Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supporting Information

to

Experimental and Computational Study of Isomerically Pure Soluble Azaphthalocyanines and their Complexes and Boron Azasubphthalocyanines of Varying Number of Aza Units

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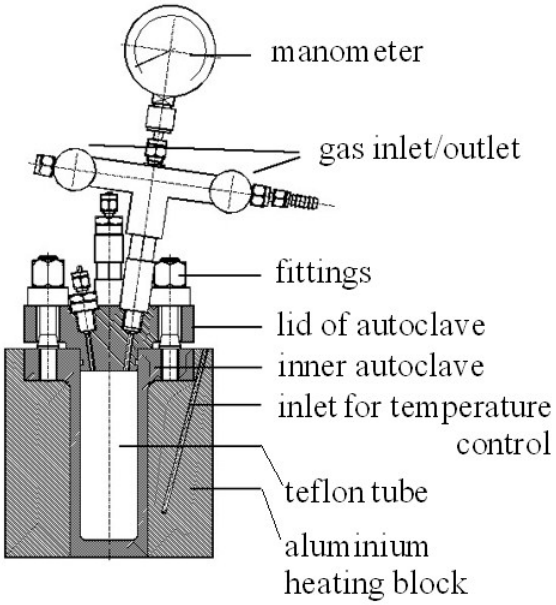
1.1 Experimental Section

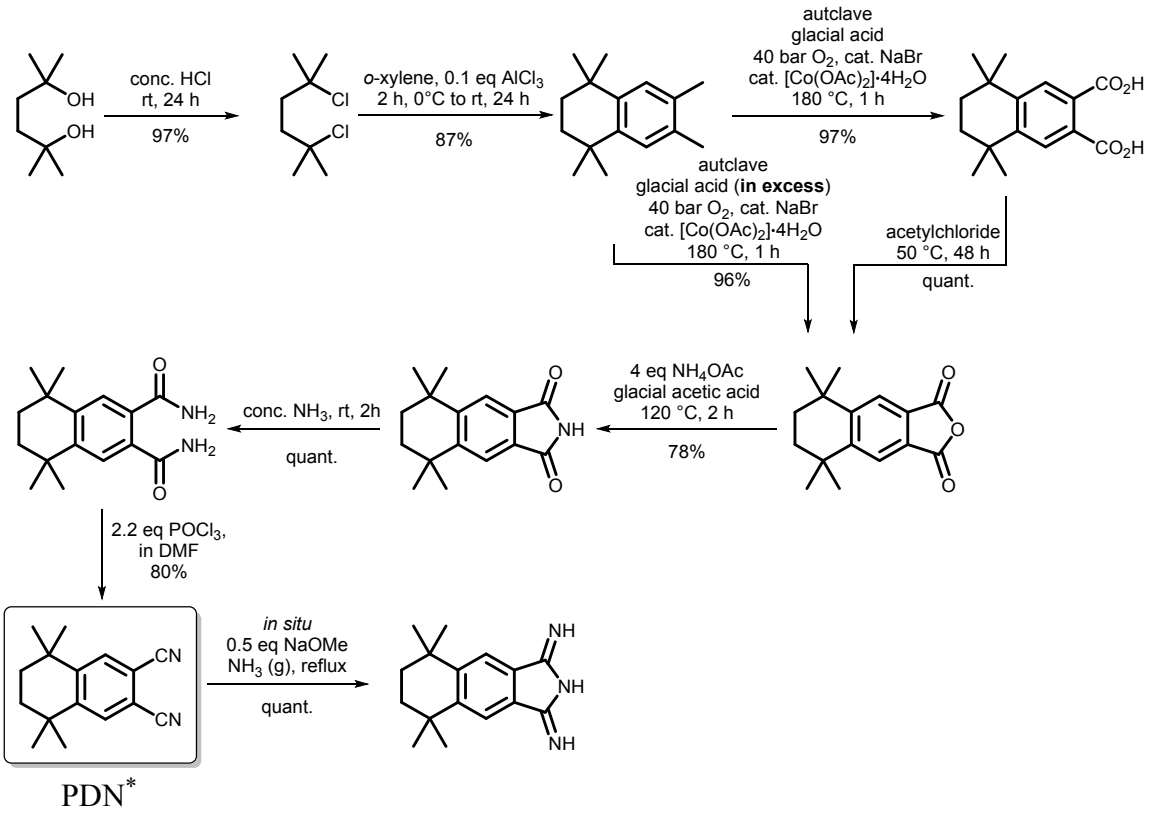
All reactions in which high pressure was needed, were carried out in an autoclave. Therefore, a glass (pressure <10 bar) or a steel autoclave (<100 bar) was used. The 100 mL stainless steel autoclaves *V4A-Edelstahlautoklaven* were constructed by the precision engineering department of the Philipps-Universität Marburg (Department of Chemistry). Solids and liquids were weighed out in a 100 mL teflon flask or in the corresponding glass flask, a magnetic stirrer was added and the autoclave was closed and sealed using EPDM-O-rings of CLEFF DICHTUNG company. The actual pressure was regulated using a manometer. The temperature was adjusted using a corresponding aluminium block in which the thermometer of the magnetic stirrer MR 3003 HEIDOLPH could be added (Pt-100-thermal element). If necessary, the heating block might be preheated (for Pc reactions). If necessary, the glass autoclaves were heated in an oil bath. A sketch of the steel autoclave is displayed below.



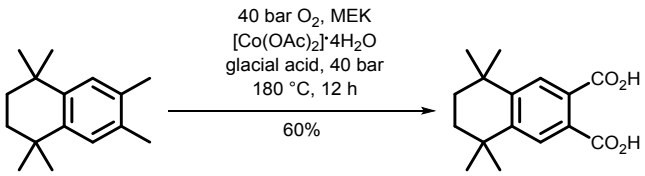
Sketch of the used steel autoclave: *V4A-stainless steel autoclave*.

1.1.1 **Synthesis of PDN***

The synthesis of the PDN* **1** was carried out according to MIKHALENKO.[1] The synthesis of 1,1,4,4-tetramethyltetralin-6,7-dicarboxylic acid (VI) was modified by using an overpressure of O_2 in a $[Co(OAc)_2]\cdot 4H_2O$ catalytic autoclave reaction.

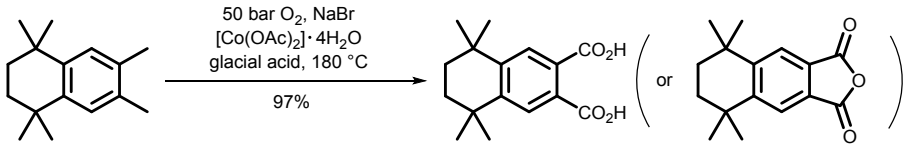


1.1.2 **Synthesis of 1,1,4,4-Tetramethyltetralin-6,7-dicarboxylic acid (TTDA)**



Method a) The reaction was carried out in an autoclave reaction as described in method b), using 50 bar O_2 and 0.1 eq $[Co(OAc)_2]\cdot 4H_2O$ as catalyst, 5 eq MEK as cocatalyst instead of NaBr, and 5 mL glacial acetic acid /g tetraline as solvent. The mixture was stirred for 12 h while the autoclave was recharged several times with O_2, until the pressure stayed constant. Workup was carried out according to method b).

Yield: 60% (only carboxylic acid was observed). - **^{1}H NMR**: according to analysis below.

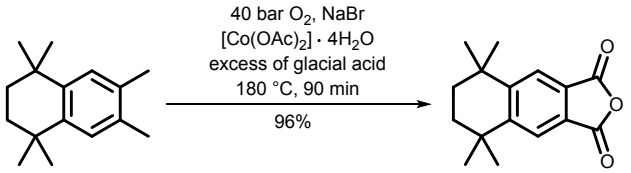


Method b) 15 g tetraline (69.3 mmol, 1 eq) were dissolved in 50 mL glacial acid in a 100 mL teflon tube and added into an autoclave. The teflon tube was additionally filled-up with 750 mg $[Co(OAc)_2]\cdot 4H_2O$ (3 mmol, 4 mol%) and 300 mg NaBr (3 mmol, 4 mol%). The mixture was briefly stirred until everything was dissolved. The autoclave was charged with O_2 to a pressure of 20 bar. With stirring, the solution was heated to 180 °C. After a short period of initiation (<30 min) the reaction started and the pressure decreased. The autoclave was recharged with O_2 to 50 bar as often as necessary, until the pressure stayed constant at about 50 bar. After 2 h, the reaction was complete. The reaction may also be stirred overnight. The resulting solution was concentrated under reduced pressure and was washed with water to remove Co-salts and NaBr traces. The product can be additionally precipitated in 20% aq. HCl (500 mL/20 g acid), followed by filtration and washing with water.

Yield: 18.5 g, 67 mmol, 97%. - **^{1}H NMR** (DMSO-d_6, 300 MHz): δ = 13.07 (s, 2 H, COO*H*), 7.57 (s, 2 H, Ar-C*H*), 1.66 (s, 4 H, -CH_2), 1.25 (s, 12 H, -CH_3) ppm. - **MS** (ESI(+), MeOH): *m/z* = 277.1436, cal. for $C_{16}H_{20}O_4$+H_1: 277.1434. - **Elemental analysis** ($C_{16}H_{20}O_4$, M = 276.33): fnd. (cal.): C 69.83% (69.55%), H 7.18% (7.30%), N 7.53% (0.00%).

Additional information: In some cases, the corresponding anhydride was detected by ^{1}H NMR spectroscopy. The amount of anhydride is dependent on the amount of glacial acid used in the reaction in ratio to the tetraline amount. No other by-products could be observed. A complete turnover was determined. The high nitrogen value in elemental analysis is caused by the measurement in closed setup in the glovebox, neither in the synthesis nor in precursor steps were nitrogen containing chemicals used.

1.1.3 **Synthesis of the Anhydride of 1,1,4,4-Tetramethyltetralin-6,7-dicarboxylic acid**



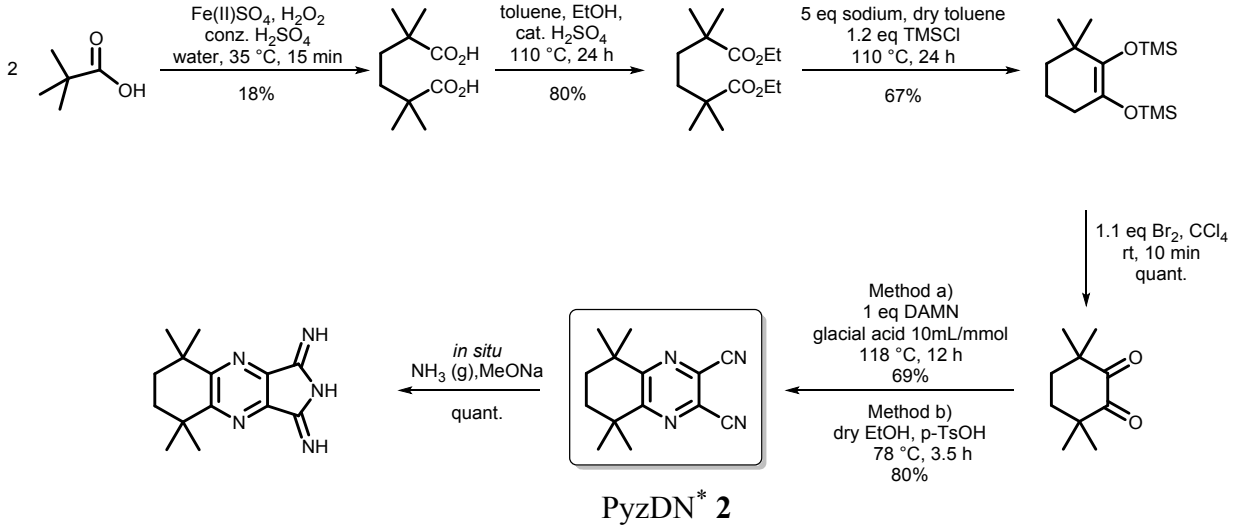
50 mg NaBr (486 µmol, ~3.5 mol%), 125 mg $[Co(OAc)_2]\cdot 4H_2O$ (502 µmol, ~3.5 mol%), 3.00 g tetraline (13.9 mmol, 1 eq) were added into an autoclave and dissolved in 10 mL glacial acid. The autoclave was charged with 20 bar O_2 and heated to 180 °C for 90 min. The pressure increased to 30 bar, dropped down to 20 bar and was recharged to 30-40 bar two

more times. The autoclave was recharged as often as needed, until the pressure stayed constant. Carboxylic acid anhydride was precipitated out of the solution and washed with water. A second/third portion was yielded overnight, filtered, washed with water and finally dried in vacuum.

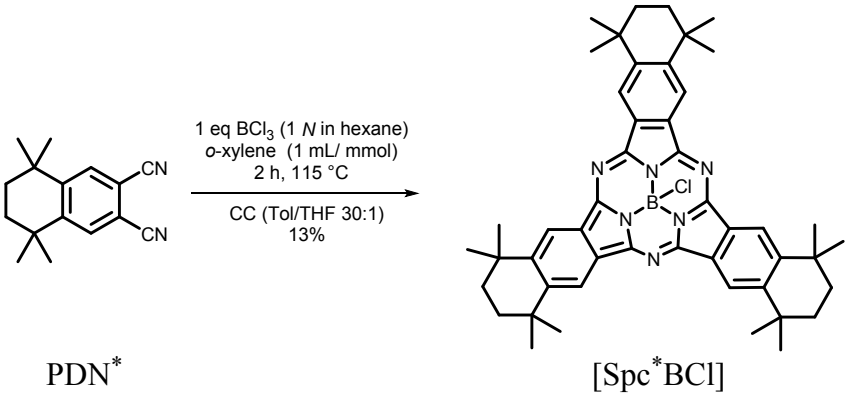
Yield: 3.43 g, 13.3 mmol, 96%. - **^{1}H NMR** ($CDCl_3$, 300 MHz): δ = 7.95 (s, 2 H, Ar-C*H*), 1.76 (s, 4 H, -CH_2), 1.36 (s, 12 H, -CH_3) ppm.

1.1.4 **Synthesis of PyzDN***

The synthesis of 3,3,6,6-tetramethylcyclohexane-1,2-dione (**XIV**) was carried out following the procedure of JONES.[2] The synthesis of PyzDN* **2** was carried out according to the procedure of SEIKEL.[3]



1.1.5 **Synthesis of [Spc*BCl]** [4,5]

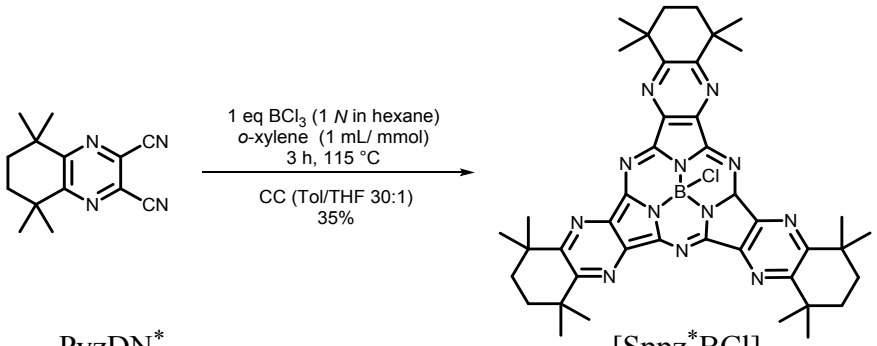


1 eq PDN was dissolved in 2 mL toluene /5 mmol PDN. Fresh BCl_3 solution (1 M in heptane or in *o*-xylene, 3 eq BCl_3 per intended [SpcBCl]) was added at once and then heated to 150 °C. The yellowish solution turned deep pink. After heating for about 5 h, the solution was loaded onto a short silica pluck, purified with DCM/EE to remove the boron compounds and then purified by CC (PE/EA 10:1).

Yield: ~5%. - R_f (PE/EE 10:1) = 0.4. - **^{1}H NMR** (C_6D_6, 300 MHz): δ = 8.91 (s, 6 H, Ar-C*H*), 1.65-1.52 (m, 12 H, -CH_2), 1.42 (s, 18 H, -CH_3), 1.10 (s, 18 H, -CH_3) ppm. - **^{1}H NMR** (CD_2Cl_2, 300 MHz): δ = 8.84 (s, 6 H, Ar-C*H*), 1.94-1.80 (m, 12 H, -CH_2), 1.66 (s, 18 H, -CH_3), 1.44 (s, 18 H, -CH_3) ppm. - **^{13}C NMR** (CD_2Cl_2, 75 MHz): δ = 149.6, 149.2, 129.4, 120.4, 36.0, 35.3, 32.9, 32.3 ppm. - **UV-Vis** (DCM): λ = 582 (s), 528 (sh), 318 (s), 267 (s) nm. - **Fluorescence** (DCM, λ_{ex} = 350 nm): λ = 592 nm. - Φ_F (λ_{ex} = 490 nm) = 0.18. - Φ_Δ = 0.64. - **MS** (APCI-HRMS(+)): *m/z* = 761.4247 $[M+H]^+$, cal. for $C_{48}H_{54}B_1Cl_1N_6+H_1$: 761.4272. - **X-ray**: Crystals could be obtained out of CD_2Cl_2 in the NMR tube at rt.

Additional information: In some cases, degradation of [Spc*BCl] in the form of a fast decolouration was observed in acidic solvents.

1.1.6 Synthesis of [Sppz*BCl] [4,5]

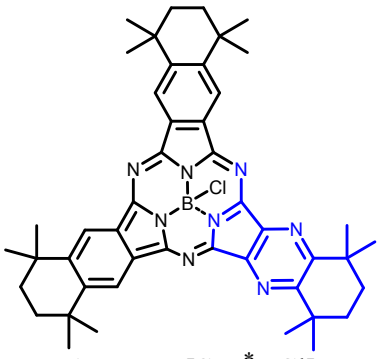


PyzDN* [Sppz*BCl]

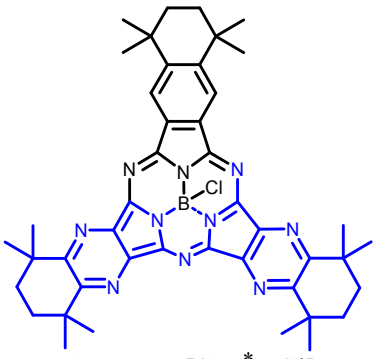
According to procedure described in 1.1.5. The pink solution was purified by CC (Tol/THF 30:1). The pink solid was dried in vacuum.

Yield: 35%. - R_f (Tol/THF 30:1) = 0.35. - R_f (DCM) = 0.6. - **^{1}H NMR** ($CDCl_3$, 300 MHz): δ = 1.94–2.07 (m, 12 H, -CH_2), 1.75 (s, 18 H, -CH_3), 1.52 (s, 18 H, -CH_3) ppm. - **^{1}H NMR** (CD_2Cl_2, 300 MHz): δ = 1.53 (s, 18 H, -CH_3), 1.78 (s, 18 H, -CH_3), 1.96–2.16 (m, 12 H, -CH_2) ppm. - **UV-Vis** (DCM): λ = 534 (s), 489 (sh), 334 (m), 303 (s) nm. - **Fluorescence** (DCM, λ_{ex} = 350 nm): λ = 546 nm. - Φ_F (λ_{ex} = 490 nm) = 0.19. - Φ_Δ = 0.88. - **MS** (APCI-HRMS(+)): *m/z* = 767.3964 $[M+H]^+$, cal. for $C_{42}H_{48}B_1Cl_1N_{12}+H_1$: 767.3980.

1.1.7 Synthesis of Azasubphthalocyanines N_x-[Spc*BCl]



A_2B; N_2-[Spc*BCl]
Bisazasubphthalocyanine



A_2B; N_4-[Spc*BCl]
Tetraazasubphthalocyanine

According to procedure described in 1.1.5 using PDN*/PyzDN* in a 1:1 ratio. After evaporation of the solvent, the solid residue was loaded onto silica and the crude product was purified via gradient CC (Tol → Tol/THF).

[Spc*BCl]: **Yield**: <1%. - The product was identified by using UV-Vis and MS. The analysis is in accordance to the one described in section 1.1.5.

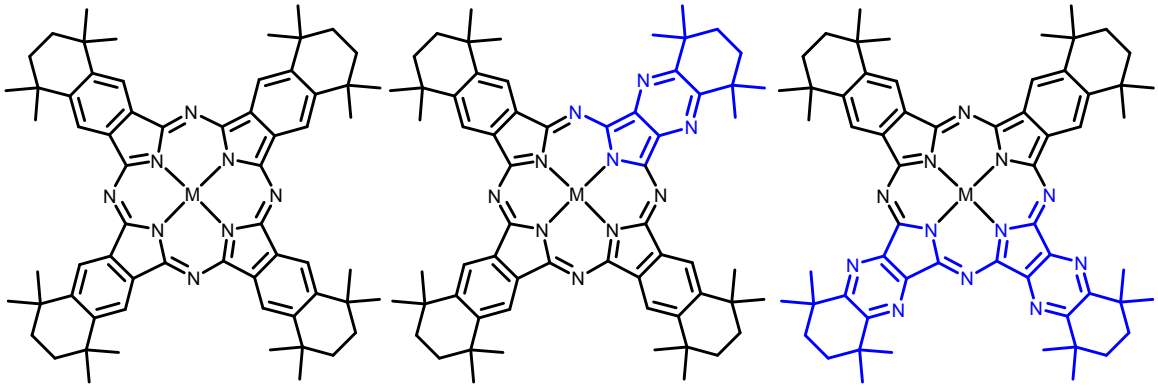
N_2-[Spc*BCl]: Yield: 8 mg, 10.5 μmol, 1%. - **^{1}H NMR** ($CDCl_3$, 300 MHz): δ = 8.87 (s, 2 H, Ar-C*H*), 8.78 (s, 2 H, Ar-C*H*), 1.77-1.55 (m, 12 H, -CH_2), 1.38 (s, 9 H, -CH_3), 1.35 (s, 9 H, -CH_3), 1.05 (s, 9 H, -CH_3), 1.03 (s, 9 H, -CH_3) ppm. - **UV-Vis** (DCM): λ = 572 (s), 519 (sh), 327 (m), 303 (s) nm. - **Fluorescence** (DCM, λ_{ex} = 350 nm): λ = 577 nm. - $\mathbf{\Phi_F}$ (λ_{ex} = 490 nm) = 0.24. - $\mathbf{\Phi_\Delta}$ = 0.67. - **MS** (APCI-HRMS(+)): *m/z* = 763.4162 $[M+H]^+$, cal. for $C_{46}H_{53}B_1Cl_1N_8+H_1$: 763.4177.

N_4-[Spc*BCl]: Yield: 12 mg, 15.7 μmol, 2%. - **^{1}H NMR** ($CDCl_3$, 300 MHz): δ = 8.78 (s, 2 H, Ar-C*H*), 1.66-1.51 (m, 12 H, -CH_2), 1.38 (s, 9 H, -CH_3), 1.38 (s, 9 H, -CH_3), 1.35 (s, 9 H, -CH_3), 1.35 (s, 9 H, -CH_3) ppm. - **UV-Vis** (DCM): λ = 557 (s), 506 (sh), 330 (s), 296 (s) nm. - **Fluorescence** (DCM, λ_{ex} = 350 nm): λ = 567 nm. - $\mathbf{\Phi_F}$ (λ_{ex} = 490 nm) = 0.22. - $\mathbf{\Phi_\Delta}$ = 0.65. - **MS** (APCI-HRMS(+)): *m/z* = 765.4069 $[M+H]^+$, cal. for $C_{44}H_{51}B_1Cl_1N_{10}+H_1$: 765.4082.

[Sppz*BCl]: **Yield**: <1%. - The analysis is in accordance to the one described in section 1.1.6.

Additional information: For the synthesis of N_x-[Spc*BCl], depending on the desired product, the corresponding ratios of dinitriles was varied. In the ^{1}H NMR spectra, dinitriles traces were observed.

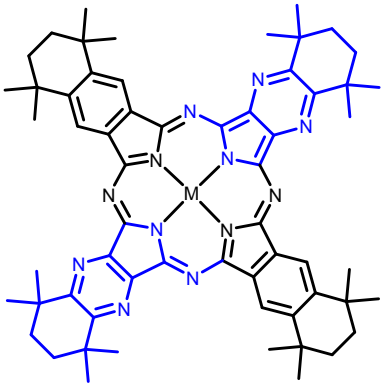
1.1.8 Synthesis of Asymmetrical Phthalocyanines: N_x-Pc^*H_2



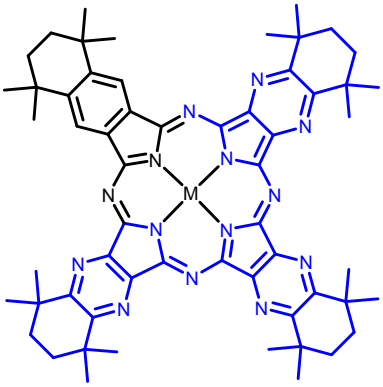
A_4; [Pc^*M]
with M = 2 H, Zn

A_3B; N_2-[Pc^*M]
with M = 2 H, Zn

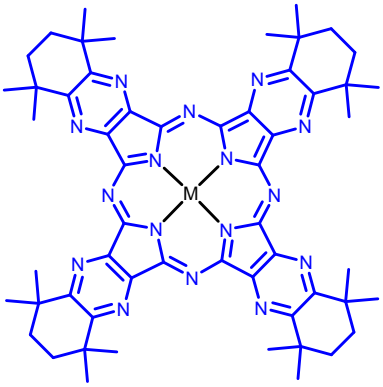
A_2B_2; N_4-[Pc^*M]
with M = 2 H, Zn



ABAB; N_4-[MPc*M]
with M = 2 H, Zn

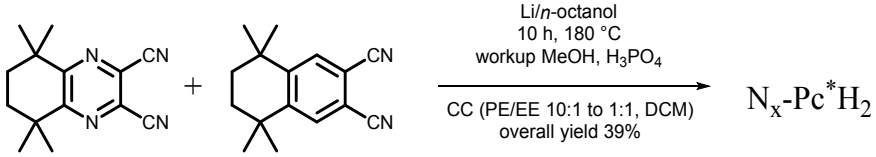


AB_3; N_6-[Pc^*M]
with M = 2 H, Zn



B_4; N_8-[Pc^*M] or [Ppz^*M]
M = 2 H, Zn

1.1.9 Synthesis of N_x-Pc^*H_2 [4]



$PyzDN^*$ PDN^*

According to the procedure described in the main paper, using $PyzDN^*$ **2**/PDN^* **1** in a 1:1 ratio. The solution turned dark green. The isomers were separated by CC (PE(40/60)/EE gradient). At first, Pc^*H_2 and N_2-Pc^*H_2 were eluted, then ABAB and the symmetrical A_2B_2 N_4-Pc^*H_2 were eluted. After changing the solvent to PE/EE 1:1 a mixture of A_2B_2 N_4-Pc^*H_2 and AB_3 N_6-Pc^*H_2 was eluted. Finally, Ppz^*H_2 was eluted with pure DCM. In a second CC (DCM), A_2B_2 N_4-Pc^*H_2 and AB_3 N_6-Pc^*H_2 were separated.

Pc^*H_2: **Yield:** 2%. - The analysis is in accordance with values in the main paper. - Φ_F (λ_{ex} = 350 nm) = 0.44; - (λ_{ex} = 598 nm) = 0.45. - Φ_Δ = 0.16.

N_2-Pc*H_2: **Yield**: 4%. - **^{1}H NMR** ($CDCl_3$, 300 MHz): δ = 9.69 (s, 2 H, Ar-C*H*), 9.65 (s, 2 H, Ar-C*H*), 9.42 (s, 2 H, Ar-C*H*), 2.19 (s, 4 H, -CH_2), 2.07 (s, 8 H, -CH_2), 2.04 (s, 4 H, -CH_2), 1.90 (s, 12 H, -CH_3), 1.83 (s, 12 H, -CH_3), 1.81 (s, 12 H, -CH_3), 1.81 (s, 12 H, -CH_3), -0.07 (s, 2 H, -N*H*) ppm. - **^{13}C NMR** (C_6D_6, 75 MHz): δ = 160.6, 149.8, 149.2, 148.6, 137.0, 133.0, 132.2, 122.2, 121.6, 39.1, 36.1, 36.1, 35.9, 35.4, 35.3, 34.7, 32.9, 32.8, 32.7, 30.9 ppm. - not all quartary atoms could be detected. - **IR** (ATR, 400-4000 cm^{-1}): $\tilde{\nu}$ = 3475 (vw), 3297 (vw), 2956 (m), 2921 (m), 2855 (m), 2555 (vw), 2348 (vw), 1711 (m), 1688 (m), 1621 (m), 1539 (m), 1498 (s), 1460 (m), 1382 (m), 1358 (m), 1328 (m), 1301 (s), 1258 (m), 1242 (m), 1188 (m), 1159 (m), 1140 (m), 1119 (m), 1089 (m), 1071 (m), 1022 (s), 999 (m), 980 (m), 891 (m), 848 (m), 804 (m), 755 (s), 722 (m), 681 (s), 622 (m), 541 (m) cm^{-1}. - **CV** (DCM, [TBA]PF_6, Fc): E_{ox1} = 0.43, E_{red1} = -1.23, E_{red2} = -1.65 V. - **UV-Vis** (DCM): λ = 687 (s), 619 (sh), 340 (s), 306 (s), 232 (s) nm. - **Φ_F** (λ_{ex} = 350 nm) = 0.31; - (λ_{ex} = 598 nm) = 0.33. - **Φ_Δ** = 0.14. - **MS** (APCI-HRMS(+)): *m/z* = 957.5992 $[M+H]^+$, cal. for $C_{62}H_{72}N_{10}+H_1$: 957.6014. - **Elemental analysis** ($C_{62}H_{72}N_{10}$, M = 957.30 g/mol): fnd. (cal.): C: 75.29% (77.79%), H: 8.92% (7.58%), N: 10.14% (14.63%).

A_2B_2 N_4-Pc*H_2: **Yield**: 17%. - **^{1}H NMR** ($CDCl_3$, 300 MHz): δ = 9.56 (s, 2 H, Ar-C*H*), 9.50 (s, 2 H, Ar-C*H*), 2.20 (s, 8 H, -CH_2), 2.05 (s, 8 H, -CH_2), 1.91 (s, 24 H, -CH_3), 1.81 (s, 12 H,
-CH_3), 1.80 (s, 12 H, -CH_3), -0.04 (s, 2 H, -N*H*) ppm. - **^{1}H NMR** (Pyridine-d_5, 300 MHz): δ = 9.87 (s, 2 H, Ar-C*H*), 9.68 (s, 2 H, Ar-C*H*), 1.94 (s, 8 H, -CH_2), 1.76 (s, 8 H, -CH_2), 1.72 (s, 12 H, -CH_3), 1.67 (s, 12 H, -CH_3), 1.46 (s, 12 H, -CH_3), 1.37 (s, 12 H, -CH_3), -0.26 (s, 2 H, -N*H*) ppm. - **^{1}H NMR** (C_6D_6, 300 MHz): δ = 9.83 (s, 2 H, Ar-C*H*), 9.82 (s, 2 H, Ar-C*H*), 1.86 (s, 8 H, -CH_2), 1.79 (s, 8 H, -CH_2), 1.75 (s, 24 H, -CH_3), 1.48 (s, 12 H, -CH_3), 1.38 (s, 12 H, -CH_3), -0.31 (s, 2 H, -N*H*) ppm. - **^{13}C NMR** (C_6D_6, 75 MHz): δ = 162.4, 150.0, 149.6, 145.1, 144.4, 135.2, 134.8, 122.7, 122.0, 39.4, 39.3, 36.1, 36.0, 35.2, 34.6, 34.5, 32.7, 32.7, 21.1, 30.8 ppm. - **IR** (ATR, 400-4000 cm^{-1}): $\tilde{\nu}$ = 3526 (w), 3284 (w), 2915 (s), 2857 (s), 1736 (w), 1638 (w), 1553 (w), 1496 (w), 1455 (s), 1381 (w), 1358 (m), 1328 (m), 1300 (s), 1254 (m), 1242 (m), 1190 (m), 1162 (m), 1148 (m), 1128 (m), 1083 (w), 1048 (w), 1019 (s), 1001 (s), 983 (s), 949 (w), 936 (w), 893 (m), 851 (m), 828 (m),761 (s), 752 (s),717 (m), 700 (m), 679 (m), 623 (w), 560 (w), 543 (m), 507 (m), 443 (w), 429 (w) cm^{-1}. - **CV** (DCM, [TBA]PF_6, Fc): E_{ox1} = 0.28, E_{red1} = -1.47, E_{red2} = -1.79 V. - **UV-Vis** (DCM): λ = 680 (s), 656 (s), 625 (sh), 348 (s), 232 (s) nm. - **Φ_F** (λ_{ex} = 350 nm) = 0.13; - (λ_{ex} = 598 nm) = 0.14. - **Φ_Δ** = 0.07. - **MS** (APCI-HRMS(+)): *m/z* = 959.5921 $[M+H]^+$, cal. for $C_{60}H_{70}N_{12}+H_1$: 959.5919. - **Elemental**

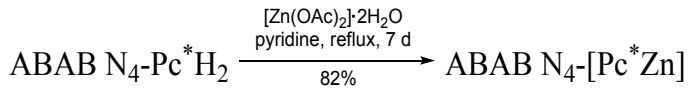
analysis ($C_{60}H_{70}N_{12}$, M = 959.28 g/mol): fnd. (cal.): C: 72.03% (75.12%), H: 7.36% (7.36%), N: 16.36% (17.52%).

N_6-Pc*H_2: **Yield**: 9%. - **^{1}H NMR** ($CDCl_3$, 300 MHz): δ = 9.75 (s, 2 H, Ar-C*H*), 2.22 (s, 4 H, -CH_2), 2.19 (s, 12 H, -CH_2), 1.93 (s, 12 H, -CH_3), 1.91 (s, 12 H, -CH_3), 1.90 (s, 12 H, -CH_3), 1.83 (s, 12 H, -CH_3), -0.53 (s, 2 H, -N*H*) ppm. - **^{13}C NMR** (C_6D_6, 75 MHz): δ = 162.0, 139.1, 131.3 134.1 (w), 132.9 (w), 132.9 (w), 131.3 (w), 127.1 (w), 123.1, 46.0, 41.3 (w), 39.7, 39.3, 36.3, 34.5, 32.8, 31.8, 31.7, 31.1, 30.9, 30.8, 29.8, 29.5, 29.3, 29.2, 28.6, 28.1, 27.5, 27.5 ppm. - 6 weak signal, marked with (w); not all quartary atoms could be detected. - **IR** (ATR, 400-4000 cm^{-1}): $\tilde{\nu}$ = 3291 (w), 2957 (s), 2924 (s), 2856 (s), 1727 (s), 1693 (s), 1637 (m), 1540 (m), 1503 (m), 1457 (s), 1411 (m), 1381 (m), 1360 (m), 1330 (m), 1305 (m), 1281 (m), 1257 (s), 1192 (s), 1157 (w), 1139 (m), 1127 (s), 1086 (m), 1072 (m), 1021 (s), 995 (s), 952 (m), 935 (w), 893 (w), 852 (m), 828 (m), 804 (m), 756 (m), 744 (s), 719 (s), 700 (w), 677 (s), 631 (m), 542 (w), 506 (w), 466 (w), 429 (w) cm^{-1}. - **CV** (DCM, [TBA]PF_6, Fc): E_{ox1} = 0.35, E_{red1} = -1.47, E_{red2} = -1.82 V. - **UV-Vis** (DCM): λ = 660 (s), 597 (sh), 343 (s), 234 (s) nm. - **Φ_F** (λ_{ex} = 350 nm) = 0.05; - (λ_{ex} = 598 nm) = 0.03. - **Φ_Δ** = 0.04. - **MS** (APCI-HRMS(+)): *m/z* = 961.5825 $[M+H]^+$, cal. for $C_{58}H_{68}N_{14}+H_1$: 961.5824. - **Elemental analysis** ($C_{58}H_{68}N_{14}$, M = 961.25 g/mol): fnd. (cal.): C: 71.99% (72.47%), H: 9.49% (7.13%), N: 12.38% (20.40%).

Ppz*H_2: **Yield:** 9%. - The analysis is in accordance with values in the main paper. - **Φ_F** (λ_{ex} = 350 nm) = 0.03; - (λ_{ex} = 598 nm) = 0.03. - **Φ_Δ** = 0.05.

N_x-Pc*H_2 in DCM

1.1.10 Synthesis of N_4-[Pc*Zn] using [$Zn(OAc)_2$]



General Procedure for the Synthesis of N_x-[Pc*Zn] using [$Zn(OAc)_2$]:

1 eq ABAB or A_2B_2 N_4-Pc*H_2 was dissolved in pyridine and 1.2 eq [$Zn(OAc)_2$]·$2H_2O$ were added. After refluxing for 1 h, the reaction was monitored by TLC (DCM), and was stirred for another 1 h. The resulting blue solutions were concentrated in vacuum, filtered, and washed with an excess of water. After washing the product off the filter paper using $CHCl_3$/MeOH 3:1, the blue product was dried in vacuum and purified by preparative TLC or CC (Tol/THF 20:1).

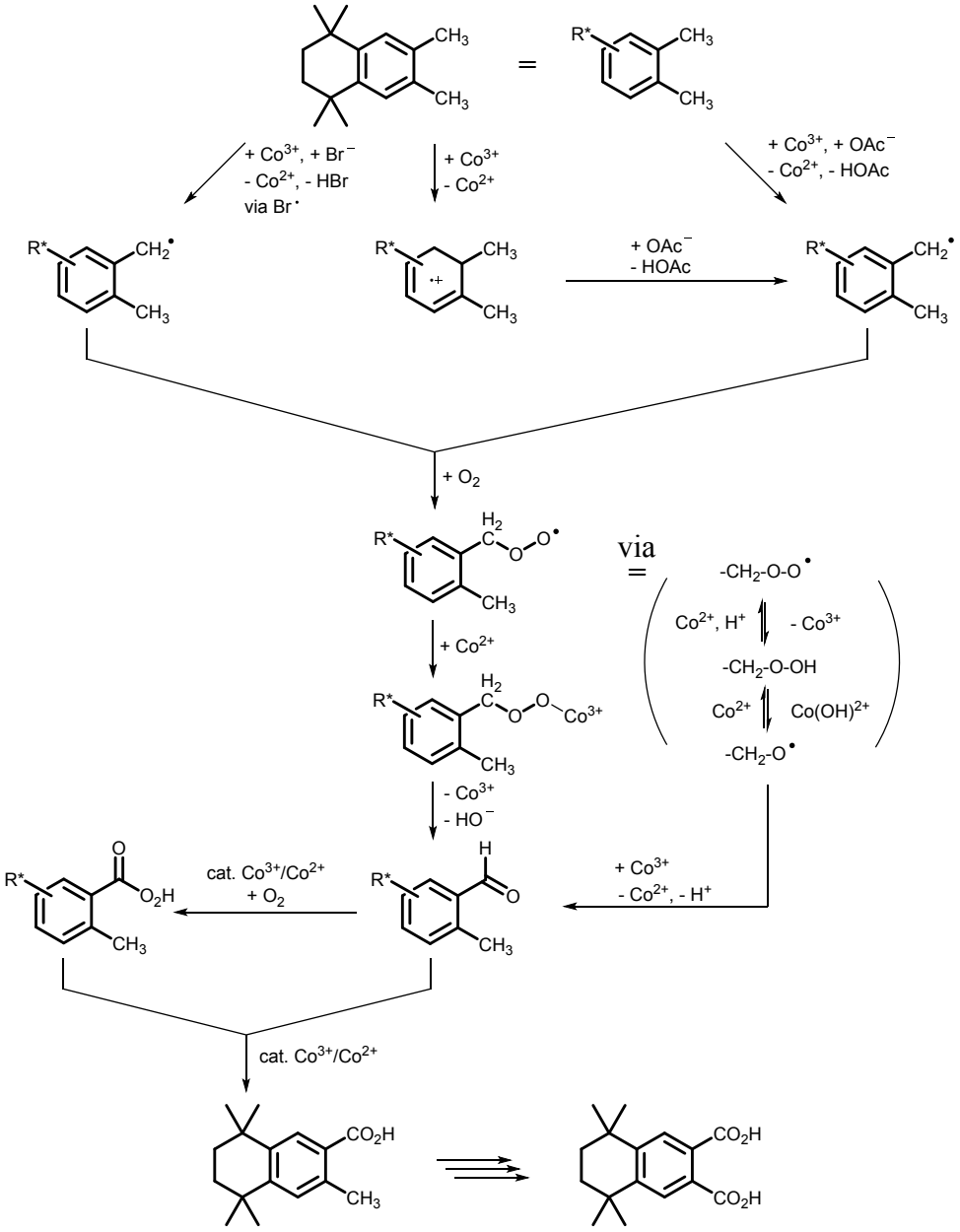
ABAB N_4-[Pc*Zn]: **Yield**: 82%. - R_f (Tol/THF 20:1) = 0.63. - **^{1}H NMR** (C_6D_6, 300 MHz): δ = 9.96 (s, 4 H, Ar-C*H*), 1.91 (s, 8 H, -CH_2), 1.85 (s, 24 H, -CH_3), 1.78 (s, 8 H, -CH_2), 1.45 (s, 24 H, -CH_3) ppm. - **UV-Vis** (DCM): λ = 687 (s), 657 (s), 631 (sh), 596 (sh), 357 (s) nm. - Φ_F (λ_{ex} = 350 nm) = 0.16; - (λ_{ex} = 598 nm) = 0.18. - Φ_Δ = 0.73. - **MS** (APCI-HRMS(+)): *m/z* = 1021.5073 $[M+H]^+$, cal. for $C_{60}H_{68}N_{12}Zn_1+H_1$: 1021.5054.

A_2B_2 N_4-[Pc*Zn]: **Yield**: 76%. - The analysis is in accordance with the data described above.

All other N_x-[Pc*Zn] are described in the Paper.

1.2 Suggested Radical Autoxidation Mechanism of Tetraline

In literature, such Co(III) or Mn(III) assisted aerobic oxidations are discussed as radical chain reactions. Rate determining step is the selective benzylic C-H activation, H abstraction by Co(III)-coordinated acetate (quasi acetyl radical ligands) or by bromine radicals generated in the presence of bromide promotor. Instead of H atom abstraction, a sequence of electron transfer followed by deprotonation of the formed radical cation is discussed. The benzylic radicals Ar-CH_2· are trapped by oxygen, the peroxy radical is reduced by Co(II). Hock cleavage leads to a carbaldehyde, which undergoes further metal catalysed autoxidation steps to the carbonic acid:



1.3 Absorbance and Emission Spectra

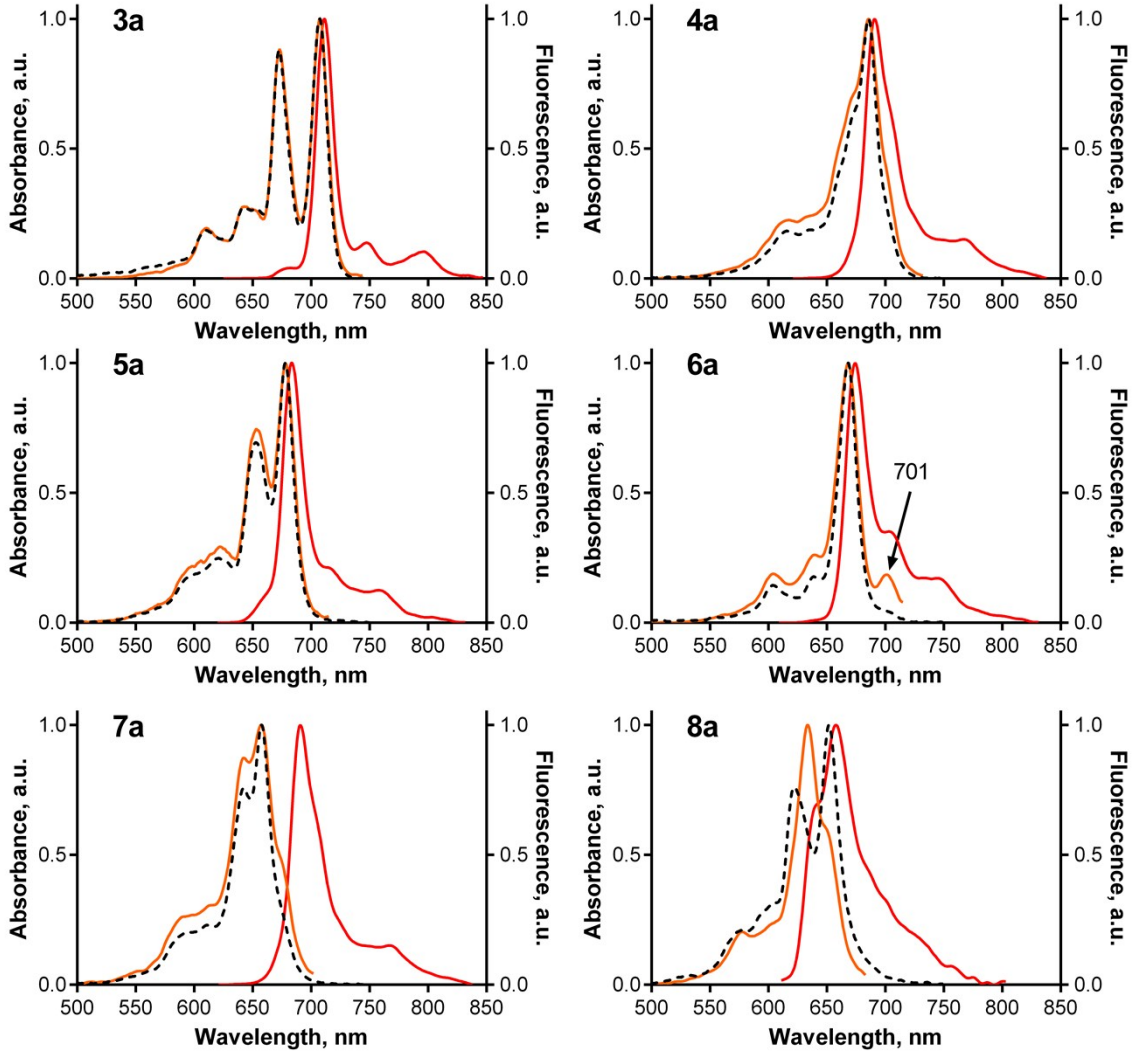


Figure SI-1. Normalized absorption (black, dashed), emission (red) and excitation (orange) spectra of N_x-Pc*H_2 in THF.

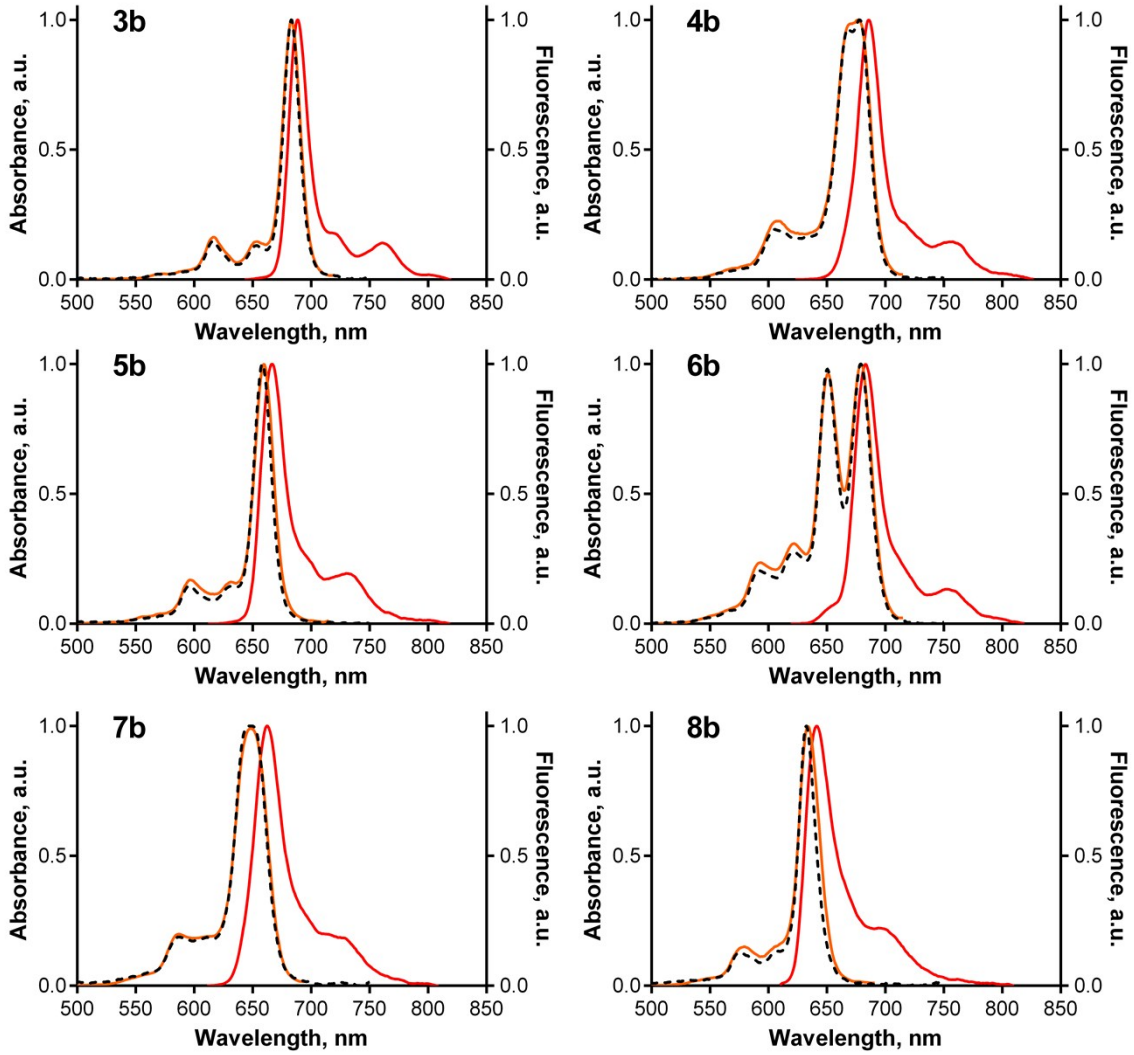


Figure SI-2. Normalized absorption (black, dashed), emission (red) and excitation (orange) spectra of N_x-Pc*Zn in THF.

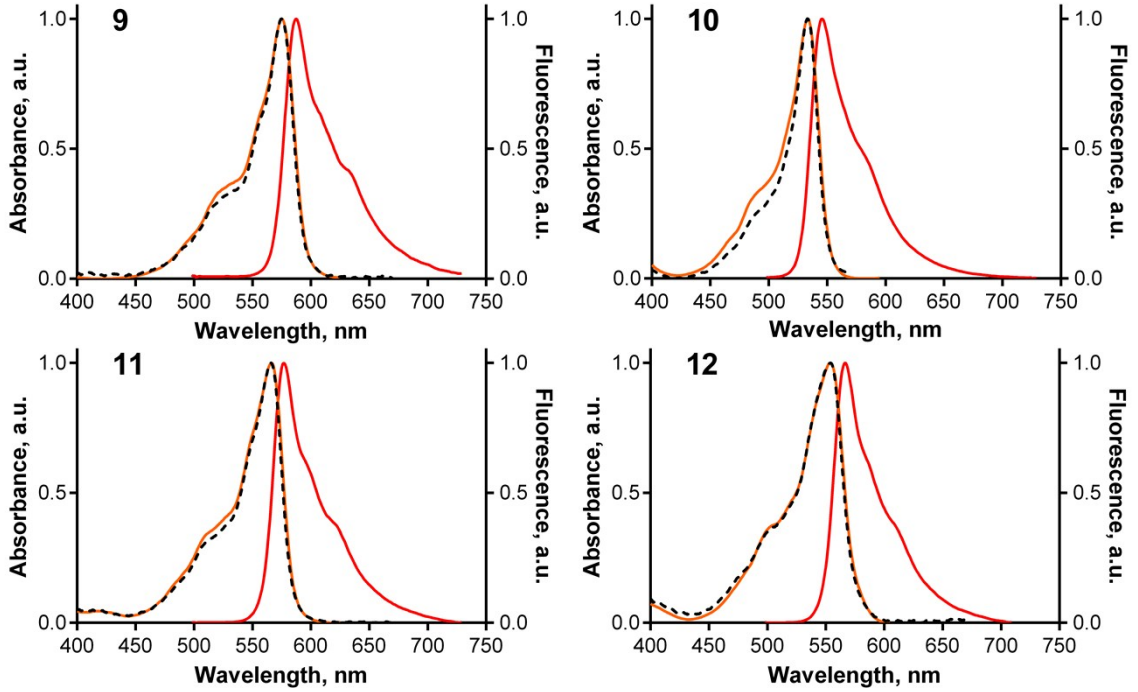


Figure SI-3. Bottom: Normalized absorption (black, dashed), emission (red) and excitation (orange) spectra of N_x-Spc*BCl in MeOH. Top: Cuvettes of a [PpzZn] (left) in THF and N_x-[Spc*BCl] in MeOH, with increasing number of [-N=] in N_x-[Spc*BCl] from x = 0, 2, 4, to 6 (left to right). Samples are illuminated with light at λ = 365 nm.

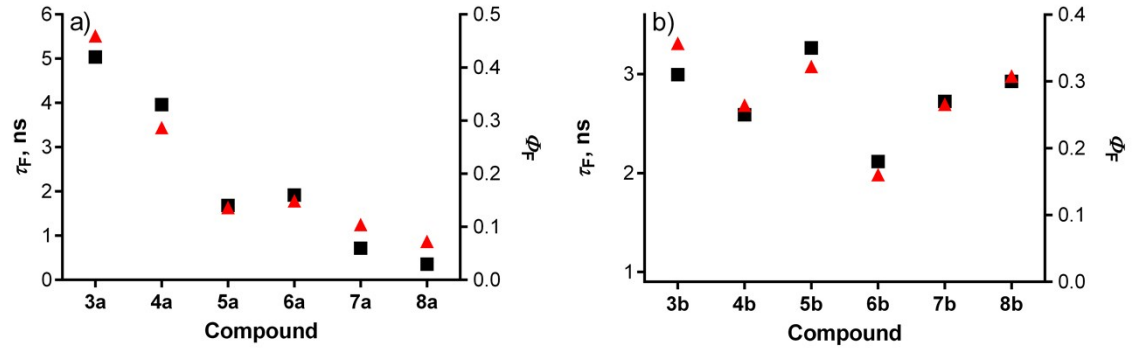


Figure SI-4. Correlation between Φ_F (black squares) and τ_F (red triangles) values for N_x-Pc*H_2 in THF (a) and N_x-Pc*Zn in THF (b). For purposes of this presentation, the relative contribution of each process to the average lifetime for compounds with two lifetime components (**7a** and **8a**) was calculated.

1.4 Computational Studies

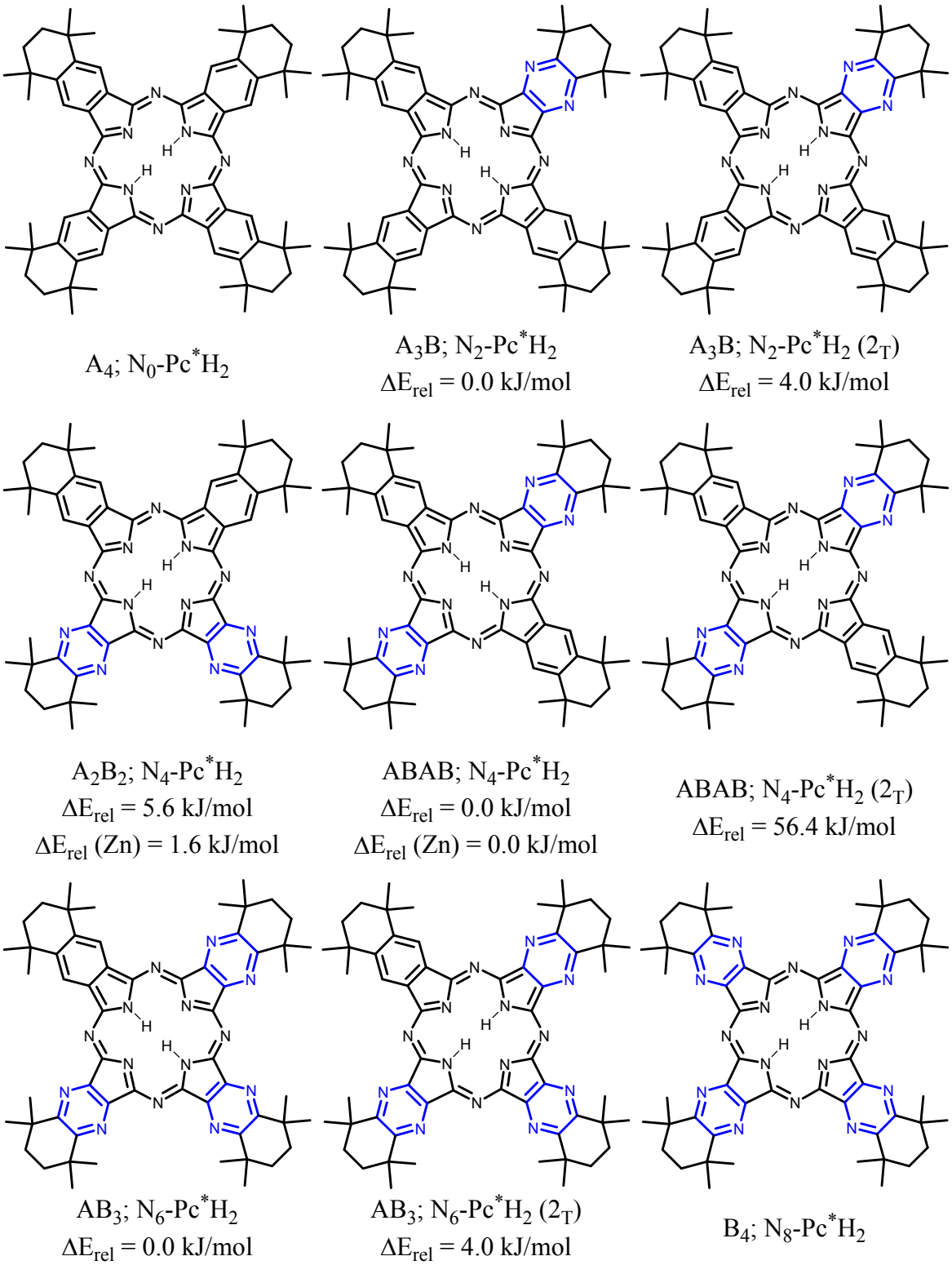


Figure SI-5. Overview of the phthalocyanines N_x-Pc*H_2 computationally investigated. Regioisomers are numbered and tautomers marked (subscript T). Energies are given relative to the most stable isomer (ΔE_{rel}). Zn-substituted phthalocyanines [Pc*Zn] are derived by substituting the two central H atoms by Zn. Relative isomer energies are given as ΔE_{rel}(Zn), no tautomers are found for [Pc*Zn].

Table SI-1. Computed excitation energies (□□in nm), oscillator strengths (*f*), frontier orbital gaps (□$_{H\text{-}L/L+1}$ in nm) and molecular orbital character of the transitions for the Q-bands. Dipole moment (□) and isotropic polarizability (□) in a.u.[a]

Molecule	λ / nm	$\Delta\lambda$ / nm	f	*Character*[b]	$\Delta_{H\text{-}L/L+1}$ [c]	μ [d]	$\Delta\alpha$ [e]
N_8-Pc*H_2	541	0	0.42	H → L+1	781	0.00	0.0
	536	0	0.53	H → L	818		
N_6-Pc*H_2	550	9	0.56	H → L	861	0.87	23.6
	549	13	0.49	H → L+1	797		
N_6-Pc*H_2 (2_T)	559	18	0.47	H → L+1	839	0.92	26.6
	552	16	0.60	H → L	848		
N_4-Pc*H_2 (A_2B_2)	563	22	0.55	H → L+1 (39%)	845	1.25	28.3
				H → L (27%)			
				H → L (41%)			
	559	23	0.63	H → L+1 (18%)			
				H-2 → L+1 (15%)			
N_4-Pc*H_2 (ABAB)	561	20	0.62	H → L	910	0.00	47.8
	560	24	0.55	H → L+1	815		
N_4-Pc*H_2 (ABAB, 2_T)	583	42	0.56	H → L+1	892	0.06	61.8
	580	44	0.54	H → L	911		
N_2-Pc*H_2	569	28	0.62	H → L+1	855	0.90	71.1
	564	28	0.72	H → L	915		
N_2-Pc*H_2 (2_T)	577	36	0.61	H → L+1	897	0.87	73.3
	571	35	0.69	H → L	900		
N_0-Pc*H_2	580	39	0.69	H → L+1	903	0.00	94.9
	568	32	0.81	H → L	923		
N_8-[Pc*Zn]	532	0	0.51	H → L	788	0.00	0.0
	532	0	0.51	H → L+1	788		
N_6-[Pc*Zn]	549	17	0.55	H → L	840	0.89	24.6
	544	12	0.59	H → L+1	810		
N_4-[Pc*Zn] (A_2B_2)	556	26	0.62	H → L	852	1.25	47.6
	554	22	0.63	H → L+1	848		
N_4-[Pc*Zn] (ABAB)	565	33	0.60	H → L	898	0.00	49.5
	557	26	0.63	H → L+1	831		
N_2-[Pc*Zn]	566	34	0.69	H → L	897	0.88	71.1
	564	32	0.69	H → L+1	863		
N_0-[Pc*Zn]	570	38	0.77	H → L	902	0.00	93.7
	570	38	0.77	H → L+1	901		

[a] Shift relative to Q1/Q2 band of N_8-Pc*H_2. [b] dominant MO transitions for the Q-bands (H: HOMO, H-2: HOMO-2, L: LUMO, L+1: LUMO+1). For N_4-Pc*H_2, relative contributions are given in percent. [c] Frontier MO gap of the orbitals given in the "character" column HOMO/LUMO and HOMO/LUMO+1 in nm. [d] All compounds exhibit an in-plane dipole moment only pointing toward the nitrogen-rich parts of the molecule. [e] Polarizabilities are given relative to B_4H_2 (α = 1091.3 a.u.) and B_4Zn (α = 1097.1 a.u.), respectively.

1.5 ^{1}H NMR Spectra

1.5.1 Subphthalocyanines

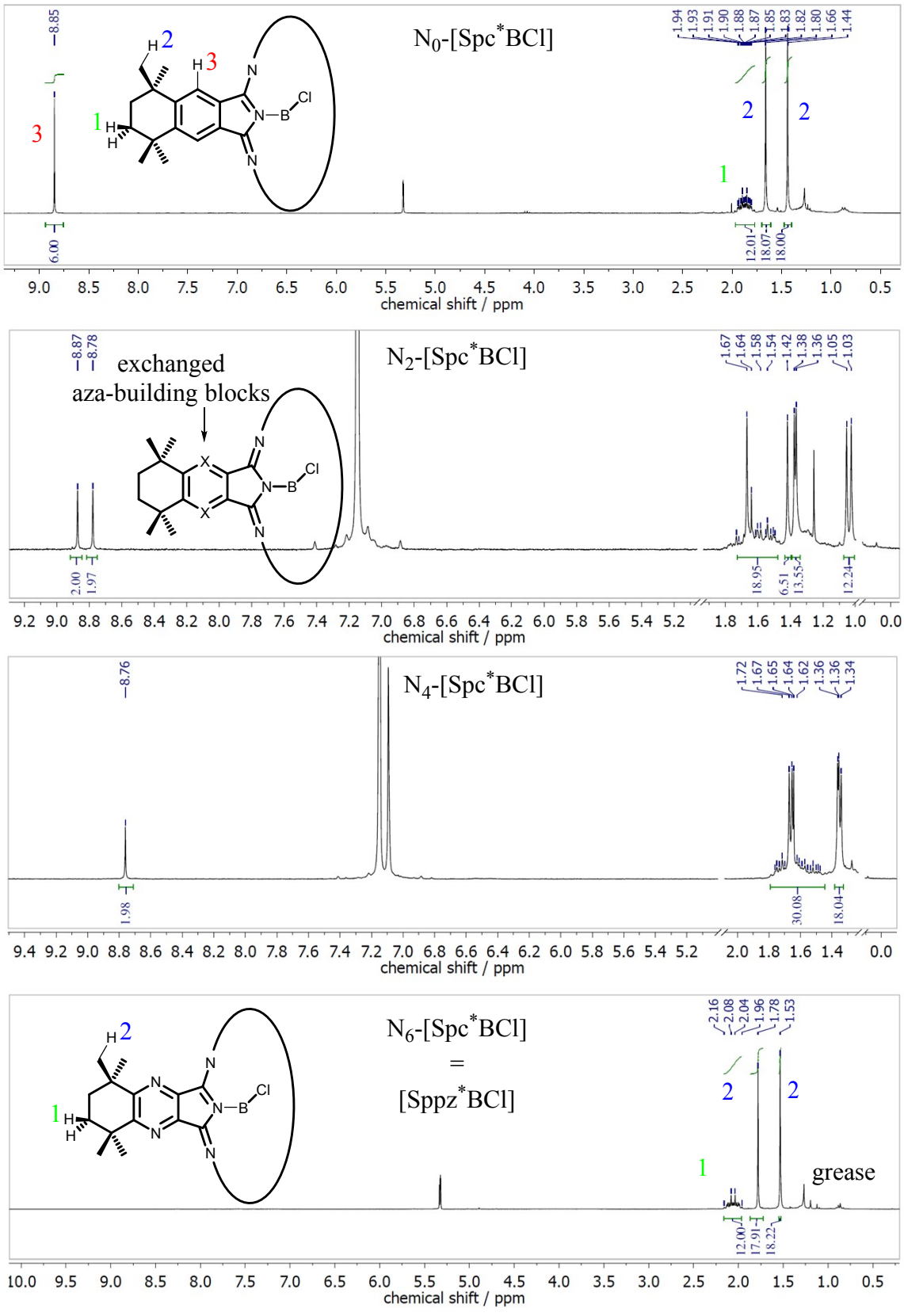
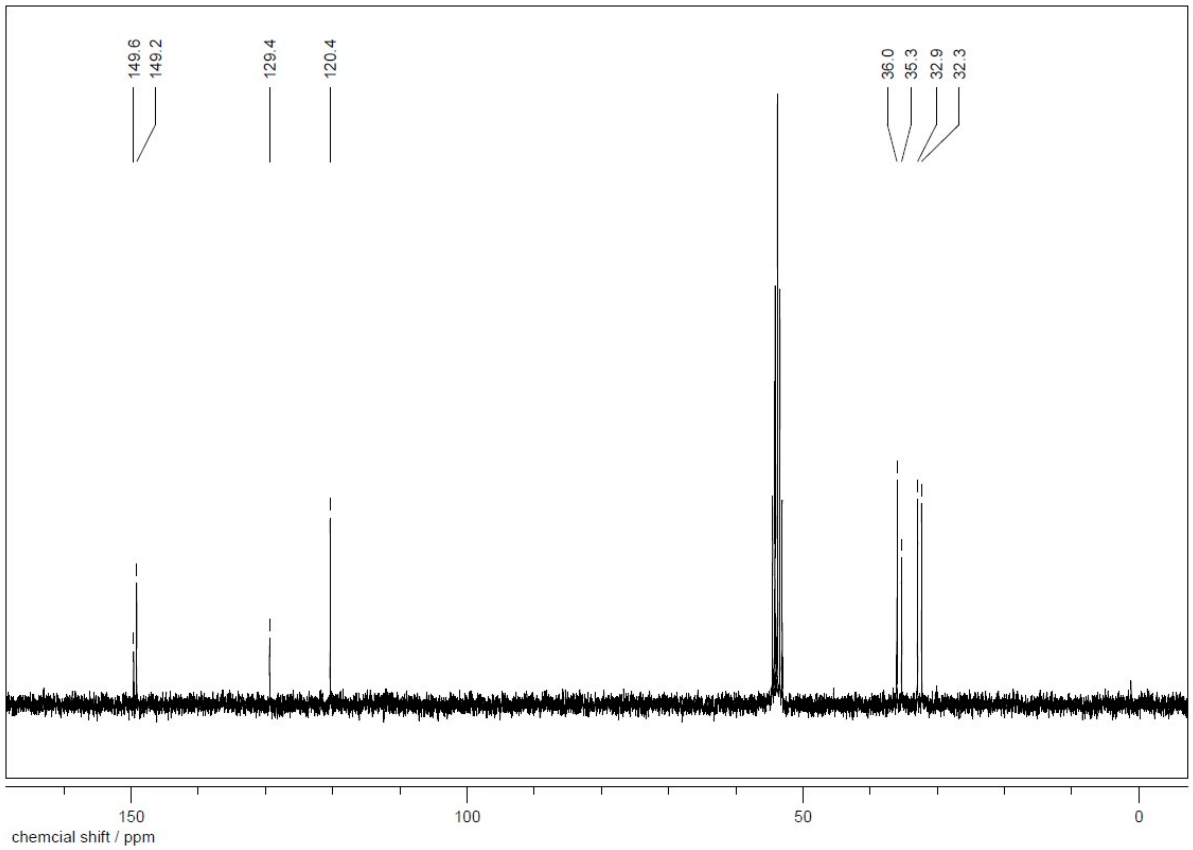


Figure SI-6. ^{1}H NMR spectrum of N_x-[Spc*BCl] in DCM-d_2, 300 MHz, or C_6D_6, respectively, with increasing number of x = N.

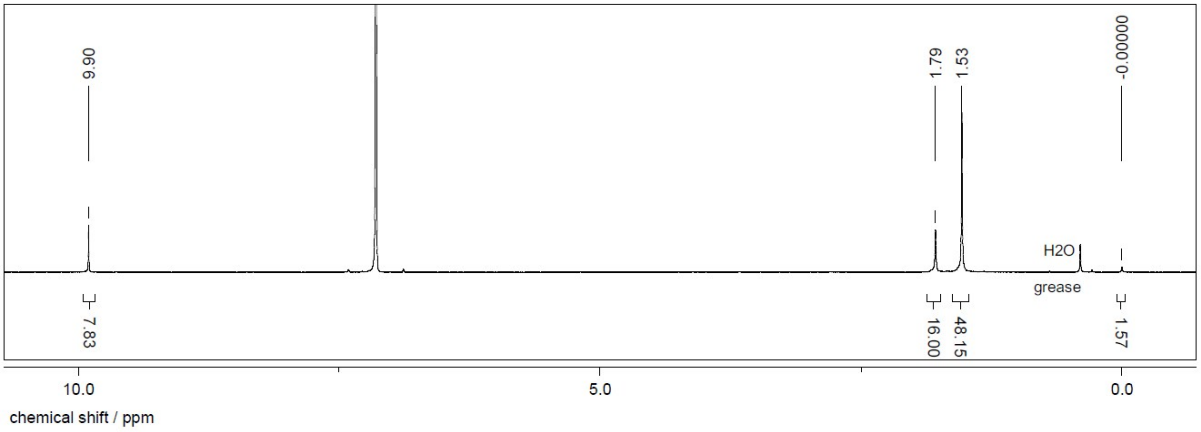
^{13}C NMR N_0-[Spc*BCl]



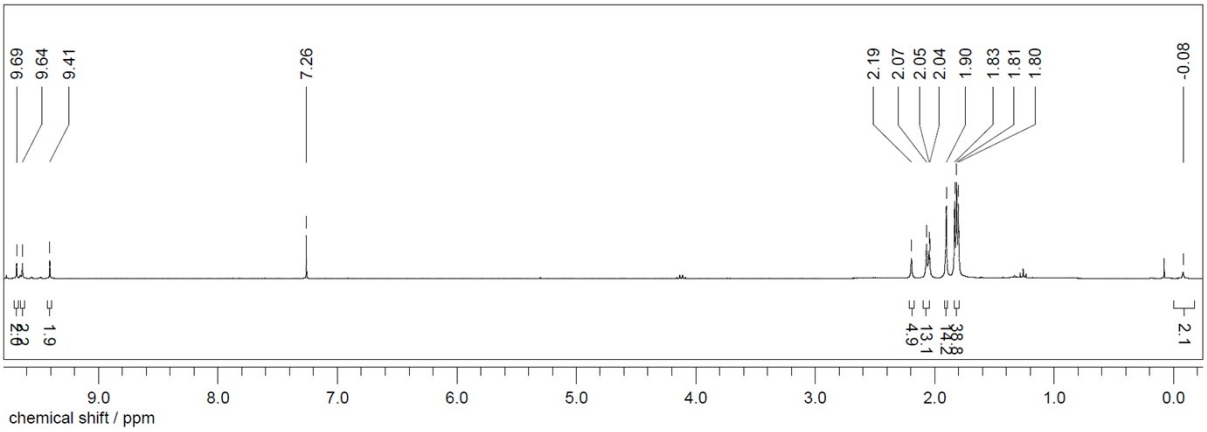
Because of the decreasing stability and solubility no ^{13}C NMR spectra in sufficient purity could be obtained of the other N_x-[Spc*BCl].

1.5.2 **Azaphthalocyanines**

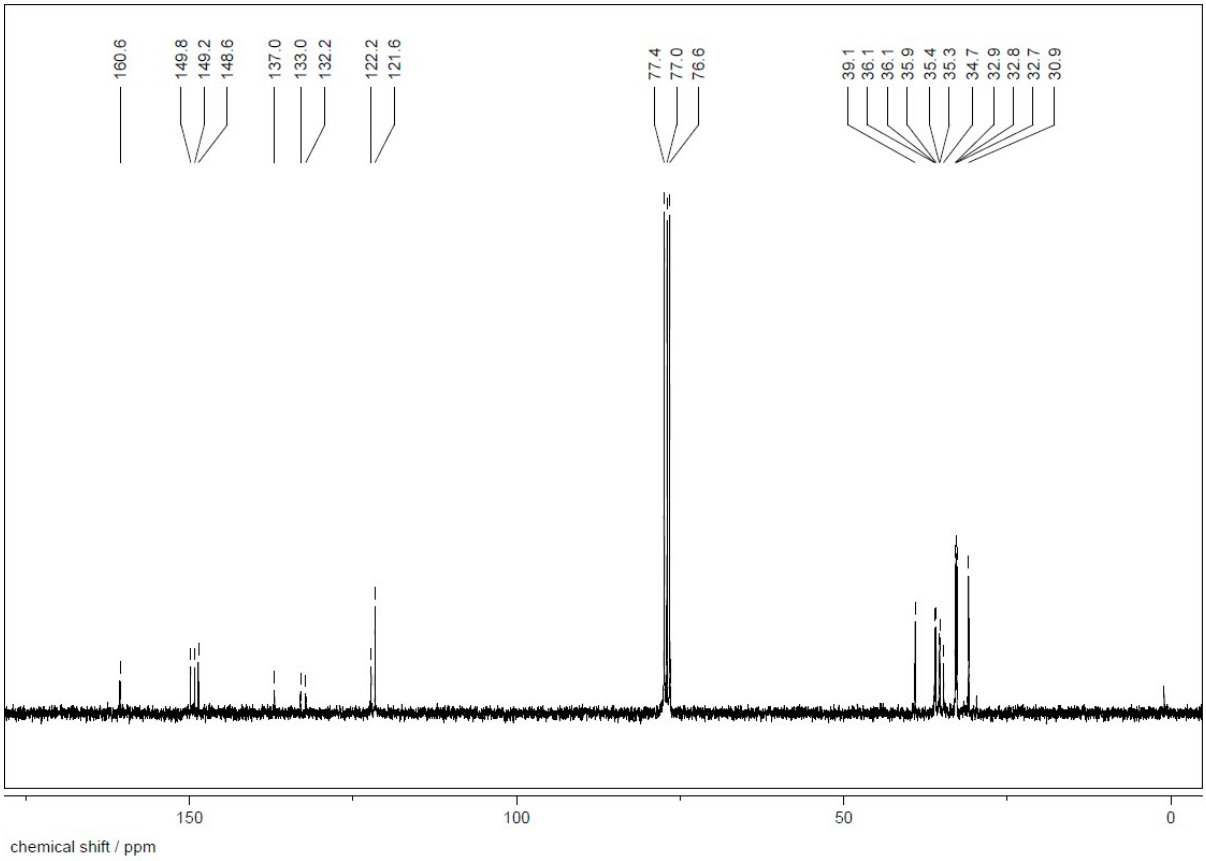
N_0-Pc*H_2 [3-5]



^{1}H NMR N_2-Pc*H_2



^{13}C NMR N_2-Pc*H_2



N_4-Pc*H_2

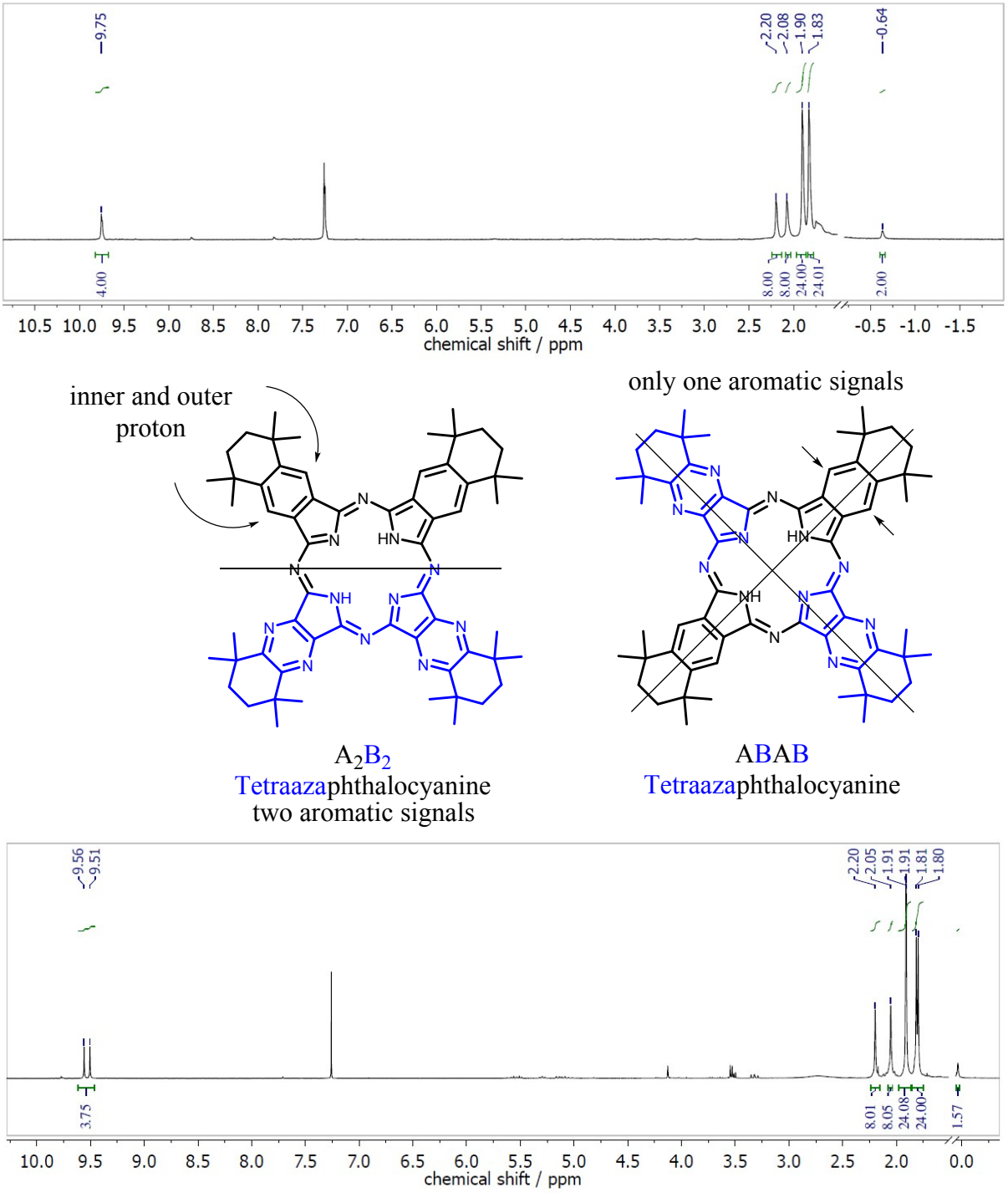
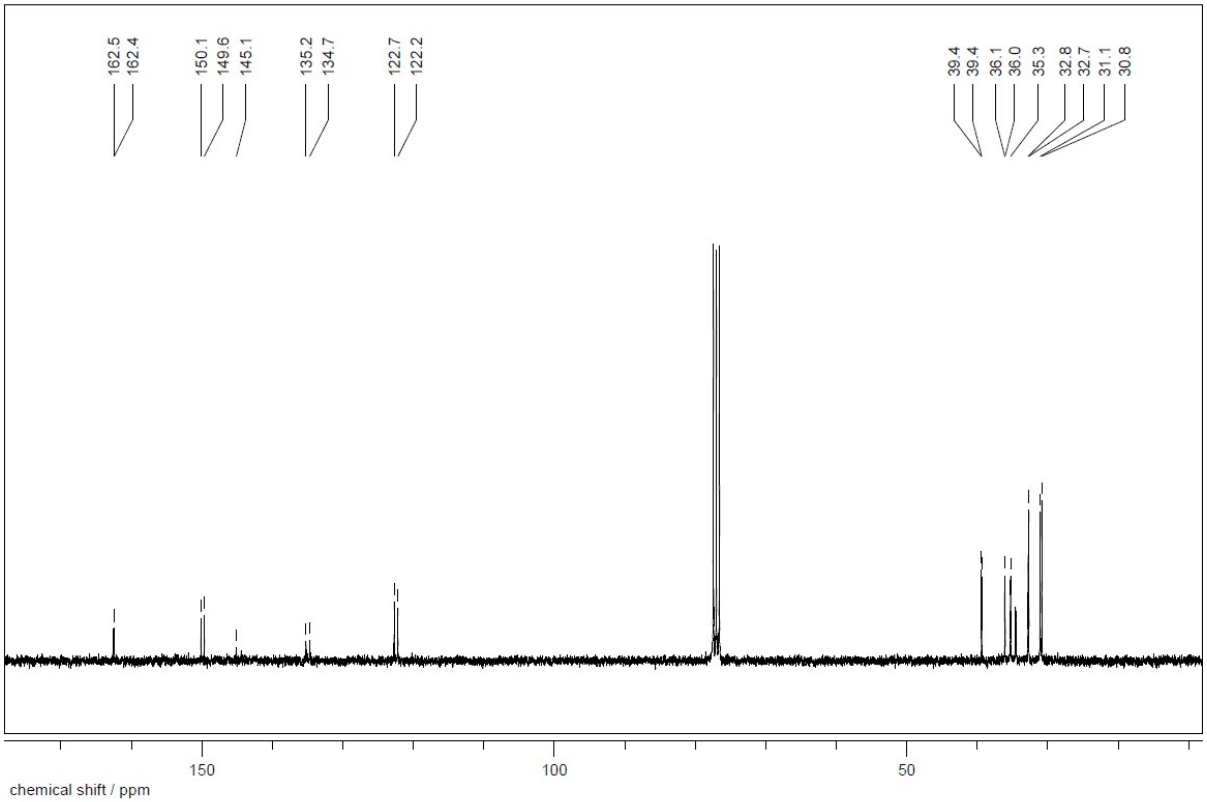


Figure SI-7b. ^{1}H NMR spectrum of ABAB (above) / A_2B_2 (below) N_4-Pc*H_2 in $CDCl_3$, 300 MHz.

^{13}C NMR A_2B_2 N_4-Pc*H_2



^{13}C NMR ABAB N_4-Pc*H_2

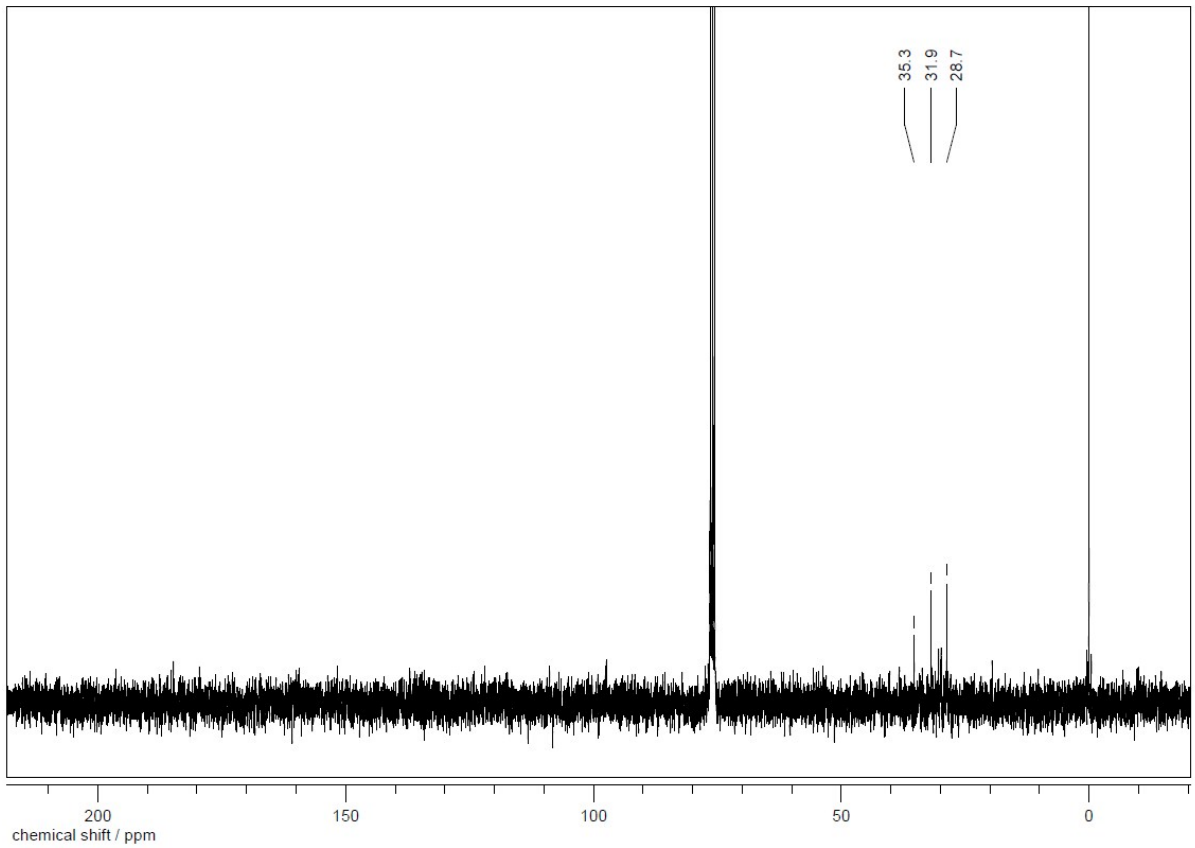
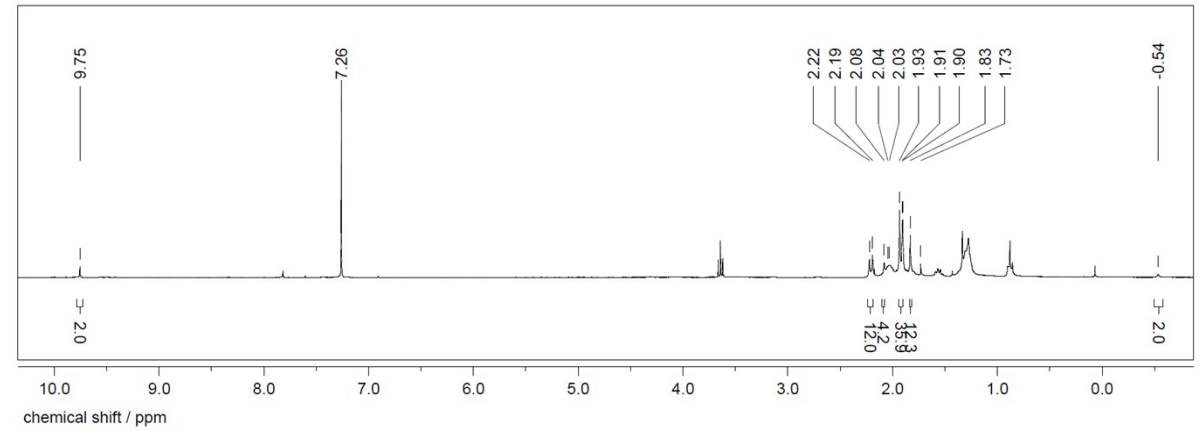
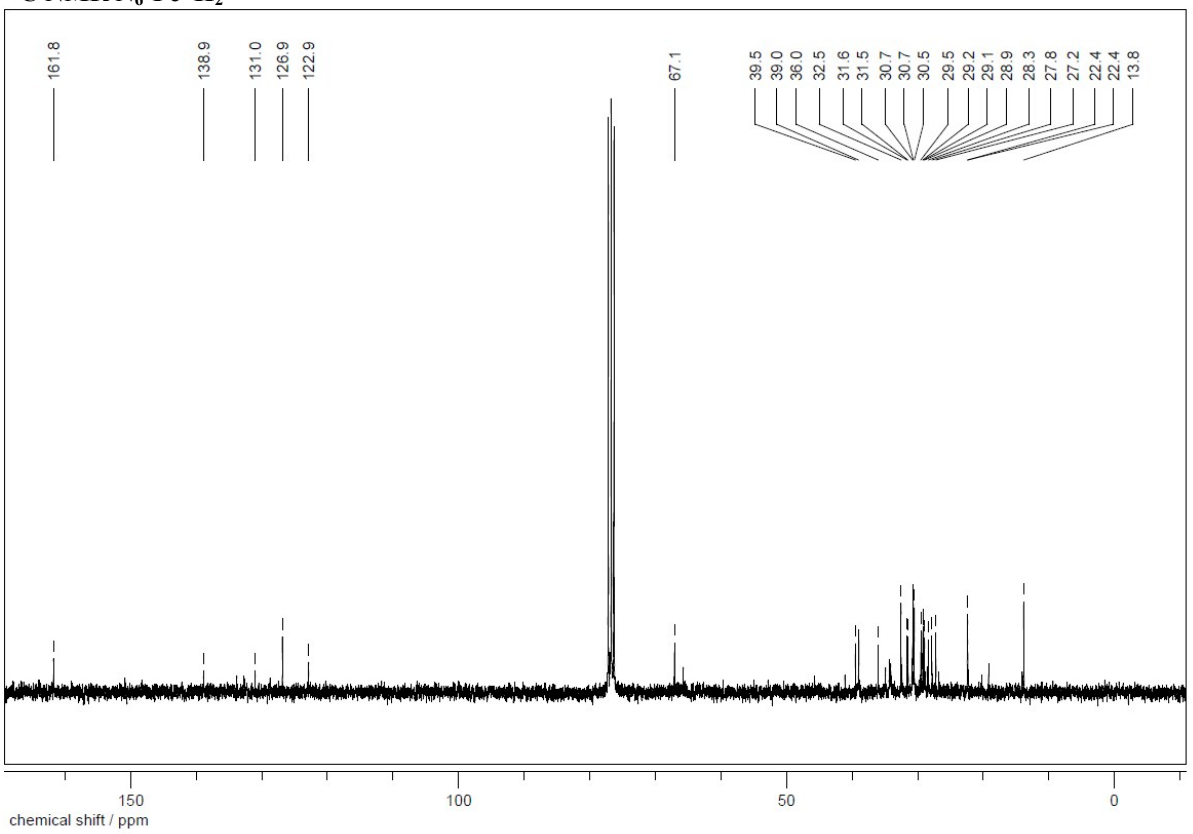


Figure SI-7c. ^{13}C NMR spectra of ABAB (above) / A_2B_2 (below) N_4-Pc*H_2 in $CDCl_3$, 75 MHz.

N_6-Pc*H_2



^{13}C NMR N_6-Pc*H_2



N_8-Pc*H_2 or Ppz*H_2 [3-5]

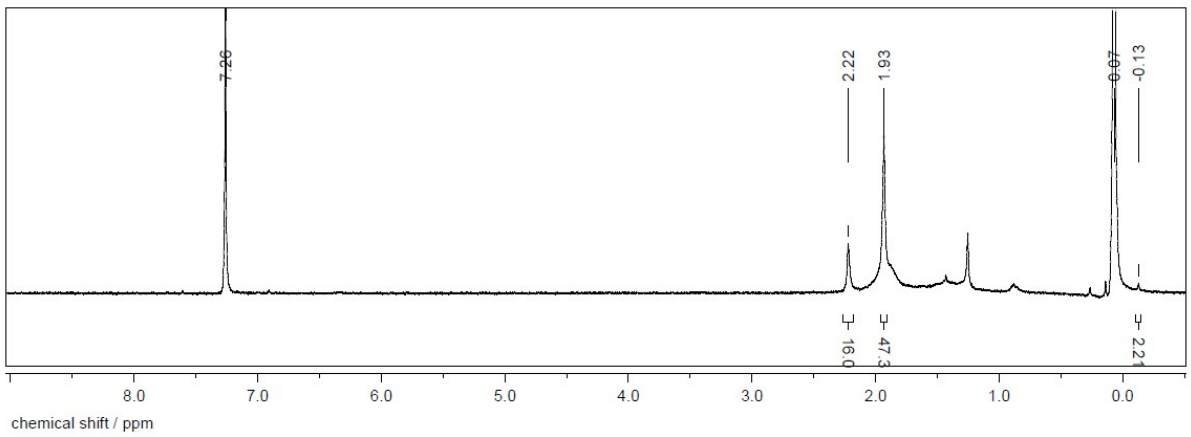
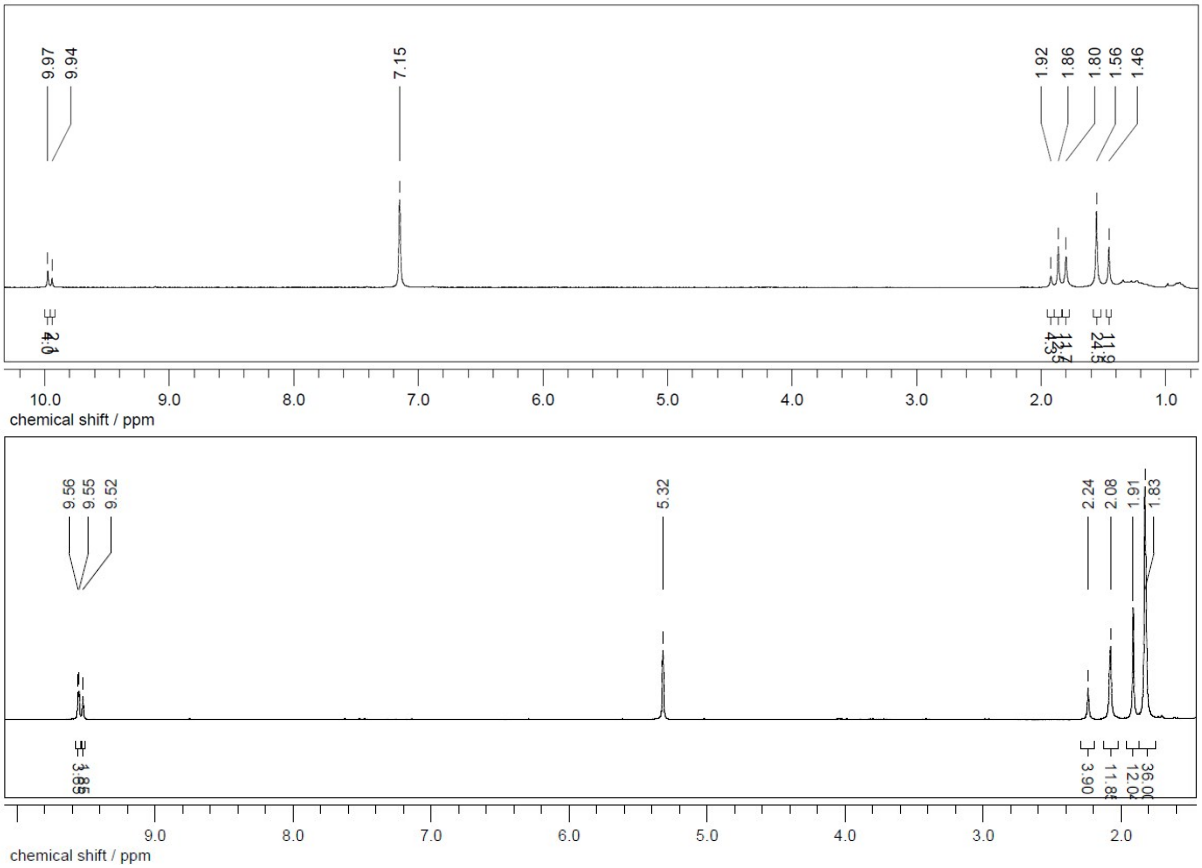


Figure SI-7a. ^{1}H/^{13}C NMR spectrum of N_x-Pc*H_2 in $CDCl_3$, 300 MHz.

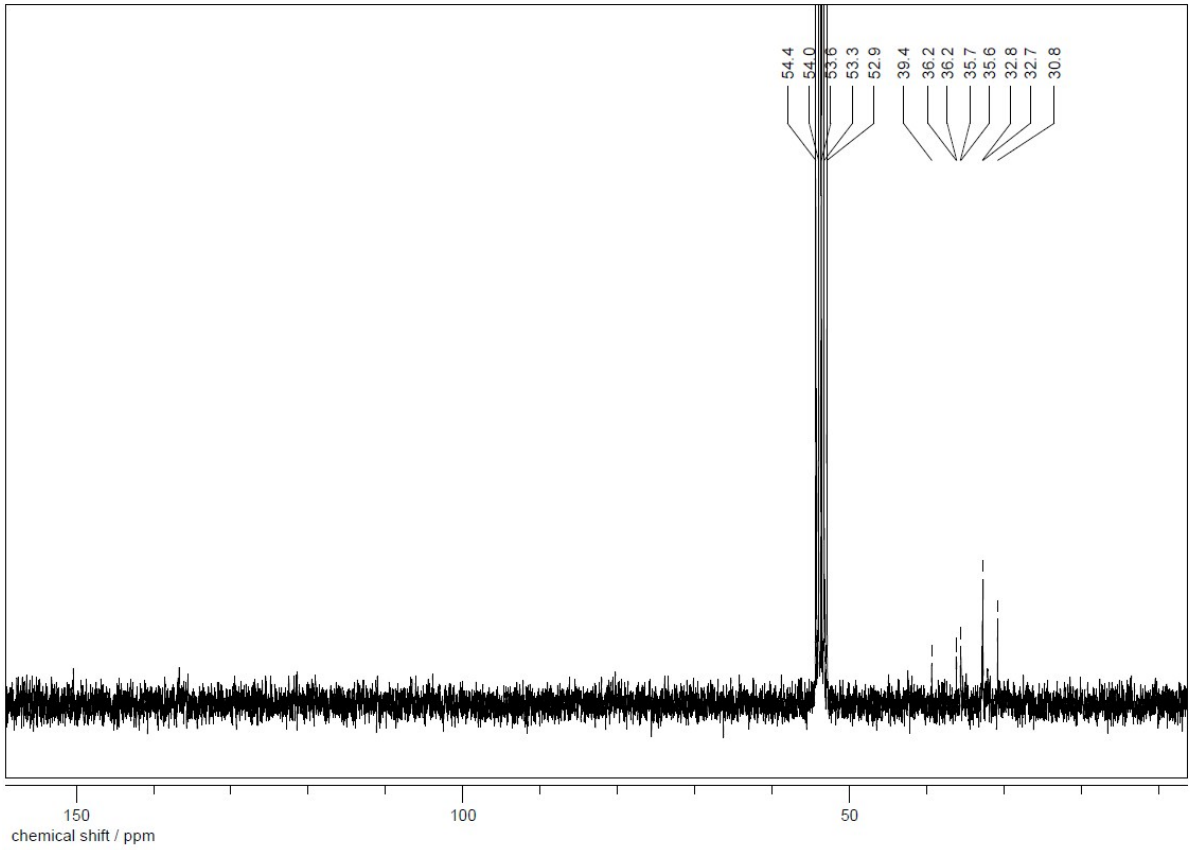
N_0-[Pc*Zn] [1, 3-5]

^{1}H NMR N_2-[Pc*Zn]

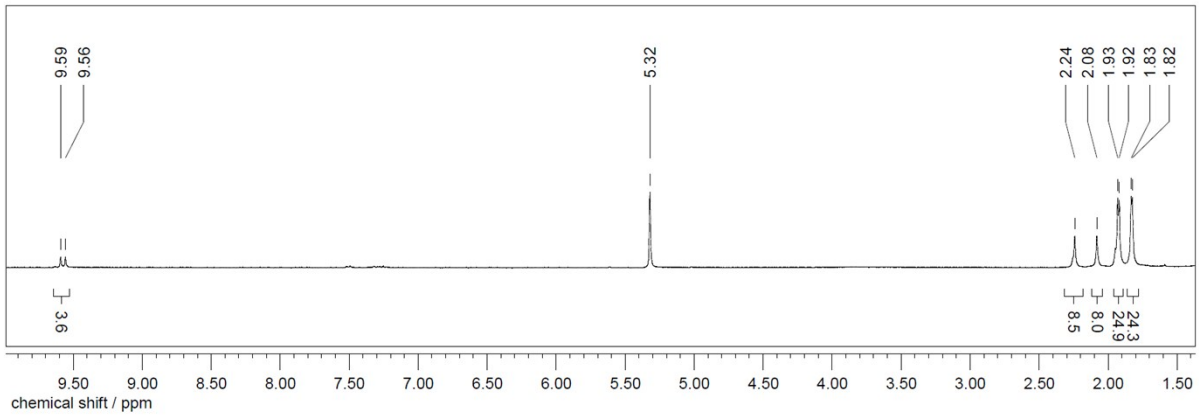


in C_6D_6 (top) or d_2-DCM (bottom).

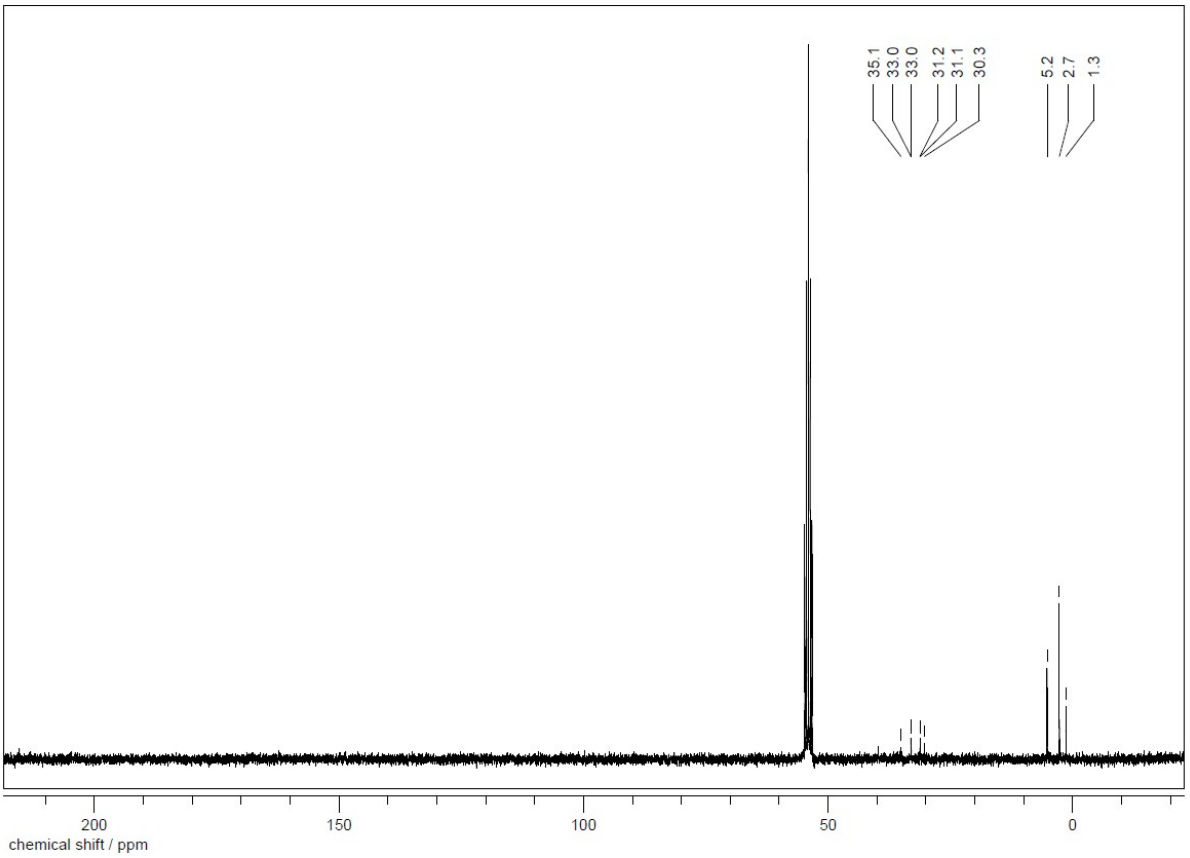
^{13}C NMR N_2-[Pc*Zn]



^{1}H NMR N_4-[Pc*Zn]



^{13}C NMR N_4-[Pc*Zn]



N_6-[Pc*Zn]

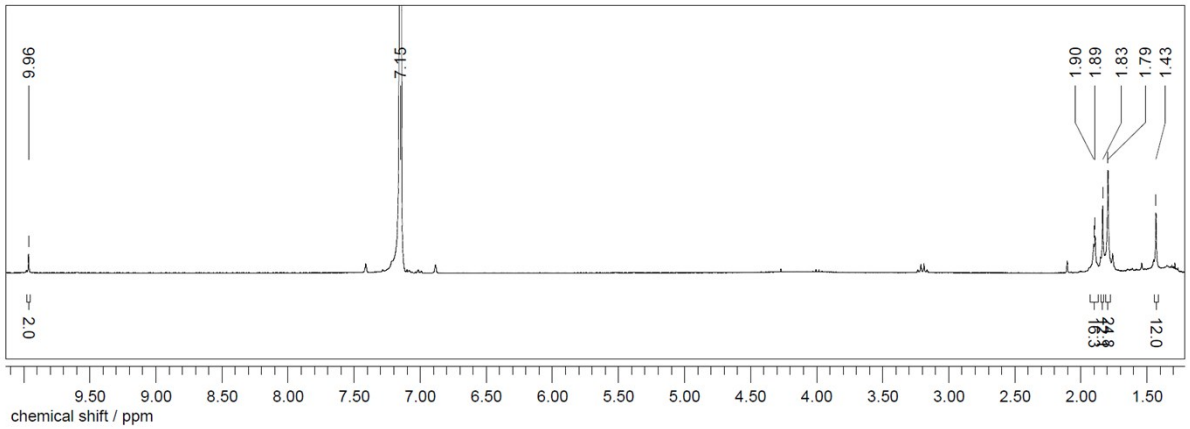
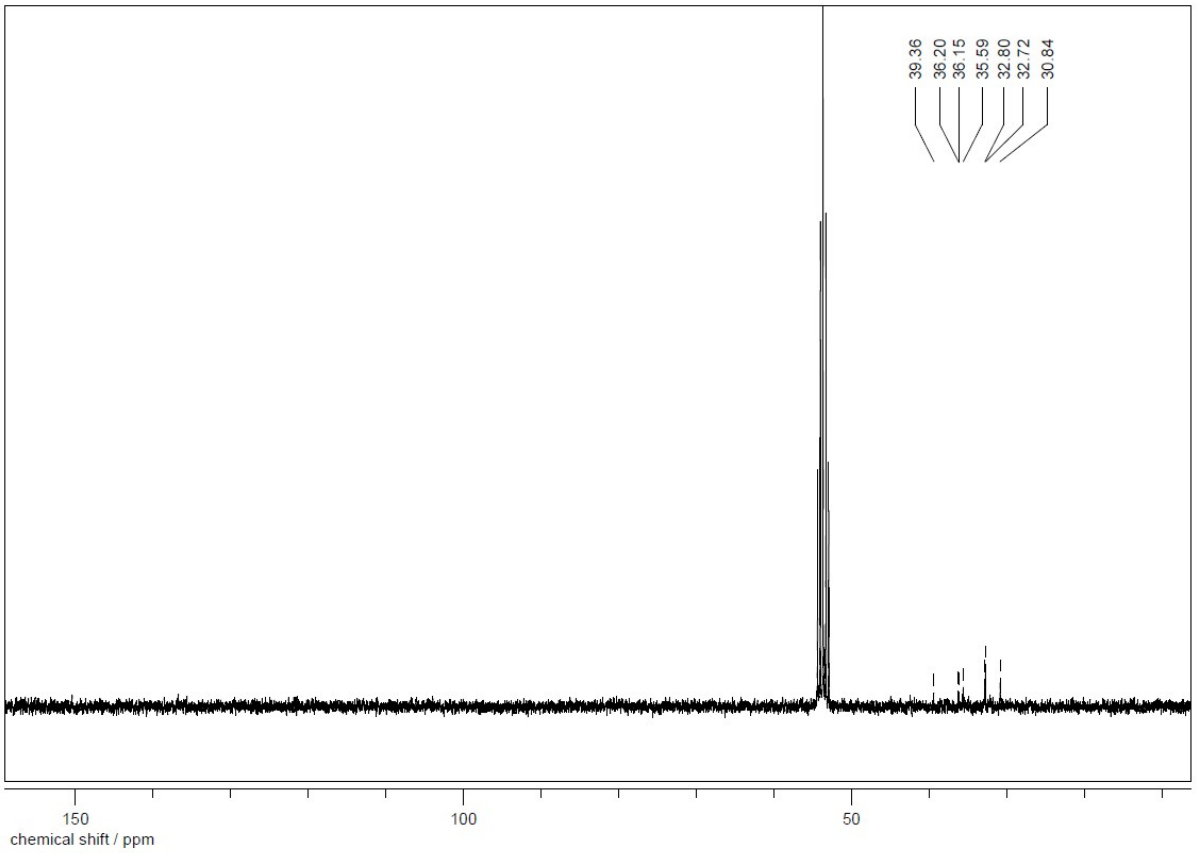


Figure SI-7c. $^{1}H/^{13}C$ NMR spectrum of N_x-[Pc*Zn] with X = 2, 4, and 6 in C_6D_6, and CD_2Cl_2, respectively, 300 MHz.

^{13}C NMR N_6-[Pc*Zn]



N_8-[Pc*Zn] [3-5]

1.6 Cylovoltammetric Measurements

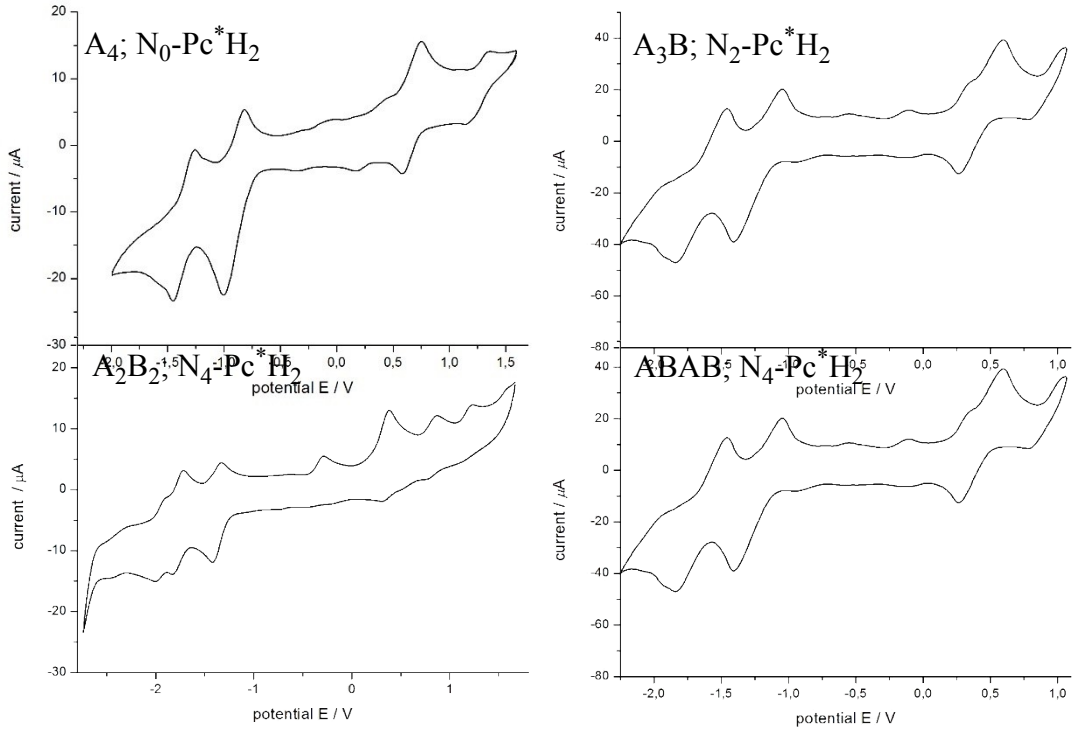


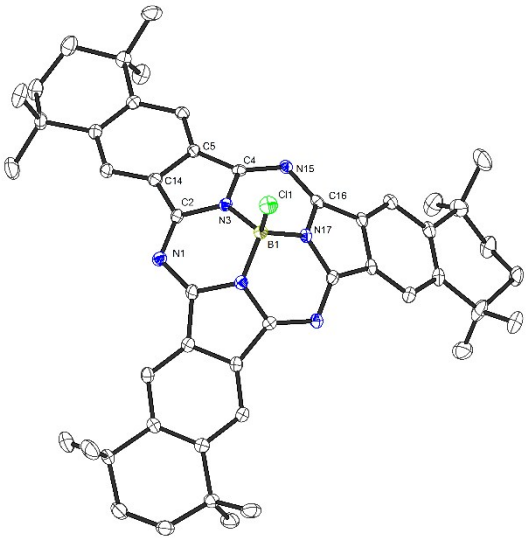
Figure SI-8. Cyclovoltammetric measurements of N_x-Pc*H_2. All measurements were carried out in DCM, except of Ppz*H_2, which was measured in THF because of solubility. The red circles mark impurities caused by used DCM. In all cases, different scan rates were tested, here, 20 mV/s measurements are shown. The spectra are calibrated using Fc in the final scan, measured in $[TBA]PF_6$.

1.7 Crystal Structures

Crystal were measured with a Bruker D8 QUEST area detector. Crystal structures were resolved and refined by Dr. K. Harms of the service Department of Chemistry of the Philipps-Universität Marburg.

Diffractometer type	Bruker D8 QUEST area detector
Wavelength	0.71073 Å
Temperature	100(2) K
Index ranges	-14<=h<=14, -28<=k<=28, -15<=l<=15
Data collection software	BRUKER APEX2 2014.9-0 [6]
Cell refinement software	BRUKER SAINT [7]
Data reduction software	SAINT V8.34A (Bruker AXS Inc., 2013) [7]
Programs used	XT V2014/1 (Bruker AXS Inc., 2014) [8,9]
	SHELXL-2014/7 (Sheldrick, 2014) [8,10]
	DIAMOND (Crystal Impact) [11]

1.7.1 **Crystal Structure of [Spc*BCl]**



Habitus, colour	prism, colourless	
Crystal size	0.22 x 0.22 x 0.09 mm^3	
Crystal system	Orthorhombic	
Space group	$Cmc2_1$	Z = 4
Unit cell dimensions	a = 24.8236(10) Å	α= 90°.
	b = 16.3090(6) Å	β= 90°.
	c = 10.9728(4) Å	γ = 90°.
Volume	4442.3(3) $Å^3$	
Cell determination	9874 peaks with Theta 2.4 to 25.4°.	
Empirical formula	C_{49} H_{56} B Cl_3 N_6	
Moiety formula	C_{48} H_{54} B Cl N_6, CH_2Cl_2	
Formula weight	846.15	
Density (calculated)	1.265 Mg/m^3	
Absorption coefficient	0.248 mm^{-1}	
F(000)	1792	

Solution and refinement:	
Reflections collected	28577
Independent reflections	4177 [R(int) = 0.0342]
Completeness to theta = 25.242°	99.9 %
Observed reflections	4031[I>2sigma(I)]
Reflections used for refinement	4177
Absorption correction	Semi-empirical from equivalents [12]
Max. and min. transmission	0.98 and 0.86
Flack parameter (absolute struct.)	0.001(14)
Largest diff. peak and hole	0.283 and -0.192 $e.Å^{-3}$
Solution	Direct methods [8]
Refinement	Full-matrix least-squares on F^2 [8]
Treatment of hydrogen atoms	Calculated positions, constr. ref.
Data / restraints / parameters	4177 / 44 / 311
Goodness-of-fit on F^2	1.049
R index (all data)	wR2 = 0.0754
R index conventional [I>2sigma(I)]	R1 = 0.0293

Table SI-2. Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for ML153F_0m. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)	Occupancy
N1	0.5000	0.08718(16)	0.7070(3)	0.0163(6)	1
N3	0.54732(7)	0.15242(11)	0.54643(17)	0.0130(4)	1
N15	0.59330(7)	0.26327(11)	0.45407(16)	0.0136(4)	1
N17	0.5000	0.24139(16)	0.4157(2)	0.0127(5)	1
C2	0.54616(9)	0.11154(13)	0.6547(2)	0.0149(4)	1
C4	0.59270(8)	0.19816(13)	0.5299(2)	0.0128(4)	1
C5	0.62944(9)	0.17210(13)	0.6260(2)	0.0138(4)	1
C6	0.68271(9)	0.19023(13)	0.6541(2)	0.0141(4)	1
C7	0.70788(9)	0.15358(13)	0.7545(2)	0.0144(4)	1
C8	0.76727(10)	0.17460(14)	0.7780(2)	0.0186(5)	1
C9	0.79202(10)	0.11748(16)	0.8738(2)	0.0253(6)	1
C10	0.75505(11)	0.10051(17)	0.9799(2)	0.0257(6)	1
C11	0.70338(10)	0.05628(15)	0.9411(2)	0.0197(5)	1
C12	0.67783(9)	0.10049(13)	0.8318(2)	0.0150(4)	1
C13	0.62411(9)	0.08414(14)	0.8058(2)	0.0162(5)	1
C14	0.60011(9)	0.11829(13)	0.7033(2)	0.0148(5)	1
C16	0.54605(9)	0.28670(13)	0.40512(19)	0.0137(4)	1
C18	0.52856(9)	0.36689(14)	0.3620(2)	0.0145(4)	1
C19	0.55637(9)	0.43836(13)	0.3359(2)	0.0174(5)	1
C20	0.52846(9)	0.51054(14)	0.3088(2)	0.0180(5)	1
C21	0.56208(11)	0.58749(16)	0.2815(3)	0.0287(6)	1
C22	0.5284(2)	0.6650(3)	0.2921(7)	0.0259(11)	0.5
C23	0.4778(2)	0.6530(3)	0.2168(6)	0.0242(11)	0.5
C24	0.66584(12)	0.05663(19)	1.0520(2)	0.0328(6)	1
C25	0.71454(12)	-0.03249(16)	0.9045(3)	0.0306(6)	1
C26	0.80131(9)	0.16592(17)	0.6619(2)	0.0267(6)	1
C27	0.77020(10)	0.26457(15)	0.8206(2)	0.0242(5)	1
C28	0.59861(12)	0.57227(19)	0.1717(3)	0.0376(7)	1
C29	0.5886(4)	0.6179(6)	0.3816(10)	0.033(2)	0.5
C29A	0.6058(3)	0.6001(6)	0.3970(9)	0.0251(17)	0.5
B1	0.5000	0.1569(2)	0.4646(3)	0.0130(7)	1
Cl1	0.5000	0.07386(5)	0.34930(7)	0.02119(19)	1
C1S	0.5136(3)	0.1520(5)	1.0477(6)	0.054(3)	0.5
Cl1S	0.56140(14)	0.22218(19)	1.1014(2)	0.0507(6)	0.5
Cl2S	0.44951(15)	0.1926(3)	1.0606(5)	0.1026(15)	0.5

Table SI-3. Bond lengths [Å] and angles [°] for ML153F_0m.

N1-C2	1.342(3)	C20-C21	1.537(3)
N1-C2#1	1.342(3)	C21-C29	1.374(10)
N3-C2	1.363(3)	C21-C22	1.521(6)
N3-C4	1.363(3)	C21-C28	1.528(4)
N3-B1	1.480(3)	C21-C29A	1.682(8)
N15-C16	1.345(3)	C22-C23	1.514(7)
N15-C4	1.349(3)	C22-C29	1.947(10)
N17-C16	1.366(3)	C22-H22A	0.9700
N17-C16#1	1.366(3)	C22-H22B	0.9700
N17-B1	1.479(4)	C23-H23A	0.9700
C2-C14	1.446(3)	C23-H23B	0.9701
C4-C5	1.457(3)	C24-H24A	0.9800
C5-C6	1.390(3)	C24-H24B	0.9800
C5-C14	1.421(3)	C24-H24C	0.9800
C6-C7	1.401(3)	C25-H25A	0.9800
C6-H6	0.9500	C25-H25B	0.9800
C7-C12	1.423(3)	C25-H25C	0.9800
C7-C8	1.536(3)	C26-H26A	0.9800
C8-C9	1.533(3)	C26-H26B	0.9800
C8-C26	1.535(3)	C26-H26C	0.9800
C8-C27	1.542(3)	C27-H27A	0.9800
C9-C10	1.508(4)	C27-H27B	0.9800
C9-H9A	0.9900	C27-H27C	0.9800
C9-H9B	0.9900	C28-H28A	0.9800
C10-C11	1.532(3)	C28-H28B	0.9800
C10-H10A	0.9900	C28-H28C	0.9800
C10-H10B	0.9900	C29-H29A	0.9800
C11-C25	1.528(4)	C29-H29B	0.9800
C11-C24	1.533(4)	C29-H29C	0.9800
C11-C12	1.537(3)	C29A-H29D	0.9800
C12-C13	1.389(3)	C29A-H29E	0.9800
C13-C14	1.390(3)	C29A-H29F	0.9800
C13-H13	0.9500	B1-N3#1	1.480(3)
C16-C18	1.457(3)	B1-Cl1	1.853(4)
C18-C19	1.385(3)	C1S-Cl2S	1.730(9)
C18-C18#1	1.418(4)	C1S-Cl1S	1.750(7)
C19-C20	1.398(3)	C1S-H1S1	0.9900
C19-H19	0.9500	C1S-H1S2	0.9900
C20-C20#1	1.413(5)		

C2-N1-C2#1	117.3(3)	C7-C6-H6	119.7
C2-N3-C4	113.63(19)	C6-C7-C12	119.6(2)
C2-N3-B1	122.4(2)	C6-C7-C8	117.7(2)
C4-N3-B1	123.3(2)	C12-C7-C8	122.6(2)
C16-N15-C4	117.41(18)	C9-C8-C26	107.0(2)
C16-N17-C16#1	113.6(3)	C9-C8-C7	111.37(19)
C16-N17-B1	122.34(13)	C26-C8-C7	111.61(19)
C16#1-N17-B1	122.34(13)	C9-C8-C27	110.59(19)
N1-C2-N3	122.4(2)	C26-C8-C27	108.3(2)
N1-C2-C14	131.0(2)	C7-C8-C27	107.97(19)
N3-C2-C14	105.34(19)	C10-C9-C8	113.4(2)
N15-C4-N3	121.43(19)	C10-C9-H9A	108.9
N15-C4-C5	131.98(19)	C8-C9-H9A	108.9
N3-C4-C5	105.18(18)	C10-C9-H9B	108.9
C6-C5-C14	119.1(2)	C8-C9-H9B	108.9
C6-C5-C4	133.9(2)	H9A-C9-H9B	107.7
C14-C5-C4	106.92(19)	C9-C10-C11	112.4(2)
C5-C6-C7	120.5(2)	C9-C10-H10A	109.1
C5-C6-H6	119.7	C11-C10-H10A	109.1

C9-C10-H10B	109.1	H24A-C24-H24C	109.5
C11-C10-H10B	109.1	H24B-C24-H24C	109.5
H10A-C10-H10B	107.9	C11-C25-H25A	109.5
C25-C11-C10	111.6(2)	C11-C25-H25B	109.5
C25-C11-C24	108.8(2)	H25A-C25-H25B	109.5
C10-C11-C24	106.7(2)	C11-C25-H25C	109.5
C25-C11-C12	108.3(2)	H25A-C25-H25C	109.5
C10-C11-C12	110.0(2)	H25B-C25-H25C	109.5
C24-C11-C12	111.6(2)	C8-C26-H26A	109.5
C13-C12-C7	119.9(2)	C8-C26-H26B	109.5
C13-C12-C11	117.8(2)	H26A-C26-H26B	109.5
C7-C12-C11	122.30(19)	C8-C26-H26C	109.5
C12-C13-C14	120.0(2)	H26A-C26-H26C	109.5
C12-C13-H13	120.0	H26B-C26-H26C	109.5
C14-C13-H13	120.0	C8-C27-H27A	109.5
C13-C14-C5	120.7(2)	C8-C27-H27B	109.5
C13-C14-C2	131.7(2)	H27A-C27-H27B	109.5
C5-C14-C2	107.56(19)	C8-C27-H27C	109.5
N15-C16-N17	122.8(2)	H27A-C27-H27C	109.5
N15-C16-C18	130.1(2)	H27B-C27-H27C	109.5
N17-C16-C18	105.30(19)	C21-C28-H28A	109.5
C19-C18-C18#1	119.90(13)	C21-C28-H28B	109.5
C19-C18-C16	132.4(2)	H28A-C28-H28B	109.5
C18#1-C18-C16	107.34(12)	C21-C28-H28C	109.5
C18-C19-C20	120.4(2)	H28A-C28-H28C	109.5
C18-C19-H19	119.8	H28B-C28-H28C	109.5
C20-C19-H19	119.8	C21-C29-C22	51.0(3)
C19-C20-C20#1	119.71(13)	C21-C29-H29A	109.5
C19-C20-C21	117.4(2)	C22-C29-H29A	159.2
C20#1-C20-C21	122.90(13)	C21-C29-H29B	109.5
C29-C21-C22	84.4(5)	C22-C29-H29B	75.8
C29-C21-C28	113.9(5)	H29A-C29-H29B	109.5
C22-C21-C28	121.5(3)	C21-C29-H29C	109.5
C29-C21-C20	113.5(5)	C22-C29-H29C	86.5
C22-C21-C20	111.4(3)	H29A-C29-H29C	109.5
C28-C21-C20	110.1(2)	H29B-C29-H29C	109.5
C28-C21-C29A	103.4(4)	C21-C29A-H29D	109.5
C20-C21-C29A	107.6(4)	C21-C29A-H29E	109.5
C23-C22-C21	107.8(4)	H29D-C29A-H29E	109.5
C23-C22-C29	149.3(5)	C21-C29A-H29F	109.5
C21-C22-C29	44.6(4)	H29D-C29A-H29F	109.5
C23-C22-H22A	110.5	H29E-C29A-H29F	109.5
C21-C22-H22A	110.3	N17-B1-N3#1	105.42(18)
C29-C22-H22A	94.7	N17-B1-N3	105.42(18)
C23-C22-H22B	109.7	N3#1-B1-N3	105.0(3)
C21-C22-H22B	109.9	N17-B1-Cl1	115.7(2)
C29-C22-H22B	76.7	N3#1-B1-Cl1	112.22(16)
H22A-C22-H22B	108.6	N3-B1-Cl1	112.22(16)
C22-C23-H23A	109.0	Cl2S-C1S-Cl1S	110.2(4)
C22-C23-H23B	109.8	Cl2S-C1S-H1S1	109.6
H23A-C23-H23B	108.2	Cl1S-C1S-H1S1	109.6
C11-C24-H24A	109.5	Cl2S-C1S-H1S2	109.6
C11-C24-H24B	109.5	Cl1S-C1S-H1S2	109.6
H24A-C24-H24B	109.5	H1S1-C1S-H1S2	108.1
C11-C24-H24C	109.5		

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,y,z

Table SI-4. Anisotropic displacement parameters (A^2) for ML153F_0m. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

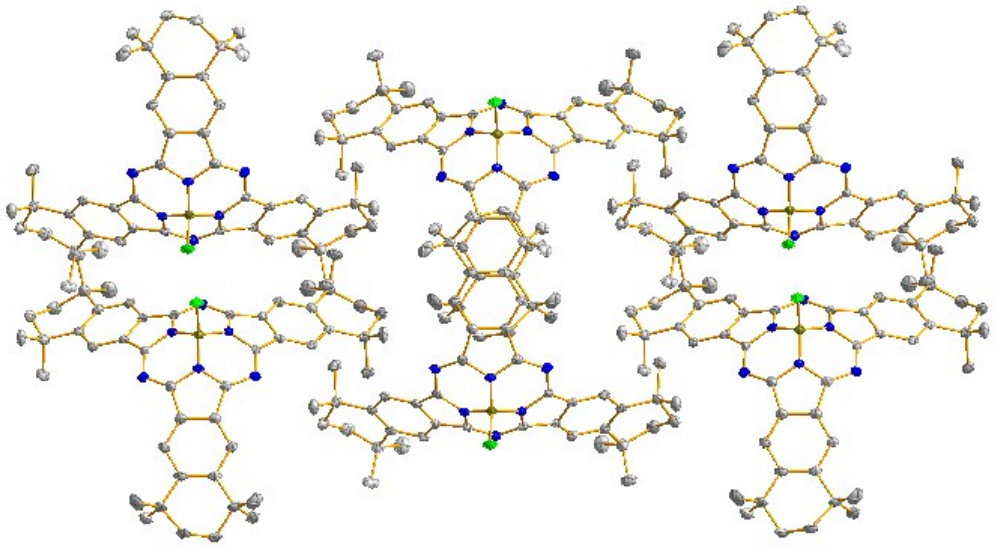
	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N1	0.0136(13)	0.0147(13)	0.0207(14)	0.0030(11)	0.000	0.000
N3	0.0135(9)	0.0100(9)	0.0155(9)	0.0009(7)	0.0006(7)	0.0013(7)
N15	0.0156(9)	0.0129(9)	0.0123(9)	-0.0002(7)	0.0014(7)	0.0011(7)
N17	0.0153(13)	0.0113(12)	0.0114(12)	0.0010(10)	0.000	0.000
C2	0.0173(11)	0.0102(10)	0.0173(11)	0.0029(9)	0.0010(9)	0.0025(9)
C4	0.0122(10)	0.0117(10)	0.0147(10)	-0.0022(9)	0.0022(9)	0.0010(8)
C5	0.0167(11)	0.0100(10)	0.0148(10)	0.0005(8)	0.0019(8)	0.0025(9)
C6	0.0153(10)	0.0122(10)	0.0148(10)	-0.0007(9)	0.0028(9)	0.0001(9)
C7	0.0164(11)	0.0109(10)	0.0161(10)	-0.0032(9)	0.0000(9)	0.0017(8)
C8	0.0185(11)	0.0173(11)	0.0199(12)	0.0001(9)	-0.0031(9)	-0.0025(9)
C9	0.0220(12)	0.0222(12)	0.0318(15)	0.0045(11)	-0.0094(11)	-0.0037(10)
C10	0.0293(13)	0.0249(13)	0.0228(13)	0.0037(10)	-0.0088(11)	-0.0007(11)
C11	0.0214(12)	0.0212(12)	0.0165(12)	0.0062(9)	-0.0038(9)	-0.0004(10)
C12	0.0191(10)	0.0128(10)	0.0132(11)	-0.0013(8)	-0.0010(9)	0.0024(8)
C13	0.0188(11)	0.0141(10)	0.0159(10)	0.0025(9)	0.0013(9)	0.0019(9)
C14	0.0157(11)	0.0118(10)	0.0168(11)	0.0001(8)	0.0017(9)	0.0014(8)
C16	0.0168(11)	0.0143(11)	0.0100(10)	-0.0016(9)	0.0027(9)	-0.0014(9)
C18	0.0201(11)	0.0139(10)	0.0094(9)	0.0008(8)	0.0016(9)	0.0012(9)
C19	0.0190(10)	0.0170(10)	0.0163(11)	0.0021(9)	0.0024(10)	-0.0019(9)
C20	0.0263(12)	0.0137(11)	0.0139(10)	0.0023(9)	0.0025(9)	-0.0004(10)
C21	0.0269(14)	0.0163(12)	0.0429(16)	0.0090(11)	0.0101(12)	-0.0015(11)
C22	0.032(3)	0.013(2)	0.033(3)	0.004(2)	-0.007(2)	-0.004(2)
C23	0.028(2)	0.015(2)	0.030(3)	0.010(2)	-0.003(2)	-0.0007(18)
C24	0.0364(15)	0.0440(17)	0.0179(13)	0.0104(12)	-0.0024(11)	-0.0013(13)
C25	0.0389(15)	0.0209(13)	0.0318(13)	0.0056(11)	-0.0133(13)	0.0037(11)
C26	0.0145(11)	0.0363(14)	0.0293(14)	-0.0023(12)	-0.0007(11)	-0.0002(10)
C27	0.0251(12)	0.0206(12)	0.0268(13)	-0.0015(10)	-0.0076(10)	-0.0041(10)
C28	0.0354(16)	0.0410(16)	0.0362(17)	0.0160(14)	0.0075(13)	-0.0115(13)
C29	0.030(5)	0.024(4)	0.046(5)	0.008(3)	-0.010(4)	-0.006(3)
C29A	0.022(4)	0.018(4)	0.035(4)	0.002(3)	-0.016(3)	-0.005(3)
B1	0.0137(17)	0.0111(16)	0.0141(17)	-0.0016(14)	0.000	0.000
Cl1	0.0270(4)	0.0151(4)	0.0215(4)	-0.0066(3)	0.000	0.000
C1S	0.081(8)	0.047(3)	0.035(3)	0.002(3)	-0.009(3)	-0.023(4)
Cl1S	0.0548(13)	0.0534(15)	0.0440(11)	0.0083(9)	-0.0010(9)	-0.0125(11)
Cl2S	0.062(2)	0.095(3)	0.151(4)	0.058(3)	-0.045(2)	-0.032(2)

Table SI-5. Hydrogen coordinates and isotropic displacement parameters ($Å^2$) for ML153F_0m.

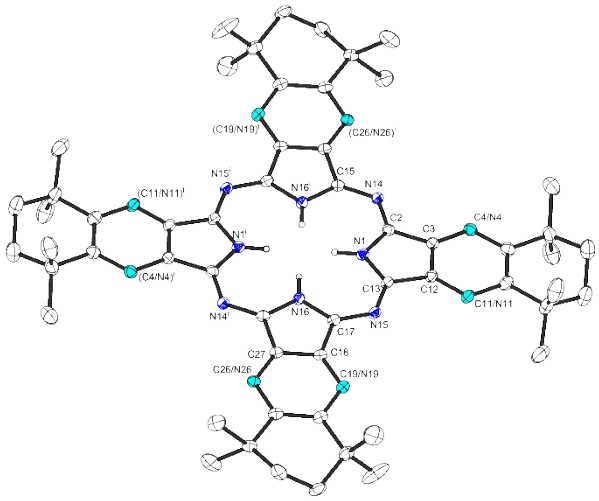
	x	y	z	U(eq)	Occupancy
H6	0.7022	0.2278	0.6048	0.017	1
H9A	0.8016	0.0648	0.8344	0.030	1
H9B	0.8257	0.1425	0.9048	0.030	1
H10A	0.7454	0.1530	1.0196	0.031	1
H10B	0.7743	0.0665	1.0405	0.031	1
H13	0.6038	0.0496	0.8582	0.019	1
H19	0.5946	0.4383	0.3364	0.021	1
H22A	0.5486	0.7120	0.2629	0.031	0.5
H22B	0.5187	0.6744	0.3766	0.031	0.5
H23A	0.4878	0.6332	0.1366	0.029	0.5
H23B	0.4593	0.7050	0.2071	0.029	0.5
H24A	0.6331	0.0256	1.0330	0.049	1
H24B	0.6562	0.1133	1.0725	0.049	1
H24C	0.6842	0.0313	1.1215	0.049	1
H25A	0.6806	-0.0596	0.8834	0.046	1
H25B	0.7315	-0.0614	0.9727	0.046	1
H25C	0.7387	-0.0334	0.8339	0.046	1
H26A	0.8392	0.1772	0.6810	0.040	1
H26B	0.7886	0.2050	0.6005	0.040	1
H26C	0.7979	0.1100	0.6302	0.040	1
H27A	0.8079	0.2797	0.8350	0.036	1
H27B	0.7497	0.2709	0.8963	0.036	1
H27C	0.7549	0.3003	0.7577	0.036	1
H28A	0.6183	0.6227	0.1519	0.056	1
H28B	0.5767	0.5558	0.1016	0.056	1
H28C	0.6243	0.5286	0.1911	0.056	1
H29A	0.6135	0.5764	0.4130	0.050	0.5
H29B	0.5623	0.6320	0.4449	0.050	0.5
H29C	0.6088	0.6671	0.3584	0.050	0.5
H29D	0.6335	0.5572	0.3933	0.038	0.5
H29E	0.5866	0.5963	0.4748	0.038	0.5
H29F	0.6230	0.6540	0.3904	0.038	0.5
H1S1	0.5212	0.1388	0.9613	0.065	0.5
H1S2	0.5160	0.1006	1.0955	0.065	0.5

Table SI-6. Torsion angles [°] for ML153F_0m.

C2#1-N1-C2-N3	-6.4(4)		
C2#1-N1-C2-C14	158.84(17)	C16#1-N17-C16-C18	-10.8(3)
C4-N3-C2-N1	156.6(2)	B1-N17-C16-C18	-176.2(2)
B1-N3-C2-N1	-14.2(3)	N15-C16-C18-C19	14.2(4)
C4-N3-C2-C14	-11.9(2)	N17-C16-C18-C19	179.0(3)
B1-N3-C2-C14	177.3(2)	N15-C16-C18-C18#1	-158.6(2)
C16-N15-C4-N3	6.9(3)	N17-C16-C18-C18#1	6.19(19)
C16-N15-C4-C5	-157.4(2)	C18#1-C18-C19-C20	-0.4(3)
C2-N3-C4-N15	-156.0(2)	C16-C18-C19-C20	-172.5(2)
B1-N3-C4-N15	14.7(3)	C18-C19-C20-C20#1	0.4(3)
C2-N3-C4-C5	12.0(2)	C18-C19-C20-C21	179.7(2)
B1-N3-C4-C5	-177.4(2)	C19-C20-C21-C29	-69.4(5)
N15-C4-C5-C6	-19.3(4)	C20#1-C20-C21-C29	109.9(4)
N3-C4-C5-C6	174.6(2)	C19-C20-C21-C22	-162.6(4)
N15-C4-C5-C14	159.3(2)	C20#1-C20-C21-C22	16.7(4)
N3-C4-C5-C14	-6.9(2)	C19-C20-C21-C28	59.7(3)
C14-C5-C6-C7	2.4(3)	C20#1-C20-C21-C28	-121.05(18)
C4-C5-C6-C7	-179.2(2)	C19-C20-C21-C29A	-52.3(4)
C5-C6-C7-C12	-3.1(3)	C20#1-C20-C21-C29A	127.0(4)
C5-C6-C7-C8	178.3(2)	C29-C21-C22-C23	-163.8(6)
C6-C7-C8-C9	-168.6(2)	C28-C21-C22-C23	81.5(5)
C12-C7-C8-C9	12.9(3)	C20-C21-C22-C23	-50.7(5)
C6-C7-C8-C26	-49.0(3)	C28-C21-C22-C29	-114.6(6)
C12-C7-C8-C26	132.4(2)	C20-C21-C22-C29	113.1(5)
C6-C7-C8-C27	69.8(3)	C28-C21-C29-C22	122.0(4)
C12-C7-C8-C27	-108.7(2)	C20-C21-C29-C22	-110.9(4)
C26-C8-C9-C10	-163.7(2)	C16-N17-B1-N3#1	137.5(2)
C7-C8-C9-C10	-41.5(3)	C16#1-N17-B1-N3#1	-26.6(3)
C27-C8-C9-C10	78.6(3)	C16-N17-B1-N3	26.6(3)
C8-C9-C10-C11	62.5(3)	C16#1-N17-B1-N3	-137.5(2)
C9-C10-C11-C25	71.0(3)	C16-N17-B1-Cl1	-98.0(2)
C9-C10-C11-C24	-170.3(2)	C16#1-N17-B1-Cl1	98.0(2)
C9-C10-C11-C12	-49.2(3)	C2-N3-B1-N17	140.7(2)
C6-C7-C12-C13	1.2(3)	C4-N3-B1-N17	-29.2(3)
C8-C7-C12-C13	179.7(2)	C2-N3-B1-N3#1	29.6(3)
C6-C7-C12-C11	178.1(2)	C4-N3-B1-N3#1	-140.25(18)
C8-C7-C12-C11	-3.4(3)	C2-N3-B1-Cl1	-92.6(2)
C25-C11-C12-C13	75.7(3)	C4-N3-B1-Cl1	97.6(2)
C10-C11-C12-C13	-162.2(2)		
C24-C11-C12-C13	-44.1(3)		
C25-C11-C12-C7	-101.3(3)		
C10-C11-C12-C7	20.8(3)		
C24-C11-C12-C7	139.0(2)		
C7-C12-C13-C14	1.3(3)		
C11-C12-C13-C14	-175.7(2)		
C12-C13-C14-C5	-2.0(3)		
C12-C13-C14-C2	179.6(2)		
C6-C5-C14-C13	0.1(3)		
C4-C5-C14-C13	-178.7(2)		
C6-C5-C14-C2	178.88(19)		
C4-C5-C14-C2	0.1(2)		
N1-C2-C14-C13	18.2(4)		
N3-C2-C14-C13	-174.7(2)		
N1-C2-C14-C5	-160.4(3)		
N3-C2-C14-C5	6.7(2)		
C4-N15-C16-N17	-9.1(3)		
C4-N15-C16-C18	153.4(2)		
C16#1-N17-C16-N15	155.38(15)		
B1-N17-C16-N15	-10.0(4)		



1.7.2 **Crystal Structure of N_2-Pc^*H_2**



Habitus, colour	plate, dark	
Crystal size	0.29 x 0.22 x 0.05 mm^3	
Crystal system	Monoclinic	
Space group	$P2_1/c$	Z = 2
Unit cell dimensions	a = 11.7078(4) Å	α= 90°.
	b = 23.2759(7) Å	β= 90.620(3)°.
	c = 12.9884(5) Å	γ = 90°.
Volume	3539.3(2) $Å^3$	
Cell determination	9908 peaks with Theta 2.3 to 25.2°.	
Empirical formula	$C_{66}\,H_{76}\,Cl_{12}\,N_{10}$	
Moiety formula	$C_{62}\,H_{72}\,N_{10}$, $4(CHCl_3)$	
Formula weight	1434.76	
Density (calculated)	1.346 Mg/m^3	
Absorption coefficient	0.516 mm^{-1}	
F(000)	1492	

Solution and refinement:	
Reflections collected	35003
Independent reflections	6438 [R(int) = 0.0640]
Completeness to theta = 25.242°	99.9 %
Observed reflections	4815[I>2sigma(I)]
Reflections used for refinement	6438
Absorption correction	Semi-empirical from equivalents [12]
Max. and min. transmission	0.97 and 0.84
Largest diff. peak and hole	0.491 and -0.364 $e.Å^{-3}$
Solution	Direct methods [8]
Refinement	Full-matrix least-squares on F^2 [8]
Treatment of hydrogen atoms	Mixture of constr. and indep. refinement
Data / restraints / parameters	6438 / 203 / 602
Goodness-of-fit on F^2	1.023
R index (all data)	wR2 = 0.1178
R index conventional [I>2sigma(I)]	R1 = 0.0489

Table SI-7. Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for ML026F1_0m. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)	Occupancy
N1	0.46545(16)	0.57666(8)	0.44525(14)	0.0153(4)	1
C2	0.3647(2)	0.60621(10)	0.45428(17)	0.0157(5)	1
C3	0.3755(2)	0.66129(10)	0.40227(17)	0.0156(5)	1
C4	0.30198(19)	0.70643(10)	0.38898(17)	0.0184(5)	0.75
N4	0.30198(19)	0.70643(10)	0.38898(17)	0.0184(5)	0.25
C5	0.3388(2)	0.75406(11)	0.33488(19)	0.0204(5)	1
C6	0.2532(2)	0.80284(11)	0.3170(2)	0.0268(6)	1
C7	0.3150(2)	0.85787(12)	0.2849(2)	0.0333(7)	1
C8	0.4002(2)	0.84750(12)	0.2011(2)	0.0338(7)	1
C9	0.4967(2)	0.80731(11)	0.2343(2)	0.0268(6)	1
C10	0.4506(2)	0.75531(11)	0.29354(18)	0.0202(5)	1
C11	0.5243(2)	0.70961(10)	0.30888(17)	0.0193(5)	0.75
N11	0.5243(2)	0.70961(10)	0.30888(17)	0.0193(5)	0.25
C12	0.4863(2)	0.66329(10)	0.36324(17)	0.0160(5)	1
C13	0.54049(19)	0.60941(10)	0.39127(17)	0.0154(5)	1
N14	0.27091(16)	0.59019(8)	0.50347(14)	0.0148(4)	1
N15	0.64678(16)	0.59652(8)	0.36288(15)	0.0171(4)	1
C15	0.26385(19)	0.54088(10)	0.55360(17)	0.0151(5)	1
N16	0.65576(16)	0.50203(8)	0.44055(14)	0.0152(4)	1
C17	0.6968(2)	0.54665(10)	0.38416(17)	0.0161(5)	1
C18	0.81001(19)	0.53126(10)	0.34750(17)	0.0154(5)	1
C19	0.88411(19)	0.55965(10)	0.28424(17)	0.0177(5)	0.75
N19	0.88411(19)	0.55965(10)	0.28424(17)	0.0177(5)	0.25
C20	0.9858(2)	0.53270(10)	0.25919(18)	0.0178(5)	1
C21	1.0653(2)	0.56474(11)	0.18526(19)	0.0230(6)	1
C22	1.1584(4)	0.5251(2)	0.1448(4)	0.0275(11)	0.8
C23	1.2118(3)	0.48884(18)	0.2312(3)	0.0250(9)	0.8
C22A	1.1861(17)	0.5330(11)	0.1886(15)	0.039(6)	0.2
C23A	1.1811(17)	0.4745(8)	0.1838(17)	0.040(4)	0.2
C24	1.1240(2)	0.44669(11)	0.27591(18)	0.0190(5)	1
C25	1.0129(2)	0.47795(10)	0.30069(17)	0.0170(5)	1
C26	0.93612(18)	0.45022(10)	0.36436(17)	0.0162(5)	0.75
N26	0.93612(18)	0.45022(10)	0.36436(17)	0.0162(5)	0.25
C27	0.83524(19)	0.47700(10)	0.38659(17)	0.0158(5)	1
C28	0.9988(3)	0.58457(17)	0.0908(2)	0.0527(10)	1
C29	1.1156(3)	0.61711(13)	0.2400(3)	0.0416(8)	1
C30	1.1785(5)	0.4210(2)	0.3759(4)	0.0294(12)	0.8
C31	1.1000(5)	0.3983(2)	0.2006(4)	0.0241(11)	0.8
C30A	1.193(2)	0.4464(8)	0.3646(18)	0.035(6)	0.2
C31A	1.0955(19)	0.3834(11)	0.2407(18)	0.031(5)	0.2
C33	0.1689(2)	0.78408(13)	0.2317(2)	0.0380(7)	1
C34	0.1873(3)	0.81629(13)	0.4147(3)	0.0427(8)	1
C35	0.5593(3)	0.78816(14)	0.1376(2)	0.0475(9)	1
C36	0.5807(3)	0.83935(13)	0.3052(3)	0.0411(8)	1
C1S	0.4189(4)	1.07467(18)	0.3759(3)	0.0589(10)	1
Cl1	0.3082(13)	0.9987(7)	0.4049(13)	0.087(4)	0.089(3)
Cl2	0.384(2)	0.9986(8)	0.3634(16)	0.080(4)	0.079(3)
Cl3	0.4567(5)	1.00427(14)	0.3302(4)	0.0668(13)	0.635(3)
Cl4	0.4849(10)	1.0172(5)	0.3321(10)	0.069(3)	0.234(3)
Cl5	0.5264(15)	1.0658(9)	0.3633(14)	0.080(4)	0.070(2)
Cl6	0.54339(12)	1.11200(7)	0.41534(12)	0.0615(4)	0.843(3)
Cl7	0.488(3)	1.1245(12)	0.411(2)	0.077(6)	0.054(3)
Cl8	0.345(2)	1.1101(9)	0.4684(17)	0.137(8)	0.103(3)
Cl9	0.31974(12)	1.07437(15)	0.47132(11)	0.0788(8)	0.794(3)
Cl10	0.3195(16)	1.0394(10)	0.4564(17)	0.098(5)	0.099(3)
C2S	0.8490(3)	0.70760(18)	0.4147(3)	0.0404(10)	0.9

C2SA	0.962(4)	0.733(2)	0.560(4)	0.078(6)	0.1
Cl11	0.844(2)	0.7483(13)	0.650(2)	0.092(6)	0.049(2)
Cl12	0.788(2)	0.8059(13)	0.5125(17)	0.090(5)	0.058(3)
Cl13	0.80543(14)	0.76779(9)	0.49037(10)	0.0609(5)	0.785(3)
Cl14	0.7662(10)	0.7308(7)	0.4884(9)	0.088(3)	0.123(3)
Cl15	0.887(2)	0.7915(12)	0.4584(19)	0.097(5)	0.058(2)
Cl16	0.7871(13)	0.6961(7)	0.4299(14)	0.090(5)	0.095(3)
Cl17	0.85946(7)	0.72932(4)	0.28604(6)	0.0343(3)	0.884(2)
Cl18	0.9371(18)	0.6712(10)	0.4653(18)	0.068(5)	0.079(3)
Cl19	0.98215(13)	0.68209(7)	0.46156(13)	0.0437(4)	0.809(3)
Cl20	0.9905(18)	0.7094(11)	0.524(2)	0.081(5)	0.061(3)

Table SI-8. Bond lengths [Å] and angles [°] for ML026F1_0m.

N1-C13	1.363(3)	C22A-H22C	0.9900
N1-C2	1.371(3)	C22A-H22D	0.9900
N1-H1	0.8800	C23A-C24	1.521(19)
C2-N14	1.330(3)	C23A-H23C	0.9900
C2-C3	1.455(3)	C23A-H23D	0.9900
C3-N4	1.368(3)	C24-C30A	1.40(3)
C3-C4	1.368(3)	C24-C31	1.516(7)
C3-C12	1.398(3)	C24-C25	1.528(3)
C4-C5	1.384(3)	C24-C30	1.561(6)
C4-H4	0.9500	C24-C31A	1.58(3)
N4-C5	1.384(3)	C25-N26	1.387(3)
C5-C10	1.421(3)	C25-C26	1.387(3)
C5-C6	1.531(3)	C26-C27	1.369(3)
C6-C34	1.524(4)	C26-H26	0.9500
C6-C7	1.532(4)	N26-C27	1.369(3)
C6-C33	1.539(4)	C27-C15#1	1.464(3)
C7-C8	1.503(4)	C28-H28A	0.9800
C7-H7A	0.9900	C28-H28B	0.9800
C7-H7B	0.9900	C28-H28C	0.9800
C8-C9	1.525(4)	C29-H29A	0.9800
C8-H8A	0.9900	C29-H29B	0.9800
C8-H8B	0.9900	C29-H29C	0.9800
C9-C35	1.527(4)	C30-H30A	0.9800
C9-C36	1.534(4)	C30-H30B	0.9800
C9-C10	1.535(3)	C30-H30C	0.9800
C10-N11	1.382(3)	C31-H31A	0.9800
C10-C11	1.382(3)	C31-H31B	0.9800
C11-C12	1.366(3)	C31-H31C	0.9800
C11-H11	0.9500	C30A-H30D	0.9800
N11-C12	1.366(3)	C30A-H30E	0.9800
C12-C13	1.450(3)	C30A-H30F	0.9800
C13-N15	1.336(3)	C31A-H31D	0.9800
N14-C15	1.323(3)	C31A-H31E	0.9800
N15-C17	1.328(3)	C31A-H31F	0.9800
C15-N16#1	1.374(3)	C33-H33A	0.9800
C15-C27#1	1.464(3)	C33-H33B	0.9800
N16-C17	1.362(3)	C33-H33C	0.9800
N16-C15#1	1.374(3)	C34-H34A	0.9800
N16-H16	0.8800	C34-H34B	0.9800
C17-C18	1.458(3)	C34-H34C	0.9800
C18-N19	1.371(3)	C35-H35A	0.9800
C18-C19	1.371(3)	C35-H35B	0.9800
C18-C27	1.392(3)	C35-H35C	0.9800
C19-C20	1.388(3)	C36-H36A	0.9800
C19-H19	0.9500	C36-H36B	0.9800
N19-C20	1.388(3)	C36-H36C	0.9800
C20-C25	1.418(3)	C1S-Cl5	1.287(17)
C20-C21	1.537(3)	C1S-Cl7	1.48(3)
C21-C28	1.518(4)	C1S-Cl4	1.648(12)
C21-C29	1.527(4)	C1S-Cl8	1.701(18)
C21-C22	1.527(6)	C1S-Cl9	1.708(4)
C21-C22A	1.60(2)	C1S-Cl6	1.768(5)
C22-C23	1.531(6)	C1S-Cl10	1.774(18)
C22-H22A	0.9900	C1S-Cl3	1.799(6)
C22-H22B	0.9900	C1S-Cl2	1.82(2)
C23-C24	1.539(5)	C1S-Cl1	2.227(18)
C23-H23A	0.9900	C1S-H1S	1.09(5)
C23-H23B	0.9900	Cl1-Cl2	1.04(3)
C22A-C23A	1.36(3)	Cl1-Cl10	1.17(3)

Cl1-Cl4	2.32(2)	C2SA-Cl18	1.92(6)
Cl2-Cl4	1.33(3)	C2SA-Cl15	2.08(6)
Cl2-Cl10	1.72(3)	C2SA-H2SA	1.0000
Cl2-Cl5	2.29(3)	Cl11-Cl14	2.32(3)
Cl4-Cl5	1.29(2)	Cl11-Cl12	2.32(4)
Cl5-Cl7	1.57(4)	Cl12-Cl15	1.40(3)
Cl7-Cl8	1.87(4)	Cl12-Cl14	1.79(3)
Cl8-Cl10	1.68(3)	Cl14-Cl16	1.138(18)
C2S-Cl17	1.751(4)	Cl14-Cl15	2.04(3)
C2S-Cl19	1.770(4)	Cl14-Cl18	2.46(2)
C2S-Cl13	1.789(5)	Cl15-Cl20	2.41(3)
C2S-H2S	1.0000	Cl16-Cl18	1.90(2)
C2SA-Cl11	1.85(6)	Cl18-Cl20	1.32(3)

C13-N1-C2	108.86(19)	C11-C10-C9	117.2(2)
C13-N1-H1	125.6	C5-C10-C9	122.4(2)
C2-N1-H1	125.6	C12-C11-C10	118.4(2)
N14-C2-N1	128.0(2)	C12-C11-H11	120.8
N14-C2-C3	123.1(2)	C10-C11-H11	120.8
N1-C2-C3	108.85(19)	C12-N11-C10	118.4(2)
N4-C3-C12	120.9(2)	N11-C12-C3	121.5(2)
C4-C3-C12	120.9(2)	C11-C12-C3	121.5(2)
N4-C3-C2	132.7(2)	N11-C12-C13	131.9(2)
C4-C3-C2	132.7(2)	C11-C12-C13	131.9(2)
C12-C3-C2	106.4(2)	C3-C12-C13	106.58(19)
C3-C4-C5	118.7(2)	N15-C13-N1	128.6(2)
C3-C4-H4	120.6	N15-C13-C12	122.1(2)
C5-C4-H4	120.6	N1-C13-C12	109.27(19)
C3-N4-C5	118.7(2)	C15-N14-C2	122.4(2)
N4-C5-C10	120.1(2)	C17-N15-C13	123.3(2)
C4-C5-C10	120.1(2)	N14-C15-N16#1	127.7(2)
N4-C5-C6	117.7(2)	N14-C15-C27#1	124.2(2)
C4-C5-C6	117.7(2)	N16#1-C15-C27#1	108.09(19)
C10-C5-C6	122.2(2)	C17-N16-C15#1	109.80(19)
C34-C6-C5	111.3(2)	C17-N16-H16	125.1
C34-C6-C7	107.4(2)	C15#1-N16-H16	125.1
C5-C6-C7	110.5(2)	N15-C17-N16	128.4(2)
C34-C6-C33	109.4(2)	N15-C17-C18	123.2(2)
C5-C6-C33	108.2(2)	N16-C17-C18	108.4(2)
C7-C6-C33	110.1(2)	N19-C18-C27	121.5(2)
C8-C7-C6	112.5(2)	C19-C18-C27	121.5(2)
C8-C7-H7A	109.1	N19-C18-C17	131.3(2)
C6-C7-H7A	109.1	C19-C18-C17	131.3(2)
C8-C7-H7B	109.1	C27-C18-C17	107.1(2)
C6-C7-H7B	109.1	C18-C19-C20	118.2(2)
H7A-C7-H7B	107.8	C18-C19-H19	120.9
C7-C8-C9	112.9(2)	C20-C19-H19	120.9
C7-C8-H8A	109.0	C18-N19-C20	118.2(2)
C9-C8-H8A	109.0	N19-C20-C25	120.4(2)
C7-C8-H8B	109.0	C19-C20-C25	120.4(2)
C9-C8-H8B	109.0	N19-C20-C21	117.0(2)
H8A-C8-H8B	107.8	C19-C20-C21	117.0(2)
C8-C9-C35	107.9(2)	C25-C20-C21	122.6(2)
C8-C9-C36	109.8(2)	C28-C21-C29	109.0(3)
C35-C9-C36	109.0(3)	C28-C21-C22	105.5(3)
C8-C9-C10	111.2(2)	C29-C21-C22	111.7(3)
C35-C9-C10	110.9(2)	C28-C21-C20	110.1(2)
C36-C9-C10	108.0(2)	C29-C21-C20	109.2(2)
N11-C10-C5	120.4(2)	C22-C21-C20	111.1(3)
C11-C10-C5	120.4(2)	C28-C21-C22A	127.5(7)
N11-C10-C9	117.2(2)	C29-C21-C22A	91.1(10)

C20-C21-C22A	107.5(8)	H29A-C29-H29C	109.5
C21-C22-C23	111.6(3)	H29B-C29-H29C	109.5
C21-C22-H22A	109.3	C24-C30-H30A	109.5
C23-C22-H22A	109.3	C24-C30-H30B	109.5
C21-C22-H22B	109.3	H30A-C30-H30B	109.5
C23-C22-H22B	109.3	C24-C30-H30C	109.5
H22A-C22-H22B	108.0	H30A-C30-H30C	109.5
C22-C23-C24	111.0(3)	H30B-C30-H30C	109.5
C22-C23-H23A	109.4	C24-C31-H31A	109.5
C24-C23-H23A	109.4	C24-C31-H31B	109.5
C22-C23-H23B	109.4	H31A-C31-H31B	109.5
C24-C23-H23B	109.4	C24-C31-H31C	109.5
H23A-C23-H23B	108.0	H31A-C31-H31C	109.5
C23A-C22A-C21	115.0(18)	H31B-C31-H31C	109.5
C23A-C22A-H22C	108.5	C24-C30A-H30D	109.5
C21-C22A-H22C	108.5	C24-C30A-H30E	109.5
C23A-C22A-H22D	108.5	H30D-C30A-H30E	109.5
C21-C22A-H22D	108.5	C24-C30A-H30F	109.5
H22C-C22A-H22D	107.5	H30D-C30A-H30F	109.5
C22A-C23A-C24	114.1(16)	H30E-C30A-H30F	109.5
C22A-C23A-H23C	108.7	C24-C31A-H31D	109.5
C24-C23A-H23C	108.7	C24-C31A-H31E	109.5
C22A-C23A-H23D	108.7	H31D-C31A-H31E	109.5
C24-C23A-H23D	108.7	C24-C31A-H31F	109.5
H23C-C23A-H23D	107.6	H31D-C31A-H31F	109.5
C30A-C24-C23A	113.4(13)	H31E-C31A-H31F	109.5
C30A-C24-C25	108.2(9)	C6-C33-H33A	109.5
C31-C24-C25	109.7(3)	C6-C33-H33B	109.5
C23A-C24-C25	110.2(8)	H33A-C33-H33B	109.5
C31-C24-C23	110.5(3)	C6-C33-H33C	109.5
C25-C24-C23	110.5(2)	H33A-C33-H33C	109.5
C31-C24-C30	108.9(3)	H33B-C33-H33C	109.5
C25-C24-C30	110.4(3)	C6-C34-H34A	109.5
C23-C24-C30	106.9(3)	C6-C34-H34B	109.5
C30A-C24-C31A	110.6(12)	H34A-C34-H34B	109.5
C23A-C24-C31A	105.2(11)	C6-C34-H34C	109.5
C25-C24-C31A	109.1(8)	H34A-C34-H34C	109.5
N26-C25-C20	120.1(2)	H34B-C34-H34C	109.5
C26-C25-C20	120.1(2)	C9-C35-H35A	109.5
N26-C25-C24	117.6(2)	C9-C35-H35B	109.5
C26-C25-C24	117.6(2)	H35A-C35-H35B	109.5
C20-C25-C24	122.4(2)	C9-C35-H35C	109.5
C27-C26-C25	118.7(2)	H35A-C35-H35C	109.5
C27-C26-H26	120.7	H35B-C35-H35C	109.5
C25-C26-H26	120.7	C9-C36-H36A	109.5
C27-N26-C25	118.7(2)	C9-C36-H36B	109.5
N26-C27-C18	121.1(2)	H36A-C36-H36B	109.5
C26-C27-C18	121.1(2)	C9-C36-H36C	109.5
N26-C27-C15#1	132.3(2)	H36A-C36-H36C	109.5
C26-C27-C15#1	132.3(2)	H36B-C36-H36C	109.5
C18-C27-C15#1	106.6(2)	Cl5-C1S-Cl7	68.5(16)
C21-C28-H28A	109.5	Cl5-C1S-Cl4	50.5(11)
C21-C28-H28B	109.5	Cl7-C1S-Cl4	118.9(14)
H28A-C28-H28B	109.5	Cl5-C1S-Cl8	132.2(13)
C21-C28-H28C	109.5	Cl7-C1S-Cl8	71.5(15)
H28A-C28-H28C	109.5	Cl4-C1S-Cl8	151.7(9)
H28B-C28-H28C	109.5	Cl9-C1S-Cl6	110.9(2)
C21-C29-H29A	109.5	Cl5-C1S-Cl10	130.5(11)
C21-C29-H29B	109.5	Cl7-C1S-Cl10	122.5(14)
H29A-C29-H29B	109.5	Cl4-C1S-Cl10	98.1(9)
C21-C29-H29C	109.5	Cl8-C1S-Cl10	57.7(9)

Cl9-C1S-Cl3	114.0(3)	Cl5-Cl7-Cl8	105.2(19)
Cl6-C1S-Cl3	109.8(3)	Cl10-Cl8-C1S	63.3(10)
Cl5-C1S-Cl2	92.9(13)	Cl10-Cl8-Cl7	107.3(15)
Cl7-C1S-Cl2	155.0(14)	C1S-Cl8-Cl7	48.8(10)
Cl4-C1S-Cl2	44.5(9)	Cl1-Cl10-Cl8	150(2)
Cl8-C1S-Cl2	114.7(11)	Cl1-Cl10-Cl2	36.5(12)
Cl10-C1S-Cl2	57.1(11)	Cl8-Cl10-Cl2	121.9(15)
Cl5-C1S-Cl1	117.8(11)	Cl1-Cl10-C1S	96.2(15)
Cl7-C1S-Cl1	152.2(11)	Cl8-Cl10-C1S	59.0(9)
Cl4-C1S-Cl1	72.0(6)	Cl2-Cl10-C1S	62.9(10)
Cl8-C1S-Cl1	87.9(9)	Cl17-C2S-Cl19	110.8(2)
Cl10-C1S-Cl1	31.4(8)	Cl17-C2S-Cl13	108.8(2)
Cl2-C1S-Cl1	27.7(8)	Cl19-C2S-Cl13	109.2(2)
Cl5-C1S-H1S	116(3)	Cl17-C2S-H2S	109.4
Cl7-C1S-H1S	99(3)	Cl19-C2S-H2S	109.4
Cl4-C1S-H1S	109(2)	Cl13-C2S-H2S	109.4
Cl8-C1S-H1S	94(3)	Cl11-C2SA-Cl18	116(3)
Cl9-C1S-H1S	103(2)	Cl11-C2SA-Cl15	88(3)
Cl6-C1S-H1S	114(2)	Cl18-C2SA-Cl15	91(2)
Cl10-C1S-H1S	109(3)	Cl11-C2SA-H2SA	118.1
Cl3-C1S-H1S	106(2)	Cl18-C2SA-H2SA	118.1
Cl2-C1S-H1S	105(2)	Cl15-C2SA-H2SA	118.1
Cl1-C1S-H1S	101(2)	C2SA-Cl11-Cl14	71.6(19)
Cl2-Cl1-Cl10	102(2)	C2SA-Cl11-Cl12	80(2)
Cl2-Cl1-C1S	54.2(13)	Cl14-Cl11-Cl12	45.5(9)
Cl10-Cl1-C1S	52.4(11)	Cl15-Cl12-Cl14	78.4(18)
Cl2-Cl1-Cl4	12.7(13)	Cl15-Cl12-Cl11	91.2(18)
Cl10-Cl1-Cl4	89.2(13)	Cl14-Cl12-Cl11	67.0(12)
C1S-Cl1-Cl4	42.4(4)	Cl16-Cl14-Cl12	140.9(17)
Cl1-Cl2-Cl4	157(2)	Cl16-Cl14-Cl15	102.1(14)
Cl1-Cl2-Cl10	41.6(14)	Cl12-Cl14-Cl15	42.2(11)
Cl4-Cl2-Cl10	115.7(15)	Cl16-Cl14-Cl11	130.2(13)
Cl1-Cl2-C1S	98.2(16)	Cl12-Cl14-Cl11	67.4(12)
Cl4-Cl2-C1S	60.7(9)	Cl15-Cl14-Cl11	77.6(11)
Cl10-Cl2-C1S	60.0(9)	Cl16-Cl14-Cl18	48.4(10)
Cl1-Cl2-Cl5	128.5(18)	Cl12-Cl14-Cl18	117.0(11)
Cl4-Cl2-Cl5	28.8(8)	Cl15-Cl14-Cl18	78.4(9)
Cl10-Cl2-Cl5	87.0(12)	Cl11-Cl14-Cl18	84.1(10)
C1S-Cl2-Cl5	34.2(6)	Cl12-Cl15-Cl14	59.4(17)
Cl5-Cl4-Cl2	121.5(13)	Cl12-Cl15-C2SA	101(2)
Cl5-Cl4-C1S	50.1(8)	Cl14-Cl15-C2SA	73.6(18)
Cl2-Cl4-C1S	74.8(9)	Cl12-Cl15-Cl20	115(2)
Cl5-Cl4-Cl1	111.6(11)	Cl14-Cl15-Cl20	74.4(11)
Cl2-Cl4-Cl1	10.0(10)	C2SA-Cl15-Cl20	18.9(14)
C1S-Cl4-Cl1	65.6(6)	Cl14-Cl16-Cl18	105.0(13)
C1S-Cl5-Cl4	79.4(13)	Cl20-Cl18-Cl16	111.4(17)
C1S-Cl5-Cl7	61.7(14)	Cl20-Cl18-C2SA	19.4(18)
Cl4-Cl5-Cl7	141.0(19)	Cl16-Cl18-C2SA	93.5(19)
C1S-Cl5-Cl2	52.8(9)	Cl20-Cl18-Cl14	86.0(15)
Cl4-Cl5-Cl2	29.6(9)	Cl16-Cl18-Cl14	26.6(6)
Cl7-Cl5-Cl2	112.6(16)	C2SA-Cl18-Cl14	67.4(17)
C1S-Cl7-Cl5	49.8(11)	Cl18-Cl20-Cl15	95.7(17)
C1S-Cl7-Cl8	59.6(13)		

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+1,-z+1

Table SI-9. Anisotropic displacement parameters (A^2) for ML026F1_0m. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N1	0.0131(10)	0.0183(10)	0.0147(10)	0.0016(8)	0.0015(8)	0.0013(8)
C2	0.0179(12)	0.0154(12)	0.0139(12)	-0.0022(9)	-0.0003(9)	0.0006(10)
C3	0.0167(12)	0.0150(12)	0.0149(12)	-0.0002(9)	0.0002(9)	0.0008(10)
C4	0.0167(12)	0.0184(12)	0.0202(12)	-0.0007(10)	0.0023(9)	0.0010(10)
N4	0.0167(12)	0.0184(12)	0.0202(12)	-0.0007(10)	0.0023(9)	0.0010(10)
C5	0.0208(13)	0.0205(13)	0.0199(13)	-0.0022(10)	0.0001(10)	-0.0006(11)
C6	0.0256(14)	0.0201(14)	0.0348(15)	0.0019(12)	0.0036(12)	0.0048(11)
C7	0.0317(16)	0.0253(15)	0.0430(17)	0.0067(13)	-0.0007(13)	0.0037(12)
C8	0.0312(16)	0.0294(16)	0.0407(17)	0.0159(13)	0.0001(13)	0.0002(13)
C9	0.0256(14)	0.0273(15)	0.0277(14)	0.0121(12)	0.0007(11)	0.0007(12)
C10	0.0206(13)	0.0229(13)	0.0170(12)	0.0025(10)	-0.0023(10)	-0.0023(11)
C11	0.0176(12)	0.0224(13)	0.0181(12)	0.0059(10)	0.0013(9)	0.0007(10)
N11	0.0176(12)	0.0224(13)	0.0181(12)	0.0059(10)	0.0013(9)	0.0007(10)
C12	0.0161(12)	0.0179(12)	0.0140(12)	0.0021(9)	-0.0001(9)	0.0012(10)
C13	0.0151(12)	0.0184(12)	0.0128(11)	0.0030(9)	0.0009(9)	-0.0005(10)
N14	0.0148(10)	0.0149(10)	0.0146(10)	0.0012(8)	0.0010(8)	0.0003(8)
N15	0.0151(10)	0.0193(11)	0.0171(10)	0.0047(8)	0.0033(8)	0.0016(8)
C15	0.0126(12)	0.0183(12)	0.0145(12)	-0.0012(10)	0.0004(9)	-0.0008(10)
N16	0.0138(10)	0.0161(10)	0.0156(10)	0.0023(8)	0.0006(8)	0.0005(8)
C17	0.0156(12)	0.0182(13)	0.0145(12)	0.0014(9)	0.0011(9)	-0.0004(10)
C18	0.0141(12)	0.0197(13)	0.0124(11)	-0.0010(9)	0.0011(9)	-0.0004(10)
C19	0.0185(12)	0.0186(12)	0.0160(12)	0.0022(9)	-0.0004(9)	-0.0016(10)
N19	0.0185(12)	0.0186(12)	0.0160(12)	0.0022(9)	-0.0004(9)	-0.0016(10)
C20	0.0158(12)	0.0227(13)	0.0147(12)	-0.0005(10)	-0.0006(10)	-0.0052(10)
C21	0.0219(13)	0.0247(14)	0.0225(13)	0.0026(11)	0.0043(11)	-0.0045(11)
C22	0.030(3)	0.031(2)	0.022(3)	0.005(2)	0.012(2)	-0.0058(18)
C23	0.013(2)	0.024(2)	0.038(3)	-0.0029(19)	0.0085(17)	-0.0014(16)
C22A	0.017(10)	0.084(18)	0.018(11)	0.024(11)	0.009(8)	0.016(10)
C23A	0.029(11)	0.038(12)	0.053(13)	0.002(10)	0.007(9)	-0.002(8)
C24	0.0164(12)	0.0230(13)	0.0178(13)	-0.0017(10)	0.0024(10)	0.0000(10)
C25	0.0148(12)	0.0231(13)	0.0130(11)	-0.0027(10)	-0.0014(9)	-0.0030(10)
C26	0.0145(11)	0.0177(12)	0.0164(11)	-0.0011(9)	0.0010(9)	-0.0007(9)
N26	0.0145(11)	0.0177(12)	0.0164(11)	-0.0011(9)	0.0010(9)	-0.0007(9)
C27	0.0151(12)	0.0192(12)	0.0130(11)	-0.0003(9)	0.0005(9)	-0.0003(10)
C28	0.0424(19)	0.086(3)	0.0302(17)	0.0246(17)	0.0032(14)	-0.0227(19)
C29	0.0400(18)	0.0344(17)	0.051(2)	-0.0028(15)	0.0123(15)	-0.0174(14)
C30	0.020(2)	0.043(3)	0.026(2)	0.007(3)	-0.0024(17)	0.009(3)
C31	0.022(2)	0.023(3)	0.027(3)	-0.004(2)	0.004(2)	-0.0021(19)
C30A	0.051(13)	0.031(12)	0.023(9)	0.015(10)	0.017(8)	0.032(12)
C31A	0.009(8)	0.038(14)	0.047(16)	-0.009(10)	0.007(10)	0.002(8)
C33	0.0272(16)	0.0336(17)	0.053(2)	0.0007(14)	-0.0085(14)	0.0079(13)
C34	0.0494(19)	0.0290(16)	0.050(2)	0.0006(14)	0.0182(16)	0.0109(15)
C35	0.056(2)	0.047(2)	0.0390(19)	0.0223(15)	0.0205(16)	0.0119(17)
C36	0.0308(16)	0.0363(17)	0.056(2)	0.0178(15)	-0.0056(15)	-0.0115(14)
C1S	0.064(2)	0.076(3)	0.0364(19)	-0.0010(17)	-0.0009(17)	0.0133(19)
Cl1	0.076(6)	0.081(7)	0.103(9)	0.023(5)	-0.001(5)	0.029(5)
Cl2	0.067(6)	0.080(6)	0.094(9)	0.007(5)	-0.005(6)	0.020(5)
Cl3	0.084(3)	0.0396(11)	0.0765(17)	0.0016(10)	-0.0378(18)	0.0096(13)
Cl4	0.049(4)	0.098(6)	0.058(4)	-0.012(4)	-0.008(3)	0.023(4)
Cl5	0.064(5)	0.101(7)	0.075(10)	-0.004(6)	-0.002(5)	0.015(5)
Cl6	0.0392(7)	0.0820(10)	0.0634(8)	0.0098(7)	0.0074(6)	-0.0053(7)
Cl7	0.086(10)	0.088(7)	0.057(11)	0.009(7)	0.005(9)	0.005(6)
Cl8	0.136(12)	0.112(8)	0.164(15)	-0.018(8)	0.074(11)	-0.011(7)
Cl9	0.0354(7)	0.154(2)	0.0474(8)	-0.0111(11)	0.0083(5)	-0.0282(11)
Cl10	0.084(8)	0.099(8)	0.112(9)	0.004(6)	0.031(7)	0.008(6)
C2S	0.027(2)	0.052(2)	0.043(2)	0.0160(17)	0.0086(17)	-0.0024(18)

C2SA	0.067(9)	0.091(12)	0.075(11)	-0.003(8)	0.003(7)	0.003(8)
Cl11	0.072(11)	0.119(14)	0.084(8)	-0.015(8)	0.004(7)	0.000(10)
Cl12	0.094(10)	0.103(9)	0.072(10)	-0.015(7)	0.009(8)	0.022(7)
Cl13	0.0700(10)	0.0714(11)	0.0415(7)	-0.0011(7)	0.0193(6)	0.0237(9)
Cl14	0.069(6)	0.107(8)	0.088(7)	-0.021(6)	0.004(5)	0.028(5)
Cl15	0.093(9)	0.112(9)	0.087(10)	-0.009(7)	0.010(7)	0.022(7)
Cl16	0.068(7)	0.091(8)	0.110(9)	-0.026(7)	-0.021(6)	0.030(6)
Cl17	0.0291(5)	0.0373(5)	0.0367(5)	0.0076(4)	0.0024(3)	0.0030(3)
Cl18	0.055(8)	0.083(9)	0.065(9)	0.003(7)	0.005(7)	0.006(7)
Cl19	0.0368(8)	0.0535(8)	0.0407(7)	0.0124(6)	-0.0020(7)	0.0067(7)
Cl20	0.064(8)	0.096(10)	0.084(11)	-0.005(8)	0.004(7)	0.000(7)

Table SI-10. Hydrogen coordinates and isotropic displacement parameters ($Å^2$) for ML026F1_0m.

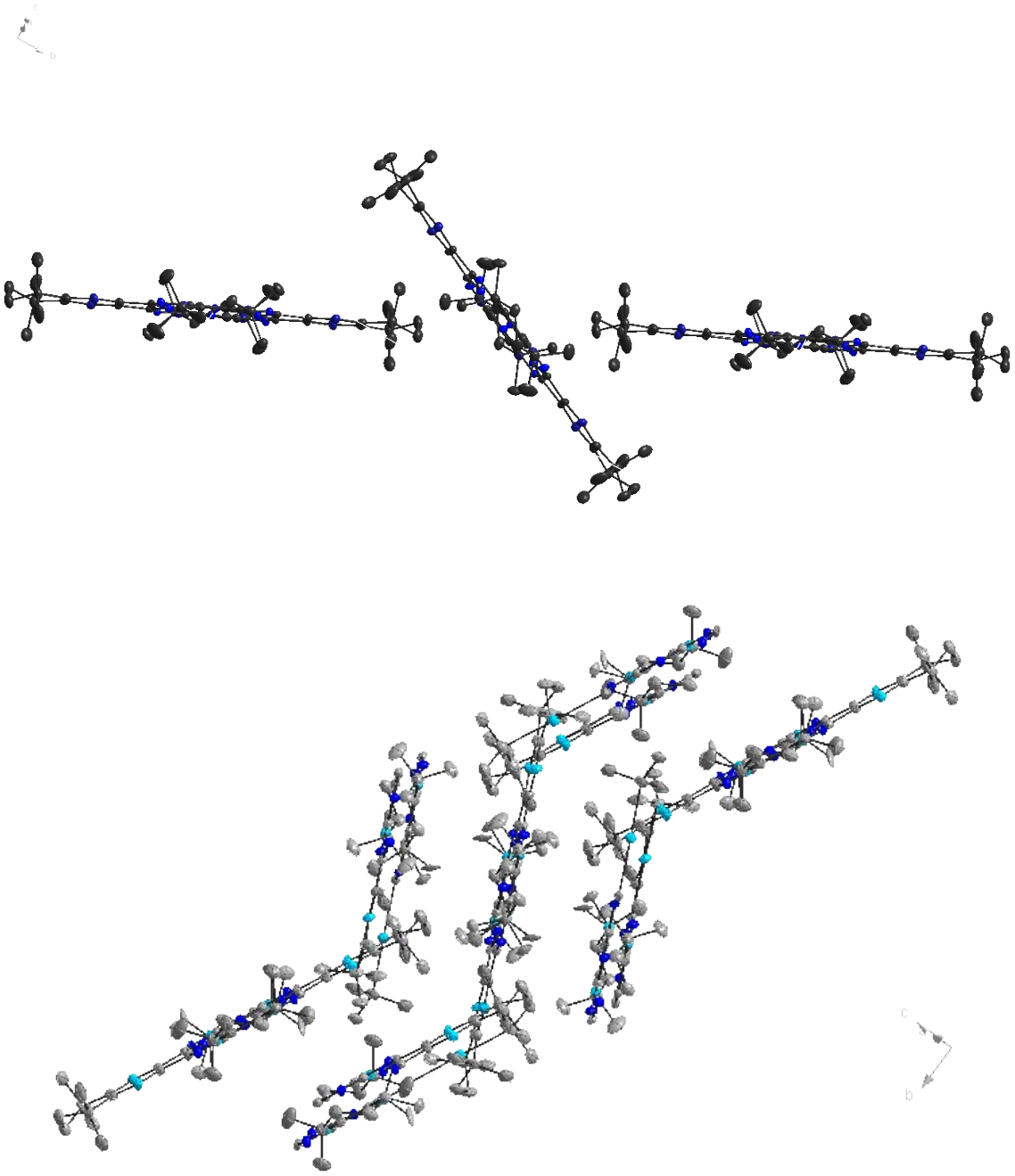
	x	y	z	U(eq)	Occupancy
H1	0.4794	0.5422	0.4702	0.018	0.5
H4	0.2271	0.7051	0.4164	0.022	0.75
H7A	0.2580	0.8864	0.2607	0.040	1
H7B	0.3550	0.8743	0.3457	0.040	1
H1S	0.373(4)	1.0953(19)	0.312(4)	0.102(15)	1
H8A	0.4332	0.8848	0.1799	0.041	1
H8B	0.3602	0.8308	0.1407	0.041	1
H11	0.5995	0.7104	0.2823	0.023	0.75
H16	0.5879	0.5008	0.4690	0.018	0.5
H19	0.8663	0.5968	0.2582	0.021	0.75
H22A	1.2186	0.5484	0.1120	0.033	0.8
H22B	1.1253	0.4993	0.0917	0.033	0.8
H23A	1.2405	0.5145	0.2865	0.030	0.8
H23B	1.2775	0.4670	0.2040	0.030	0.8
H22C	1.2323	0.5470	0.1303	0.047	0.2
H22D	1.2265	0.5440	0.2529	0.047	0.2
H23C	1.2597	0.4592	0.1783	0.048	0.2
H23D	1.1388	0.4633	0.1205	0.048	0.2
H26	0.9532	0.4134	0.3920	0.019	0.75
H28A	1.0514	0.6018	0.0414	0.079	1
H28B	0.9417	0.6131	0.1111	0.079	1
H28C	0.9603	0.5516	0.0589	0.079	1
H29A	1.1697	0.6364	0.1945	0.062	1
H29B	1.1553	0.6048	0.3031	0.062	1
H29C	1.0540	0.6438	0.2577	0.062	1
H30A	1.1319	0.3888	0.3999	0.044	0.8
H30B	1.1820	0.4506	0.4294	0.044	0.8
H30C	1.2559	0.4074	0.3613	0.044	0.8
H31A	1.0472	0.3708	0.2317	0.036	0.8
H31B	1.1716	0.3788	0.1839	0.036	0.8
H31C	1.0655	0.4141	0.1375	0.036	0.8
H30D	1.1548	0.4244	0.4188	0.052	0.2
H30E	1.2052	0.4859	0.3880	0.052	0.2
H30F	1.2664	0.4285	0.3491	0.052	0.2
H31D	1.0643	0.3619	0.2988	0.047	0.2
H31E	1.1654	0.3646	0.2169	0.047	0.2
H31F	1.0392	0.3844	0.1844	0.047	0.2
H33A	0.1170	0.8159	0.2154	0.057	1
H33B	0.1247	0.7510	0.2555	0.057	1
H33C	0.2114	0.7734	0.1700	0.057	1
H34A	0.1391	0.8502	0.4031	0.064	1
H34B	0.2413	0.8240	0.4712	0.064	1
H34C	0.1392	0.7834	0.4325	0.064	1
H35A	0.6271	0.7659	0.1574	0.071	1
H35B	0.5826	0.8220	0.0982	0.071	1
H35C	0.5084	0.7643	0.0952	0.071	1
H36A	0.6457	0.8143	0.3217	0.062	1
H36B	0.5421	0.8502	0.3689	0.062	1
H36C	0.6081	0.8740	0.2704	0.062	1
H2S	0.7907	0.6764	0.4201	0.048	0.9
H2SA	1.0422	0.7411	0.5841	0.093	0.1

Table SI-11. Torsion angles [°] for ML026F1_0m.

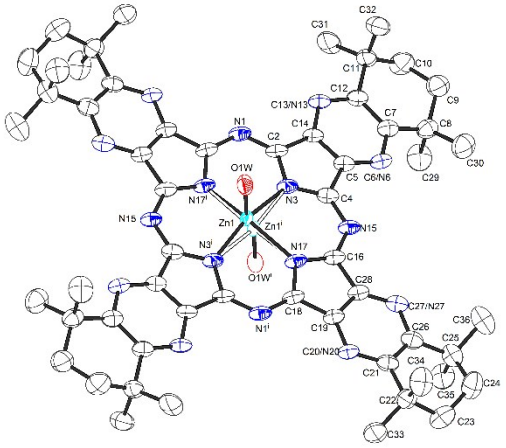
C13-N1-C2-N14	-178.1(2)	C2-C3-C12-C11	179.5(2)
C13-N1-C2-C3	0.4(3)	N4-C3-C12-C13	179.6(2)
N14-C2-C3-N4	-1.0(4)	C4-C3-C12-C13	179.6(2)
N1-C2-C3-N4	-179.5(2)	C2-C3-C12-C13	0.5(2)
N14-C2-C3-C4	-1.0(4)	C2-N1-C13-N15	-178.1(2)
N1-C2-C3-C4	-179.5(2)	C2-N1-C13-C12	-0.1(3)
N14-C2-C3-C12	178.0(2)	N11-C12-C13-N15	-1.0(4)
N1-C2-C3-C12	-0.5(3)	C11-C12-C13-N15	-1.0(4)
C12-C3-C4-C5	0.8(3)	C3-C12-C13-N15	177.9(2)
C2-C3-C4-C5	179.7(2)	N11-C12-C13-N1	-179.2(2)
C12-C3-N4-C5	0.8(3)	C11-C12-C13-N1	-179.2(2)
C2-C3-N4-C5	179.7(2)	C3-C12-C13-N1	-0.3(3)
C3-N4-C5-C10	0.5(3)	N1-C2-N14-C15	0.8(4)
C3-N4-C5-C6	177.4(2)	C3-C2-N14-C15	-177.5(2)
C3-C4-C5-C10	0.5(3)	N1-C13-N15-C17	0.5(4)
C3-C4-C5-C6	177.4(2)	C12-C13-N15-C17	-177.4(2)
N4-C5-C6-C34	44.4(3)	C2-N14-C15-N16#1	-3.8(4)
C4-C5-C6-C34	44.4(3)	C2-N14-C15-C27#1	176.5(2)
C10-C5-C6-C34	-138.8(3)	C13-N15-C17-N16	-3.7(4)
N4-C5-C6-C7	163.7(2)	C13-N15-C17-C18	176.0(2)
C4-C5-C6-C7	163.7(2)	C15#1-N16-C17-N15	-178.2(2)
C10-C5-C6-C7	-19.5(3)	C15#1-N16-C17-C18	2.1(3)
N4-C5-C6-C33	-75.7(3)	N15-C17-C18-N19	-3.4(4)
C4-C5-C6-C33	-75.7(3)	N16-C17-C18-N19	176.3(2)
C10-C5-C6-C33	101.0(3)	N15-C17-C18-C19	-3.4(4)
C34-C6-C7-C8	169.3(3)	N16-C17-C18-C19	176.3(2)
C5-C6-C7-C8	47.8(3)	N15-C17-C18-C27	178.6(2)
C33-C6-C7-C8	-71.7(3)	N16-C17-C18-C27	-1.7(3)
C6-C7-C8-C9	-62.9(3)	C27-C18-C19-C20	0.3(3)
C7-C8-C9-C35	166.0(3)	C17-C18-C19-C20	-177.4(2)
C7-C8-C9-C36	-75.4(3)	C27-C18-N19-C20	0.3(3)
C7-C8-C9-C10	44.1(3)	C17-C18-N19-C20	-177.4(2)
N4-C5-C10-N11	-1.4(4)	C18-N19-C20-C25	-1.7(3)
C6-C5-C10-N11	-178.1(2)	C18-N19-C20-C21	178.0(2)
C4-C5-C10-C11	-1.4(4)	C18-C19-C20-C25	-1.7(3)
C6-C5-C10-C11	-178.1(2)	C18-C19-C20-C21	178.0(2)
N4-C5-C10-C9	-179.1(2)	N19-C20-C21-C28	-50.0(3)
C4-C5-C10-C9	-179.1(2)	C19-C20-C21-C28	-50.0(3)
C6-C5-C10-C9	4.2(4)	C25-C20-C21-C28	129.7(3)
C8-C9-C10-N11	166.5(2)	N19-C20-C21-C29	69.7(3)
C35-C9-C10-N11	46.4(3)	C19-C20-C21-C29	69.7(3)
C36-C9-C10-N11	-72.9(3)	C25-C20-C21-C29	-110.6(3)
C8-C9-C10-C11	166.5(2)	C19-C20-C21-C22	-166.6(3)
C35-C9-C10-C11	46.4(3)	C25-C20-C21-C22	13.1(4)
C36-C9-C10-C11	-72.9(3)	N19-C20-C21-C22A	167.3(9)
C8-C9-C10-C5	-15.7(3)	C25-C20-C21-C22A	-13.0(10)
C35-C9-C10-C5	-135.9(3)	C28-C21-C22-C23	-164.4(3)
C36-C9-C10-C5	104.8(3)	C29-C21-C22-C23	77.3(4)
C5-C10-C11-C12	0.9(4)	C20-C21-C22-C23	-45.0(4)
C9-C10-C11-C12	178.7(2)	C21-C22-C23-C24	65.6(4)
C5-C10-N11-C12	0.9(4)	C28-C21-C22A-C23A	-89.0(17)
C9-C10-N11-C12	178.7(2)	C29-C21-C22A-C23A	155.8(16)
C10-N11-C12-C3	0.5(4)	C20-C21-C22A-C23A	45.2(18)
C10-N11-C12-C13	179.3(2)	C21-C22A-C23A-C24	-65(2)
C10-C11-C12-C3	0.5(4)	C22A-C23A-C24-C30A	-75(2)
C10-C11-C12-C13	179.3(2)	C22A-C23A-C24-C25	46.6(19)
N4-C3-C12-N11	-1.4(4)	C22A-C23A-C24-C31A	164.1(18)
C2-C3-C12-N11	179.5(2)	C22-C23-C24-C31	72.6(4)
C4-C3-C12-C11	-1.4(4)	C22-C23-C24-C25	-48.9(4)

C22-C23-C24-C30	-169.0(4)	Cl8-C1S-Cl2-Cl5	-139.9(13)
N19-C20-C25-N26	1.9(3)	Cl10-C1S-Cl2-Cl5	-137.8(12)
C21-C20-C25-N26	-177.8(2)	Cl1-C1S-Cl2-Cl5	-155.2(16)
C19-C20-C25-C26	1.9(3)	Cl1-Cl2-Cl4-Cl5	-4(6)
C21-C20-C25-C26	-177.8(2)	Cl10-Cl2-Cl4-Cl5	-6(2)
N19-C20-C25-C24	-179.7(2)	C1S-Cl2-Cl4-Cl5	18.9(14)
C19-C20-C25-C24	-179.7(2)	Cl1-Cl2-Cl4-C1S	-23(5)
C21-C20-C25-C24	0.6(3)	Cl10-Cl2-Cl4-C1S	-24.9(13)
C30A-C24-C25-N26	-71.5(9)	Cl5-Cl2-Cl4-C1S	-18.9(14)
C23A-C24-C25-N26	164.0(9)	Cl10-Cl2-Cl4-Cl1	-2(4)
C31A-C24-C25-N26	49.0(9)	C1S-Cl2-Cl4-Cl1	23(5)
C31-C24-C25-C26	73.7(3)	Cl5-Cl2-Cl4-Cl1	4(6)
C23-C24-C25-C26	-164.2(3)	Cl7-C1S-Cl4-Cl5	-2.7(17)
C30-C24-C25-C26	-46.3(3)	Cl8-C1S-Cl4-Cl5	-108(2)
C30A-C24-C25-C20	110.0(9)	Cl10-C1S-Cl4-Cl5	-137.0(14)
C31-C24-C25-C20	-104.8(3)	Cl2-C1S-Cl4-Cl5	-158.9(16)
C23A-C24-C25-C20	-14.4(9)	Cl1-C1S-Cl4-Cl5	-154.6(12)
C23-C24-C25-C20	17.3(3)	Cl5-C1S-Cl4-Cl2	158.9(16)
C30-C24-C25-C20	135.2(3)	Cl7-C1S-Cl4-Cl2	156.2(15)
C31A-C24-C25-C20	-129.5(9)	Cl8-C1S-Cl4-Cl2	51(2)
C20-C25-C26-C27	-0.6(3)	Cl10-C1S-Cl4-Cl2	21.8(13)
C24-C25-C26-C27	-179.1(2)	Cl1-C1S-Cl4-Cl2	4.2(10)
C20-C25-N26-C27	-0.6(3)	Cl5-C1S-Cl4-Cl1	154.6(12)
C24-C25-N26-C27	-179.1(2)	Cl7-C1S-Cl4-Cl1	152.0(13)
C25-N26-C27-C18	-0.8(3)	Cl8-C1S-Cl4-Cl1	47(2)
C25-N26-C27-C15#1	177.3(2)	Cl10-C1S-Cl4-Cl1	17.6(9)
C25-C26-C27-C18	-0.8(3)	Cl2-C1S-Cl4-Cl1	-4.2(10)
C25-C26-C27-C15#1	177.3(2)	Cl7-C1S-Cl5-Cl4	177.5(16)
N19-C18-C27-N26	0.9(4)	Cl8-C1S-Cl5-Cl4	142.4(14)
C17-C18-C27-N26	179.1(2)	Cl10-C1S-Cl5-Cl4	62.4(18)
C19-C18-C27-C26	0.9(4)	Cl2-C1S-Cl5-Cl4	14.7(11)
C17-C18-C27-C26	179.1(2)	Cl1-C1S-Cl5-Cl4	27.4(13)
N19-C18-C27-C15#1	-177.6(2)	Cl4-C1S-Cl5-Cl7	-177.5(16)
C19-C18-C27-C15#1	-177.6(2)	Cl8-C1S-Cl5-Cl7	-35.0(18)
C17-C18-C27-C15#1	0.6(2)	Cl10-C1S-Cl5-Cl7	-115.0(18)
Cl10-Cl1-Cl2-Cl4	-3(6)	Cl2-C1S-Cl5-Cl7	-162.8(13)
C1S-Cl1-Cl2-Cl4	20(4)	Cl1-C1S-Cl5-Cl7	-150.1(12)
C1S-Cl1-Cl2-Cl10	22.8(17)	Cl7-C1S-Cl5-Cl2	162.8(13)
Cl4-Cl1-Cl2-Cl10	3(6)	Cl4-C1S-Cl5-Cl2	-14.7(11)
Cl10-Cl1-Cl2-C1S	-22.8(17)	Cl8-C1S-Cl5-Cl2	127.8(15)
Cl4-Cl1-Cl2-C1S	-20(4)	Cl10-C1S-Cl5-Cl2	47.8(15)
Cl10-Cl1-Cl2-Cl5	-5(2)	Cl1-C1S-Cl5-Cl2	12.7(9)
C1S-Cl1-Cl2-Cl5	17.6(10)	Cl2-Cl4-Cl5-C1S	-24.1(18)
Cl4-Cl1-Cl2-Cl5	-2(4)	Cl1-Cl4-Cl5-C1S	-24.8(11)
Cl5-C1S-Cl2-Cl1	155.2(16)	Cl2-Cl4-Cl5-Cl7	-21(4)
Cl7-C1S-Cl2-Cl1	115(3)	C1S-Cl4-Cl5-Cl7	4(2)
Cl4-C1S-Cl2-Cl1	171(2)	Cl1-Cl4-Cl5-Cl7	-21(3)
Cl8-C1S-Cl2-Cl1	15.3(19)	C1S-Cl4-Cl5-Cl2	24.1(18)
Cl10-C1S-Cl2-Cl1	17.3(14)	Cl1-Cl4-Cl5-Cl2	-0.7(11)
Cl5-C1S-Cl2-Cl4	-16.2(12)	Cl4-C1S-Cl7-Cl5	2.2(14)
Cl7-C1S-Cl2-Cl4	-57(3)	Cl8-C1S-Cl7-Cl5	153.4(14)
Cl8-C1S-Cl2-Cl4	-156.1(13)	Cl10-C1S-Cl7-Cl5	125.1(14)
Cl10-C1S-Cl2-Cl4	-154.0(15)	Cl2-C1S-Cl7-Cl5	44(3)
Cl1-C1S-Cl2-Cl4	-171(2)	Cl1-C1S-Cl7-Cl5	109(3)
Cl5-C1S-Cl2-Cl10	137.8(12)	Cl5-C1S-Cl7-Cl8	-153.4(14)
Cl7-C1S-Cl2-Cl10	97(3)	Cl4-C1S-Cl7-Cl8	-151.2(11)
Cl4-C1S-Cl2-Cl10	154.0(15)	Cl10-C1S-Cl7-Cl8	-28.2(17)
Cl8-C1S-Cl2-Cl10	-2.1(15)	Cl2-C1S-Cl7-Cl8	-109(3)
Cl1-C1S-Cl2-Cl10	-17.3(14)	Cl1-C1S-Cl7-Cl8	-44(3)
Cl7-C1S-Cl2-Cl5	-41(3)	Cl4-Cl5-Cl7-C1S	-4(2)
Cl4-C1S-Cl2-Cl5	16.2(12)	Cl2-Cl5-Cl7-C1S	-14.8(11)

C1S-Cl5-Cl7-Cl8	23.6(13)
Cl4-Cl5-Cl7-Cl8	20(3)
Cl2-Cl5-Cl7-Cl8	9(2)
Cl5-C1S-Cl8-Cl10	-117.6(17)
Cl7-C1S-Cl8-Cl10	-151.8(17)
Cl4-C1S-Cl8-Cl10	-35(3)
Cl2-C1S-Cl8-Cl10	2.1(15)
Cl1-C1S-Cl8-Cl10	9.1(11)
Cl5-C1S-Cl8-Cl7	34.3(19)
Cl4-C1S-Cl8-Cl7	117(2)
Cl10-C1S-Cl8-Cl7	151.8(17)
Cl2-C1S-Cl8-Cl7	153.9(14)
Cl1-C1S-Cl8-Cl7	160.9(13)
C1S-Cl7-Cl8-Cl10	26.2(16)
Cl5-Cl7-Cl8-Cl10	5(2)
Cl5-Cl7-Cl8-C1S	-20.8(11)
Cl2-Cl1-Cl10-Cl8	55(4)
C1S-Cl1-Cl10-Cl8	31(3)
Cl4-Cl1-Cl10-Cl8	54(4)
C1S-Cl1-Cl10-Cl2	-23.4(18)
Cl4-Cl1-Cl10-Cl2	-0.6(13)
Cl2-Cl1-Cl10-C1S	23.4(17)
Cl4-Cl1-Cl10-C1S	22.8(9)
C1S-Cl8-Cl10-Cl1	-37(4)
Cl7-Cl8-Cl10-Cl1	-59(5)
C1S-Cl8-Cl10-Cl2	-2.3(17)
Cl7-Cl8-Cl10-Cl2	-24(3)
Cl7-Cl8-Cl10-C1S	-21.8(13)
Cl4-Cl2-Cl10-Cl1	179(2)
C1S-Cl2-Cl10-Cl1	154(2)
Cl5-Cl2-Cl10-Cl1	175.9(19)
Cl1-Cl2-Cl10-Cl8	-151(3)
Cl4-Cl2-Cl10-Cl8	27(3)
C1S-Cl2-Cl10-Cl8	2.2(17)
Cl5-Cl2-Cl10-Cl8	24(2)
Cl1-Cl2-Cl10-C1S	-154(2)
Cl4-Cl2-Cl10-C1S	25.1(14)
Cl5-Cl2-Cl10-C1S	22.2(6)
Cl5-C1S-Cl10-Cl1	-77(2)
Cl7-C1S-Cl10-Cl1	-165.6(18)
Cl4-C1S-Cl10-Cl1	-33.5(15)
Cl8-C1S-Cl10-Cl1	162(2)
Cl2-C1S-Cl10-Cl1	-15.4(12)
Cl5-C1S-Cl10-Cl8	120.4(18)
Cl7-C1S-Cl10-Cl8	32(2)
Cl4-C1S-Cl10-Cl8	164.1(13)
Cl2-C1S-Cl10-Cl8	-177.8(16)
Cl1-C1S-Cl10-Cl8	-162(2)
Cl5-C1S-Cl10-Cl2	-61.8(18)
Cl7-C1S-Cl10-Cl2	-150.2(17)
Cl4-C1S-Cl10-Cl2	-18.1(10)
Cl8-C1S-Cl10-Cl2	177.8(16)
Cl1-C1S-Cl10-Cl2	15.4(12)
Cl18-C2SA-Cl11-Cl14	-42(3)
Cl15-C2SA-Cl11-Cl14	48.2(15)
Cl18-C2SA-Cl11-Cl12	-89(3)
Cl15-C2SA-Cl11-Cl12	1.9(17)
Cl15-Cl12-Cl14-Cl16	-30(3)
Cl11-Cl12-Cl14-Cl16	-127(2)
Cl11-Cl12-Cl14-Cl15	-96.4(16)
Cl15-Cl12-Cl14-Cl11	96.4(16)
Cl15-Cl12-Cl14-Cl18	26.1(18)
Cl11-Cl12-Cl14-Cl18	-70.3(12)
Cl11-Cl12-Cl15-Cl14	66.3(11)
Cl14-Cl12-Cl15-C2SA	-64(2)
Cl11-Cl12-Cl15-C2SA	3(2)
Cl14-Cl12-Cl15-Cl20	-51.3(17)
Cl11-Cl12-Cl15-Cl20	15(2)
Cl12-Cl14-Cl16-Cl18	83(2)
Cl15-Cl14-Cl16-Cl18	62.3(15)
Cl11-Cl14-Cl16-Cl18	-22(3)
Cl16-Cl18-Cl20-Cl15	-27.6(18)
C2SA-Cl18-Cl20-Cl15	-52(6)
Cl14-Cl18-Cl20-Cl15	-35.9(11)



1.7.3 **Crystal Structure of A_2B_2 N_4-[Pc*Zn·H_2O]**



Habitus, colour	prism, dark	
Crystal size	0.27 x 0.06 x 0.03 mm^3	
Crystal system	Monoclinic	
Space group	$P2_1/c$	Z = 2
Unit cell dimensions	a = 6.0419(5) Å	α= 90°.
	b = 16.2175(13) Å	β= 95.305(3)°.
	c = 31.008(2) Å	γ = 90°.
Volume	3025.3(4) $Å^3$	
Cell determination	9556 peaks with Theta 2.3 to 25.2°.	
Empirical formula	C_{60} H_{70} N_{12} O Zn	
Moiety formula	C_{60} H_{70} N_{12} O Zn	
Formula weight	1040.65	
Density (calculated)	1.142 Mg/m^3	
Absorption coefficient	0.454 mm^{-1}	
F(000)	1104	

Solution and refinement:	
Reflections collected	32818
Independent reflections	5598 [R(int) = 0.0711]
Completeness to theta = 25.242°	99.9 %
Observed reflections	4276[I > 2(I)]
Reflections used for refinement	5598
Absorption correction	Numerical Mu Calculated[12]
Max. and min. transmission	0.99 and 0.89
Largest diff. peak and hole	0.288 and -0.347 e.$Å^{-3}$
Solution	Direct methods
Refinement	Full-matrix least-squares on F^2
Treatment of hydrogen atoms	Calculated positions, constr. ref.
Programs used	XT V2014/1 (Bruker AXS Inc., 2014)[13]
	SHELXL-2014/7 (Sheldrick, 2014)[14]
	DIAMOND (Crystal Impact)[11]
	ShelXle (Hübschle, Sheldrick, Dittrich, 2011)[15]
Data / restraints / parameters	5598 / 0 / 353
Goodness-of-fit on F^2	1.021
R index (all data)	wR2 = 0.1467
R index conventional [I>2sigma(I)]	R1 = 0.0580

Table SI-12. Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for mL105c2_0m_sq. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)	Occupancy
Zn1	1.49975(18)	0.51807(4)	0.50622(3)	0.0242(2)	0.5
N1	1.5282(5)	0.39227(14)	0.59501(8)	0.0354(6)	1
C2	1.3557(6)	0.37918(17)	0.56599(9)	0.0336(7)	1
N3	1.3123(5)	0.41696(14)	0.52645(8)	0.0330(6)	1
C4	1.1271(6)	0.38191(18)	0.50470(10)	0.0357(8)	1
C5	1.0459(5)	0.31799(17)	0.53226(9)	0.0324(7)	1
C6	0.8816(5)	0.26266(17)	0.52335(9)	0.0369(7)	0.5
N6	0.8816(5)	0.26266(17)	0.52335(9)	0.0369(7)	0.5
C7	0.8475(6)	0.20533(19)	0.55472(10)	0.0378(8)	1
C8	0.6829(6)	0.1355(2)	0.54251(11)	0.0459(9)	1
C9	0.6011(7)	0.0982(3)	0.58286(13)	0.0594(11)	1
C10	0.7865(8)	0.0790(2)	0.61729(13)	0.0609(11)	1
C11	0.9179(6)	0.1542(2)	0.63326(11)	0.0446(9)	1
C12	0.9761(6)	0.20836(19)	0.59537(10)	0.0362(8)	1
C13	1.1473(5)	0.26387(16)	0.60328(9)	0.0362(7)	0.5
N13	1.1473(5)	0.26387(16)	0.60328(9)	0.0362(7)	0.5
C14	1.1822(5)	0.31757(16)	0.57052(9)	0.0306(7)	1
N15	1.0358(5)	0.39883(15)	0.46520(8)	0.0350(6)	1
C16	1.1103(6)	0.45652(18)	0.43907(9)	0.0345(7)	1
N17	1.2882(5)	0.50688(15)	0.44710(8)	0.0348(6)	1
C18	1.3091(6)	0.55471(17)	0.41116(9)	0.0335(7)	1
C19	1.1260(6)	0.53481(17)	0.37847(9)	0.0339(7)	1
C20	1.0650(5)	0.56503(17)	0.33820(9)	0.0357(7)	0.5
N20	1.0650(5)	0.56503(17)	0.33820(9)	0.0357(7)	0.5
C21	0.8899(6)	0.52815(19)	0.31471(10)	0.0392(8)	1
C22	0.8002(6)	0.5685(2)	0.27201(11)	0.0448(8)	1
C23	0.6709(8)	0.5058(3)	0.24279(13)	0.0640(11)	1
C24	0.5072(8)	0.4553(3)	0.26589(15)	0.0672(12)	1
C25	0.6171(6)	0.4051(2)	0.30292(12)	0.0492(9)	1
C26	0.7813(6)	0.4578(2)	0.33098(11)	0.0417(8)	1
C27	0.8404(5)	0.43133(18)	0.37254(9)	0.0404(7)	0.5
N27	0.8404(5)	0.43133(18)	0.37254(9)	0.0404(7)	0.5
C28	1.0081(6)	0.47124(18)	0.39565(10)	0.0347(7)	1
C29	0.8078(7)	0.0725(2)	0.51705(15)	0.0657(12)	1
C30	0.4821(7)	0.1666(3)	0.51310(14)	0.0660(12)	1
C31	1.1256(7)	0.1267(3)	0.66111(13)	0.0644(12)	1
C32	0.7765(7)	0.2076(3)	0.66089(12)	0.0589(11)	1
C33	0.9850(7)	0.6044(3)	0.24761(13)	0.0650(12)	1
C34	0.6459(7)	0.6390(2)	0.28378(15)	0.0665(12)	1
C35	0.7495(7)	0.3332(2)	0.28583(14)	0.0601(11)	1
C36	0.4342(8)	0.3688(3)	0.32869(17)	0.0783(14)	1
O1W	1.3888(7)	0.6241(3)	0.53911(14)	0.0403(11)	0.5

Table SI-13. Bond lengths [Å] and angles [°] for mL105c2_0m_sq.

Zn1-Zn1#1	0.7019(11)	C20-H20	0.9400
Zn1-N17#1	1.886(3)	C21-C26	1.431(5)
Zn1-N3#1	1.908(3)	C21-C22	1.531(5)
Zn1-N3	2.121(3)	C22-C33	1.521(5)
Zn1-O1W	2.138(4)	C22-C23	1.528(5)
Zn1-N17	2.143(3)	C22-C34	1.540(5)
N1-C2	1.330(4)	C23-C24	1.514(6)
N1-C18#1	1.333(4)	C23-H23A	0.9800
C2-N3	1.374(4)	C23-H23B	0.9800
C2-C14	1.464(4)	C24-C25	1.510(6)
N3-C4	1.375(4)	C24-H24A	0.9800
N3-Zn1#1	1.908(3)	C24-H24B	0.9800
C4-N15	1.325(4)	C25-C26	1.521(5)
C4-C5	1.457(4)	C25-C35	1.537(5)
C5-C6	1.348(4)	C25-C36	1.540(6)
C5-C14	1.380(4)	C26-C27	1.373(5)
C6-C7	1.375(4)	C27-C28	1.351(4)
C6-H6	0.9400	C27-H27	0.9400
C7-C12	1.419(5)	C29-H29A	0.9700
C7-C8	1.531(5)	C29-H29B	0.9700
C8-C9	1.513(5)	C29-H29C	0.9700
C8-C29	1.531(5)	C30-H30A	0.9700
C8-C30	1.534(5)	C30-H30B	0.9700
C9-C10	1.507(6)	C30-H30C	0.9700
C9-H9A	0.9800	C31-H31A	0.9700
C9-H9B	0.9800	C31-H31B	0.9700
C10-C11	1.514(5)	C31-H31C	0.9700
C10-H10A	0.9800	C32-H32A	0.9700
C10-H10B	0.9800	C32-H32B	0.9700
C11-C31	1.523(5)	C32-H32C	0.9700
C11-C32	1.533(5)	C33-H33A	0.9700
C11-C12	1.533(4)	C33-H33B	0.9700
C12-C13	1.376(4)	C33-H33C	0.9700
C13-C14	1.369(4)	C34-H34A	0.9700
C13-H13	0.9400	C34-H34B	0.9700
N15-C16	1.343(4)	C34-H34C	0.9700
C16-N17	1.355(4)	C35-H35A	0.9700
C16-C28	1.448(4)	C35-H35B	0.9700
N17-C18	1.373(4)	C35-H35C	0.9700
N17-Zn1#1	1.886(3)	C36-H36A	0.9700
C18-N1#1	1.333(4)	C36-H36B	0.9700
C18-C19	1.465(5)	C36-H36C	0.9700
C19-C20	1.360(4)	O1W-H1WA	0.8643
C19-C28	1.387(4)	O1W-H1WB	0.8644
C20-C21	1.366(5)		

Zn1#1-Zn1-N17#1	101.9(2)	N3-Zn1-N17	83.97(10)
Zn1#1-Zn1-N3#1	97.8(2)	O1W-Zn1-N17	106.71(14)
N17#1-Zn1-N3#1	97.51(12)	C2-N1-C18#1	123.2(2)
Zn1#1-Zn1-N3	63.01(17)	N1-C2-N3	127.3(3)
N17#1-Zn1-N3	87.16(11)	N1-C2-C14	124.6(3)
N3#1-Zn1-N3	160.86(4)	N3-C2-C14	108.1(3)
Zn1#1-Zn1-O1W	162.0(2)	C2-N3-C4	109.4(3)
N17#1-Zn1-O1W	91.56(14)	C2-N3-Zn1#1	130.3(2)
N3#1-Zn1-O1W	92.15(14)	C4-N3-Zn1#1	117.73(19)
N3-Zn1-O1W	106.33(14)	C2-N3-Zn1	123.1(2)
Zn1#1-Zn1-N17	59.45(17)	C4-N3-Zn1	127.40(19)
N17#1-Zn1-N17	161.30(4)	Zn1#1-N3-Zn1	19.14(4)
N3#1-Zn1-N17	85.97(11)	N15-C4-N3	128.2(3)

N15-C4-C5	123.8(3)	C19-C20-H20	121.2
N3-C4-C5	108.0(3)	C21-C20-H20	121.2
C6-C5-C14	122.9(3)	C20-C21-C26	121.3(3)
C6-C5-C4	129.4(3)	C20-C21-C22	118.0(3)
C14-C5-C4	107.5(3)	C26-C21-C22	120.6(3)
C5-C6-C7	117.4(3)	C33-C22-C23	108.5(3)
C5-C6-H6	121.3	C33-C22-C21	112.1(3)
C7-C6-H6	121.3	C23-C22-C21	110.4(3)
C6-C7-C12	120.0(3)	C33-C22-C34	108.8(3)
C6-C7-C8	117.5(3)	C23-C22-C34	110.3(3)
C12-C7-C8	122.3(3)	C21-C22-C34	106.6(3)
C9-C8-C29	111.9(3)	C24-C23-C22	113.6(3)
C9-C8-C7	110.2(3)	C24-C23-H23A	108.9
C29-C8-C7	106.3(3)	C22-C23-H23A	108.9
C9-C8-C30	108.8(3)	C24-C23-H23B	108.9
C29-C8-C30	108.2(3)	C22-C23-H23B	108.9
C7-C8-C30	111.3(3)	H23A-C23-H23B	107.7
C10-C9-C8	112.9(3)	C25-C24-C23	113.0(4)
C10-C9-H9A	109.0	C25-C24-H24A	109.0
C8-C9-H9A	109.0	C23-C24-H24A	109.0
C10-C9-H9B	109.0	C25-C24-H24B	109.0
C8-C9-H9B	109.0	C23-C24-H24B	109.0
H9A-C9-H9B	107.8	H24A-C24-H24B	107.8
C9-C10-C11	113.5(3)	C24-C25-C26	110.5(3)
C9-C10-H10A	108.9	C24-C25-C35	110.7(3)
C11-C10-H10A	108.9	C26-C25-C35	106.9(3)
C9-C10-H10B	108.9	C24-C25-C36	108.4(4)
C11-C10-H10B	108.9	C26-C25-C36	112.3(3)
H10A-C10-H10B	107.7	C35-C25-C36	108.1(3)
C10-C11-C31	109.2(3)	C27-C26-C21	119.5(3)
C10-C11-C32	109.6(3)	C27-C26-C25	117.4(3)
C31-C11-C32	108.7(3)	C21-C26-C25	122.8(3)
C10-C11-C12	111.2(3)	C28-C27-C26	117.7(3)
C31-C11-C12	111.5(3)	C28-C27-H27	121.1
C32-C11-C12	106.5(3)	C26-C27-H27	121.1
C13-C12-C7	121.5(3)	C27-C28-C19	122.6(3)
C13-C12-C11	117.4(3)	C27-C28-C16	130.4(3)
C7-C12-C11	121.0(3)	C19-C28-C16	106.8(3)
C14-C13-C12	116.6(3)	C8-C29-H29A	109.5
C14-C13-H13	121.7	C8-C29-H29B	109.5
C12-C13-H13	121.7	H29A-C29-H29B	109.5
C13-C14-C5	121.4(3)	C8-C29-H29C	109.5
C13-C14-C2	131.8(3)	H29A-C29-H29C	109.5
C5-C14-C2	106.8(2)	H29B-C29-H29C	109.5
C4-N15-C16	124.6(3)	C8-C30-H30A	109.5
N15-C16-N17	127.9(3)	C8-C30-H30B	109.5
N15-C16-C28	122.6(3)	H30A-C30-H30B	109.5
N17-C16-C28	109.5(3)	C8-C30-H30C	109.5
C16-N17-C18	108.8(3)	H30A-C30-H30C	109.5
C16-N17-Zn1#1	118.9(2)	H30B-C30-H30C	109.5
C18-N17-Zn1#1	129.6(2)	C11-C31-H31A	109.5
C16-N17-Zn1	127.5(2)	C11-C31-H31B	109.5
C18-N17-Zn1	123.7(2)	H31A-C31-H31B	109.5
Zn1#1-N17-Zn1	18.69(4)	C11-C31-H31C	109.5
N1#1-C18-N17	127.2(3)	H31A-C31-H31C	109.5
N1#1-C18-C19	124.2(3)	H31B-C31-H31C	109.5
N17-C18-C19	108.5(3)	C11-C32-H32A	109.5
C20-C19-C28	121.0(3)	C11-C32-H32B	109.5
C20-C19-C18	132.7(3)	H32A-C32-H32B	109.5
C28-C19-C18	106.2(3)	C11-C32-H32C	109.5
C19-C20-C21	117.5(3)	H32A-C32-H32C	109.5

H32B-C32-H32C	109.5	C25-C35-H35B	109.5
C22-C33-H33A	109.5	H35A-C35-H35B	109.5
C22-C33-H33B	109.5	C25-C35-H35C	109.5
H33A-C33-H33B	109.5	H35A-C35-H35C	109.5
C22-C33-H33C	109.5	H35B-C35-H35C	109.5
H33A-C33-H33C	109.5	C25-C36-H36A	109.5
H33B-C33-H33C	109.5	C25-C36-H36B	109.5
C22-C34-H34A	109.5	H36A-C36-H36B	109.5
C22-C34-H34B	109.5	C25-C36-H36C	109.5
H34A-C34-H34B	109.5	H36A-C36-H36C	109.5
C22-C34-H34C	109.5	H36B-C36-H36C	109.5
H34A-C34-H34C	109.5	Zn1-O1W-H1WA	109.6
H34B-C34-H34C	109.5	Zn1-O1W-H1WB	109.6
C25-C35-H35A	109.5	H1WA-O1W-H1WB	109.2

Symmetry transformations used to generate equivalent atoms:
#1 -x+3,-y+1,-z+1

Table SI-14. Anisotropic displacement parameters ($Å^2$) for mL105c2_0m_sq. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Zn1	0.0235(3)	0.0261(6)	0.0219(6)	0.0052(4)	-0.0039(4)	-0.0076(5)
N1	0.0602(19)	0.0240(13)	0.0228(14)	0.0029(10)	0.0085(13)	0.0018(13)
C2	0.058(2)	0.0241(15)	0.0201(16)	-0.0001(12)	0.0107(15)	0.0024(15)
N3	0.0509(17)	0.0247(12)	0.0239(13)	0.0044(10)	0.0071(12)	0.0008(12)
C4	0.053(2)	0.0245(15)	0.0316(18)	0.0031(13)	0.0125(15)	0.0041(15)
C5	0.048(2)	0.0214(15)	0.0295(17)	0.0023(12)	0.0100(14)	0.0044(14)
C6	0.0522(19)	0.0354(15)	0.0234(14)	0.0011(12)	0.0041(13)	0.0099(15)
N6	0.0522(19)	0.0354(15)	0.0234(14)	0.0011(12)	0.0041(13)	0.0099(15)
C7	0.046(2)	0.0348(17)	0.0340(18)	0.0005(14)	0.0079(15)	0.0119(15)
C8	0.049(2)	0.049(2)	0.0392(19)	-0.0031(16)	0.0024(16)	0.0106(17)
C9	0.065(3)	0.060(2)	0.053(2)	-0.0006(19)	0.007(2)	-0.012(2)
C10	0.079(3)	0.048(2)	0.054(2)	0.0135(18)	0.000(2)	-0.007(2)
C11	0.045(2)	0.052(2)	0.0362(19)	0.0154(16)	0.0047(16)	-0.0002(17)
C12	0.046(2)	0.0317(16)	0.0312(18)	0.0041(13)	0.0082(15)	0.0086(15)
C13	0.0548(19)	0.0303(15)	0.0248(15)	0.0056(12)	0.0104(13)	0.0044(14)
N13	0.0548(19)	0.0303(15)	0.0248(15)	0.0056(12)	0.0104(13)	0.0044(14)
C14	0.049(2)	0.0201(14)	0.0241(16)	0.0008(12)	0.0118(14)	0.0019(13)
N15	0.0520(18)	0.0293(13)	0.0243(14)	0.0046(11)	0.0072(12)	0.0039(12)
C16	0.055(2)	0.0250(15)	0.0249(16)	0.0013(12)	0.0090(15)	0.0038(15)
N17	0.0569(18)	0.0264(13)	0.0212(13)	0.0039(10)	0.0037(12)	0.0007(13)
C18	0.056(2)	0.0241(15)	0.0205(15)	0.0010(12)	0.0042(14)	0.0065(15)
C19	0.052(2)	0.0241(15)	0.0260(16)	-0.0009(12)	0.0054(14)	0.0025(14)
C20	0.0510(19)	0.0328(15)	0.0237(15)	0.0030(12)	0.0052(13)	0.0021(14)
N20	0.0510(19)	0.0328(15)	0.0237(15)	0.0030(12)	0.0052(13)	0.0021(14)
C21	0.048(2)	0.0360(18)	0.0354(18)	-0.0011(14)	0.0137(16)	0.0086(16)
C22	0.043(2)	0.048(2)	0.042(2)	0.0088(16)	-0.0002(16)	0.0076(17)
C23	0.080(3)	0.062(3)	0.047(2)	0.0016(19)	-0.009(2)	0.003(2)
C24	0.063(3)	0.058(2)	0.077(3)	0.000(2)	-0.014(2)	-0.010(2)
C25	0.047(2)	0.0400(19)	0.062(2)	-0.0024(17)	0.0103(18)	-0.0003(17)
C26	0.049(2)	0.0364(18)	0.042(2)	-0.0015(15)	0.0149(16)	0.0072(16)
C27	0.055(2)	0.0325(15)	0.0356(17)	0.0016(13)	0.0148(15)	0.0020(14)
N27	0.055(2)	0.0325(15)	0.0356(17)	0.0016(13)	0.0148(15)	0.0020(14)
C28	0.051(2)	0.0276(15)	0.0260(16)	0.0002(13)	0.0055(14)	0.0036(15)
C29	0.063(3)	0.052(2)	0.083(3)	-0.023(2)	0.011(2)	0.011(2)
C30	0.056(3)	0.078(3)	0.063(3)	-0.005(2)	-0.002(2)	0.015(2)
C31	0.057(3)	0.076(3)	0.061(3)	0.043(2)	0.007(2)	0.000(2)
C32	0.061(3)	0.071(3)	0.047(2)	0.002(2)	0.0188(19)	0.000(2)
C33	0.058(3)	0.092(3)	0.044(2)	0.029(2)	-0.0033(19)	0.003(2)
C34	0.058(3)	0.051(2)	0.089(3)	0.003(2)	-0.005(2)	0.016(2)
C35	0.064(3)	0.046(2)	0.070(3)	-0.0147(19)	0.008(2)	0.003(2)
C36	0.055(3)	0.081(3)	0.102(4)	0.003(3)	0.024(3)	-0.007(2)
O1W	0.027(2)	0.046(3)	0.047(3)	-0.007(2)	0.003(2)	-0.001(2)

Table SI-15. Hydrogen coordinates and isotropic displacement parameters ($Å^2$) for mL105c2_0m_sq.

	x	y	z	U(eq)	Occupancy
H6	0.7937	0.2632	0.4967	0.044	0.5
H9A	0.4972	0.1366	0.5947	0.071	1
H9B	0.5197	0.0473	0.5750	0.071	1
H10A	0.8878	0.0393	0.6056	0.073	1
H10B	0.7234	0.0529	0.6419	0.073	1
H13	1.2358	0.2649	0.6298	0.043	0.5
H20	1.1406	0.6097	0.3269	0.043	0.5
H23A	0.5900	0.5351	0.2186	0.077	1
H23B	0.7766	0.4684	0.2307	0.077	1
H24A	0.3981	0.4925	0.2771	0.081	1
H24B	0.4270	0.4181	0.2450	0.081	1
H27	0.7666	0.3870	0.3845	0.049	0.5
H29A	0.7083	0.0278	0.5076	0.099	1
H29B	0.9329	0.0508	0.5355	0.099	1
H29C	0.8614	0.0991	0.4920	0.099	1
H30A	0.3726	0.1229	0.5088	0.099	1
H30B	0.5300	0.1829	0.4853	0.099	1
H30C	0.4169	0.2136	0.5265	0.099	1
H31A	1.2093	0.1748	0.6717	0.097	1
H31B	1.2170	0.0931	0.6439	0.097	1
H31C	1.0829	0.0947	0.6854	0.097	1
H32A	0.8638	0.2541	0.6725	0.088	1
H32B	0.7291	0.1749	0.6846	0.088	1
H32C	0.6470	0.2276	0.6431	0.088	1
H33A	0.9209	0.6314	0.2215	0.098	1
H33B	1.0830	0.5604	0.2399	0.098	1
H33C	1.0691	0.6441	0.2658	0.098	1
H34A	0.5716	0.6623	0.2575	0.100	1
H34B	0.7330	0.6814	0.2995	0.100	1
H34C	0.5359	0.6176	0.3018	0.100	1
H35A	0.8144	0.3006	0.3100	0.090	1
H35B	0.8668	0.3547	0.2697	0.090	1
H35C	0.6510	0.2988	0.2670	0.090	1
H36A	0.5014	0.3338	0.3517	0.118	1
H36B	0.3323	0.3364	0.3095	0.118	1
H36C	0.3536	0.4132	0.3412	0.118	1
H1WA	1.4889	0.6385	0.5594	0.060	0.5
H1WB	1.2668	0.6126	0.5504	0.060	0.5

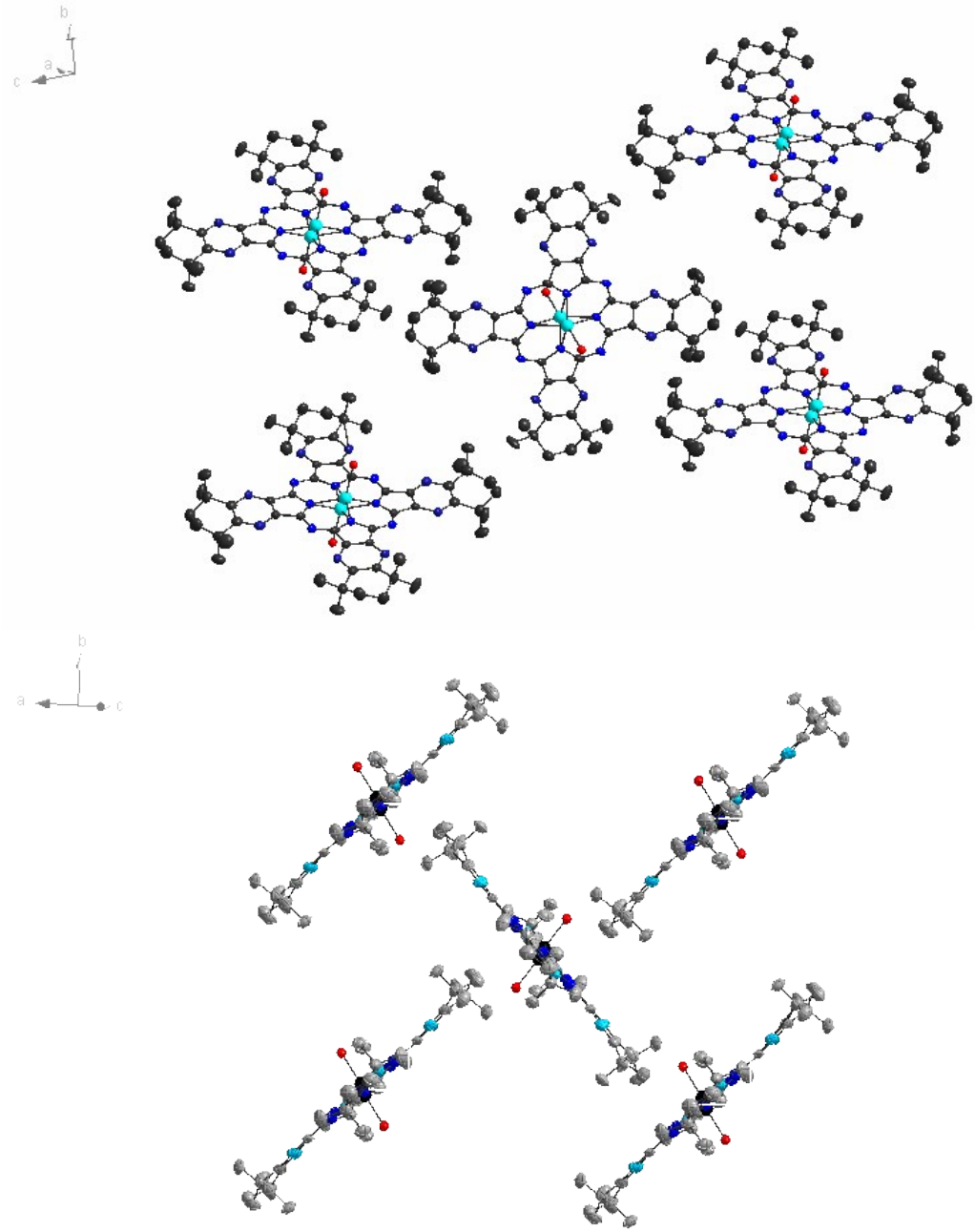
Table SI-16. Torsion angles [°] for mL105c2_0m_sq.

C18#1-N1-C2-N3	-1.2(5)	C4-N15-C16-N17	0.7(5)
C18#1-N1-C2-C14	175.7(3)	C4-N15-C16-C28	178.3(3)
N1-C2-N3-C4	175.4(3)	N15-C16-N17-C18	178.1(3)
C14-C2-N3-C4	-2.0(3)	C28-C16-N17-C18	0.2(3)
N1-C2-N3-Zn1#1	14.4(5)	N15-C16-N17-Zn1#1	15.1(4)
C14-C2-N3-Zn1#1	-163.0(2)	C28-C16-N17-Zn1#1	-162.8(2)
N1-C2-N3-Zn1	-7.8(4)	N15-C16-N17-Zn1	-4.8(5)
C14-C2-N3-Zn1	174.78(18)	C28-C16-N17-Zn1	177.3(2)
C2-N3-C4-N15	-177.5(3)	C16-N17-C18-N1#1	-174.9(3)
Zn1#1-N3-C4-N15	-13.8(4)	Zn1#1-N17-C18-N1#1	-14.3(4)
Zn1-N3-C4-N15	5.9(5)	Zn1-N17-C18-N1#1	7.9(4)
C2-N3-C4-C5	0.4(3)	C16-N17-C18-C19	1.9(3)
Zn1#1-N3-C4-C5	164.15(19)	Zn1#1-N17-C18-C19	162.5(2)
Zn1-N3-C4-C5	-176.16(19)	Zn1-N17-C18-C19	-175.29(19)
N15-C4-C5-C6	4.4(5)	N1#1-C18-C19-C20	-5.1(5)
N3-C4-C5-C6	-173.6(3)	N17-C18-C19-C20	177.9(3)
N15-C4-C5-C14	179.4(3)	N1#1-C18-C19-C28	173.5(3)
N3-C4-C5-C14	1.4(3)	N17-C18-C19-C28	-3.4(3)
C14-C5-C6-C7	1.9(4)	C28-C19-C20-C21	-2.8(4)
C4-C5-C6-C7	176.1(3)	C18-C19-C20-C21	175.7(3)
C5-C6-C7-C12	2.9(4)	C19-C20-C21-C26	-3.0(5)
C5-C6-C7-C8	-171.9(3)	C19-C20-C21-C22	172.1(3)
C6-C7-C8-C9	-159.1(3)	C20-C21-C22-C33	37.8(4)
C12-C7-C8-C9	26.2(4)	C26-C21-C22-C33	-147.2(3)
C6-C7-C8-C29	79.4(4)	C20-C21-C22-C23	159.0(3)
C12-C7-C8-C29	-95.3(4)	C26-C21-C22-C23	-26.0(4)
C6-C7-C8-C30	-38.3(4)	C20-C21-C22-C34	-81.2(4)
C12-C7-C8-C30	147.0(3)	C26-C21-C22-C34	93.9(4)
C29-C8-C9-C10	70.3(4)	C33-C22-C23-C24	170.3(3)
C7-C8-C9-C10	-47.8(4)	C21-C22-C23-C24	47.0(4)
C30-C8-C9-C10	-170.1(3)	C34-C22-C23-C24	-70.6(4)
C8-C9-C10-C11	61.1(5)	C22-C23-C24-C25	-60.7(5)
C9-C10-C11-C31	-169.2(3)	C23-C24-C25-C26	46.8(5)
C9-C10-C11-C32	71.8(4)	C23-C24-C25-C35	-71.4(4)
C9-C10-C11-C12	-45.7(5)	C23-C24-C25-C36	170.3(4)
C6-C7-C12-C13	-5.0(5)	C20-C21-C26-C27	6.1(5)
C8-C7-C12-C13	169.6(3)	C22-C21-C26-C27	-168.8(3)
C6-C7-C12-C11	170.3(3)	C20-C21-C26-C25	-167.9(3)
C8-C7-C12-C11	-15.1(5)	C22-C21-C26-C25	17.2(5)
C10-C11-C12-C13	-160.9(3)	C24-C25-C26-C27	159.3(3)
C31-C11-C12-C13	-38.7(4)	C35-C25-C26-C27	-80.1(4)
C32-C11-C12-C13	79.8(4)	C36-C25-C26-C27	38.2(4)
C10-C11-C12-C7	23.6(4)	C24-C25-C26-C21	-26.5(5)
C31-C11-C12-C7	145.8(3)	C35-C25-C26-C21	94.0(4)
C32-C11-C12-C7	-95.7(4)	C36-C25-C26-C21	-147.7(3)
C7-C12-C13-C14	2.1(4)	C21-C26-C27-C28	-3.2(5)
C11-C12-C13-C14	-173.4(3)	C25-C26-C27-C28	171.1(3)
C12-C13-C14-C5	2.7(4)	C26-C27-C28-C19	-2.5(5)
C12-C13-C14-C2	-174.4(3)	C26-C27-C28-C16	-178.1(3)
C6-C5-C14-C13	-4.8(5)	C20-C19-C28-C27	5.8(5)
C4-C5-C14-C13	179.8(3)	C18-C19-C28-C27	-173.1(3)
C6-C5-C14-C2	172.9(3)	C20-C19-C28-C16	-177.7(3)
C4-C5-C14-C2	-2.5(3)	C18-C19-C28-C16	3.4(3)
N1-C2-C14-C13	2.8(5)	N15-C16-C28-C27	-4.3(5)
N3-C2-C14-C13	-179.8(3)	N17-C16-C28-C27	173.8(3)
N1-C2-C14-C5	-174.6(3)	N15-C16-C28-C19	179.6(3)
N3-C2-C14-C5	2.8(3)	N17-C16-C28-C19	-2.4(3)
N3-C4-N15-C16	-1.3(5)		
C5-C4-N15-C16	-178.9(3)		

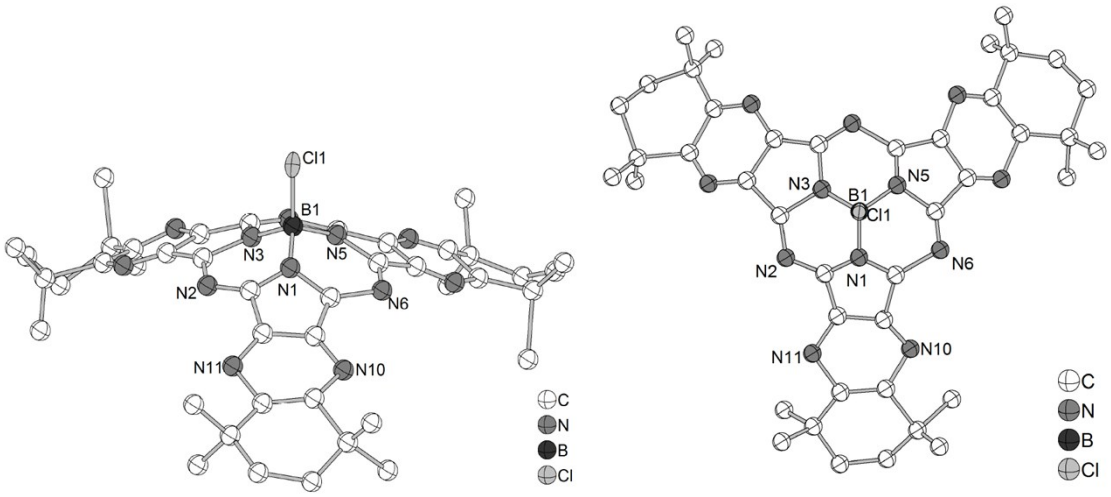
Table SI-17. Hydrogen bonds for mL105c2_0m_sq [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O1W-H1WB...N15#2	0.86	1.86	2.583(5)	140.6
O1W-H1WB...N27#2	0.86	2.63	3.307(5)	135.7

Symmetry transformations used to generate equivalent atoms:
#1 -x+3,-y+1,-z+1 #2 -x+2,-y+1,-z+1



1.7.4 **Crystal Structure of [Sppz*BCl]** Crystallographer: Dr. Benjamin Oelkers



Empirical formula	C49 H56 B Cl N12	
Formula weight	859.32	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 7.253(3) Å	α= 90°.
	b = 25.008(5) Å	β= 98.83(3)°.
	c = 25.698(7) Å	γ = 90°.
Volume	4606(2) $Å^3$	
Z	4	
Density (calculated)	1.239 Mg/m^3	
Absorption coefficient	0.132 mm^{-1}	
F(000)	1824	
Crystal size	0.3 x 0.06 x 0.03 mm^3	
Theta range for data collection	1.14 to 20.00°.	
Index ranges	-6<=h<=6, -24<=k<=24, -24<=l<=24	
Reflections collected	13040	
Independent reflections	4273 [R(int) = 0.2894]	
Completeness to theta = 20.00°	99.8 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4273 / 0 / 197	
Goodness-of-fit on F^2	0.841	
Final R indices [I>2sigma(I)]	R1 = 0.1654, wR2 = 0.3401	
R indices (all data)	R1 = 0.4135, wR2 = 0.4094	
Largest diff. peak and hole	0.382 and -0.431 $e.Å^{-3}$	

Note: Because of the poor diffraction of the crystal, no satisfying refinement could be obtained. To gain a preliminary crystal structure of low resolution only refelexes up to theta = 20° were used. All deflection coefficients C, N, and B were hold constant isotropic and refined with common parameters. The interpretation and orientation of the solvent molecules are, in contrast to the general figure of the complex molecule, not of sufficient quality for a discussion. Because of the poor data, no detailed discussion of bond lengths is possible however a documentation of the unit cell is possible.

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