{(H,H)}$ = 5.01 Hz, 9/13+8/14), 7.92, 7.74, 7.67 (A_2M_2X, (2+2+1)H, Ph), 7.16 (s,

2H, 5-Mes), 7.13 (s, 2H, 3-Mes), 6.07, 6.52, 4.87 (AM_2X_2, (1+2+2)H, Ph'), 2.47 (s, 6H, 4-Me), 1.79 (s, 6H, 2-Me), 1.69 ppm (s, 6H, 6-Me).**^{13}C NMR** ($CDCl_3$, 298 K): *d* = 150.4, 146.0, 140.6, 140.3, 139.6, 138.8, 133.4, 132.6, 132.0, 131.3, 129.9, 129.8, 129.6, 129.5, 129.4, 129.0, 128.7, 128.0, 127.4, 117.2, 21.7, 21.5, 21.0 ppm. **UV-Vis** (CH_2Cl_2) λ_{max} (log ε) = 358 (4.46), 485 (3.54), 523 (3.43), 687 nm (3.85). **HRMS** (ESI, *m*/*z*): 644.32356 (644.32316 for $[C_{46}H_{39}N_3B]^+$).

***syn*/*anti*-2-etoksy-6,16-dimesityl-11-phenyl-subpyriporphyrin-phenylboron 10**. 5 μl of diluted CH_3CH_2ONa (in CH_3CH_2OH) was added to the solution of **9** in CH_2Cl_2 (CD_2Cl_2) . Conversion into **10** was complete. After addition of 50% HBF_4 (5 μl), washing with water, drying with Na_2SO_4, filtration and evaporation **9** was quantitatively recovered.

***syn*-10** (major): **^{1}H NMR** (CD_2Cl_2, 298 K): *d* = 8.08, 7.68, 7.60(A_2M_2X, (2+2+1)H, Ph), 8.03 (**A**B, 1H, $^3J_{(H,H)}$ = 4.31 Hz, 9), 7.98 (**A'**B', 1H, $^3J_{(H,H)}$ = 4.31 Hz, 13), 7.34 (A**B**, 1H, $^3J_{(H,H)}$ = 4.31 Hz, 8), 7.29 (A'**B'**, 1H, $^3J_{(H,H)}$ = 4.31 Hz, 14), 7.13 (s, 2H, "6"/"16"-3-Mes), 7.07 (s, 1H, "16"-5-Mes), 7.05 (s, 1H, "6"-5-Mes), 7.06 , 6.49, 4.46 (AMX: (1+1+1)H, $^3J_{(H,H)}$ = 9.54 Hz, $^3J_{(H,H)}$ = 5.01 Hz, 4/3/2), 6.57, 6.44, 5.27 (AM_2X_2 (1+2+2)H, Ph'), 3.31/2.94, 0.96 (AA'B, (1+1+3)H, O-HCH-CH_3), 2.44 (s, 3H, "6"-4-Me), 2.43 (s, 3H, "16"-4-Me), 2.06 (s, 3H, "6"-2-Me). 2.03 (s, 3H, "16"-2-Me). 1.65 (s, 3H, "16"-6-Me). 1.50 ppm (s, 3H, "6"-6-Me). **^{13}C NMR** (CD_2Cl_2, 298 K, partially data from HMCQ map): *d* = 133.3 (*o*-Ph), 129.6 (o-Ph'), 129.1 (*m*-Ph), *m*-Mes: 129.0, 128.5, 128.4; 128.4 (*p*-Ph), 126.9 (3), 126.3 (*m*-Ph'), 126.1 (*p*-Ph'), 123.4 (9), 123.1 (4), 122.5 (12), 118.3 (8), 116.8 (13), 67.6 (2), 63.9 (O-**C**H_2-CH_3), 15.6 ppm (O-CH_2-**C**H_3). ***anti*-10** (minor, from COSY map)**: 1H NMR** (CD_2Cl_2, 298 K): *d* = Pyrrole 1: 8.17, 7.46; Ph: 8.13, 7.72, 7.63; Pyrrole 2: 8.02, 7.35; m-Mes: 7.13, 7.07, 7.08; 4/3/2-Py: 7.35, 6.69, 5.96; Ph': 6.52, 6.38, 5.05, 2/4/6-Me: 2.43, 1.90, 1.87, 1.73, 1.71 ppm. ***syn*/*anti*-10: UV-Vis** (CH_2Cl_2) λ_{max} (log ε) = 382 (4.75), 365 (4.61), 530 nm (4.34).

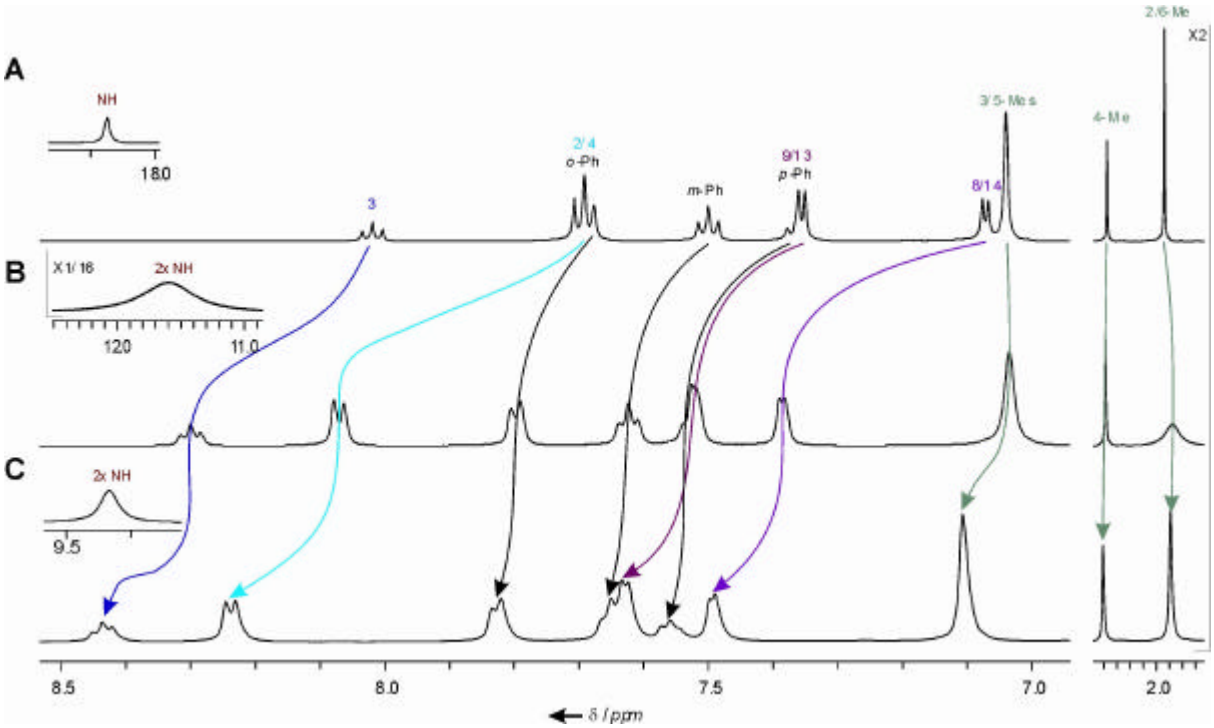

Figure 1s. ^{1}H NMR spectra (downfield regions presented): (A) **5**, (B) **5**-H , (C) **5**-H_2 as obtained in the course of titration of **5** with TFA in (dichloromethane-D_2, 203 K). NH resonances are shown in the associated insets. The inner N(17)H resonances of **5**-H_2 in exchange the COOH resonance of TFA are not shown in Trace C. Resonance assignments follow the numbering given in Scheme 2.

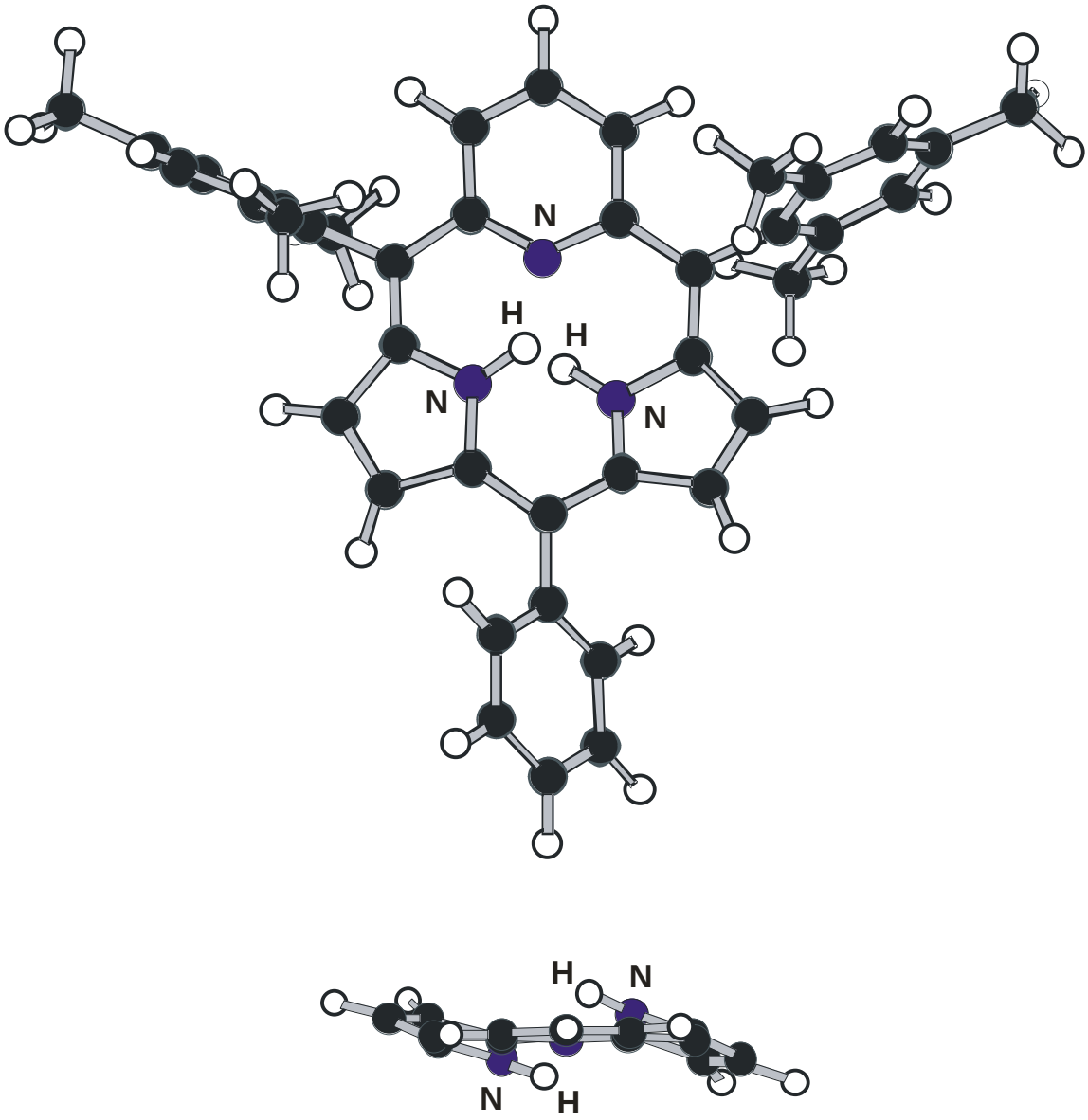

Figure 2s. The DFT optimized structure of **5**-H (bottom: view from pyridine side, *mezo* substituents omitted for clarity).

Computational details

The calculations have been performed with program Gaussian 03[1] using standars 6-31G** basis set[2] at the hybrid Hartree-Fock density functionally method (B3LYP).[3] All systems considered in this study were fully optimised. Additionally Bader`s theory[4] is applied here to get more detailed insight into the nature of hydrogen-bond. PROAIM package[5] was used to localize bond critical points and ring critical points (BCPs and RCPs). The electron densities at BCPs (ρ) and Laplacians of these densities were calculated ($\nabla^2\rho$).

[1] Gaussian 03, Revision C.02, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Wallingford CT, 2004.

[2] P. J. Hay; W. R. Wadt, *J. Chem. Phys.* **1985**, *82*, 270, 284, 299.

[3] A. D. Becke *J. Chem. Phys.* **1993**, *98*, 5648-5652.

[4] R. F. W. Bader, *Atoms in Molecules. A Quantum Theory*, Oxford University Press, New York, **1990.**

[5] F. W. Biegler- Koenig, R. W.Bader, T. H.Tang, *J. Comput. Chem.* **1982**, *3*, 317.

Table 1s.

The topological (in a.u.) parameters of selected Bond Critical points (BCPs) obtained from the AIB Analyses of.**5**.

	ρ	∇^2_ρ	H	ε
N(17) - H	0.0450	0.1473	-0.0014	0.2384
N(19) - H	0.0781	0.1655	-0.0188	0.0302
N(18) - H	0.2986	-1.5315	-0.4441	0.0172

Explanation of symbols: ρ, electron density at BCP; ∇^2_ρ, Laplacian; H, total energy density; ε, ellipcity.

Structure **5**: B3LYP optimized geometry (xyz format)

Tautomer with hydrogen on pyrrole

C	-1.097245	-1.698619	-0.398049
C	-1.073147	-3.110293	-0.401811
H	-1.993657	-3.683331	-0.423049
C	0.167298	-3.754442	-0.371546
H	0.205605	-4.840058	-0.376889
C	1.356573	-3.025490	-0.322594
H	2.315392	-3.530585	-0.274113
C	1.278010	-1.614252	-0.330770
C	2.472649	-0.735808	-0.237085
C	2.336280	0.649147	-0.265976
C	3.236281	1.775609	0.004374
H	4.294269	1.691989	0.212512
C	2.493515	2.926230	-0.010369
H	2.860711	3.927376	0.163933
C	1.095874	2.565230	-0.285987
C	-0.155870	3.237880	-0.260234
C	-1.354804	2.427538	-0.380031
C	-2.737807	2.658105	0.102566
H	-3.138054	3.594853	0.466939
C	-3.374055	1.453790	0.062722
H	-4.380567	1.234580	0.393865
C	-2.381221	0.466136	-0.409507
C	-2.369050	-0.922097	-0.329126
N	0.067418	-1.036225	-0.385411
N	1.128521	1.232223	-0.499243
H	0.226709	0.720297	-0.667365
N	-1.253442	1.155562	-0.751788
C	3.826836	-1.344885	-0.042585
C	4.269031	-1.713260	1.246052
C	5.539771	-2.281744	1.396394
H	5.874782	-2.560862	2.392945
C	6.386805	-2.496740	0.307866
C	5.931898	-2.125119	-0.961540
H	6.574476	-2.285743	-1.824876
C	4.672049	-1.553170	-1.157018
C	3.398980	-1.494071	2.463098
H	3.919868	-1.798941	3.374610
H	2.465915	-2.064694	2.402125
H	3.115385	-0.441807	2.568391
C	7.757393	-3.105935	0.488363
H	7.927897	-3.406891	1.525591
H	8.547887	-2.397839	0.213009
H	7.887399	-3.991374	-0.144001
C	4.232068	-1.167653	-2.551538
H	3.259426	-1.603148	-2.802402
H	4.958508	-1.504080	-3.296086

H	4.123232	-0.082495	-2.653639
C	-0.264818	4.685771	0.014242
C	0.499549	5.319311	1.012850
H	1.166760	4.724182	1.627820
C	0.378496	6.687070	1.250400
H	0.975884	7.150784	2.030489
C	-0.519598	7.456141	0.507628
H	-0.616172	8.521095	0.697134
C	-1.296494	6.841947	-0.476008
H	-1.997541	7.429541	-1.062147
C	-1.168907	5.476042	-0.721512
H	-1.757362	5.009847	-1.505984
C	-3.642051	-1.658568	-0.043250
C	-3.966990	-2.049721	1.276692
C	-5.162381	-2.733986	1.509926
H	-5.408397	-3.026120	2.528826
C	-6.049128	-3.049906	0.474970
C	-5.711204	-2.655217	-0.820373
H	-6.385632	-2.890789	-1.640567
C	-4.527402	-1.961370	-1.099436
C	-3.052570	-1.722251	2.435582
H	-2.843159	-0.649054	2.488415
H	-2.084753	-2.226998	2.343024
H	-3.501051	-2.029364	3.384095
C	-7.334601	-3.790629	0.759469
H	-7.890533	-3.994000	-0.159793
H	-7.988523	-3.213602	1.423727
H	-7.142609	-4.749521	1.254276
C	-4.217804	-1.554370	-2.522858
H	-3.224638	-1.894294	-2.834457
H	-4.224787	-0.465554	-2.639914
H	-4.953408	-1.972436	-3.215278

Structure **5'**: B3LYP optimized geometry (xyz format)

Tautomer with hydrogen on pyridine

H	-0.000123	0.034146	-0.000135
C	-1.227214	-1.631123	-0.086836
C	-1.217036	-3.036927	-0.090515
H	-2.152289	-3.578940	-0.162374
C	-0.000163	-3.716899	0.000288
H	-0.000193	-4.802864	0.000416
C	1.216750	-3.036983	0.090947
H	2.151959	-3.579051	0.162951
C	1.227042	-1.631177	0.086969
C	2.446818	-0.827159	0.121369
C	2.371601	0.575587	0.181548
C	3.344396	1.644751	-0.127785
H	4.398210	1.514318	-0.336870
C	2.631737	2.806366	-0.168308
H	3.004486	3.788362	-0.428011
C	1.219197	2.455419	0.120028
C	0.000127	3.204027	-0.000107
C	-1.218985	2.455487	-0.120192
C	-2.631494	2.806571	0.168081
H	-3.004159	3.788620	0.427702
C	-3.344261	1.645014	0.127629
H	-4.398101	1.514695	0.336651
C	-2.371560	0.575739	-0.181586
C	-2.446919	-0.826990	-0.121310
N	-0.000071	-1.028046	0.000030
N	1.167925	1.149188	0.388962
N	-1.167823	1.149222	-0.389008
C	3.773951	-1.513064	0.017915
C	4.552438	-1.716308	1.179208
C	5.794354	-2.350486	1.067555
H	6.383633	-2.511990	1.967634
C	6.296064	-2.782134	-0.162669
C	5.515066	-2.567570	-1.301597
H	5.888173	-2.892701	-2.270492
C	4.266361	-1.941282	-1.236057
C	4.062317	-1.267688	2.537755
H	4.736753	-1.609865	3.327271
H	3.060513	-1.653206	2.753202
H	3.995826	-0.176328	2.600536
C	7.654494	-3.434740	-0.264776
H	7.937420	-3.919898	0.674017
H	8.432604	-2.696883	-0.497410
H	7.678075	-4.188913	-1.057442
C	3.474956	-1.721171	-2.505809
H	2.555562	-2.317025	-2.521549
H	4.065055	-1.996958	-3.383809

H	3.172368	-0.674700	-2.611658
C	0.000178	4.675742	-0.000173
C	0.887684	5.403737	0.818146
H	1.557620	4.864354	1.480276
C	0.890335	6.796562	0.813418
H	1.580344	7.334238	1.457703
C	0.000293	7.500813	-0.000286
H	0.000332	8.586827	-0.000329
C	-0.889805	6.796567	-0.813935
H	-1.579768	7.334249	-1.458264
C	-0.887267	5.403742	-0.818550
H	-1.557245	4.864360	-1.480641
C	-3.774110	-1.512791	-0.017837
C	-4.266895	-1.940182	1.236282
C	-5.515609	-2.566411	1.301862
H	-5.889004	-2.890921	2.270855
C	-6.296260	-2.781755	0.162821
C	-5.794173	-2.350954	-1.067528
H	-6.383161	-2.513062	-1.967688
C	-4.552218	-1.716819	-1.179217
C	-3.475801	-1.719216	2.506077
H	-3.174683	-0.672332	2.612119
H	-2.555567	-2.313759	2.521668
H	-4.065510	-1.995968	3.384033
C	-7.654709	-3.434308	0.265018
H	-7.937714	-3.919478	-0.673743
H	-8.432770	-2.696404	0.497674
H	-7.678272	-4.188444	1.057719
C	-4.061661	-1.269097	-2.537899
H	-3.060291	-1.655797	-2.753296
H	-3.993939	-0.177835	-2.600950
H	-4.736486	-1.610745	-3.327310

Structure **5-H**: B3LYP optimized geometry (xyz format)

Monocation

C	-1.180301	-1.667497	-0.142312
C	-1.188890	-3.073677	-0.260689
H	-2.120223	-3.603377	-0.425313
C	0.022320	-3.760595	-0.167666
H	0.032705	-4.843486	-0.240171
C	1.222393	-3.069536	0.009420
H	2.163983	-3.600619	0.089579
C	1.191340	-1.660354	0.075840
C	2.427882	-0.848874	0.159947
C	2.361122	0.537977	0.274374
C	3.289789	1.601687	-0.071543
H	4.330965	1.450530	-0.318639
C	2.587035	2.778973	-0.145016
H	2.964801	3.741143	-0.458758
C	1.194262	2.500568	0.158845
C	-0.013357	3.244407	-0.000510
C	-1.222260	2.499506	-0.161668
C	-2.599522	2.751436	0.213675
H	-2.970735	3.698211	0.577928
C	-3.290308	1.565807	0.143488
H	-4.313203	1.391652	0.445647
C	-2.370070	0.523757	-0.274516
C	-2.424955	-0.865957	-0.179686
N	-0.002692	-1.030796	0.022612
N	1.172609	1.188346	0.518710
H	0.359981	0.629001	0.747547
N	-1.203440	1.198825	-0.564954
C	3.761643	-1.507332	0.026568
C	4.563642	-1.696452	1.175928
C	5.806388	-2.320723	1.035263
H	6.414705	-2.479277	1.922118
C	6.286763	-2.748244	-0.205807
C	5.479854	-2.541916	-1.329481
H	5.838402	-2.860691	-2.305120
C	4.225886	-1.932487	-1.241023
C	4.100906	-1.261172	2.549300
H	4.780021	-1.631803	3.320215
H	3.097376	-1.633932	2.780356
H	4.064240	-0.169945	2.640243
C	7.646805	-3.388494	-0.336103
H	7.957118	-3.864484	0.597778
H	8.407728	-2.640783	-0.590717
H	7.659138	-4.144432	-1.126372
C	3.413714	-1.717218	-2.499457
H	2.513997	-2.342500	-2.522736
H	4.003601	-1.962618	-3.385274

H	3.082950	-0.677687	-2.595652
C	-0.020226	4.714836	0.015556
C	0.850673	5.432360	0.859387
H	1.510386	4.892891	1.532039
C	0.843163	6.824392	0.868416
H	1.515930	7.361170	1.529888
C	-0.038871	7.528199	0.045163
H	-0.045893	8.613449	0.056601
C	-0.912039	6.830542	-0.792390
H	-1.592549	7.372153	-1.441891
C	-0.901166	5.438557	-0.812369
H	-1.555134	4.904376	-1.494907
C	-3.746604	-1.536957	-0.026797
C	-4.123587	-2.094572	1.219460
C	-5.374318	-2.706379	1.333863
H	-5.669394	-3.116002	2.296605
C	-6.259076	-2.797035	0.255054
C	-5.866698	-2.237051	-0.964958
H	-6.540642	-2.297014	-1.815906
C	-4.633679	-1.601563	-1.129191
C	-3.230512	-2.008079	2.438324
H	-2.813198	-1.004439	2.567587
H	-2.384781	-2.702442	2.379452
H	-3.790810	-2.256182	3.342506
C	-7.588394	-3.496142	0.395175
H	-8.355761	-3.025184	-0.225593
H	-7.936231	-3.492412	1.431508
H	-7.513381	-4.543670	0.078825
C	-4.276240	-1.023964	-2.482070
H	-3.264556	-1.302807	-2.793534
H	-4.321132	0.070787	-2.484590
H	-4.971110	-1.379899	-3.245932
H	-0.391683	0.691311	-0.878672

Structure 9: B3LYP optimized geometry (xyz format)

Complex with phenylboron.

C	-0.077414	0.243694	2.182667
C	-0.202072	1.409576	2.961847
C	-0.242823	1.370628	4.355877
C	-0.161452	0.146814	5.025013
C	-0.042173	-1.026666	4.281032
C	-0.001889	-0.972233	2.883686
H	-0.341059	2.294735	4.922282
H	-0.193540	0.110080	6.111734
H	0.018288	-1.988276	4.786828
H	0.086058	-1.902094	2.327645
H	-0.273720	2.373423	2.463207
B	-0.007118	0.351559	0.543872
C	0.182838	4.639877	-0.657603
C	1.046127	5.463827	0.090048
C	1.145207	6.829690	-0.170510
C	0.380279	7.412362	-1.182622
C	-0.478486	6.609246	-1.936348
C	-0.573093	5.242320	-1.681308
H	1.629599	5.016255	0.888162
H	1.816291	7.442344	0.426346
H	0.454138	8.477842	-1.383716
H	-1.069601	7.046990	-2.736964
H	-1.217309	4.619400	-2.292107
C	0.100663	3.190264	-0.373641
C	2.386675	0.442777	-0.212915
C	1.291429	2.432143	-0.244752
C	-3.245480	1.656495	-0.615648
C	-2.497643	2.832275	-0.628595
C	-1.143523	2.503859	-0.321549
H	-4.292079	1.548898	-0.865100
H	-2.864896	3.819043	-0.873341
C	-2.459683	-0.837713	-0.268592
C	-3.813249	-1.454514	-0.412306
C	-4.685716	-1.511255	0.700981
C	-5.959704	-2.071721	0.557819
C	-6.408487	-2.584447	-0.662065
C	-5.547181	-2.508450	-1.758995
C	-4.267736	-1.949716	-1.657696
C	-3.392003	-1.866058	-2.885694
C	-4.254803	-0.969186	2.043984
H	-6.616278	-2.113123	1.425816
C	-7.773074	-3.223310	-0.784027
H	-5.882454	-2.882916	-2.725260
H	-2.515900	-2.518289	-2.792367
H	-3.945755	-2.159741	-3.783401
H	-3.010791	-0.849938	-3.026582

H -4.973758 -1.238694 2.824581
H -3.267021 -1.343385 2.327932
H -4.169268 0.123142 2.023168
C -1.303388 -3.068074 -0.461480
C 1.131937 -3.133556 -0.446708
C -0.106900 -3.766857 -0.512203
H -2.257492 -3.574998 -0.516679
H 2.056631 -3.692698 -0.494339
H -0.136248 -4.850412 -0.618704
C 2.410738 -0.973566 -0.233168
C 3.727698 -1.659935 -0.398506
C 4.606235 -1.777388 0.704789
C 5.846826 -2.404536 0.542609
C 6.257620 -2.921805 -0.688108
C 5.387638 -2.793287 -1.773662
C 4.141461 -2.168053 -1.653764
C 3.257781 -2.030162 -2.870779
C 4.218986 -1.231956 2.059784
H 6.505861 -2.497408 1.404746
C 7.614061 -3.569601 -0.848479
H 5.689506 -3.180844 -2.745754
H 2.932256 -0.993553 -3.002521
H 3.784465 -2.348853 -3.776116
H 4.225622 -0.135840 2.062929
H 2.347921 -2.632997 -2.769802
C 2.653093 2.673924 -0.609925
H 3.051449 3.629279 -0.923546
C 3.331423 1.463084 -0.586518
C -1.277985 -1.652070 -0.280835
H 3.203312 -1.528833 2.336303
H 4.912606 -1.576279 2.833851
H 4.359132 1.285870 -0.872052
N -1.144989 1.142101 -0.052679
N -0.030237 -1.061824 -0.105055
C 1.180112 -1.725269 -0.261559
N 1.219093 1.078706 0.049828
C -2.356755 0.581490 -0.277945
H -8.505295 -2.735900 -0.131192
H -7.749263 -4.284957 -0.503212
H -8.149750 -3.170129 -1.810909
H 7.946357 -4.039114 0.083469
H 8.382122 -2.837131 -1.131720
H 7.601688 -4.339357 -1.627403