Electronic Supporting Information

Aromaticity switching via azulene transformations in azulene-bridged A,D-dithiahexaphyrin

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Instrumentation

NMR spectra were measured on Bruker Avance 500 MHz and Bruker Avance III 600 MHz spectrometers. ^{1}H and ^{13}C shifts were referenced to the residual resonances of deuterated solvents. Mass spectra (High Resolution and Accurate Mass) were recorded on Bruker micrOTOF-Q and Apex Ultra spectrometers using the electrospray technique. UV-vis spectra were collected with Jasco V-770 spectrometer.

Synthetic Procedures

*5,15,20,30-tetratolyl-A,D-dithia[26]hexaphyrin[1.1.1.1.1.1] with 10,25-azulene bridge (**1**)*

1,3-Diformylazulene[1] (40.0 mg, 0.217 mmol), 5,10-ditolyl-16-thiatripyrrane[2] (190 mg, 0.450 mmol), and TFA (100 µl) were added to degased DCM (300 ml) and mixed under nitrogen atmosphere protected from light for 16 h. Next, DDQ (0.50 g, 2.2 mmol) was added and, after one hour, Et_3N (0.5 ml). The mixture was evaporated and separated by column chromatography [basic Al_2O_3, 4% water (w/w)]. Violet byproduct and unreacted 1,3-diformylazulene were eluted before the product with DCM–hexanes mixtures (up to pure DCM). After fraction evaporation **1** was crystallized from DCM–*n*-hexan system.

67 mg (31%; consideration of unreacted recovered 1,3-diformylazulene gives more than 50% of yield); **^{1}H NMR** (600 MHz, $CDCl_3$, 250 K) δ 10.03 (d, *J* = 4.4 Hz, 4H, 8,12,23,27), 9.52 (s, 4H, 2,3,17,18), 8.71 (d, *J* = 4.1 Hz, 4H, 7,13,22,28), 8.43 (d, *J* = 7.1 Hz, 4H, *o*Tol), 7.89 (d, *J* = 7.2 Hz, 4H, *o*Tol'), 7.71 (d, *J* = 7.3 Hz, 4H, *m*Tol), 7.56 (d, *J* = 7.3 Hz, 4H, *m*Tol'), 5.76 (t, *J* = 9.3 Hz, 1H, 42), 5.37 (t, *J* = 9.9 Hz, 2H, 41,43), 4.64 (d, *J* = 10.4 Hz, 2H, 40,44), 2.68 (s, 12H, CH_3), −1.62 (s, 1H, 37) ppm; *[1-H_2]*$^{2+}$ (600 MHz, CD_2Cl_2 + TFA, 190 K) δ 10.10 (s, 2H, 2,3), 9.83 (br d, *J* = 3 Hz, 2H, 12,23), 9.67 (br s, 2H, 8,27), 8.94 (s, 2H, 17,18), 8.77 (br d, *J* = 6 Hz, 2H, 5,30-*o*Tol), 8.74 (br d, *J* = 3.5 Hz, 2H, 13,22), 8.65 (br s, 2H, 7,28), 8.60 (br d, *J* = 5.5 Hz, 2H, 5,30-*o*Tol), 8.20 (d, *J* = 6.6 Hz, 2H, 15,20-*o*Tol), 8.01 (d, *J* = 6.8 Hz, 2H, 5,30-*m*Tol), 7.95 (d, *J* = 6.7 Hz, 2H, 5,30-*m*Tol), 7.77 (br d, *J* = 5.5 Hz, 2H, 15,20-*o*Tol), 7.71 (d, *J* = 6.9 Hz, 2H, 15,20-*m*Tol), 7.60 (d, *J* = 6.8 Hz, 2H, 15,20-*m*Tol), 6.68 (t, *J* = 9.1 Hz, 1H, 42), 6.47 (t, *J* = 8.9 Hz, 2H, 41,43), 5.91 (d, *J* = 9.2 Hz, 2H, 40,44), 2.79 (br s, 2H, overlapped with CH_3, 32,36), 2.79 (s, 6H, 5,30-CH_3), 2.64 (s, 6H, 15,20-CH_3), −2.89 (s, 1H, 37) ppm; **^{13}C NMR** (151 MHz, $CDCl_3$, 250 K) δ 159.5, 156.8, 150.3, 145.7, 138.0, 137.7, 137.5, 137.0 (37), 136.4 (40,44), 135.5 (42), 135.4 (2,3,17,18), 135.0 (7,13,22,28), 134.7 (*o*Tol'), 134.6 (*o*Tol), 131.8 (8,12,23,27), 128.4 (*m*Tol), 128.3 (*m*Tol'), 127.0, 125.2 (41,43), 120.2, 21.6 (CH_3) ppm; **HRMS** (ESI) calcd for $C_{68}H_{47}N_4S_2$ ([M+H]$^+$): 983.3237; found: 983.3192 (*m/z*); **UV-vis** (CH_2Cl_2 + 0.1% Et_3N, 293 K) λ_{max} ($\log\varepsilon_{mol}$) 364 (4.61), 455 (4.78), 565 (5.25), 607 (4.66), 673 (4.43), 1038 (4.44), *[1-H_2]*$^{2+}$ (CH_2Cl_2 + 0.1% TFA, 293 K) 428 (4.81), 461 (4.77), 587 (5.22), 960 (4.60) nm; *[1-H_3]*$^{3+}$ (CH_2Cl_2 + TFA, 293 K) 452, 503, 581, 811, 973, 1101 nm, *[1-H_4]*$^{4+}$ (CH_2Cl_2 + 2% TFA, 293 K) 371 (4.49), 470 (4.90), 582 (5.25), 678 (4.35), 1016 (4.98) nm.

[1] K. Hafner, C. Bernhard, *Liebigs Ann. Chem.* 1959, **625**, 108.
[2] R. R. Malakalapalli, R. Mangalampalli, *Tetrahedron* 2012, **68**, 1306.

*5,15,20,30-tetratolyl-A,D- dithia[28]hexaphyrin[1.1.1.1.1.1] with 10,25-azulene bridge (**2**)*

HexAz **1** (15 mg) was added to degased DCM (10 mL). The suspension was acidified by passing gasous HCl (solution became blue-green). To such a mixture zinc powder (0.10 g) was added and the mixture was stirred under nitrogen. The solution changed color to dark blue and was mixed for additional 15 min. The mixture was passed through short alumina column [basic Al_2O_3, 4% water (w/w)] with DCM + 1% Et_3N. Product **2** was obtained quantitatively after evaporation of solvent.

^{1}H NMR (600 MHz, $CDCl_3$, 280 K) δ 18.26 (s, 2H, 32,35), 16.37 (s, 1H, 37), 11.13 (d, *J* = 9.3 Hz, 2H, 40,44), 9.25 (t, *J* = 9.9 Hz, 1H, 42), 9.04 (d, *J* = 9.7 Hz, 2H, 41,43), 6.80 (d, *J* = 8.0 Hz, 4H, *m*Tol), 6.78 (d, *J* = 8.1 Hz, 4H, *m*Tol'), 6.43 (s, 4H, *o*Tol), 6.37 (br d, *J* = 7.1 Hz, 4H, *o*Tol'), 5.47 (d, *J* = 4.5 Hz, 2H, 13,28), 4.98 (d, *J* = 3.7 Hz, 2H, 7,22), 4.89 (d, *J* = 4.4 Hz, 2H, 12,27), 4.36 (d, *J* = 6.1 Hz, 2H, 3,18/2,17), 4.28 (d, *J* = 6.0 Hz, 2H, 3,18/2,17), 4.25 (br d, *J* = 3 Hz, 2H, 8,23), 2.11 (s, 6H, CH_3), 2.10 (s, 6H, CH_3') ppm; *[2-H_2]*$^{2+}$ (600 MHz, CD_2Cl_2 + TFA, 190 K) δ 21.61 (s, 4H, 32,33,35,36), 18.17 (s, 37), 11.92 (br s, 2H, 40,44), 9.78 (br s, 1H, 42), 9.61 (br s, 2H, 41,43), 6.58 (br s, 8H, Tol), 6.01 (br s, 4H, Tol), 5.69 (br s, 4H, Tol), 4.61 (br s, 4H, pyrr/th), 4.57 (br s, 4H, pyrr/th), 4.41 (br s, 4H, pyrr/th), 1.98 (s, 12H, CH_3); **^{13}C NMR** (151 MHz, $CDCl_3$, 250 K, partial data from HSQC) 151.2 (37), 145.8 (40,44), 142.1 (42), 134.0 (3,18/2,17), 131.8 (41,43), 133.0 (3,18/2,17), 126.3 (13,28), 126.3 (12,27), 116.5 (7,22), 119.0 (8,23), 20.8 (CH_3) ppm; **MS** (ESI) calcd for $C_{68}H_{49}N_4S_2$ ([M+H]$^+$): 985.3393; found: 985.3372 (*m/z*); **UV-vis** (CH_2Cl_2 + 0.1% Et_3N, 293 K) λ_{max} (logε_{mol}) 446 (4.62), 534 (4.81), 738 (3.88), *[2-H_2]*$^{2+}$ (CH_2Cl_2 + 0.1% TFA, 293 K) 609 (4.96), 877 (4.04) nm.

[Pd(HexAz)]$^+$ ***(1-Pd**$^+$**)***

HexAz **1** (15 mg, 15.2 μmol) and $PdCl_2$ (40 mg, 226 μmol) were added to a degased mixture of DCM (15 mL) and MeCN (15 mL). The solution was mixed for ca. 6 h under nitrogen atmosphere and evaporated partialy in a nitrogen stream, then put on chromatographic column (silica gel, DCM). Gray-red fractions eluted with DCM-MeCN 3:1 and with MeOH addition contain product **1-Pd**$^+$. By analogy to cationic palladium(II) complex of 23-thiaazuliporphyrin[3] obtained in the same conditions, asummed counterion should be $[PdCl_3(H_2O)]^-$ obtained from hydrolysis of $[Pd_2Cl_4]^{2-}$.

10.2 mg (51%); **^{1}H NMR** (600 MHz, $CDCl_3$ + CD_3CN, 280 K) δ 10.13 (d, *J* = 4.7 Hz, 2H, 8,27), 9.19 (s, 2H, 2,3) 8.98 (d, *J* = 4.3 Hz, 2H, 12,23), 8.88 (d, *J* = 4.7 Hz, 2H, 7,28), 8.66 (br s, 2H, *o*Tol), 8.12 (d, *J* = 4.3 Hz, 2H, 13,22), 7.91 (s, 2H, 17,18), 7.79 – 7.71 (m, 8H, Tol), 7.50 (br s, 6H, Tol), 6.70 (br s, 3H, 41,42,43), 6.29 (br s, 2H, 40,44), 2.72 (s, 6H, 5,30-CH_3), 2.59 (s, 6H, 15,20-CH_3) ppm; **^{13}C NMR** (151 MHz, $CDCl_3$ + CD_3CN 2:1, 300 K, partial data from HMQC) 146.2 (40,44), 144.9 (41,43/42), 144.1 (13,22), 143.5 (2,3), 142.7 (41,43/42), 141.8 (17,18), 139.7 (7,28), 135.9 (8,27), 134.4 (12,23); **HRMS** (ESI) calcd for $C_{68}H_{45}N_4PdS_2$ ([M]$^+$): 1087.2136; found: 1087.2121 (*m/z*); **UV-vis** (CH_2Cl_2 + MeCN 2:1, 293 K) λ_{max} (logε_{mol}) 386 (4.73), 412 (4.73), 570 (4.76), 910 (4.28) nm.

[($PdCl_2$)$_2$(rHexAz)] ***(2-Pd$_2$)***

rHexAz **2** (10 mg, 10.1 μmol) and $PdCl_2$ (30 mg, 169 μmol) were added to degased DCM (10 mL). The solution was mixed for ca. 4 h under nitrogen atmosphere and reduced

[3] M. J. Białek, L. Latos-Grażyński, *Inorg. Chem.* 2016, **55**, 1758.

with nitrogen stream. The residue was separated on a TLC plate (silica gel, DCM). One of first fractions, the pink-violet one, was identified as product **2-Pd$_2$**.[4] It is also observable as byproduct of **1-Pd$^+$** synthesis.

1.4 mg (9%); **^{1}H NMR** (500 MHz, $CDCl_3$, 300 K, $PdCl_2$ attached to S31,N36 and S33,N34) δ 13.48 (s, 1H, 35), 12.67 (s, 1H, 32), 10.92 (s, 1H, 37), 9.57 (d, *J* = 10.0 Hz, 1H, 44), 8.78 (t, *J* = 9.8 Hz, 1H, 42), 8.61 (t, *J* = 9.8 Hz, 1H, 43), 8.51 (d, *J* = 9.9 Hz, 1H, 40), 8.37 (t, *J* = 9.8 Hz, 1H, 41), 7.20–7.04 (m, 14H, Tol), 7.01 (dd, *J* = 4.4, 1.8 Hz, 1H, 8), 6.79 (d, *J* = 4.6 Hz, 1H, 27), 6.72 (d, *J* = 4.2 Hz, 1H, 12), 6.70 (br s, 1H, oTol), 6.61 (br s, 1H, oTol), 6.47 (d, *J* = 6.0 Hz, 1H, 2/3), 6.43 (dd, *J* = 4.1, 1.6 Hz, 1H, 23), 6.363 (d, *J* = 6.0 Hz, 1H, 2/3), 6.362 (d, *J* = 4.7 Hz, 1H, 28), 6.22 (dd, *J* = 4.4, 1.8 Hz, 1H, 7), 6.11 (d, *J* = 4.1 Hz, 1H, 13), 5.56 (d, *J* = 6.2 Hz, 1H, 17/18), 5.55 (dd, *J* = 4.1, 2.2 Hz, 1H, 22), 5.46 (d, *J* = 6.2 Hz, 1H, 17/18), 2.38 (s, 3H, CH_3), 2.35 (s, 3H, CH_3), 2.31 (s, 3H, CH_3), 2.26 (s, 3H, CH_3) ppm; **^{13}C NMR** (151 MHz, $CDCl_3$, 300 K, some signals are overlapped and broadened) δ 157.46, 156.58, 155.62, 153.53, 150.11, 150.07 (37), 149.32 (44), 149.13, 147.80, 147.65, 146.96, 146.17, 145.88, 144.41 (40), 143.68 (42), 142.65, 140.65, 140.64, 140.44, 140.40, 139.76, 139.10, 139.00, 138.35, 138.15, 137.88 (2/3), 137.07 (43), 136.86 (41), 136.47 (17/18), 135.19, 134.45 (27), 133.92, 133.56, 133.55, 133.42, 133.41, 133.25, 133.24, 133.13 (2/3), 132.95, 132.83, 132.36, 131.41 (17/18), 131.40, 130.51, 130.50, 130.45, 130.44, 129.37, 129.28, 129.27, 128.91 (12), 128.29 (8), 128.07 (28), 126.08 (7), 124.84 (13), 121.70 (22), 120.83 (23), 21.44 (CH_3), 21.37 (CH_3), 21.32 (CH_3), 21.21 (CH_3) ppm; **MS** (ESI) calcd for $C_{68}H_{49}Cl_2PdN_4S_2$ ([M−$PdCl_2$+H]$^+$): 1163.1810; found: 1163.1838 (*m/z*); **UV-vis** (CH_2Cl_2, 293 K) λ_{max} (logε_{mol}) 402 (4.56), 417 (4.57), 557 (4.81), 867 (4.15) nm.

Contraction/rearrangement

HexAz **1** (10 mg, 10.2 μmol) and $Pd(OAc)_2$ (10 mg, 45.6 μmol) were added to degased DMF (25 mL) and refluxed for 1 h in nitrogen athmosphere.[5] Next, the mixture was evaporated and solved in DCM to separate it on a TLC plate (silica gel, DCM). Fractions have been extracted with DCM-ethyl acetate 2:1 (and addition of MeOH for latter fractions) and evaporated. As first fractions formylated thiabenzocarbaporphyrin complexes were acqired in trace amounts. Next, brown band of thianaphthiporphyrin complex **4-Pd** and at the starting line **3-Pd**. **3-Pd** was subsequently purified with TLC (silica gel, DCM-ethyl acetate 2:1) and collected as a redish-brown band.

[Pd(SBzc)] ***3-Pd***

Less than 1%; **^{1}H NMR** (600 MHz, $CDCl_3$, 250 K) δ 9.77 (d, *J* = 5.0 Hz, 2H, 8,27), 8.98 (s, 2H, 2,3), 8.80 (d, *J* = 7.6 Hz, 2H, 5,30-oTol), 8.73 (d, *J* = 4.9 Hz, 2H, 7,28), 8.52 (d, *J* = 4.3 Hz, 2H, 12,23), 7.82 (d, *J* = 7.9 Hz, 2H, 15,20-oTol), 7.78 (d, *J* = 4.1 Hz, 2H, 13,22), 7.76 (d, *J* = 7.8 Hz, 2H, 5,30-mTol), 7.72 (d, *J* = 7.3 Hz, 2H, 5,30-oTol), 7.60 (d, *J* = 7.8 Hz, 2H, 5,30-mTol), 7.48 (d, *J*

[4] The dipalladium(II) form easily demetalates to form a monocoordinated species.

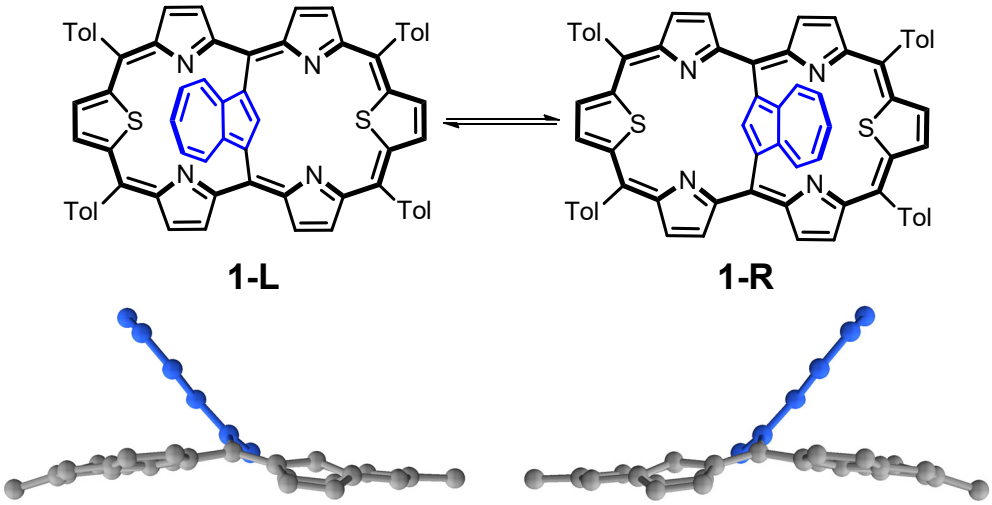
[5] Nucleophilic attack resulting in formyl or carbonyl formation (**3-Pd**/**4-Pd**; Scheme 5) is assumed to be caused by OH^- derived from solvents residual water or DMF thermal decomposition (W. Liu, C. Chen, P. Zhou *J. Org. Chem*. 2017, **82**, 2219−2222) rather than atmospheric oxygen. At this stage the internal electron and accompanying proton transfer afforded the transient species presented in Scheme 5. The subsequent oxidation is performed either by the molecular oxygen accessible during the further procedures (evaporation) or by the palladium source used in excess.

= 7.5 Hz, 2H, 15,20-oTol), 7.44 (d, *J* = 7.2 Hz, 2H, 15,20-mTol), 7.43 (s, 2H, 17,18), 7.36 (d, *J* = 7.0 Hz, 2H, 15,20-mTol), 6.51 (d, *J* = 11 Hz, 2H, 40,43), 6.38 (d, *J* = 11 Hz, 2H, 41,42), 2.69 (s, 6H, 5,30-CH_3), 2.53 (s, 6H, 15,20-CH_3) ppm; **^{13}C NMR** (151 MHz, $CDCl_3$, 250 K, partial data from HSQC) 128.0 (8,27), 135.7 (2,3), 133.7 (5,30-oTol), 131.3 (7,28), 128.1 (12,23), 132.1 (15,20-oTol), 137.5 (13,22), 129.1 (5,30-mTol), 137.0 (5,30-oTol), 129.2 (5,30-mTol), 132.5 (15,20-oTol), 128.3 (15,20-mTol), 134.9 (17,18), 128.3 (15,20-mTol), 136.9 (40,43), 133.6 (41,42), 21.4 (5,30-CH_3), 21.3 (15,20-CH_3); **MS** (ESI) calcd for $C_{67}H_{45}N_4PdS_2$ ($[M+H]^+$): 1075.2135; found: 1075.2124 (*m/z*); **UV-vis** (CH_2Cl_2, 293 K) λ_{max} ($\log\varepsilon_{mol}$) 378 (4.59), 424 (4.61), 479 (4.59), 929 (3.93) nm.

[Pd(SNaph)] ***4-Pd***

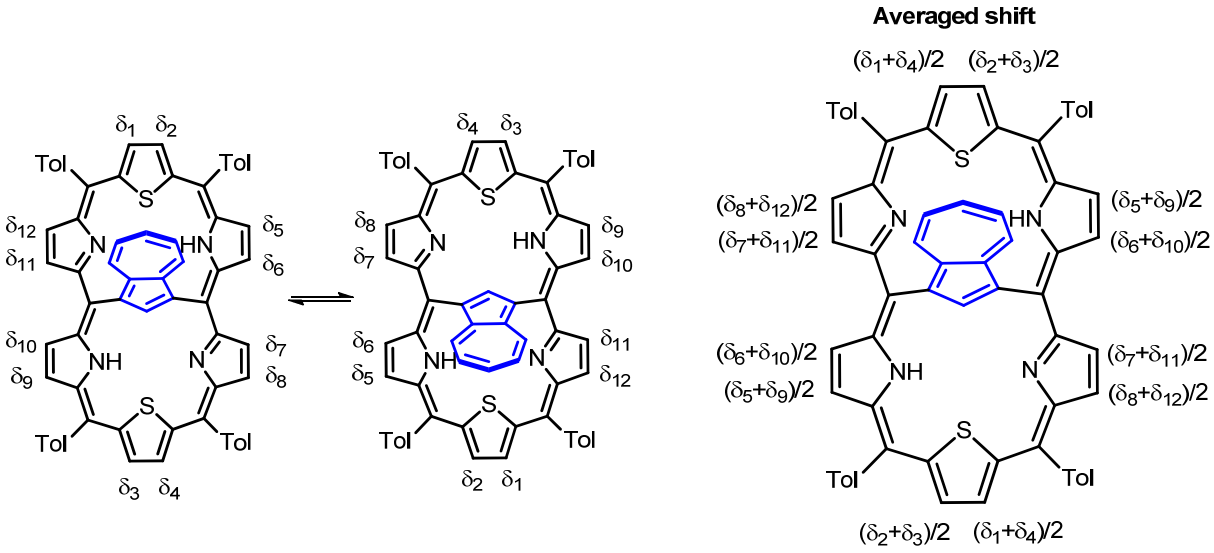
1.3 mg (12%); **^{1}H NMR** (600 MHz, $CDCl_3$, 300 K) δ 9.28 (s, 1H, 35), 8.44 (d, *J* = 4.4 Hz, 1H, 8), 8.20 (br s, Tol), 7.98 (d, *J* = 5.5 Hz, 1H, 2/3), 7.93 (dd, *J* = 7.5, 1.2 Hz, 1H, 43), 7.86 (dd, *J* = 8.0, 1.2 Hz, 1H, 41), 7.81 (d, *J* = 4.6 Hz, 1H, 27), 7.79 (d, *J* = 5.5 Hz, 1H, 2/3), 7.67 (d, *J* = 8.0 Hz, Tol), 7.50 (d, *J* = 4.4 Hz, 1H, 28), 7.45 (d, *J* = 4.5 Hz, 1H, 7), 7.41 (br s, Tol), 7.30 (d, *J* = 7.9 Hz, Tol), 7.24 (br s, overlapped with $CHCl_3$, Tol), 7.18 (d, *J* = 6.8 Hz, Tol), 7.14 (dd, *J* = 3.9, 2.4 Hz, 2H, 23), 7.05 (t, *J* = 7.8 Hz, 1H, 42), 6.83 (d, *J* = 5.8 Hz, 1H, 17/18), 6.64 (d, *J* = 4.1 Hz, 1H, 13), 6.52 (d, *J* = 4.1 Hz, 1H, 12), 6.31 (d, *J* = 5.8 Hz, 1H, 17/18), 6.20 – 6.09 (m, t-like, 1H, 22), 2.51 (s, 6H, 5,30-CH_3), 2.45 (s, 3H, 15/20-CH_3), 2.39 (s, 3H, 15/20-CH_3) ppm; **^{13}C NMR** (151 MHz, $CDCl_3$, 300 K, partial data from broadened ^{13}C) δ 190.01 (45), 164.95, 154.87, 149.04, 143.24, 141.02, 138.98, 138.65, 138.07, 138.00, 137.49, 137.34, 137.23, 137.13 (2/3), 136.73, 136.08, 134.85 (17/18), 133.28, 133.23 (2/3), 131.29, 131.20, 131.07, 130.89, 130.49 (27), 130.42 (17/18), 129.55, 129.44 (7), 128.80, 128.23, 126.97, 126.87, 126.71 (8), 126.55, 126.11 (28), 125.80 (42), 124.97 (13), 124.30, 123.81 (43), 123.61, 121.06 (12), 119.21 (22), 119.00 (41), 114.08 (23), 21.43 (CH_3), 21.42 (CH_3), 21.39 (CH_3), 21.30 (CH_3) ppm; **MS** (ESI) calcd for $C_{68}H_{44}N_4OPdS_2$ ($[M]^+$): 1075,2007; found: 1102.1980 (*m/z*); **UV-vis** (CH_2Cl_2, 293 K) λ_{max} ($\log\varepsilon_{mol}$) 444 (4.64), 534 (4.48), 896 (4.25) nm.

Additional information



Scheme S1. Two energetically equivalent conformers of **1** transforming into each other in solution. The side projection of the X-ray model (without substituents and H atoms) shown at the bottom.

Structure and Protonation of **2**



Scheme S2. The reason for the observation of three pyrr/th AB systems in the ^{1}H NMR spectrum of **2**. Due to the presence of two conformers in equilibrium the appropriate chemical are averaged affording the ^{1}H NMR pattern consistent with the effective symmetry C_2.

The presence of two NH hydrogens lowered the effective symmetry to C_2 consistently with the (N32–**H**,N33,N35–**H**,N36) distribution as one NH resides in each porphyrin-like cavity (Scheme 3,S2). In particular, such a symmetry is confirmed by the AB pattern of thiophene resonances (4.36 and 4.28 ppm, J_{HH} = 6.0 Hz) accompanied by two β-H pyrrolic AB sets. The effective high symmetry of **2** implies the fast conformational rearrangement described already for **1** (Schemes S1,S2). In the presence of TFA in excess the formation of dication **[2-H$_2$]$^{2+}$** was achieved (Figure S1b).

NMR spectra

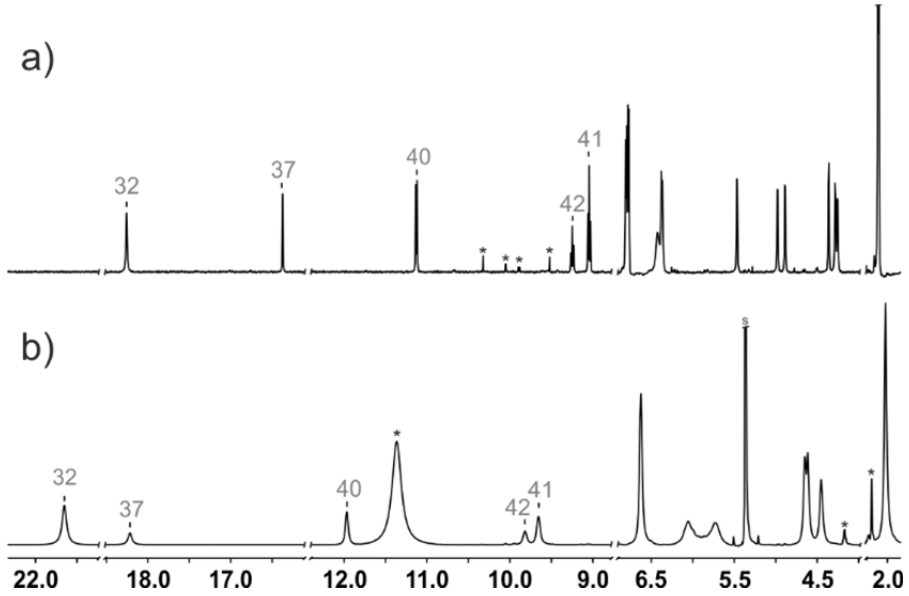


Figure S1. ^{1}H NMR spectra of a) **2** (600 MHz, $CDCl_3$, 280 K), b) **[2-H$_2$]$^{2+}$** (600 MHz, CD_2Cl_2 + TFA, 190 K).

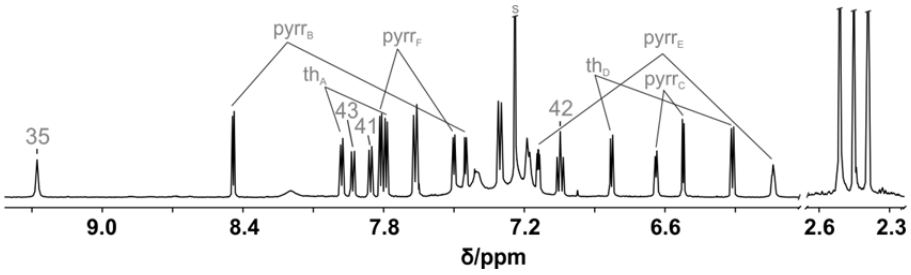


Figure S2. ^{1}H NMR spectrum of **4-Pd** (600 MHz, $CDCl_3$, 300 K). One can see two subsets of thiatripyrrolic frame protons: 'aromatic' A, B, F and 'nonaromatic' C, D, E.

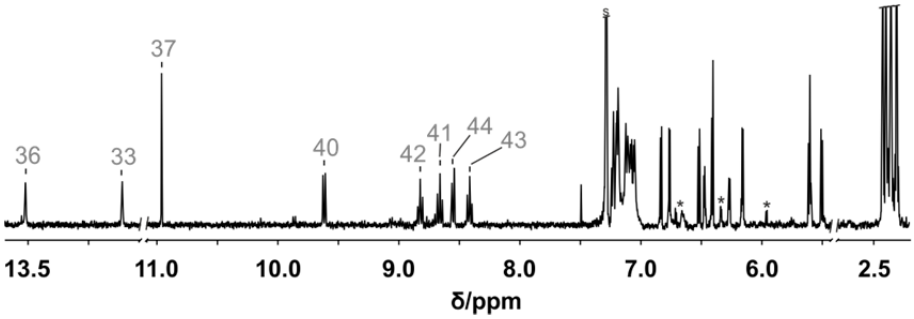


Figure S3. ^{1}H NMR spectrum of **2-Pd$_2$** (500 MHz, $CDCl_3$, 300 K).

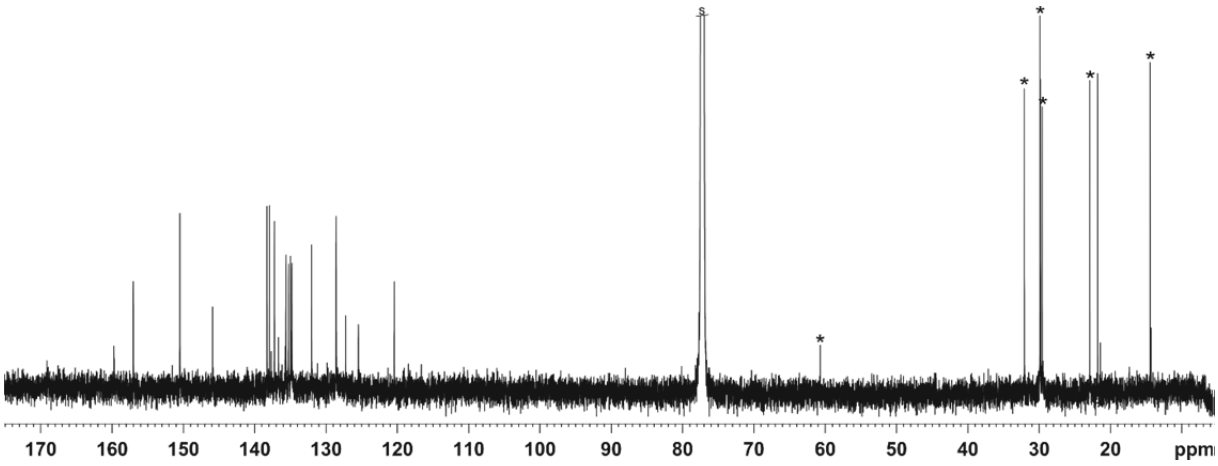


Figure S4. ^{13}C NMR spectrum of **1** (151 MHz, $CDCl_3$, 250 K).

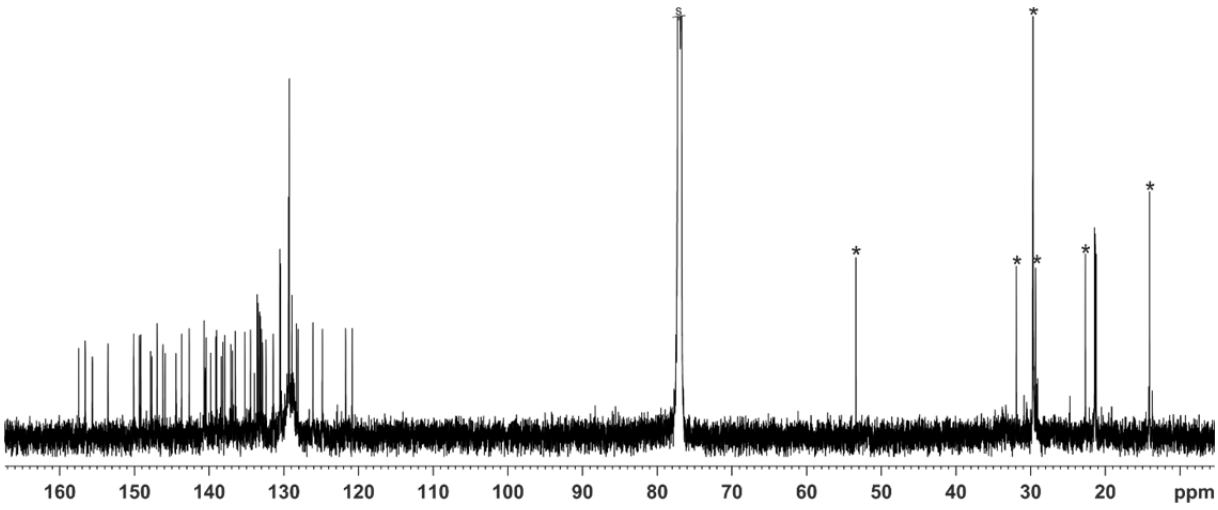


Figure S5. ^{13}C NMR spectrum of **2-Pd$_2$** (151 MHz, $CDCl_3$, 300 K).

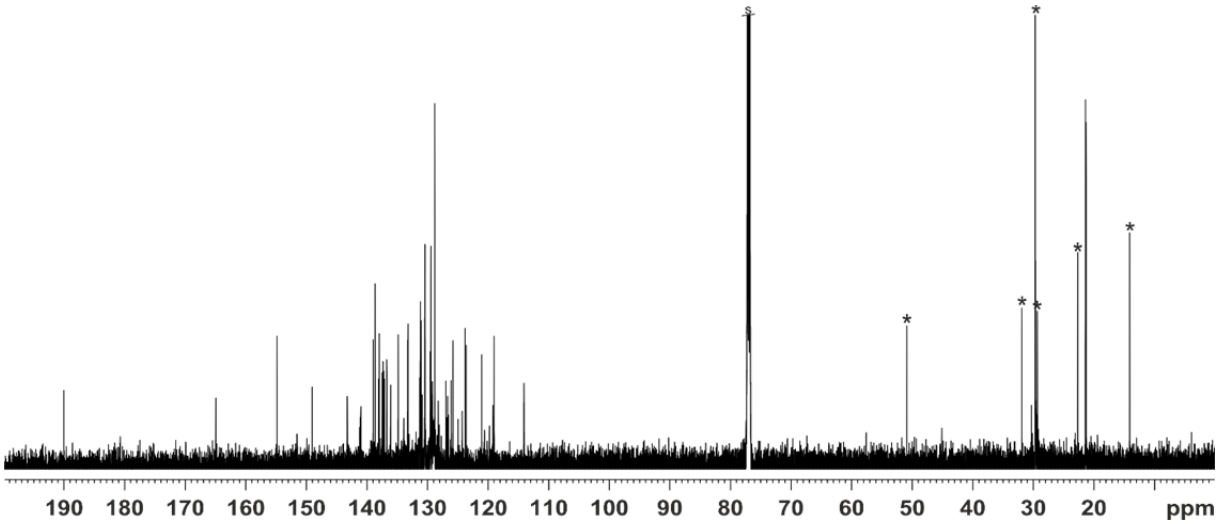


Figure S6. ^{13}C NMR spectrum of **4-Pd** (151 MHz, $CDCl_3$, 300 K).

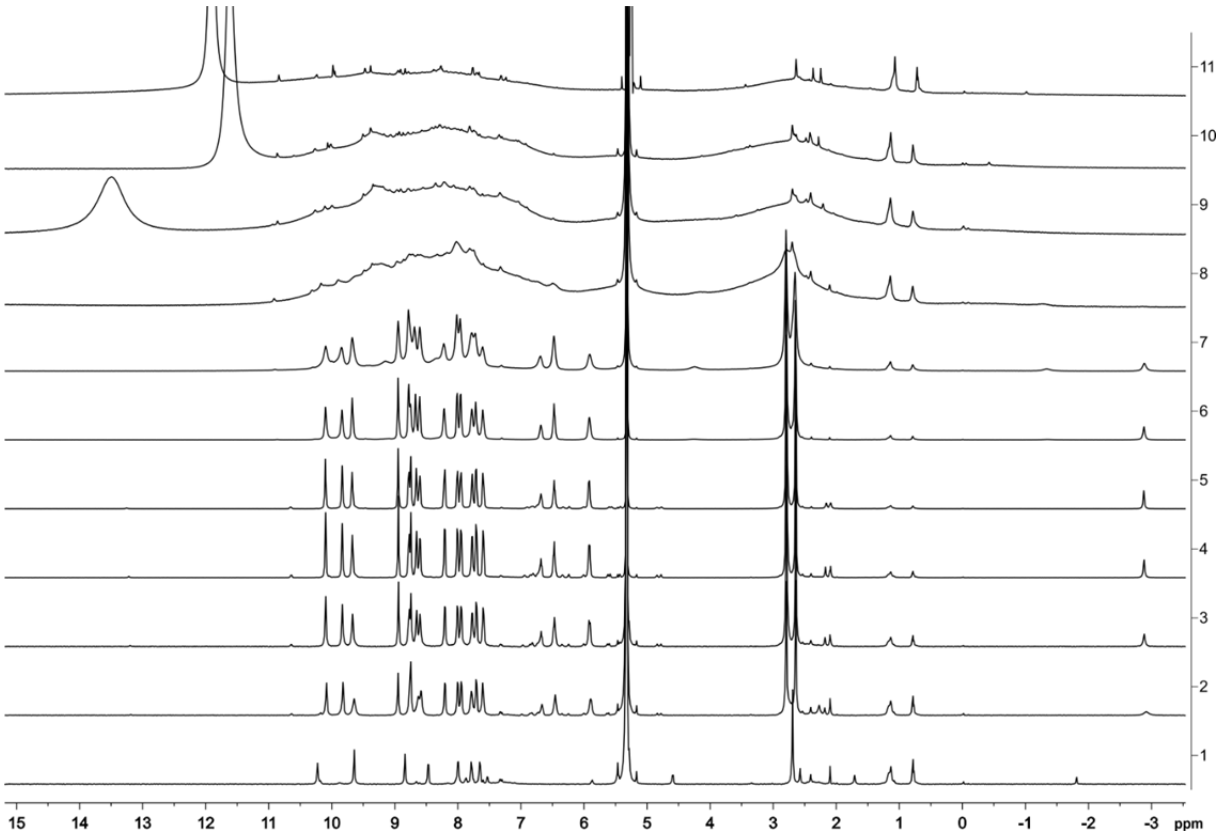


Figure S7. ^{1}H NMR spectra of acid titration (with TFA) of **1** (600 MHz, CD_2Cl_2, 190 K). Trace 1 – HexAz **1**; from Trace 2 to 7 – $[HexAzH_2]^{2+}$; from Trace 8 – the resonances of $[HexAzH_2]^{3+}$ and $[HexAzH_2]^{4+}$ are broadened beyond detection because of exchange presumably forming hydrogen bonds with TFA associates. Residual sharp signals come from the contamination of the sample with 23-thiaazuliporphyrin.

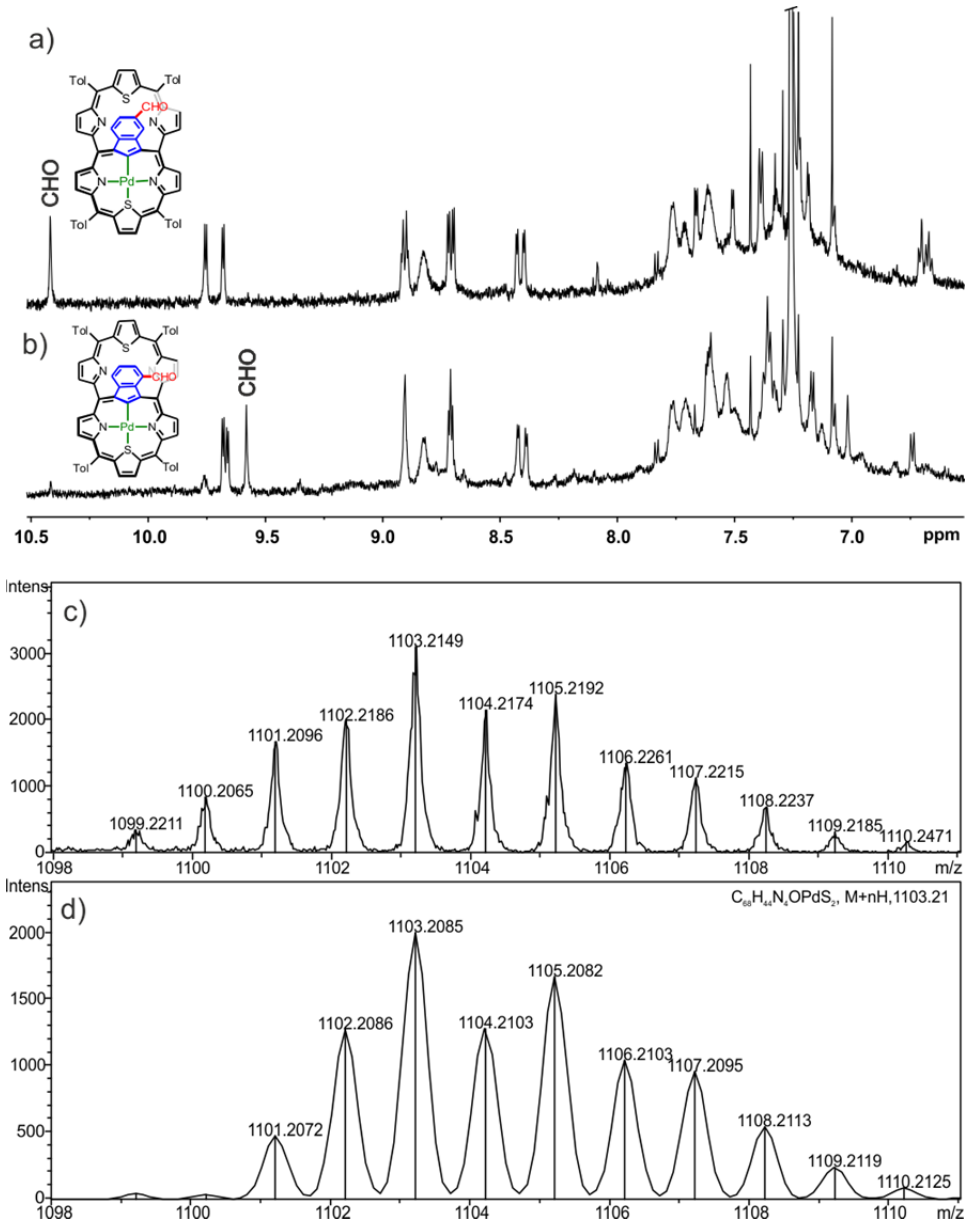


Figure S8. a,b) ^{1}H NMR spectra (600 MHz, $CDCl_3$, 300 K) of formylated **3-Pd$_{a/b}$** obtained in trace amount from coordination reactions. c,d) MS (ESI; obtained and simulated) of the formylated complex sample.

UV-vis spectra

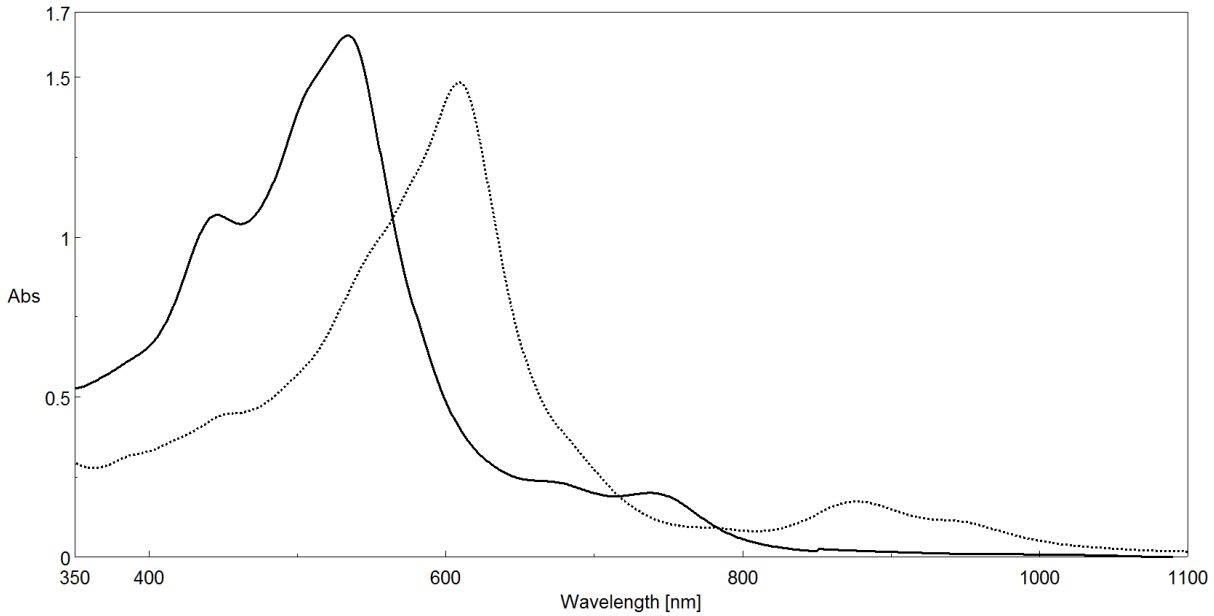


Figure S9. Electronic spectra of **2** (CH_2Cl_2, 293 K, solid line) and **[2-H$_2$]$^{2+}$** (CH_2Cl_2 + TFA, 293 K, dotted line). Arbitrary concentrations.

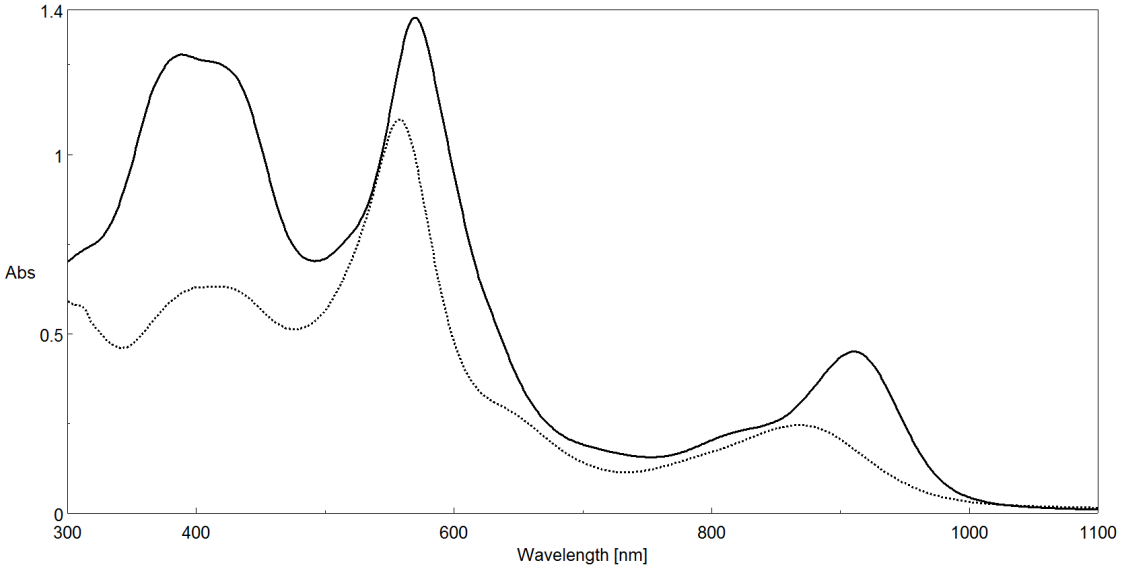


Figure S10. Electronic spectra of **1-Pd^{+}** (CH_2Cl_2 – CH_3CN 2:1, 293 K, solid line) and **2-Pd$_2$** (CH_2Cl_2, 293 K, dotted line). Arbitrary concentrations.

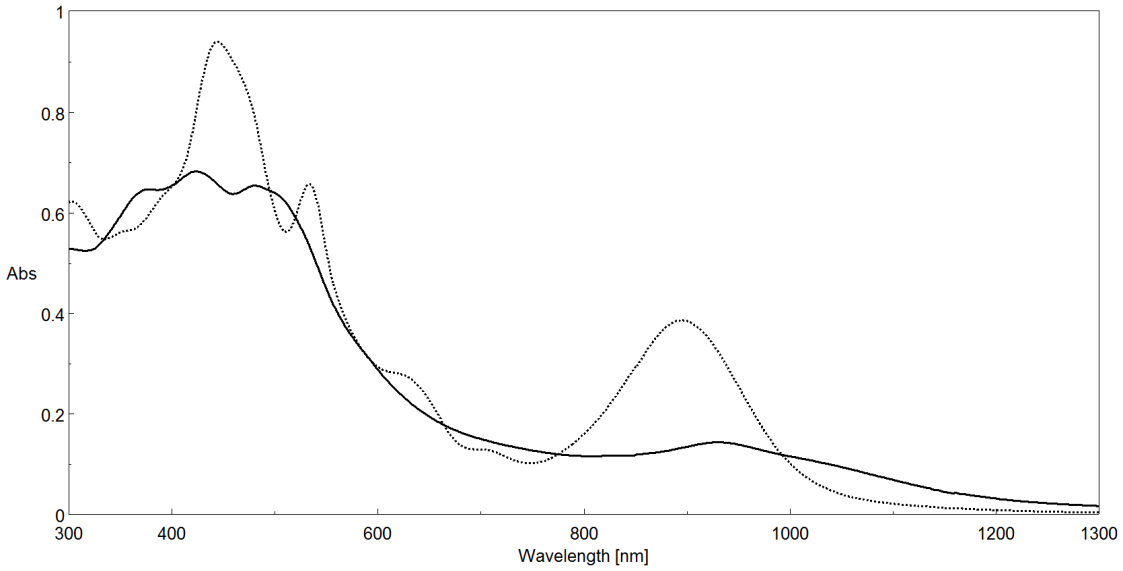


Figure S11. Electronic spectra of **3-Pd** (CH_2Cl_2, 293 K, solid line) and **4-Pd** (CH_2Cl_2, 293 K, dotted line). Arbitrary concentrations.

X-ray crystallography

Crystals for **1** were obtained with a diffusion method of *n*-hexane into DCM solution, while standing in a fridge. These of **4-Pd** crystallized from cooled deuterated toluene solution. The X-ray diffraction data were collected on Oxford Diffraction Xcalibur with a Ruby detector (Mo-K_α radiation; λ = 0.71073 Å). Data reduction and analysis were carried out with the CrysAlis Pro program.[6] An analytical absorption correction was applied for Pd complex. Structures were solved by direct methods using the SHELXS program and refined using all F^2 data, as implemented by the SHELXL program.[7] The SQUEEZE procedure[8] implemented into the PLATON program[9] was applied for disordered lattice solvent molecules. See Table S1 for detailed data. Both structures were drawn with the use of displacement ellipsoids at a 30% probability level.

[6] *CrysAlis Pro RED; Oxford Diffraction (Poland) v. 38.34a*, Wrocław, 2015.
[7] G. M. Sheldrick, *Acta Cryst. A* 2008, **64**, 112.
[8] A. L. Spek, *Acta Cryst. C* 2015, **71**, 9.
[9] A. L. Spek, *Acta Cryst. D* 2009, **65**, 148.

Table S1. Crystal and structure refinement data for **1** and **4-Pd**.

symbol of the structure	**1**	**4-Pd**
empirical formula	$C_{68}H_{46}N_4S_2$	$C_{82}H_{44}D_{16}N_4OPdS_2$
formula weight	983.21	1303.95
crystal size [mm³]	0.20 x 0.14 x 0.11	0.20 x 0.02 x 0.02
crystal system	triclinic	triclinic
space group	$P\bar{1}$	$P\bar{1}$
a [Å]	13.296(3)	11.111(2)
b [Å]	13.957(3)	16.969(3)
c [Å]	17.986(4)	18.186(3)
α [°]	87.92(5)	106.13(3)
β [°]	79.12(4)	93.46(2)
γ [°]	75.01(3)	90.79(2)
V [Å³]	3165.9(14)	3286.2(11)
Z	2	2
density (calcd) [Mg·m⁻³]	1.031	1.318
F(000)	1028	1332
coeff, μ [mm⁻¹]	0.123	0.40
abs. correction	-	analytical
$T_{min/max}$	-	0.966/0.994
T [K]	168(2)	79.9(6)
λ [Å]	0.71073	0.71073
reflections coll., independ., obs.	19968, 10727, 5865	26208, 12892, 5184
R_{int}	0.0548	0.1539
data/parameters	10727/671	12892/817
final R indices (I > 2σ(I))	R_1 = 0.0722, wR = 0.1213	R_1 = 0.0883, wR = 0.1503
R indices (all data)	R_1 = 0.1672, wR = 0.1902	R_1 = 0.2224, wR = 0.2101
GOF on F²	0.954	0.967
Completness	0.961	0.998
peak, hole [e·Å⁻³]	0.50, −0.38	0.65, −0.67
CCDC numbers	1577493	1577494

DFT studies

Geometry optimizations were carried out within unconstrained C_1 symmetry in vacuo, with starting coordinates derived from preoptimized models or crystal structures using Gaussian software.[10] Harmonic frequencies were calculated using analytical second derivatives as a verification of local minimum achievement, with no imaginary frequencies observed. Optimized model names are marked with 'o' as a subscript. Calculations were performed at B3LYP/6-31G(d,p) level of theory[11] and pseudopotential LANL2DZ for Pd atoms. NMR shifts were calculated for optimized structures using the GIAO method and B3LYP/6-31G(d,p)/LANL2DZ(Pd) set with TMS shieldings as a reference. NICS(0)[12] points were determined as a center between four *meso*-C atoms. Total electron density surfaces were derived from population analysis and mapped with electrostatic potential (ESP). Relative energies were calculated including zero-point correction.

*Protonation of **1***

The small energy differences between **[1-H$_2$]$^{2+}$-A$_o$**, **[1-H$_2$]$^{2+}$-B$_o$**, and **[1-H$_2$]$^{2+}$-C$_o$** (Table S2) seem to allows for their simultaneous presence in equilibrium. Presumably the formation of the **[1-H$_2$]$^{2+}$-A$_o$** isomer is directed by generation of a complex with the TFA anion. In fact, the structural model of the least stable tautomer **[1-H$_2$]$^{2+}$-A$_o$** reproduces all structural constraints determined by COSY and ROESY measurements. Importantly, the satisfactory agreement between the experimental and calculated ^{1}H NMR chemical shifts has been found for **[1-H$_2$]$^{2+}$-A$_o$** albeit to account for the peculiar observed chemical shift of NH (2.79 ppm) the formation of the hydrogen bonds with TFA anion had to be included into the modeled structure (Figure S10).

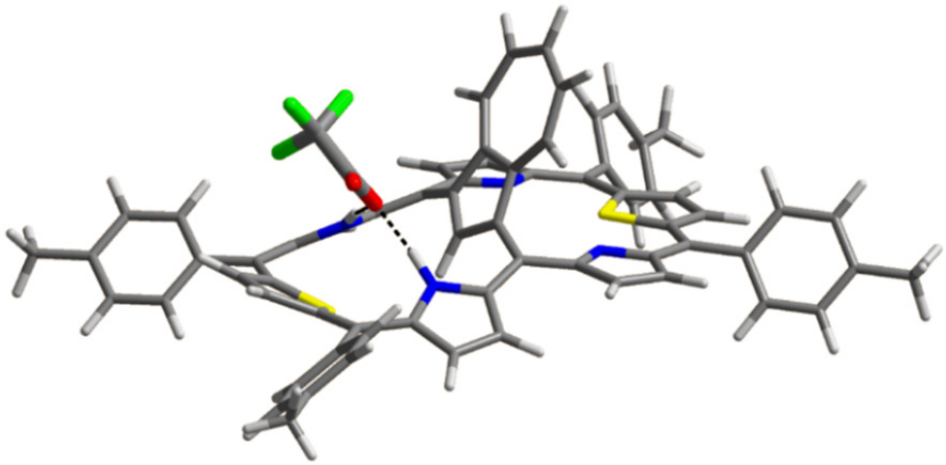


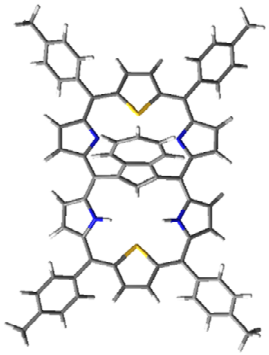
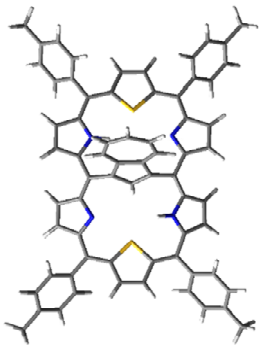
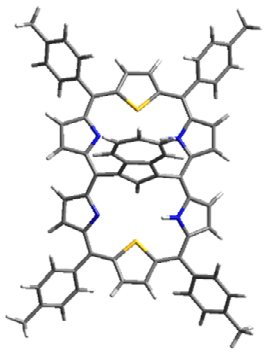
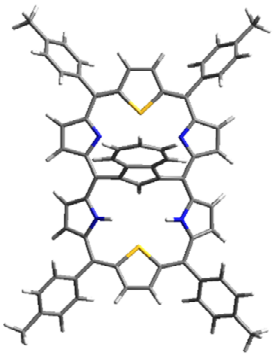
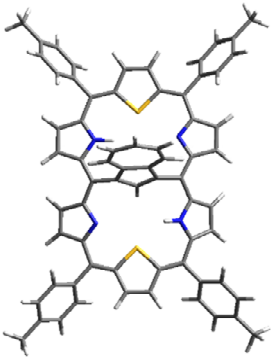
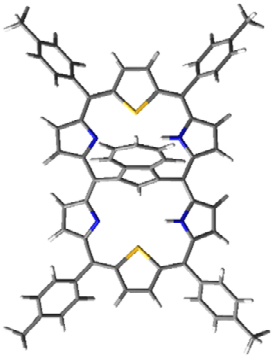
Figure S12. DFT-optimized model of **[1-H$_2$]$^{2+}$-TFA$_o$** with O···H–N hydrogen bonds shown as dashed lines.

[10] Frisch, M. J. T., G. W.; Schlegel, H. B.; Scuseria, G. E.;Robb, M. A.; Cheeseman, J. R.; et al. *Gaussian 09*, Revision E.01; Gaussian, Inc.: Wallingford CT, 2009.

[11] Lee, C.; Yang, W.; Parr, R. G., *Phys. Rev. B* 1988, **37**, 785-789; Becke, A. D., *J. Chem. Phys.* 1993, **98**, 5648-5652.

[12] Chen, Z.; Wannere, C. S.; Corminboeuf, C.; Puchta, R.; Schleyer, P. v. R., *Chem. Rev.* 2005, **105**, 3842-3888.

Table S2. Energy comparison between three $[1\text{-}H_2]^{2+}$ tautomers and respective **2** isomers.

Isomer HexAz dication, $[1\text{-}H_2]^{2+}{}_o$			
	$[1\text{-}H_2]^{2+}\text{-}A_o$	$[1\text{-}H_2]^{2+}\text{-}B_o$	$[1\text{-}H_2]^{2+}\text{-}C_o$
Energy [kcal/mol]	**1.4**	**0.0**	**0.7**
Isomer rHexAz, $\mathbf{2}_o$			
Energy [kcal/mol]	**2.3**	**0.0**	**3.2**

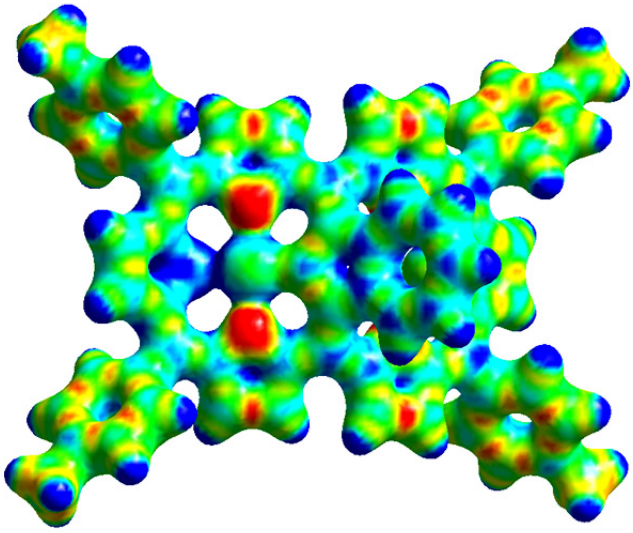


Figure S13. Electrostatic potential (ESP) mapped on a total electron density surface (isovalue = 0.05 e/a.u.^{3}) for $\mathbf{1\text{-}Pd}^+{}_o$. Color code: (scale 0.15-0.30 a.u.) red – the most negative, blue – the most positive charge.

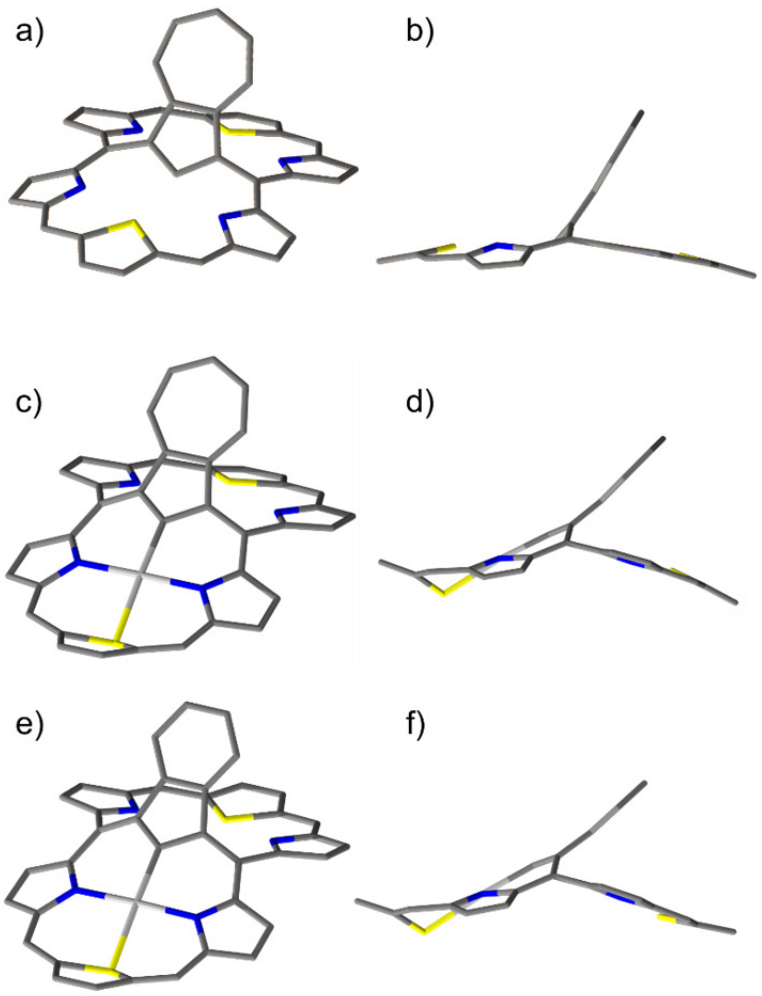


Figure S14. DFT models (without substituents and H atoms) with side projections showing hexaphyrin framework deformations for a,b) $\mathbf{1_o}$, c,d) $\mathbf{1\text{-}Pd^{+}_o}$, e,f) $\mathbf{3\text{-}Pd_o}$.

Table S3. Conformation determining angles and NICS(0) for selected models.

DFT model	$NICS(0)_I$	$NICS(0)_{II}$	Angle C_{Bridge}-$C_{4meso(I)}$	Angle $C_{4meso(I)}$-$C_{4meso(II)}$
$\mathbf{1_o}$	−13.5	−16.7	49.5	17.6
$\mathbf{[1\text{-}H_2]^{2+}_o}$	−12.7	−11.1	50.1	16.9
2	+13.3	+11.2	58.6	12.8
$\mathbf{1\text{-}Pd^{+}_o}$	–	−7.2	29.7	18.9
$\mathbf{3\text{-}Pd_o}$	–	−1.6	25.2	31.3
$\mathbf{4\text{-}Pd_o}$	–	−2.7	32.6*	21.4

*with the 6-membered bridging ring

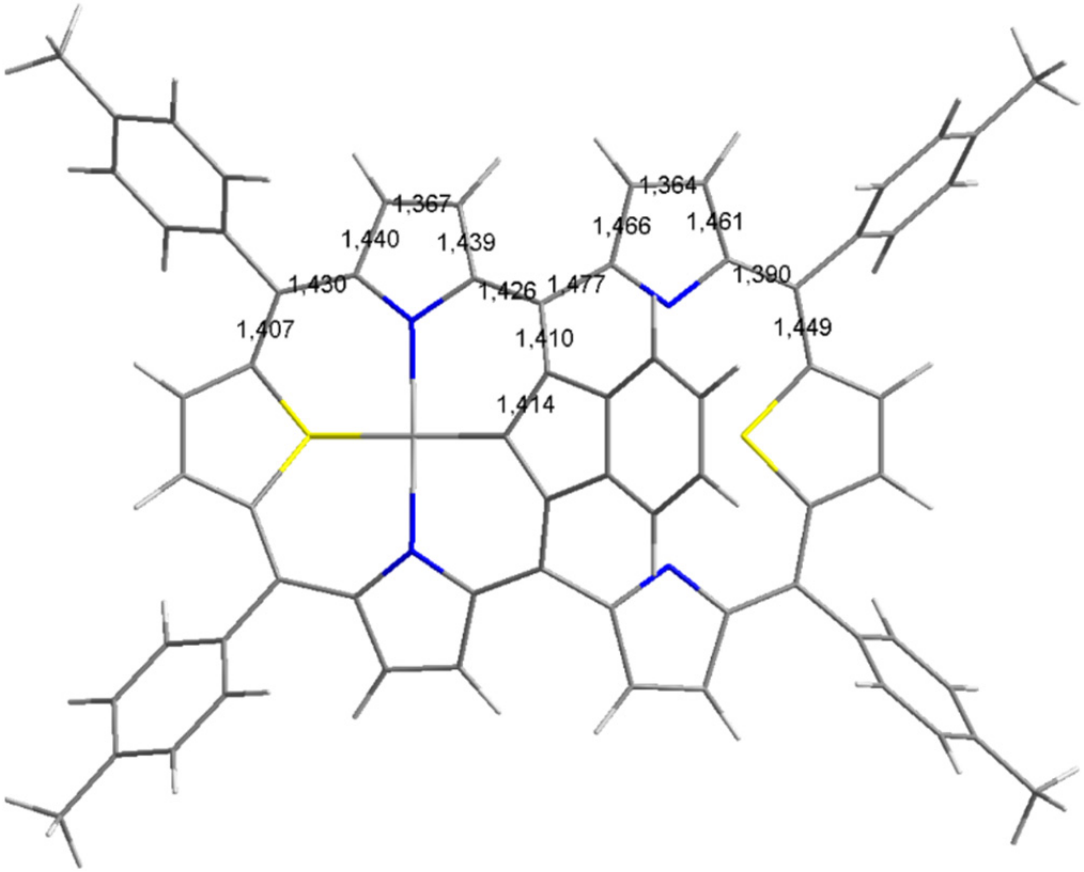


Figure S15. Significant bond distances for **3-Pd$_o$**. One can see marked equalization of values in the cavity I (coordinated), with preserved macrocyclic aromaticity.

Correlations of calculated and observed ^{1}H NMR shifts

(internal signals and those from sunstituents are not included)

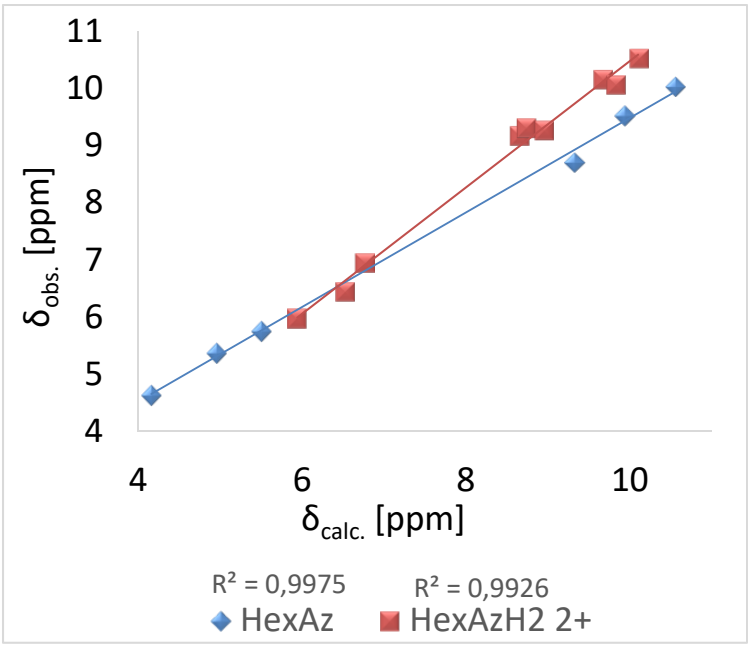


Figure S16. Correlations of DFT calculated and observed ^{1}H NMR shifts of **1$_o$** and **[1-H$_2$]$^{2+}_o$**.

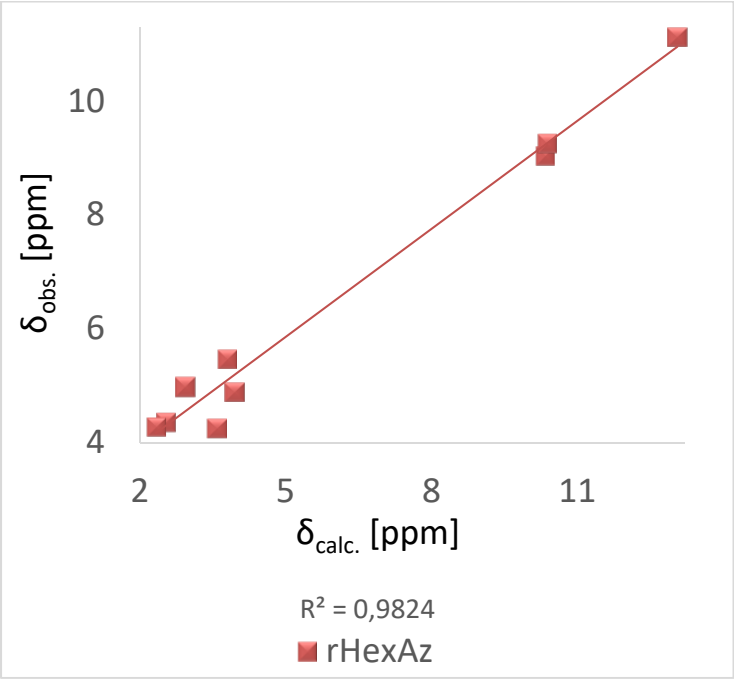


Figure S17. Correlation of DFT calculated and observed ^{1}H NMR shifts of $\mathbf{2}_{o}$.

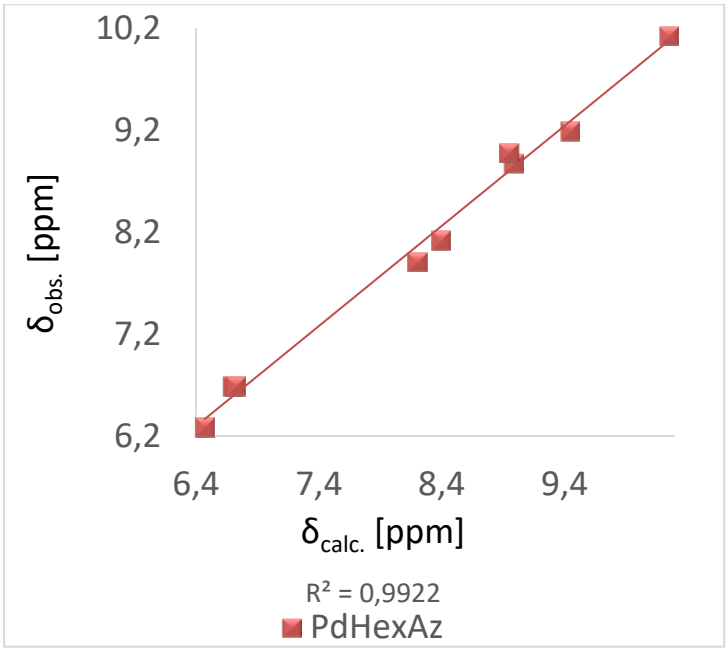


Figure S18. Correlation of DFT calculated and observed ^{1}H NMR shifts of $\mathbf{1\text{-}Pd^{+}}_{o}$.

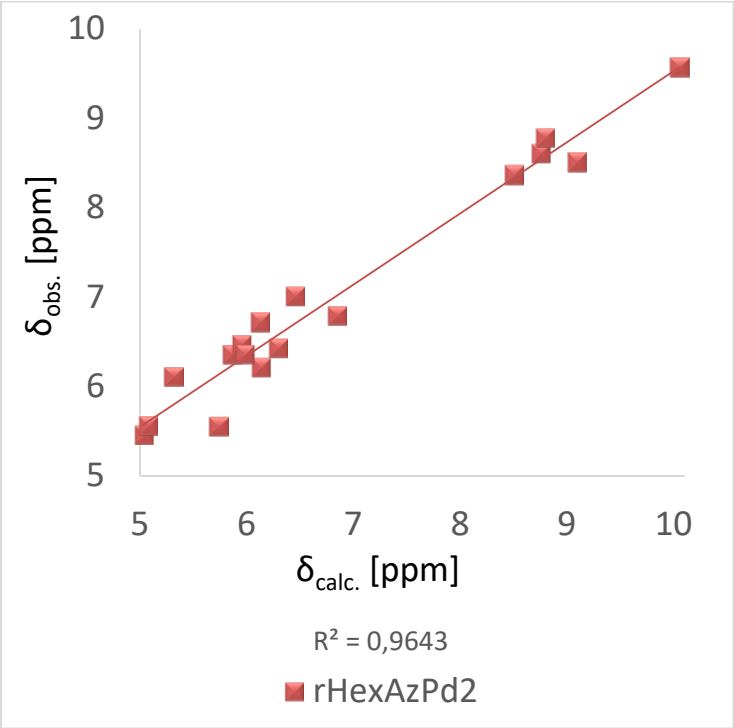


Figure S19. Correlation of DFT calculated and observed ^{1}H NMR shifts of **2-Pd$_{2o}$**.

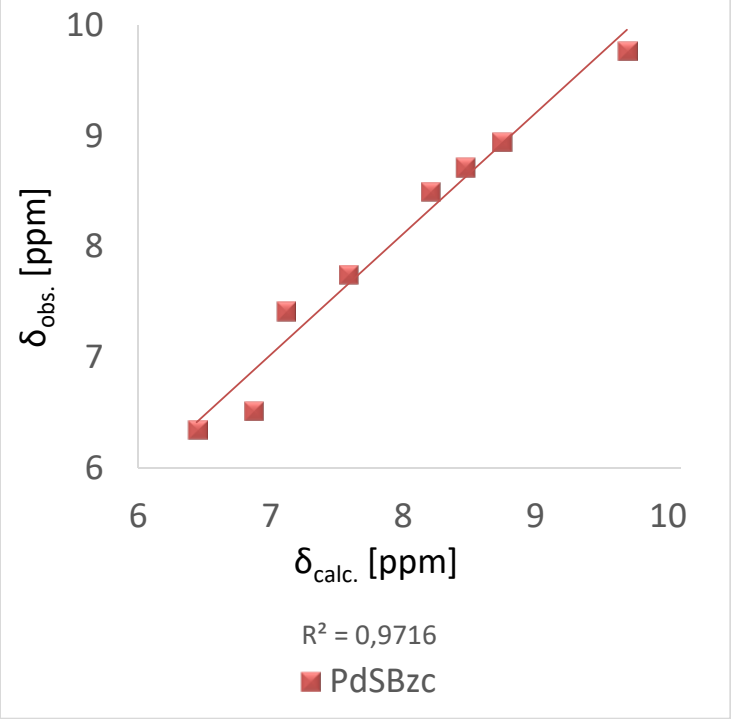


Figure S20. Correlation of DFT calculated and observed ^{1}H NMR shifts of **3-Pd$_{o}$**.

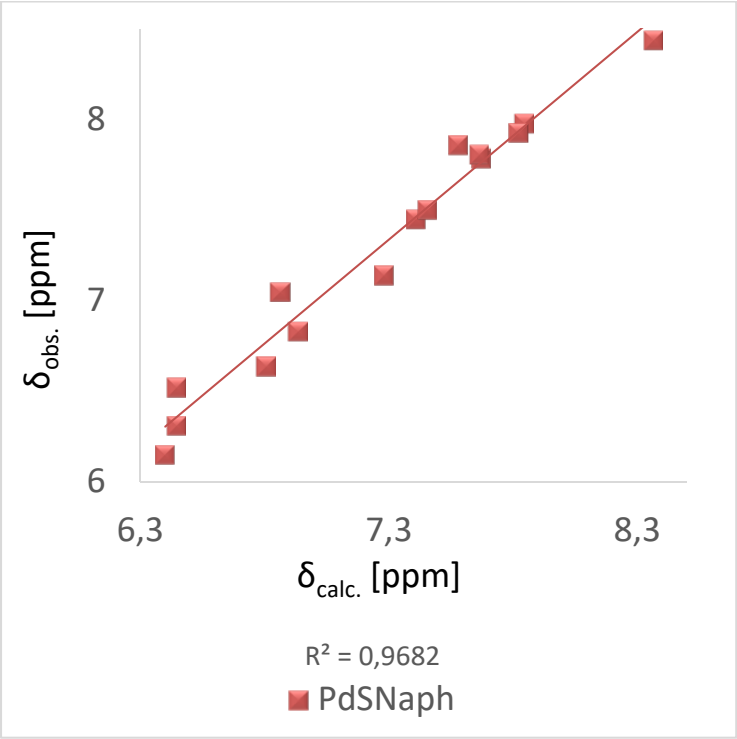


Figure S21. Correlation of DFT calculated and observed ^{1}H NMR shifts of **4-Pd$_o$**.

DFT Coordinates

Azulene-bridged A,D-dithia[26]hexaphyrin, **1$_o$**

C	8.02759500	4.74122800	0.38404200
C	8.12157000	5.42618600	-0.83429000
C	7.14120800	5.17472700	-1.80247500
C	6.09986000	4.27984000	-1.56193500
C	6.00377400	3.60011700	-0.33800400
C	6.98991600	3.84415400	0.63041000
H	8.77600800	4.91409600	1.15364200
H	6.93459800	3.33050900	1.58559900
C	4.88924900	2.64163700	-0.06844300
C	6.48226700	0.68929800	-0.13884300
C	6.48230000	-0.68890900	-0.13919500
C	5.20083100	-1.26736700	0.06489100
S	3.99523200	0.00001600	0.31767800
H	7.36235600	1.28938400	-0.33204100
C	3.56197900	3.13078900	-0.02280200
C	3.08485600	4.46915300	-0.37671300
H	3.69596900	5.30840900	-0.67691700
H	5.36086500	4.09078000	-2.33457300
H	7.19672100	5.68073600	-2.76327900
C	9.22946800	6.42109900	-1.08597200
H	10.14081300	6.15184600	-0.54365900
H	9.47493300	6.48650100	-2.15014000
H	8.94127800	7.42734100	-0.75657500
C	1.72958200	4.42504200	-0.27825700
C	1.39503900	3.07967100	0.19536300
N	2.52319800	2.34116800	0.33426500
C	0.02855400	1.15156900	0.98117700
C	0.56774500	-0.00005900	0.38620800
C	0.02860300	-1.15199200	0.98063000
C	-0.76773500	-0.73471700	2.09709900
C	-0.76775200	0.73373300	2.09745900
C	-1.34243300	1.57915500	3.04200200
C	-2.06638600	1.25818900	4.19329200
C	-1.34239300	-1.58061500	3.04122900
H	-1.20779000	2.64148800	2.85751500
C	0.12790900	-2.52257200	0.50014900
C	1.72979500	-4.42486700	-0.28015500
C	3.08507600	-4.46891100	-0.37850200
C	3.56212400	-3.13061200	-0.02423700
N	2.52331400	-2.34120900	0.33324000
C	4.88936200	-2.64138100	-0.06972800
C	6.00396900	-3.59970400	-0.33951100
C	6.10027800	-4.27926200	-1.56309900
C	6.99009500	-3.84390300	0.62940800
C	8.02753300	-4.74080300	0.38340500
C	8.12180600	-5.42586900	-0.83527800
C	7.14189700	-5.17446100	-1.80338500
H	5.36152400	-4.09042100	-2.33601900
H	7.19748400	-5.68051600	-2.76411800
C	9.23068400	-6.42011400	-1.08529600
H	10.16090400	-6.11462800	-0.59647900
H	8.97000500	-7.41152500	-0.69391600
H	9.43155800	-6.53545100	-2.15438800
H	8.77581700	-4.91375300	1.15316500
H	6.93426200	-3.33027800	1.58457700
H	7.36243000	-1.28883200	-0.33271100
H	1.03648900	5.21914200	-0.51166200
H	1.21542400	0.00015700	-0.47641300
H	-2.42397600	2.10674600	4.77151300
H	-1.20771600	-2.64285500	2.85622500
H	1.03674100	-5.21890700	-0.51388300
H	3.69624800	-5.30803700	-0.67894500
C	-1.13606800	-3.16515000	0.26839400
C	-1.13622600	3.16500700	0.26990400
N	-2.21730500	2.38113900	0.08105900
C	-3.28267400	3.19709000	-0.12382200
C	-2.86416300	4.59692700	-0.02476600
C	-1.52039800	4.57649000	0.19803500
N	-2.21718100	-2.38123900	0.07991700
C	-3.28250900	-3.19714200	-0.12537000
C	-2.86391900	-4.59701100	-0.02707000
C	-1.52016700	-4.57661800	0.19580500
C	-4.56061100	-2.67044900	-0.39307200
C	-4.82754000	-1.26929900	-0.45001200
S	-3.64057700	-0.00003300	-0.12133800
C	-4.82761000	1.26932800	-0.44940000
C	-6.06015000	0.69170200	-0.83371000
C	-6.06011100	-0.69155700	-0.83404400
C	-4.56075400	2.67046400	-0.39177400

C	-5.68328700	3.62109600	-0.64086700
C	-6.82783200	3.62656100	0.17341800
C	-7.86275700	4.53077500	-0.05362600
C	-7.79957200	5.45979100	-1.10077500
C	-6.66096100	5.44861800	-1.91620300
C	-5.61915500	4.55068400	-1.69119600
C	-5.68308800	-3.62101300	-0.64267300
C	-5.61890200	-4.55006700	-1.69339500
C	-6.66071200	-5.44797700	-1.91883700
C	-7.79929000	-5.45957900	-1.10347600
C	-7.86253000	-4.53103100	-0.05583300
C	-6.82768600	-3.62691700	0.17163100
C	-8.91094000	-6.45626100	-1.32886100
C	-8.91105000	6.45673000	-1.32586500
H	-3.50439300	5.46488700	-0.09900600
H	-0.87792500	5.42888500	0.36617700
H	-3.50409700	-5.46496700	-0.10180200
H	-0.87765300	-5.42906900	0.36351100
H	-6.91523400	1.28819000	-1.12426400
H	-6.91516200	-1.28795200	-1.12489000
H	-6.89697700	2.92311100	0.99751200
H	-8.73412200	4.51688800	0.59656900
H	-6.58990700	6.14905100	-2.74469400
H	-4.75271400	4.55304900	-2.34510500
H	-4.75245300	-4.55212100	-2.34729500
H	-6.58960800	-6.14804200	-2.74762600
H	-8.73390000	-4.51748600	0.59437600
H	-6.89684100	-2.92385800	0.99605900
C	1.39519200	-3.07968800	0.19398200
C	5.20077300	1.26759000	0.06555200
H	-8.75009600	7.36884700	-0.73748300
H	-8.97426000	6.75546300	-2.37632400
H	-8.75709700	-7.36313500	-0.73056600
H	-8.96585300	-6.76451200	-2.37699400
H	-9.88355800	-6.04301900	-1.04516300
H	-9.88202500	6.04822500	-1.03009900
C	-2.06635100	-1.26023100	4.19267700
C	-2.38788300	-0.00115000	4.70246600
H	-2.96632700	-0.00138200	5.62415400
H	-2.42391200	-2.10908100	4.77048700
C	0.12779100	2.52237600	0.50132600

Azulene-bridged A,D-dithia[26]hexaphyrin dication, two protons in I cavity, **[1-H_2]$^{2+}_o$**

C	-7.00488500	-5.80696200	0.26074600
C	-8.09642700	-5.57977100	-0.59231000
C	-8.13417600	-4.36924000	-1.30384400
C	-7.12743200	-3.42185600	-1.17023100
C	-6.02920300	-3.65315300	-0.31562600
C	-5.98687900	-4.87060200	0.39486800
H	-6.96024600	-6.72735600	0.83567100
H	-5.17042400	-5.06174000	1.08404400
C	-4.94839400	-2.66086200	-0.17333900
C	-6.50739300	-0.69248000	0.27895200
C	-6.50751300	0.69215800	0.27907700
C	-5.26649800	1.28339500	-0.06033100
S	-4.10533500	0.00013600	-0.41364200
H	-7.36508900	-1.29089500	0.55860500
C	-3.60119300	-3.12514800	-0.18622500
C	-3.05717400	-4.31067200	-0.77173000
H	-3.63998500	-5.05852900	-1.28835600
H	-7.16737200	-2.51117700	-1.75912900
H	-8.96139600	-4.17468500	-1.98041200
C	-9.18011200	-6.61184100	-0.76101000
H	-9.27467400	-7.24361700	0.12565800
H	-10.14944300	-6.14688300	-0.95930600
H	-8.95624500	-7.27016800	-1.60947700
C	-1.68472200	-4.26991500	-0.64284400
C	-1.33625800	-3.07449800	0.05799800
N	-2.52706800	-2.42575400	0.31089200
C	-0.04268000	-1.15421600	0.95644800
C	-0.55804000	0.00035000	0.33682300
C	-0.04287300	1.15552800	0.95545800
C	0.73404200	0.72898700	2.09426500
C	0.73415700	-0.72655100	2.09492200
C	1.28867900	-1.57871400	3.05048900
C	2.00325000	-1.25861800	4.20561500
C	1.28840800	1.58209300	3.04908100
H	1.14986000	-2.64086800	2.86875400
C	-0.09936200	2.51287100	0.43741900
C	-1.68568200	4.26956700	-0.64631700
C	-3.05821900	4.31020700	-0.77442900
C	-3.60187300	3.12531500	-0.18729200
N	-2.52743400	2.42642900	0.30988500
C	-4.94901900	2.66088000	-0.17320100
C	-6.03053300	3.65255500	-0.31423200
C	-7.12770900	3.42197200	-1.17030500
C	-5.98618500	4.87192100	0.39295900
C	-7.00144400	5.81050300	0.25463700
C	-8.09494300	5.58156400	-0.59553000
C	-8.13182200	4.37167700	-1.30813800
H	-7.16522700	2.51318800	-1.76230400
H	-8.95419400	4.18083800	-1.99157300
C	-9.20480800	6.59134600	-0.72376700
H	-10.00485700	6.37758000	-0.00427800
H	-8.85046800	7.60577100	-0.52433200
H	-9.65193300	6.57100100	-1.72108400
H	-6.95148700	6.73578500	0.82128500
H	-5.16657600	5.06600400	1.07753900
H	-7.36535000	1.29040500	0.55864000
H	-0.97812400	-4.97869200	-1.04706200
H	-1.10395900	-0.00008500	-0.59816800
H	2.35015600	-2.10538200	4.79135700
H	1.14940700	2.64406800	2.86641300
H	-0.97935400	4.97788600	-1.05180100
H	-3.64131300	5.05744400	-1.29166000
C	1.16841700	3.15924100	0.23729500
C	1.16889300	-3.15851800	0.24055000
N	2.24973100	-2.37250700	0.07353800
C	3.31345000	-3.19870200	-0.11152100
C	2.88602900	-4.59598200	-0.01291700
C	1.53730600	-4.56930200	0.18098500
N	2.24937100	2.37311500	0.07124000
C	3.31288900	3.19918500	-0.11528800
C	2.88526900	4.59656500	-0.01882100
C	1.53662700	4.56999100	0.17557600
C	4.60069000	2.67902600	-0.36623000
C	4.86430600	1.26410500	-0.41737300
S	3.71110400	0.00034900	0.00036300
C	4.86458400	-1.26372000	-0.41584300
C	6.05825900	-0.69417800	-0.90298400
C	6.05808100	0.69419800	-0.90391700
C	4.60121300	-2.67863300	-0.36290000
C	5.72185300	-3.61274300	-0.60496700
C	6.92059100	-3.51370700	0.12904200
C	7.95952900	-4.41228800	-0.08453300
C	7.85865000	-5.42770400	-1.04833500
C	6.67052900	-5.51268200	-1.79035900
C	5.61568300	-4.63405100	-1.56904700
C	5.72121000	3.61305300	-0.60957000
C	5.61482700	4.63313000	-1.57516000
C	6.66934800	5.51158800	-1.79755100
C	7.85759700	5.42788100	-1.05517000
C	7.95859900	4.41395200	-0.09014000
C	6.91971100	3.51528000	0.12460800
C	8.98015300	6.40895400	-1.27285700
C	8.98217800	-6.40817800	-1.26373500
H	3.52374100	-5.46643700	-0.06197900
H	0.88265000	-5.41581500	0.33578900
H	3.52280400	5.46705800	-0.06946700
H	0.88196700	5.41667900	0.32939300
H	6.87772200	-1.29049400	-1.28079700
H	6.87739200	1.29022500	-1.28250200
H	7.02069500	-2.74857900	0.89235700
H	8.86626500	-4.32720500	0.50765200
H	6.57507700	-6.27428800	-2.55899100
H	4.71898200	-4.70685100	-2.17591300
H	4.71809600	4.70487200	-2.18211300
H	6.57377600	6.27211700	-2.56728100
H	8.86526200	4.32987700	0.50224800
H	7.02002000	2.75119600	0.88894200
C	-1.33677800	3.07490600	0.05558700
C	-5.26624800	-1.28344800	-0.06054500
H	8.87587400	-7.27087200	-0.59458100
H	8.99085300	-6.78989600	-2.28787200
H	8.84678800	7.29543800	-0.64066500
H	9.01661500	6.75263500	-2.30995800
H	9.94985100	5.97243600	-1.02009900
H	9.95531200	-5.95524400	-1.05640000
C	2.00303600	1.26313400	4.20448700
C	2.32372600	0.00251600	4.71448100
H	2.89240100	0.00298600	5.64110100
H	2.34979100	2.11048000	4.78948100

C	-0.09904000	-2.51205000	0.43975500
H	-2.58781800	-1.59674800	0.88311000
H	-2.58785200	1.59812500	0.88315300

Azulene-bridged A,D-dithia[26]hexaphyrin dication, two protons in I cavity H-bound to TFA-, **[1-H_2]-TFA^+_o**

C	6.43957100	5.94503400	-0.16109000
C	7.57084400	5.78628500	-0.97606000
C	7.67852200	4.60793700	-1.73097800
C	6.69585800	3.62723800	-1.67958700
C	5.55372500	3.79195500	-0.86906200
C	5.44718400	4.97388900	-0.10692300
H	6.34516200	6.83652800	0.45263800
H	4.60376900	5.10100800	0.56326600
C	4.50865200	2.75877300	-0.81076100
C	6.07124100	0.82866500	-0.27082500
C	6.08919300	-0.55615300	-0.28292300
C	4.91540400	-1.13668100	-0.81414000
S	3.85059100	0.11623500	-1.40956400
H	6.83450600	1.44117500	0.19147700
C	3.14716600	3.16049600	-0.76284900
C	2.56542100	4.36054800	-1.28968900
H	3.11389200	5.12768600	-1.81584900
H	6.79182900	2.73664600	-2.29218500
H	8.54282400	4.46328900	-2.37327500
C	8.62782000	6.85796100	-1.05415900
H	8.71159100	7.40674000	-0.11215800
H	9.60799500	6.43823000	-1.29586500
H	8.38395100	7.58829500	-1.83573400
C	1.20861300	4.29092100	-1.09369000
C	0.92773100	3.06986700	-0.39602600
N	2.12482400	2.41444400	-0.22589900
C	-0.35992900	1.19203200	0.57543500
C	0.12877500	0.04379100	-0.05732200
C	-0.31737700	-1.10145400	0.61179600
C	-1.01041800	-0.67642900	1.80146800
C	-1.04194400	0.77851800	1.77654200
C	-1.53084400	1.63727300	2.75839400
C	-2.13073400	1.32323000	3.97922700
C	-1.45462800	-1.52269400	2.81446400
H	-1.43030200	2.69791900	2.54599000
C	-0.23468400	-2.45144900	0.10262400
C	1.31105500	-4.12975100	-1.11622500
C	2.66571900	-4.15294800	-1.33882800
C	3.22410300	-2.95361500	-0.79044300
N	2.18711800	-2.25423700	-0.21312100
C	4.57357000	-2.51602600	-0.85447200
C	5.64427400	-3.52055600	-0.94929300
C	6.77053900	-3.30650900	-1.77078800
C	5.57759800	-4.72558700	-0.21971800
C	6.59176400	-5.67100900	-0.31465700
C	7.71020900	-5.45964400	-1.13499700
C	7.77588400	-4.26079400	-1.86228300
H	6.83261800	-2.40083300	-2.36531000
H	8.62341500	-4.08057800	-2.51779900
C	8.82140400	-6.47514600	-1.21072400
H	9.59020900	-6.26616300	-0.45651000
H	8.45285400	-7.48790900	-1.02684500
H	9.31255900	-6.45965900	-2.18754300
H	6.52292700	-6.58545300	0.26797600
H	4.74208500	-4.89725000	0.45060800
H	6.87090900	-1.15650800	0.16459800
H	0.46467500	4.99191200	-1.44011100
H	0.65701100	0.03986400	-1.00112100
H	-2.44413400	2.17412100	4.57819800
H	-1.30257500	-2.58367800	2.63783900
H	0.58464000	-4.84090300	-1.47693100
H	3.22497900	-4.88722800	-1.89936200
C	-1.49233400	-3.13523300	-0.02937200
C	-1.57891400	3.18498500	-0.08739500
N	-2.65992800	2.38775500	-0.17028800
C	-3.74890900	3.19521200	-0.27075800
C	-3.33366100	4.59941200	-0.22338300
C	-1.97363300	4.59192300	-0.13422800
N	-2.60647300	-2.37766400	-0.03224600
C	-3.65846200	-3.20878200	-0.25314000
C	-3.18673000	-4.59120700	-0.36398700
C	-1.83227500	-4.54355600	-0.22642000
C	-4.95636800	-2.69967100	-0.45042300
C	-5.24761400	-1.29539700	-0.45066900
S	-4.04438800	-0.01089500	-0.30548200
C	-5.28838300	1.23887600	-0.41573800
C	-6.56024200	0.64588200	-0.56595500
C	-6.53985000	-0.74010000	-0.56760800
C	-5.04118000	2.65153500	-0.38663400
C	-6.19723700	3.58441500	-0.48835000
C	-7.22872100	3.57494800	0.46619900
C	-8.29088300	4.47008200	0.37354300
C	-8.37148200	5.39836000	-0.67420300
C	-7.34521000	5.39928400	-1.62825200
C	-6.27198000	4.51601100	-1.53691700
C	-6.06720700	-3.66182500	-0.68185100
C	-6.84865000	-3.61152000	-1.84943400
C	-7.86775500	-4.53516000	-2.06275100
C	-8.15409900	-5.53430700	-1.12136300
C	-7.37822000	-5.57688700	0.04478300
C	-6.34778500	-4.66514200	0.26085800
C	-9.24578800	-6.54555400	-1.36969000
C	-9.51361600	6.38078600	-0.75628200
H	-3.98618100	5.46061600	-0.24220100
H	-1.32045600	5.44821700	-0.03746200
H	-3.79870900	-5.46405200	-0.54055600
H	-1.14964500	-5.38155800	-0.21913300
H	-7.46571100	1.22829000	-0.67128700
H	-7.43033300	-1.34891100	-0.64920700
H	-7.18492500	2.87584000	1.29572200
H	-9.07057700	4.44981500	1.13032900
H	-7.38864800	6.09840300	-2.45905000
H	-5.49725300	4.52757200	-2.29729000
H	-6.63879300	-2.85797100	-2.60213100
H	-8.44993200	-4.48187100	-2.97885600
H	-7.58677900	-6.33193100	0.79795900
H	-5.77030700	-4.71135200	1.17900100
C	1.00335000	-2.93985400	-0.37985300
C	4.88325600	1.38804500	-0.79241200
H	-9.29200500	7.28790100	-0.18069900
H	-9.70408200	6.68844000	-1.78804900
H	-8.86856500	-7.39275600	-1.95552000
H	-10.07644500	-6.10852100	-1.93120100
H	-9.64080800	-6.94730400	-0.43273600
H	-10.43656100	5.95711900	-0.35033000
C	-2.06615500	-1.19524300	4.02595300
C	-2.36978900	0.06690300	4.54023200
H	-2.84940000	0.07274600	5.51606100
H	-2.33456600	-2.03829000	4.65698900
C	-0.30283400	2.53760400	0.05304900
H	2.27524600	1.57231500	0.39339800
H	2.31564200	-1.42937400	0.41403900
O	2.57026900	0.12026300	1.28499800
O	3.89010400	1.44899900	2.55232400
C	3.37826800	0.37678100	2.25115400
C	3.71115700	-0.88268900	3.09821400
F	2.59080900	-1.41506300	3.64107200
F	4.25992500	-1.85226700	2.30796300
F	4.57408000	-0.63751100	4.08864700

Azulene-bridged A,D-dithia[26]hexaphyrin dication, two protons in both cavities, **[1-H_2]$^{2+}$$B_o$**

C	-6.91587700	-5.86957900	0.15339300
C	-7.95587500	-5.64777300	-0.76326100
C	-7.96079800	-4.43474400	-1.47201600
C	-6.97356600	-3.47876100	-1.27333100
C	-5.92542600	-3.70518900	-0.35586600
C	-5.91459900	-4.92661100	0.35017100
H	-6.89931100	-6.79095600	0.72818800
H	-5.13996500	-5.11280100	1.08711100
C	-4.86480300	-2.70524500	-0.14201100
C	-6.48610000	-0.78167000	0.22478700
C	-6.51598700	0.60449700	0.21858600
C	-5.26650600	1.21397700	-0.03749500
S	-4.03983000	-0.02099300	-0.23780100
H	-7.34779600	-1.39961700	0.44164000
C	-3.51987900	-3.16396800	-0.09744100
C	-2.95867900	-4.35144100	-0.66190500
H	-3.52663200	-5.10649800	-1.18429400
H	-6.98648900	-2.56523400	-1.85861500
H	-8.74729500	-4.24454100	-2.19665400
C	-9.01942900	-6.68716300	-0.99982800
H	-9.15661700	-7.32793900	-0.12532700

H	-9.98051200	-6.22840000	-1.24687500
H	-8.74372500	-7.33544900	-1.84078900
C	-1.58880400	-4.30129600	-0.51060600
C	-1.26123600	-3.09700900	0.18282700
N	-2.45560100	-2.45495800	0.41524600
C	-0.01099300	-1.12218800	1.01250900
C	-0.55010400	-0.01307400	0.33495600
C	-0.09657000	1.18101700	0.91991000
C	0.65873300	0.83034700	2.09710800
C	0.71299500	-0.62713500	2.15558700
C	1.27009000	-1.42064100	3.15662300
C	1.92789800	-1.03181100	4.32610500
C	1.15203500	1.73611600	3.03870100
H	1.17820100	-2.49317400	3.00862600
C	-0.23105800	2.53223900	0.38765200
C	-1.82767800	4.35868100	-0.54857400
C	-3.18154400	4.39254500	-0.65044000
C	-3.65778700	3.09210400	-0.16860900
N	-2.61929200	2.32450300	0.23805900
C	-4.99248500	2.60800000	-0.17173200
C	-6.11274700	3.55091500	-0.33499000
C	-7.16880000	3.29472400	-1.23385000
C	-6.14417600	4.75526200	0.39839000
C	-7.19379200	5.65265900	0.24534300
C	-8.24459500	5.39978000	-0.65092000
C	-8.20468000	4.20745600	-1.39113000
H	-7.14810700	2.39837600	-1.84537200
H	-8.99267700	3.99937800	-2.10919400
C	-9.38998700	6.36698200	-0.79669300
H	-10.18397100	6.13587600	-0.07583300
H	-9.07241300	7.39618600	-0.61004200
H	-9.83251100	6.31764100	-1.79489000
H	-7.20409900	6.56491100	0.83494800
H	-5.35740200	4.96497200	1.11585600
H	-7.40603800	1.18618300	0.41984700
H	-0.87323700	-5.00916900	-0.89948600
H	-1.11460800	-0.05953400	-0.58615900
H	2.28495200	-1.84343500	4.95399000
H	0.97568600	2.78553300	2.81654800
H	-1.13072600	5.12441900	-0.85730600
H	-3.79424500	5.18301400	-1.05890800
C	1.01455100	3.20832700	0.17301000
C	1.24411100	-3.13067000	0.38452800
N	2.33418900	-2.34477100	0.23296000
C	3.39031100	-3.17319700	0.03077400
C	2.95961100	-4.57326200	0.11839400
C	1.61422800	-4.54454700	0.31325400
N	2.13154400	2.43661800	-0.03592400
C	3.26997000	3.19762600	-0.16244900
C	2.83523500	4.55360900	0.00513500
C	1.46454800	4.56080500	0.18321000
C	4.57188100	2.68052600	-0.39127700
C	4.89240000	1.28902800	-0.38990300
S	3.82397800	-0.00674300	0.17406700
C	4.93776200	-1.26367900	-0.34321500
C	6.08903100	-0.66612000	-0.90180000
C	6.06516400	0.71906700	-0.93415300
C	4.67572900	-2.66849000	-0.26630500
C	5.78430900	-3.60378500	-0.56608300
C	7.00966300	-3.51370600	0.12179300
C	8.04057600	-4.40815600	-0.14516200
C	7.90114000	-5.41232100	-1.11547300
C	6.68472300	-5.48839000	-1.81081600
C	5.64057900	-4.61028300	-1.53958500
C	5.65281200	3.65040100	-0.67780400
C	5.49536700	4.64655100	-1.66146300
C	6.51817000	5.55125200	-1.92407900
C	7.72590100	5.51412400	-1.21005700
C	7.87862500	4.52156200	-0.22869400
C	6.87012400	3.60111600	0.03044600
C	8.81601200	6.52006600	-1.47256900
C	9.01435400	-6.39112400	-1.38669400
H	3.59776800	-5.44278700	0.05932300
H	0.95701400	-5.39019000	0.45984700
H	3.49261200	5.40950800	0.02999200
H	0.84730700	5.42328300	0.38636500
H	6.89481500	-1.25881100	-1.31379400
H	6.84458100	1.31770300	-1.38649700
H	7.13997700	-2.75848300	0.89084700
H	8.97025400	-4.32940900	0.41123300
H	6.55797100	-6.24186600	-2.58297800
H	4.72075000	-4.67579500	-2.11200800
H	4.58431500	4.68110100	-2.25039300
H	6.38281900	6.29396600	-2.70500000
H	8.80127800	4.47416100	0.34261400
H	7.00873800	2.85634300	0.80779100
C	-1.49742000	3.05699600	0.03590500
C	-5.20798500	-1.32632100	-0.03445200
H	8.92012900	-7.27254400	-0.74065400
H	8.99568600	-6.74312100	-2.42139300
H	8.70523400	7.38977500	-0.81330100
H	8.78524400	6.88588100	-2.50198000
H	9.80632200	6.09635500	-1.28619600
H	9.99459700	-5.94866500	-1.19105000
C	1.83349100	1.48592400	4.23001600
C	2.17842500	0.25690500	4.80069400
H	2.70832700	0.31299100	5.74832000
H	2.12571600	2.36624000	4.79588000
C	-0.02831300	-2.50336100	0.55775400
H	-2.52934300	-1.60737200	0.96108000
H	2.07150300	1.44517000	-0.22667700

Azulene-bridged A,D-dithia[26]hexaphyrin dication, two protons in both cavities, **[1-H_2]$^{2+}$$C_o$**

C	7.22019500	5.66516600	0.18033300
C	8.25257300	5.38774300	-0.72924900
C	8.19695900	4.17583400	-1.43805800
C	7.15792800	3.27488800	-1.24704200
C	6.11656200	3.55833000	-0.33787100
C	6.16825900	4.77706100	0.37031800
H	7.25008500	6.58549500	0.75627000
H	5.40128800	5.00308800	1.10419400
C	5.00010700	2.61865200	-0.13462900
C	6.50737200	0.60742600	0.26478100
C	6.46539500	-0.78160400	0.25077500
C	5.19642800	-1.32093500	-0.04581000
S	4.04678600	-0.02317900	-0.28550800
H	7.39278700	1.17907900	0.51122700
C	3.68612700	3.14060600	-0.09047700
C	3.17915200	4.36387600	-0.63858800
H	3.78578800	5.10770800	-1.13300400
H	7.12698100	2.36076900	-1.83075200
H	8.97796000	3.94258800	-2.15608200
C	9.37387600	6.36668500	-0.95755700
H	9.51834300	7.02113700	-0.09455700
H	10.31721700	5.85403600	-1.16441600
H	9.15676100	7.00628500	-1.82195900
C	1.80753400	4.36273100	-0.51641700
C	1.42144200	3.15564900	0.14767300
N	2.58274000	2.46727900	0.39459900
C	0.07741000	1.22075900	0.96767200
C	0.54440900	0.05901700	0.32499100
C	0.02993400	-1.08555600	0.95621000
C	-0.69401200	-0.65549000	2.12161100
C	-0.66253100	0.80471700	2.13593700
C	-1.17426100	1.66100000	3.10890300
C	-1.84803100	1.34941500	4.29280300
C	-1.22257500	-1.50022500	3.10000300
H	-1.02357700	2.72223500	2.92530900
C	0.08895200	-2.44569200	0.45594400
C	1.60794200	-4.30771200	-0.55036400
C	2.95752100	-4.38830900	-0.68304100
C	3.49007200	-3.11884800	-0.18703700
N	2.48663900	-2.31617500	0.24910500
C	4.84641200	-2.69972500	-0.18908100
C	5.91811000	-3.69355900	-0.35779400
C	7.00010700	-3.47065700	-1.23566900
C	5.87933900	-4.91400200	0.34992000
C	6.88593300	-5.85780800	0.19257700
C	7.96095000	-5.63850800	-0.68427200
C	7.99105800	-4.43032900	-1.39921000
H	7.03248900	-2.56190200	-1.82782300
H	8.79856000	-4.24717000	-2.10215300
C	9.05849300	-6.65845400	-0.83512000
H	9.84289000	-6.49358900	-0.08605000
H	8.68344000	-7.67533600	-0.69252600
H	9.53015800	-6.59851500	-1.81918900
H	6.84339600	-6.78121700	0.76299500
H	5.07306500	-5.09907800	1.05201300
H	7.31708800	-1.40942500	0.47796200
H	1.12606500	5.10802700	-0.89873400
H	1.10332200	0.03958800	-0.60043900
H	-2.16057200	2.20007200	4.89215400

H	-1.10702100	-2.56380000	2.91128400
H	0.87906500	-5.03897400	-0.86532600
H	3.53124100	-5.19105100	-1.12286500
C	-1.18264800	-3.09877600	0.30687700
C	-1.08133100	3.24754100	0.25144100
N	-2.18249700	2.46048700	0.02945800
C	-3.33174700	3.20610100	-0.11769800
C	-2.91455100	4.57094100	0.04897700
C	-1.54948400	4.59718700	0.24870900
N	-2.28081100	-2.32682100	0.15305800
C	-3.33438900	-3.17131400	-0.01937400
C	-2.88906700	-4.56213700	0.09103500
C	-1.54095200	-4.51588300	0.26774100
C	-4.62829800	-2.68372800	-0.30050900
C	-4.91559800	-1.27949800	-0.36924900
S	-3.83514400	-0.01002800	0.18182300
C	-4.91561700	1.27162900	-0.38287600
C	-6.06580000	0.69083500	-0.95429900
C	-6.06559700	-0.69809200	-0.93892600
C	-4.61762200	2.67391900	-0.36273200
C	-5.71452600	3.62539600	-0.65381700
C	-6.93485400	3.55154700	0.04683600
C	-7.95764700	4.45538700	-0.21434500
C	-7.81676700	5.45484800	-1.19073000
C	-6.60648200	5.51543600	-1.89789400
C	-5.56966200	4.62662400	-1.63350700
C	-5.72662900	-3.63119200	-0.58857500
C	-5.56880800	-4.65562200	-1.54223300
C	-6.60447800	-5.54566800	-1.80378400
C	-7.82574100	-5.46650200	-1.11649400
C	-7.97922900	-4.44566400	-0.16563300
C	-6.95791900	-3.53751400	0.08964700
C	-8.92882100	-6.45933100	-1.37617600
C	-8.92397200	6.44167300	-1.45503900
H	-3.58358900	5.41816500	0.05809000
H	-0.94550500	5.46856900	0.45597100
H	-3.51846700	-5.43949100	0.06270200
H	-0.87503500	-5.35199800	0.42435300
H	-6.84817200	1.28136200	-1.41211000
H	-6.85396200	-1.29898300	-1.37224900
H	-7.06568000	2.80001300	0.81904300
H	-8.88284100	4.38897100	0.35100300
H	-6.47983800	6.26317300	-2.67547400
H	-4.65679700	4.67784200	-2.21852500
H	-4.64525500	-4.72404200	-2.10789800
H	-6.46766800	-6.31175900	-2.56163100
H	-8.91254600	-4.36492700	0.38425100
H	-7.09871000	-2.76973200	0.84408700
C	1.33492300	-3.00619200	0.06114600
C	5.27061200	1.21673900	-0.02905500
H	-8.85815700	7.29020600	-0.76303700
H	-8.87056400	6.84315600	-2.46999800
H	-8.81863400	-7.33706500	-0.72757900
H	-8.91264300	-6.81542300	-2.40956100
H	-9.91297100	-6.02828000	-1.17522700
H	-9.90820700	5.98652500	-1.31554100
C	-1.87525100	-1.17199900	4.28827300
C	-2.15638800	0.09234900	4.81542800
H	-2.68131600	0.09638900	5.76748300
H	-2.20576600	-2.01538200	4.88822200
C	0.16761900	2.59848600	0.48268400
H	2.61052100	1.60256900	0.91727100
H	-2.10430500	1.47000300	-0.15986100

Azulene-bridged A,D-dithia[28]hexaphyrin, two protons in both cavities, **2**$_o$

C	6.88974100	5.88850600	0.26588600
C	7.91379400	5.75786400	-0.68276900
C	7.92150500	4.60630800	-1.47909000
C	6.94557800	3.62157600	-1.33640900
C	5.92431800	3.74727400	-0.37986400
C	5.91195800	4.90896900	0.41263600
H	6.86128800	6.76908000	0.90324000
H	5.13372200	5.03293900	1.15939200
C	4.87408300	2.70371900	-0.21717800
C	6.54374500	0.81495600	0.07025700
C	6.58783900	-0.54621800	0.10732700
C	5.31214300	-1.20746900	-0.01395700
S	4.03729100	0.02997000	-0.07071400
H	7.42048200	1.44451600	0.15375600
C	3.49901400	3.16863900	-0.27887300
C	2.97207800	4.30319700	-0.93459700
H	3.56279100	5.03559700	-1.46430000
H	6.96155700	2.75046300	-1.98375100
H	8.69711400	4.48176700	-2.23085000
C	8.95258100	6.83919600	-0.85982800
H	9.21179500	7.30553200	0.09575400
H	9.87058300	6.44400600	-1.30426500
H	8.58754100	7.63634100	-1.51970300
C	1.58015800	4.25545500	-0.84248800
C	1.22809100	3.10637400	-0.10519100
N	2.42235600	2.48719800	0.22324800
C	-0.00517500	1.13089600	0.76643400
C	0.48474500	-0.00148900	0.08796500
C	0.13839100	-1.17892900	0.77638500
C	-0.51033600	-0.79557500	1.98567600
C	-0.60406500	0.68054100	1.98066900
C	-1.12673500	1.49781000	2.97637100
C	-1.68594000	1.14069100	4.20782400
C	-0.92396300	-1.66815500	2.99245400
H	-1.09914900	2.56293100	2.76213100
C	0.26045100	-2.55654200	0.25913700
C	1.89004100	-4.33554500	-0.66776300
C	3.25338100	-4.35067200	-0.71814200
C	3.69430900	-3.06912900	-0.17502500
N	2.65815200	-2.32924600	0.20887200
C	5.05596600	-2.56192500	-0.12000600
C	6.17342900	-3.53840600	-0.21787200
C	7.20865800	-3.39166100	-1.15648300
C	6.20684400	-4.66863800	0.61847200
C	7.24093100	-5.59641100	0.53065900
C	8.28121600	-5.44100800	-0.39607400
C	8.24072800	-4.32460100	-1.24015000
H	7.18645800	-2.55174800	-1.84382100
H	9.02183100	-4.18902300	-1.98437300
C	9.41541700	-6.43519100	-0.46719800
H	10.19630200	-6.19988400	0.26706600
H	9.07093800	-7.45234800	-0.25632200
H	9.88685900	-6.43495100	-1.45430300
H	7.24208000	-6.45695300	1.19548000
H	5.41580700	-4.81024500	1.34848200
H	7.50387400	-1.11257500	0.21882300
H	0.88124300	4.93527700	-1.30508900
H	0.97784500	0.01607400	-0.87527900
H	-2.03230600	1.96868500	4.82110800
H	-0.75189300	-2.72290600	2.78941300
H	1.21691400	-5.09722600	-1.03392000
H	3.89028500	-5.12784300	-1.11786200
C	-0.99640600	-3.23264100	0.04755000
C	-1.27625700	3.11934600	0.09657000
N	-2.41351800	2.32991000	0.08846800
C	-3.44871500	3.13721000	-0.13281500
C	-3.00915900	4.52298500	-0.24950700
C	-1.64795700	4.50529600	-0.11407300
N	-2.14734200	-2.46871700	-0.02194400
C	-3.25444600	-3.22278600	-0.29670100
C	-2.79076400	-4.55773800	-0.38938000
C	-1.40912700	-4.56151800	-0.17698300
C	-4.59224900	-2.68962800	-0.46465800
C	-4.92475900	-1.34287600	-0.47184500
S	-3.75390300	0.00470500	-0.36106000
C	-5.03139200	1.24271000	-0.36318600
C	-6.30653200	0.57409700	-0.43663600
C	-6.25519100	-0.78560600	-0.49903100
C	-4.78919300	2.60383200	-0.29763100
C	-5.92275000	3.56449200	-0.40726400
C	-6.14915600	4.52468400	0.59385700
C	-7.20385500	5.42874700	0.49577900
C	-8.07084300	5.41812800	-0.60544300
C	-7.84385300	4.46392400	-1.60463700
C	-6.78984700	3.55644200	-1.51184600
C	-5.67847300	-3.70261400	-0.63985200
C	-6.45479700	-3.73710100	-1.80823900
C	-7.47041900	-4.67889300	-1.96733900
C	-7.74579500	-5.62428600	-0.97193200
C	-6.96978600	-5.58965800	0.19467600
C	-5.95406800	-4.65061800	0.35897900
C	-8.82396600	-6.66499100	-1.15895800
C	-9.19264500	6.42217200	-0.72302700
H	-3.64064800	5.38457100	-0.41672300
H	-0.98252400	5.35739100	-0.10522900
H	-3.41374900	-5.41594500	-0.59008200
H	-0.76940700	-5.43051700	-0.15216600

H	-7.23141600	1.13655800	-0.41966000
H	-7.13513000	-1.41505200	-0.53535000
H	-5.49854800	4.54768600	1.46284000
H	-7.36122600	6.15220000	1.29231000
H	-8.49678900	4.43455800	-2.47367200
H	-6.62408900	2.83939100	-2.31004100
H	-6.25272600	-3.02107700	-2.59910400
H	-8.05508800	-4.68212000	-2.88408200
H	-7.16866500	-6.30427800	0.98983500
H	-5.37340700	-4.63930600	1.27644900
C	1.51703100	-3.06662600	-0.06479700
C	5.22089800	1.36959600	-0.08282100
H	-8.84428600	7.35507700	-1.18404900
H	-10.00950400	6.03970800	-1.34208200
H	-8.41271900	-7.59165400	-1.57880900
H	-9.60289500	-6.31642400	-1.84339900
H	-9.29940100	-6.92455300	-0.20810700
H	-9.60319700	6.68077700	0.25790300
C	-1.52474300	-1.37875400	4.21770700
C	-1.86022600	-0.13116800	4.75347000
H	-2.32546200	-0.15694200	5.73686300
H	-1.76209400	-2.23870000	4.83881100
C	-0.02162900	2.51085000	0.25866300
H	-2.13808000	-1.46753500	0.10799500
H	2.47223100	1.65135800	0.78955400

Azulene-bridged A,D-dithia[28]hexaphyrin, two protons in both cavities, **2B$_o$**

C	-7.29033200	-5.55841700	0.61968800
C	-8.30527000	-5.41904600	-0.33735800
C	-8.23507100	-4.32359100	-1.20650600
C	-7.19271500	-3.40186700	-1.12630200
C	-6.18029400	-3.53503900	-0.16133400
C	-6.24712500	-4.64087800	0.70493900
H	-7.32146000	-6.39551400	1.31311600
H	-5.47822900	-4.76906300	1.46074000
C	-5.05915300	-2.55932300	-0.06439900
C	-6.58787500	-0.53907200	0.08788500
C	-6.53317000	0.82083300	0.03445000
C	-5.21266300	1.38030900	-0.11881500
S	-4.03056800	0.05181200	-0.08788200
H	-7.50786100	-1.09698800	0.20723100
C	-3.72021900	-3.12094900	-0.09635100
C	-3.27051900	-4.32363200	-0.68653100
H	-3.91103300	-5.05076100	-1.16289400
H	-7.15031100	-2.57536600	-1.82863500
H	-9.00231400	-4.19425900	-1.96604900
C	-9.41723400	-6.43473700	-0.44591000
H	-9.70297200	-6.82204400	0.53702900
H	-10.30818600	-6.00500500	-0.91282400
H	-9.11212600	-7.29459400	-1.05563600
C	-1.87724200	-4.35401600	-0.61328900
C	-1.44667500	-3.18454100	0.04879300
N	-2.59854100	-2.48214800	0.36013000
C	-0.10935200	-1.23104200	0.84192700
C	-0.48744900	-0.08077200	0.11627600
C	-0.03082700	1.08065500	0.75881200
C	0.57964600	0.68514100	1.98283400
C	0.52480300	-0.79248200	2.04393000
C	0.96124600	-1.61921300	3.07518200
C	1.55217400	-1.27305200	4.29362900
C	1.08070500	1.54854900	2.95441100
H	0.81938900	-2.68479300	2.90603900
C	-0.06781600	2.44374300	0.20945100
C	-1.57334700	4.25126700	-0.85017200
C	-2.93254400	4.33880400	-0.94958200
C	-3.46090800	3.11417400	-0.36296200
N	-2.48136400	2.33046200	0.08076600
C	-4.85714000	2.70204400	-0.30060000
C	-5.90309600	3.74634600	-0.46604400
C	-6.93845500	3.61700700	-1.40672100
C	-5.86594700	4.92145700	0.30619700
C	-6.83461700	5.90938100	0.15605100
C	-7.87585700	5.77276100	-0.77307100
C	-7.90444400	4.61123400	-1.55384200
H	-6.96763800	2.74030100	-2.04617200
H	-8.68706100	4.48718100	-2.29846300
C	-8.93803100	6.83684700	-0.91233000
H	-9.71615500	6.72396300	-0.14681000
H	-8.51729000	7.84079400	-0.79761700
H	-9.43063800	6.78562400	-1.88759500
H	-6.78276200	6.80382200	0.77237100
H	-5.07164400	5.05081100	1.03473900
H	-7.40625700	1.45762100	0.10248400
H	-1.23248700	-5.10711600	-1.04013900
H	-0.97886200	-0.08830300	-0.84773000
H	1.81068800	-2.10564800	4.94299500
H	1.02592500	2.60485500	2.70504200
H	-0.84381700	4.95313900	-1.22680700
H	-3.51122400	5.13040500	-1.40552500
C	1.22203000	3.08882400	0.07329300
C	1.06334000	-3.24921400	0.12067800
N	2.22799300	-2.48521800	0.09274300
C	3.32633500	-3.21507400	-0.26131800
C	2.84289800	-4.56149800	-0.43050600
C	1.48413900	-4.57636300	-0.20652900
N	2.32965200	2.31492400	0.00904800
C	3.39233000	3.15342900	-0.13897400
C	2.94542700	4.52841800	-0.15523000
C	1.57844800	4.48674600	-0.02025600
C	4.70863000	2.63480400	-0.29044900
C	4.99287100	1.25883400	-0.36404400
S	3.75238500	-0.00677600	-0.41223000
C	4.95193300	-1.31367000	-0.45006000
C	6.25481500	-0.74175000	-0.44057700
C	6.26780000	0.63658000	-0.38985500
C	4.63399500	-2.69348700	-0.45779200
C	5.73241100	-3.67967900	-0.68192200
C	6.00784100	-4.68904700	0.25502300
C	7.02860600	-5.61358900	0.03864800
C	7.81772100	-5.56654900	-1.11709700
C	7.54871000	-4.55525600	-2.04952400
C	6.52631000	-3.63291500	-1.84058200
C	5.84381600	3.59703000	-0.37331800
C	6.71394400	3.60747700	-1.47552000
C	7.76460100	4.51968600	-1.54843500
C	7.99020300	5.45086700	-0.52672700
C	7.12410700	5.43590500	0.57469900
C	6.06675600	4.53250900	0.65043500
C	9.11191000	6.45709500	-0.62198000
C	8.90534700	-6.58461100	-1.36417200
H	3.46255800	-5.40089300	-0.70735500
H	0.83939100	-5.44190600	-0.24257300
H	3.56665600	5.40768100	-0.25314300
H	0.90474800	5.32878800	0.05221200
H	7.15105500	-1.34818800	-0.43902000
H	7.17995900	1.21854900	-0.34657700
H	5.42322600	-4.73749700	1.16901700
H	7.22236100	-6.37845000	0.78694500
H	8.14412800	-4.49367900	-2.95741700
H	6.33081700	-2.86695900	-2.58497700
H	6.55156600	2.90456800	-2.28658900
H	8.41823000	4.51056700	-2.41724100
H	7.28205000	6.13997300	1.38806000
H	5.41282700	4.53537500	1.51652400
C	-1.29080800	2.99315600	-0.18245900
C	-5.30770100	-1.19697900	-0.01980400
H	8.53938400	-7.41586200	-1.98004800
H	9.75586300	-6.14258000	-1.89231000
H	8.77196100	7.38471700	-1.09946600
H	9.94567600	6.07297300	-1.21709300
H	9.49542800	6.72424600	0.36730900
H	9.27384700	-7.01222600	-0.42713700
C	1.64453000	1.24797700	4.19641700
C	1.85057000	-0.00148200	4.78704000
H	2.31327000	0.01927200	5.77176000
H	1.96927400	2.10451900	4.78160000
C	-0.17086900	-2.62458000	0.35845500
H	-2.58998900	-1.60739300	0.86714900
H	2.22969200	-1.49624900	0.29510000

Azulene-bridged A,D-dithia[28]hexaphyrin, two protons in I cavity, **2C$_o$**

C	6.93878000	5.79092900	0.50974200
C	8.08729700	5.64895700	-0.28225200
C	8.19121300	4.50283700	-1.07996800
C	7.18976200	3.53431100	-1.08839700
C	6.04276700	3.67070300	-0.28710200
C	5.93414200	4.82859100	0.50511100
H	6.83257900	6.66789500	1.14373500

H	5.05780000	4.96203000	1.13133000
C	4.96794500	2.64487500	-0.28618900
C	6.54099000	0.68043800	0.11690500
C	6.54081700	-0.68234000	0.11677800
C	5.27944900	-1.30246900	-0.20610400
S	4.09540500	-0.00063100	-0.52172500
H	7.40721700	1.27622900	0.37553000
C	3.60010100	3.12982600	-0.41070000
C	3.09800300	4.25976800	-1.07900300
H	3.70264600	4.98240800	-1.60713900
H	7.28327700	2.67039100	-1.73869000
H	9.06385900	4.37130700	-1.71502500
C	9.15718900	6.71382600	-0.29845400
H	9.28533600	7.16741200	0.68926400
H	10.12262100	6.30729900	-0.61310500
H	8.90110700	7.52262600	-0.99438400
C	1.69879100	4.23326700	-0.99622600
C	1.32638100	3.10009000	-0.25197400
N	2.50564200	2.46395000	0.08472900
C	0.05676600	1.15662900	0.66955700
C	0.46951800	-0.00047800	-0.01973100
C	0.05653900	-1.15810900	0.66859600
C	-0.55171500	-0.73727500	1.88950400
C	-0.55147000	0.73489400	1.89017000
C	-1.00761900	1.58233300	2.89626400
C	-1.57052700	1.25961700	4.13267800
C	-1.00813200	-1.58555300	2.89476800
H	-0.91664200	2.64393600	2.68134500
C	0.06455500	-2.53078600	0.14307300
C	1.69823000	-4.23281100	-1.00085300
C	3.09747800	-4.25975600	-1.08294100
C	3.59968300	-3.13102800	-0.41265900
N	2.50521400	-2.46544200	0.08315900
C	4.96760100	-2.64644500	-0.28694400
C	6.04296000	-3.67166300	-0.28720300
C	7.18922400	-3.53523400	-1.08977200
C	5.93232700	-4.83264600	0.50003200
C	6.93518500	-5.79696900	0.50045600
C	8.08613400	-5.65156400	-0.28722300
C	8.18884700	-4.50557300	-1.08546500
H	7.27983900	-2.67347200	-1.74333500
H	9.05753800	-4.37720200	-1.72654100
C	9.18271100	-6.68869700	-0.26195000
H	9.87446700	-6.51350700	0.57172400
H	8.77760200	-7.69768500	-0.13792300
H	9.77235600	-6.67065500	-1.18302900
H	6.82382200	-6.67993300	1.12513200
H	5.05226100	-4.97095300	1.11991700
H	7.40692100	-1.27838800	0.37521900
H	1.01519800	4.92292000	-1.46679000
H	0.91762500	-0.00012700	-1.00611900
H	-1.85717900	2.10563400	4.75225100
H	-0.91745100	-2.64697700	2.67883000
H	1.01454200	-4.92125800	-1.47306100
H	3.70209300	-4.98165400	-1.61214600
C	-1.18128700	-3.14763000	-0.00610300
C	-1.18077200	3.14694500	-0.00335600
N	-2.32287700	2.37037300	0.07147200
C	-3.35914500	3.16874600	-0.16395600
C	-2.90966500	4.54931500	-0.37517400
C	-1.54941900	4.52847900	-0.28204100
N	-2.32331000	-2.37099600	0.06952600
C	-3.35966300	-3.16905000	-0.16660200
C	-2.91039200	-4.54943400	-0.37911100
C	-1.55010000	-4.52885400	-0.28591000
C	-4.70360000	-2.64617800	-0.27111600
C	-4.97442400	-1.28073400	-0.24282000
S	-3.73778400	-0.00009300	-0.13314800
C	-4.97421300	1.28081200	-0.24180100
C	-6.28297400	0.68148700	-0.27898400
C	-6.28307600	-0.68115000	-0.27952500
C	-4.70316100	2.64623000	-0.26895800
C	-5.81750000	3.62428700	-0.43427600
C	-6.03512200	4.63331500	0.51939000
C	-7.06734600	5.55629000	0.36727800
C	-7.92082700	5.51540400	-0.74338500
C	-7.70384300	4.51167700	-1.69529600
C	-6.67200100	3.58604500	-1.54802000
C	-5.81813900	-3.62389000	-0.43729700
C	-6.67264200	-3.58446700	-1.55101000
C	-7.70464000	-4.50977400	-1.69910700
C	-7.92178100	-5.51433300	-0.74808400
C	-7.06831200	-5.55637900	0.36252000
C	-6.03589100	-4.63372600	0.51544900
C	-9.01942800	-6.53620300	-0.92649700
C	-9.01830200	6.53763700	-0.92076400
H	-3.54024000	5.40444900	-0.57639800
H	-0.87781500	5.37295800	-0.35055800
H	-3.54106100	-5.40431900	-0.58109100
H	-0.87862100	-5.37338900	-0.35506200
H	-7.18474000	1.28056000	-0.29226900
H	-7.18492900	-1.28008400	-0.29332600
H	-5.39536300	4.68020400	1.39567900
H	-7.21771800	6.31821300	1.12865000
H	-8.34765800	4.45677900	-2.56998600
H	-6.51488200	2.82798800	-2.30922100
H	-6.51540500	-2.82572400	-2.31150100
H	-8.34844200	-4.45398800	-2.57375400
H	-7.21884300	-6.31894700	1.12321000
H	-5.39611600	-4.68152200	1.39167700
C	1.32585000	-3.10079300	-0.25484800
C	5.27972700	1.30087300	-0.20582200
H	-8.64512800	7.43942600	-1.42264700
H	-9.83806100	6.14393300	-1.52896300
H	-8.64747700	-7.43565600	-1.43346100
H	-9.84119500	-6.14020900	-1.53050800
H	-9.43017400	-6.85521300	0.03644300
H	-9.43212000	6.85236100	0.04228900
C	-1.57093500	-1.26386400	4.13150500
C	-1.81984600	-0.00234200	4.67643900
H	-2.27575800	-0.00271600	5.66457600
H	-1.85781800	-2.11038900	4.75027400
C	0.06497200	2.52983000	0.14534600
H	2.53587000	1.63550000	0.66033800
H	2.53546400	-1.63847500	0.66087700

Palladium complex of azulene-bridged A,D-dithia[26]hexaphyrin, monocationic, **1-Pd$^{+}_{o}$**

C	6.61711900	5.68819700	0.63050200
C	7.67687600	5.75619000	-0.28614100
C	7.75098200	4.76720500	-1.27805400
C	6.80261900	3.75188300	-1.35597000
C	5.73302700	3.69097700	-0.44290200
C	5.66058200	4.68029100	0.55609800
H	6.54715900	6.43062400	1.42114500
H	4.86398100	4.63875900	1.29209600
C	4.73917500	2.59190300	-0.51858600
C	6.46075100	0.69575600	-0.27015800
C	6.46080500	-0.69603000	-0.27012000
C	5.23017800	-1.28199200	-0.65163100
S	4.20379400	-0.00027200	-1.28493200
H	7.28287800	1.29064600	0.10875600
C	3.34903200	2.90820800	-0.37684500
C	2.81022700	4.22694100	-0.60295800
H	3.37627700	5.06749400	-0.97552300
H	6.87354000	3.00850600	-2.14427700
H	8.55986600	4.79762100	-2.00329700
C	8.69098200	6.87107000	-0.22172500
H	8.82742200	7.23003300	0.80228600
H	9.66395900	6.55118800	-0.60517700
H	8.36843000	7.72759600	-0.82674300
C	1.48063700	4.18825900	-0.29979500
C	1.19382800	2.86242700	0.18510300
N	2.32812500	2.08772000	0.08047000
C	-0.14841400	1.14495200	1.38059600
C	0.59138600	-0.00094800	1.02721700
C	-0.14848400	-1.14714800	1.37947700
C	-1.18349200	-0.72599600	2.31070300
C	-1.18344100	0.72295100	2.31142700
C	-1.91698500	1.57569300	3.13917100
C	-2.82063800	1.25435800	4.15372800
C	-1.91710500	-1.57952100	3.13758700
H	-1.75518800	2.63737700	2.98151900
C	-0.02428300	-2.42208500	0.75720500
C	1.48089900	-4.18906500	-0.30317900
C	2.81068000	-4.22753500	-0.60557800
C	3.34937800	-2.90900100	-0.37799700
N	2.32822500	-2.08889300	0.07939700
C	4.73958100	-2.59243000	-0.51865600
C	5.73419900	-3.69071100	-0.44183200
C	5.65964900	-4.68231900	0.55485100
C	6.80213800	-3.75317800	-1.35660500
C	7.74782400	-4.77139400	-1.28169500

C	7.67538800	-5.75866400	-0.28809700
C	6.61338300	-5.69292900	0.62624700
H	4.85929000	-4.64472200	1.28695700
H	6.53747500	-6.44156800	1.41050200
C	8.72058100	-6.84188900	-0.18894400
H	9.16393300	-7.06154500	-1.16413900
H	9.53613700	-6.53794700	0.47907600
H	8.30087700	-7.76845200	0.21298600
H	8.55110500	-4.80731300	-2.01284500
H	6.86967800	-3.01318600	-2.14839300
H	7.28302500	-1.29082700	0.10872100
H	0.77055100	4.99526900	-0.38679700
H	-3.26276300	2.10475500	4.66705800
H	-1.75538100	-2.64105600	2.97886200
H	0.77085500	-4.99598400	-0.39136100
H	3.37687200	-5.06774600	-0.97873800
C	-1.28968900	-3.12292500	0.50979100
C	-1.28958900	3.12163700	0.51298200
N	-2.33909100	2.35622900	0.21286700
C	-3.40401100	3.19333900	-0.01607200
C	-2.98925500	4.57678800	0.19655200
C	-1.66002300	4.53408400	0.50829200
N	-2.33915600	-2.35713300	0.21048700
C	-3.40406000	-3.19395200	-0.01956800
C	-2.98935400	-4.57766500	0.19146200
C	-1.66016100	-4.53535900	0.50339400
C	-4.65194200	-2.68212100	-0.38713600
C	-4.91507700	-1.26439600	-0.49579700
S	-3.78600900	-0.00029800	-0.02624100
C	-4.91507400	1.26433800	-0.49436000
C	-6.07885300	0.69761800	-1.03941200
C	-6.07884900	-0.69705300	-1.04021400
C	-4.65194200	2.68193700	-0.38407100
C	-5.75587000	3.62813400	-0.69044100
C	-6.99247100	3.54603200	-0.02508700
C	-8.01021000	4.45458600	-0.30094600
C	-7.84273100	5.46749000	-1.25684400
C	-6.61415800	5.53862800	-1.92777000
C	-5.58450800	4.64329300	-1.64781900
C	-5.75581000	-3.62797200	-0.69479400
C	-5.58433100	-4.64188100	-1.65340600
C	-6.61396300	-5.53692700	-1.93458800
C	-7.84255600	-5.46667600	-1.26372200
C	-8.01017000	-4.45494700	-0.30652400
C	-6.99251800	-3.54674100	-0.02943500
C	-8.94274500	-6.46030900	-1.54485200
C	-8.94276900	6.46162700	-1.53678600
H	-3.62158200	5.45151600	0.14116400
H	-1.02729300	5.37058000	0.77123100
H	-3.62169300	-5.45231100	0.13496100
H	-1.02748400	-5.37218400	0.76540600
H	-6.88615100	1.29363100	-1.44447800
H	-6.88614500	-1.29260300	-1.44596700
H	-7.14559600	2.77813200	0.72692200
H	-8.95211200	4.37771200	0.23602700
H	-6.46298700	6.30212700	-2.68633100
H	-4.64902600	4.70762700	-2.19449900
H	-4.64879700	-4.70552400	-2.20007800
H	-6.46269300	-6.29947300	-2.69407800
H	-8.95213000	-4.37877100	0.23045800
H	-7.14571700	-2.77979300	0.72353200
C	1.19386700	-2.86367500	0.18280000
C	5.23003200	1.28156300	-0.65166200
H	-8.87914500	7.31811500	-0.85411000
H	-8.87967300	6.85266200	-2.55604600
H	-8.88613700	-7.31210000	-0.85571600
H	-8.87320600	-6.85846300	-2.56089400
H	-9.93160700	-6.00926600	-1.42141600
H	-9.93168200	6.01370900	-1.40313400
C	-2.82073000	-1.25914400	4.15246600
C	-3.22924400	-0.00260200	4.60406800
H	-3.95136700	-0.00298300	5.41682600
H	-3.26291500	-2.11002300	4.66494200
C	-0.02418300	2.42043500	0.75949600
Pd	2.28667800	-0.00060600	0.07248200

Palladium complex of meso-linked 23-thiabenzocarbaporphyrin, **3-Pd$_o$**

C	6.60877600	5.69315600	0.58664300
C	7.63260400	5.76648600	-0.36843300
C	7.66954900	4.78113600	-1.36440000
C	6.71760700	3.76558500	-1.41006500
C	5.68428100	3.69678400	-0.45839500
C	5.65249400	4.68201200	0.54583100
H	6.56643600	6.43346700	1.38197400
H	4.88205200	4.63665500	1.30876000
C	6.42476900	0.69712400	-0.31480900
C	6.42483800	-0.69675100	-0.31475800
C	5.18184400	-1.28485300	-0.64608600
S	4.13440600	0.00003500	-1.23582000
H	7.26436300	1.28991100	0.02827800
C	3.30533700	2.91110700	-0.31428800
C	2.75750000	4.22798900	-0.51316900
H	3.31061400	5.07669800	-0.88739000
H	6.76070400	3.02135500	-2.19958600
H	8.45145300	4.81341800	-2.11938300
C	8.64695600	6.88437900	-0.33814800
H	8.85246800	7.21094400	0.68585500
H	9.59350900	6.57984300	-0.79449900
H	8.28607700	7.76081500	-0.89136800
C	1.43288600	4.18021700	-0.17914000
C	1.15936000	2.84713500	0.28971000
N	2.28924600	2.08420000	0.15464000
C	-0.16582000	1.14530500	1.53728800
C	0.59715600	-0.00004600	1.21246800
C	-0.16574600	-1.14547400	1.53718800
C	-1.25897700	-0.70533600	2.44089200
C	-1.25900200	0.70503400	2.44097300
C	-2.09542600	1.41196200	3.30060300
C	-2.93751500	0.69875300	4.16161700
C	-2.09537100	-1.41238300	3.30045400
H	-2.09638900	2.49760400	3.30991400
C	-0.05069000	-2.39418700	0.89304800
C	1.43342000	-4.18044900	-0.17863700
C	2.75807500	-4.22812700	-0.51251300
C	3.30569100	-2.91109600	-0.31400400
N	2.28939600	-2.08419700	0.15458300
C	4.68758100	-2.59376000	-0.49776600
C	5.68473500	-3.69643100	-0.45802800
C	6.71791900	-3.76529000	-1.40984900
C	5.65324500	-4.68141500	0.54643000
C	6.60969300	-5.69240900	0.58733400
C	7.63337100	-5.76580900	-0.36788800
C	7.67001700	-4.78068800	-1.36409800
H	6.76078700	-3.02122100	-2.19953600
H	8.45181600	-4.81302400	-2.11918900
C	8.64789700	-6.88354500	-0.33755500
H	8.85230900	-7.21109400	0.68634600
H	8.28781100	-7.75948200	-0.89208300
H	9.59491100	-6.57838800	-0.79254500
H	6.56759700	-6.43254000	1.38284400
H	4.88289600	-4.63599500	1.30945200
H	7.26449200	-1.28942800	0.02836300
H	0.71975400	4.98675900	-0.23978000
H	-3.59310700	1.23830400	4.83975300
H	-2.09629400	-2.49802600	3.30964900
H	0.72044000	-4.98714000	-0.23905100
H	3.31135900	-5.07687000	-0.88640400
C	-1.31975500	-3.10397200	0.63239100
C	-1.31997300	3.10380200	0.63261200
N	-2.35685000	2.35198100	0.29919400
C	-3.42018000	3.19441300	0.05098600
C	-2.99725600	4.57844700	0.24898900
C	-1.68473300	4.52331800	0.61796000
N	-2.35664500	-2.35212500	0.29902800
C	-3.41993100	-3.19454600	0.05064000
C	-2.99701100	-4.57859800	0.24855200
C	-1.68449000	-4.52349500	0.61752300
C	-4.65180400	-2.68217500	-0.33883400
C	-4.91426300	-1.26283100	-0.46354200
S	-3.70213200	-0.00004300	-0.27843700
C	-4.91437000	1.26266500	-0.46341200
C	-6.18455300	0.69794400	-0.64823500
C	-6.18449300	-0.69820700	-0.64832300
C	-4.65203500	2.68202000	-0.33853600
C	-5.77438700	3.62517300	-0.60998100
C	-6.22304000	4.51530400	0.37839700
C	-7.26245500	5.40721400	0.11707500
C	-7.88521700	5.44963900	-1.13657900
C	-7.43803100	4.55659300	-2.12067300
C	-6.40614300	3.65696500	-1.86467600
C	-5.77410700	-3.62536700	-0.61038600
C	-6.40587700	-3.65699300	-1.86509700

C	-7.43768600	-4.55664300	-2.12123200
C	-7.88480500	-5.44988900	-1.13725800
C	-7.26204000	-5.40762800	0.11637600
C	-6.22267400	-4.51567000	0.37784200
C	-8.98711100	-6.43991600	-1.42955100
C	-8.98752700	6.43972900	-1.42863900
H	-3.60974000	5.46107500	0.12976200
H	-1.05274400	5.35583300	0.89589000
H	-3.60948200	-5.46122000	0.12921700
H	-1.05253300	-5.35605700	0.89538300
H	-7.08349900	1.29375700	-0.74157300
H	-7.08338200	-1.29409200	-0.74175800
H	-5.76488300	4.49048100	1.36218100
H	-7.59909300	6.07743400	0.90430100
H	-7.90398000	4.56669900	-3.10314800
H	-6.07403600	2.97907500	-2.64506700
H	-6.07381700	-2.97894700	-2.64537300
H	-7.90364400	-4.56662100	-3.10370700
H	-7.59861700	-6.07801100	0.90348600
H	-5.76448700	-4.49100400	1.36161700
C	1.15964800	-2.84727700	0.28979400
C	5.18172500	1.28510600	-0.64616900
H	-8.58884800	7.34889600	-1.89626700
H	-9.72977100	6.02220100	-2.11604500
H	-8.58904800	-7.34697100	-1.90177500
H	-9.73183600	-6.02056600	-2.11318000
H	-9.50155900	-6.74825400	-0.51472700
H	-9.50504000	6.74428400	-0.51426000
C	-2.93748500	-0.69929600	4.16154400
H	-3.59305900	-1.23894400	4.83962000
C	-0.05085400	2.39402200	0.89314400
Pd	2.24704100	-0.00000100	0.16917600
C	4.68731500	2.59396500	-0.49799100

Palladium complex of meso-linked 23-thiabenzocarbaporphyrin, CHO in position 2[2] of indene, **3-Pd$_{a,o}$**

C	-6.63690300	-5.74080700	0.54510400
C	-7.68755400	-5.81480800	-0.38044300
C	-7.76527200	-4.81832800	-1.36297300
C	-6.82706800	-3.79094200	-1.42409300
C	-5.76707200	-3.72164500	-0.50227700
C	-5.69374300	-4.71827600	0.48842000
H	-6.56270900	-6.48988200	1.32974000
H	-4.90166000	-4.67299600	1.22886600
C	-6.53756400	-0.73492100	-0.29504500
C	-6.55401700	0.65807100	-0.27239600
C	-5.32772900	1.26641800	-0.63055400
S	-4.28324400	0.00422900	-1.27256800
H	-7.35913600	-1.34353700	0.06347800
C	-3.39383300	-2.91037200	-0.41985300
C	-2.83823900	-4.21801000	-0.65344300
H	-3.39273600	-5.06704400	-1.02476500
H	-6.90183700	-3.03819900	-2.20311600
H	-8.56857000	-4.85111600	-2.09504600
C	-8.68761500	-6.94482200	-0.33393100
H	-8.85928100	-7.28559600	0.69162000
H	-9.65042200	-6.64637900	-0.75912600
H	-8.33254900	-7.81026300	-0.90776200
C	-1.50549000	-4.16087400	-0.35517400
C	-1.23325100	-2.83220900	0.12588100
N	-2.37430400	-2.07897100	0.03297900
C	0.10632000	-1.13219300	1.35784300
C	-0.67485200	0.00885600	1.06693700
C	0.07980900	1.16015100	1.38930300
C	1.19848100	0.72341800	2.25548800
C	1.21708700	-0.68889300	2.23593300
C	2.08742800	-1.38834700	3.06100300
C	2.94768800	-0.67301000	3.91213300
C	2.04945400	1.43687200	3.10525600
H	2.11291600	-2.47503400	3.06185000
C	-0.06669300	2.42012400	0.77017600
C	-1.60235600	4.20127600	-0.23398000
C	-2.93683700	4.23634800	-0.52640600
C	-3.46172500	2.90968400	-0.32935100
N	-2.42293900	2.08952600	0.09735600
C	-4.84552100	2.57825400	-0.47543400
C	-5.85337100	3.66787000	-0.38474000
C	-6.91659800	3.74096100	-1.30256400
C	-5.80099500	4.63526000	0.63583500
C	-6.76722100	5.63367300	0.72499600
C	-7.82127700	5.71163700	-0.19632300
C	-7.87812300	4.74402200	-1.20868900
H	-6.97567400	3.01090700	-2.10421000
H	-8.68352400	4.78056100	-1.93828000
C	-8.84694100	6.81638700	-0.11399900
H	-9.02299100	7.12293800	0.92155800
H	-8.51386900	7.70623400	-0.66316700
H	-9.80404900	6.50833700	-0.54518900
H	-6.70854200	6.36001000	1.53201200
H	-5.00660700	4.58566900	1.37355100
H	-7.38974000	1.23524900	0.10488000
H	-0.78593700	-4.95859300	-0.44750100
H	2.03013500	2.52180300	3.12601900
H	-0.90177200	5.01777500	-0.30528000
H	-3.51195200	5.08267600	-0.87164400
C	1.18801400	3.14485300	0.48966100
C	1.25737500	-3.06990800	0.40852700
N	2.28249300	-2.30195100	0.07217500
C	3.34825900	-3.12968700	-0.21044500
C	2.94145700	-4.52040500	-0.03009800
C	1.63446800	-4.48467300	0.36165500
N	2.22881500	2.40437600	0.13805200
C	3.27716300	3.25939500	-0.12750400
C	2.84199900	4.63766300	0.08135700
C	1.53613000	4.56761000	0.47119500
C	4.50791200	2.76462700	-0.54536800
C	4.78428600	1.35038200	-0.69057800
S	3.58867400	0.07180200	-0.50926500
C	4.81248400	-1.17486800	-0.72380300
C	6.07430600	-0.59328200	-0.91437800
C	6.05876800	0.80241000	-0.89610100
C	4.56821800	-2.59838100	-0.61450100
C	5.69564400	-3.52474900	-0.91800600
C	6.16720000	-4.42666000	0.04896300
C	7.21245700	-5.30217100	-0.24200300
C	7.81761000	-5.31668700	-1.50497300
C	7.34704300	-4.41221500	-2.46757400
C	6.30982600	-3.52792500	-2.18185600
C	5.61405300	3.72310000	-0.82712700
C	6.22627900	3.77098000	-2.09104500
C	7.24333300	4.68469900	-2.35579900
C	7.69513500	5.57543600	-1.37162300
C	7.09216400	5.51651500	-0.10891900
C	6.06692600	4.61115200	0.16135200
C	8.78192600	6.57977700	-1.67252800
C	8.92654600	-6.28916400	-1.82882500
H	3.55970400	-5.39491000	-0.17606500
H	1.01565800	-5.32841000	0.63509400
H	3.44229700	5.52731900	-0.04676800
H	0.90069800	5.39293300	0.76194300
H	6.97880100	-1.17780400	-1.02327600
H	6.94996900	1.40958700	-0.98941900
H	5.72434600	-4.42265100	1.03998700
H	7.56811800	-5.98076500	0.52938800
H	7.79917000	-4.40070200	-3.45642500
H	5.95969400	-2.84051500	-2.94587500
H	5.89038300	3.09498800	-2.87147100
H	7.69423600	4.70750200	-3.34501700
H	7.43371700	6.18384800	0.67852300
H	5.62536300	4.57296600	1.15223800
C	-1.29821200	2.86601700	0.20912300
C	-5.29768700	-1.30240700	-0.67257800
H	8.53095900	-7.19525100	-2.30495200
H	9.65367600	-5.85231000	-2.52029900
H	8.36636400	7.48653900	-2.12997900
H	9.51982000	6.17456400	-2.37184200
H	9.30766600	6.88541600	-0.76330800
H	9.46079100	-6.60205600	-0.92705700
C	2.92196800	0.73403300	3.92961600
H	3.59665900	1.24946200	4.60578900
C	-0.01195700	-2.37519200	0.70360700
Pd	-2.35642200	0.00530600	0.07677400
C	-4.78459800	-2.60672400	-0.55760800
C	3.87103800	-1.40927300	4.79041400
H	3.80125500	-2.51823700	4.69820300
O	4.66319700	-0.90338500	5.56833800

Palladium complex of meso-linked 24-thiaoxynaphthiporphyrin, **4-Pd$_o$**

C	6.77653500	5.62595800	0.34841400
C	7.88321000	5.64024000	-0.51337500
C	8.00223800	4.59794800	-1.44169100
C	7.05136700	3.58186800	-1.51146100
C	5.94079000	3.56814600	-0.64950100
C	5.82188000	4.61540700	0.28323100
H	6.66591500	6.41504900	1.08841900
H	4.98250700	4.62089700	0.97113900
C	6.64232300	0.56272000	-0.36685300
C	6.60498500	-0.80902100	-0.24933300
C	5.34085800	-1.40802200	-0.55503200
S	4.33577500	-0.14958300	-1.28539600
H	7.49232400	1.16351100	-0.06720700
C	3.53876000	2.81595600	-0.63800400
C	3.00922500	4.08530300	-1.03834000
H	3.58184800	4.87526500	-1.50253300
H	7.15648900	2.79481100	-2.25219300
H	8.84685700	4.58586700	-2.12644600
C	8.89635400	6.75837700	-0.45809700
H	9.06327800	7.09664100	0.56940400
H	9.85922900	6.44811400	-0.87430700
H	8.55702600	7.62911500	-1.03342900
C	1.66729500	4.08593900	-0.74484700
C	1.38693800	2.84516700	-0.09207900
N	2.52502700	2.06468500	-0.08067800
C	0.06113700	1.25595300	1.33593600
C	0.57608300	0.02423500	0.89509600
C	-0.28477300	-1.09808600	0.98950800
C	-1.54941900	-0.94819000	1.70402200
C	-1.73304200	0.08860200	2.63902700
C	-2.84973500	0.10582100	3.47807100
C	-3.82296600	-0.88598100	3.35742400
C	-2.62478200	-1.82392600	1.48622800
H	-2.94656000	0.92076600	4.18765500
C	-0.08392900	-2.33550800	0.30514400
C	1.52657200	-4.22681700	-0.23063000
C	2.89730900	-4.30455700	-0.34378900
C	3.41432500	-2.97840500	-0.24833400
N	2.35126900	-2.10577500	-0.05925300
C	4.82513800	-2.66511600	-0.28196300
C	5.78861900	-3.75202400	0.04827600
C	6.89939700	-4.00379700	-0.77403600
C	5.63486100	-4.53913200	1.20404600
C	6.55824000	-5.53137000	1.52021300
C	7.66561300	-5.78537600	0.69727800
C	7.81828400	-5.00187600	-0.45338500
H	7.03148900	-3.41910400	-1.67958300
H	8.66449100	-5.17950100	-1.11274100
C	8.64444900	-6.88558000	1.03131800
H	8.82693500	-6.94519900	2.10904300
H	8.26353300	-7.86463500	0.71426400
H	9.60567300	-6.73218400	0.53237400
H	6.42179600	-6.11558900	2.42722100
H	4.79172200	-4.35522500	1.86225100
H	7.42510900	-1.39345800	0.14965800
H	0.95548200	4.87276800	-0.94140700
H	-4.68110300	-0.89608100	4.02218700
H	0.82320800	-5.04588100	-0.20885200
H	3.49428700	-5.19343400	-0.48427300
C	-1.26584700	-3.04130500	-0.11699500
C	-1.04326100	3.20155200	0.39382100
N	-2.19097400	2.44795200	0.23444800
C	-3.28676700	3.23158000	-0.03467300
C	-2.80948100	4.56014800	-0.03809700
C	-1.43094200	4.53747600	0.21560700
N	-2.51706800	-2.62052900	0.33716000
C	-3.51903600	-3.10983200	-0.48935000
C	-2.89010400	-3.97859700	-1.39467200
C	-1.50736000	-3.92750800	-1.18020500
C	-4.87730800	-2.56763500	-0.55792600
C	-5.12801700	-1.20060200	-0.54261000
S	-3.87171300	0.04811100	-0.76879400
C	-4.98802300	1.39714000	-0.41686300
C	-6.30812600	0.83976600	-0.27827400
C	-6.38095400	-0.52203800	-0.33865800
C	-4.62884000	2.72795800	-0.23810100
C	-5.71857100	3.74869500	-0.20996500
C	-5.87581700	4.61524600	0.88586200
C	-6.90027800	5.55820500	0.90914800
C	-7.80103900	5.68129700	-0.15875000
C	-7.64288500	4.81812900	-1.25022700
C	-6.62142500	3.86966200	-1.27856600
C	-5.97264300	-3.54600900	-0.74849300
C	-7.04427500	-3.30992500	-1.63152100
C	-8.05813000	-4.24925400	-1.79969900
C	-8.04681300	-5.46714400	-1.10605100
C	-6.96795800	-5.71605300	-0.24572000
C	-5.95146600	-4.78186500	-0.07222000
C	-9.16274000	-6.47059700	-1.26948100
C	-8.88816700	6.72935600	-0.14130600
H	-3.41771700	5.43636800	-0.20432900
H	-0.78676500	5.39694600	0.32497100
H	-3.40013200	-4.49196500	-2.19739400
H	-0.74447200	-4.37922700	-1.79550800
H	-7.15998900	1.47105700	-0.05958300
H	-7.29605500	-1.07529700	-0.16881700
H	-5.19681500	4.53429300	1.72900000
H	-7.00713900	6.20655500	1.77563500
H	-8.32471500	4.89253500	-2.09401200
H	-6.51124300	3.21900400	-2.14091200
H	-7.06085900	-2.39449800	-2.21404400
H	-8.86498600	-4.04063500	-2.49834300
H	-6.92381900	-6.65735100	0.29703000
H	-5.12581600	-5.00526600	0.59671200
C	1.20563700	-2.85184400	-0.03681900
C	5.40396600	1.16166300	-0.76178100
H	-8.50868600	7.69945700	-0.48644000
H	-9.72081300	6.45427500	-0.79530500
H	-8.80114300	-7.49622100	-1.14764900
H	-9.63232800	-6.39081700	-2.25452300
H	-9.94983700	-6.31354700	-0.52076500
H	-9.28402000	6.87893700	0.86810800
C	-3.73224000	-1.83460700	2.33664700
H	-4.52487700	-2.55696800	2.18148700
C	0.20992500	2.47626100	0.59664000
Pd	2.34507900	-0.02892500	-0.03498300
C	4.94368800	2.46723600	-0.71002300
C	-0.85167900	1.27024200	2.52106500
O	-0.90374000	2.22374400	3.29417100
H	-2.20875800	1.43971900	0.28985900

Bis(dichloropalladium) complex of azulene-bridged A,D-dithia[28]hexaphyrin, **2-Pd$_{2,o}$**

C	7.16165400	5.52293500	-0.41084000
C	8.15808100	5.27658600	-1.36668300
C	8.08847400	4.08008200	-2.09289300
C	7.07072400	3.15652800	-1.86634900
C	6.07983800	3.39897400	-0.89877100
C	6.13866500	4.60798300	-0.18071100
H	7.18939200	6.44495300	0.16450700
H	5.38480100	4.81635800	0.57210200
C	4.98535000	2.43276500	-0.64464700
C	6.50113400	0.39492600	-0.35484000
C	6.41410100	-0.96204700	-0.22203600
C	5.08819500	-1.51450400	-0.28767800
S	3.93642500	-0.14931300	-0.48454500
H	7.43485900	0.94063700	-0.30387900
C	3.62905800	2.94631900	-0.55441900
C	3.07539700	4.07886000	-1.24227500
H	3.62519500	4.73389700	-1.90300500
H	7.02130600	2.25242300	-2.46550600
H	8.83399500	3.87463700	-2.85706700
C	9.27935400	6.26196600	-1.59132700
H	10.09438000	6.10090200	-0.87441700
H	9.70382800	6.16463200	-2.59473700
H	8.93746900	7.29371000	-1.46455700
C	1.72691700	4.09343400	-0.97190000
C	1.45603300	2.97952500	-0.10941300
N	2.65131300	2.32713400	0.14337000
C	0.05496800	1.14296400	0.83691300
C	0.47211200	-0.04564600	0.20524500
C	-0.09815200	-1.15844100	0.85571200
C	-0.79931100	-0.67733700	2.01885800
C	-0.69172700	0.77517700	2.01242400
C	-1.09881100	1.66550000	3.00582200
C	-1.77241200	1.40013900	4.19942800
C	-1.38644200	-1.48301600	2.99463900
H	-0.85344800	2.70713700	2.82759100
C	-0.11026600	-2.52772900	0.38009200
C	1.34829900	-4.25541300	-0.85675700
C	2.72284100	-4.34642900	-1.04052100
C	3.32799300	-3.27524100	-0.33456800
N	2.32851500	-2.57736400	0.28029500
C	4.71207900	-2.84624200	-0.34379500

C	5.73562800	-3.91244700	-0.50556500
C	6.73692200	-3.83389300	-1.48851500
C	5.69932400	-5.05764700	0.31015500
C	6.64300600	-6.06945900	0.16079200
C	7.65085800	-5.98660900	-0.81107200
C	7.67432000	-4.85411800	-1.63563600
H	6.76054500	-2.98108300	-2.15984500
H	8.42966500	-4.77491500	-2.41347800
C	8.68638600	-7.07612900	-0.95027100
H	9.50268500	-6.93767600	-0.23020100
H	8.25556500	-8.06457300	-0.76313700
H	9.13028000	-7.08199500	-1.94985400
H	6.59787100	-6.93943000	0.81121900
H	4.93262800	-5.14221400	1.07401700
H	7.27367600	-1.60058400	-0.06275000
H	0.97573900	4.75271100	-1.38404200
H	-1.99189000	2.26979000	4.81332300
H	-1.34972200	-2.55153300	2.80305100
H	0.58004000	-4.84326800	-1.33742800
H	3.25144600	-5.04089600	-1.67699200
C	-1.40269900	-3.13640600	0.29405800
C	-1.01898400	3.23993000	0.25087500
N	-2.16829400	2.51299700	-0.01563200
C	-3.27857300	3.31167900	0.03788200
C	-2.82615200	4.60318400	0.39424800
C	-1.42818300	4.56169100	0.50507400
N	-2.48976800	-2.33984700	-0.00459200
C	-3.62288300	-3.06975400	0.17421400
C	-3.25783400	-4.38633800	0.58990700
C	-1.86991500	-4.43438200	0.63646700
C	-4.95113900	-2.50533600	0.00087600
C	-5.19302000	-1.14189700	-0.05401400
S	-3.92464100	0.09798800	0.28075700
C	-4.98204400	1.47458100	-0.20870800
C	-6.26550000	0.91759300	-0.54901600
C	-6.37781700	-0.44040000	-0.45877700
C	-4.61804500	2.81240200	-0.19520700
C	-5.66748900	3.84827100	-0.42728000
C	-6.80456500	3.93279200	0.39068200
C	-7.77251600	4.91196500	0.16895900
C	-7.64063500	5.83883100	-0.87233500
C	-6.50274900	5.75179000	-1.68820400
C	-5.52939700	4.78075600	-1.46988000
C	-6.08884300	-3.45205100	-0.14099000
C	-6.02972300	-4.50646400	-1.07066700
C	-7.09532800	-5.39048200	-1.21206000
C	-8.25273700	-5.26866100	-0.42863800
C	-8.30681000	-4.22269300	0.50106300
C	-7.24605200	-3.32982800	0.64550100
C	-9.39044800	-6.25125100	-0.56961400
C	-8.67588900	6.91441700	-1.09951100
H	-3.46337300	5.45264800	0.59193400
H	-0.77902600	5.36339100	0.82895100
H	-3.94752000	-5.17029000	0.86950400
H	-1.25228500	-5.25587800	0.97430500
H	-7.07252300	1.55598000	-0.88475100
H	-7.27881000	-0.97847100	-0.72484000
H	-6.92323700	3.23284600	1.21263700
H	-8.64199400	4.95931300	0.82000700
H	-6.38060300	6.45136800	-2.51155700
H	-4.66271400	4.72461900	-2.12118000
H	-5.14972100	-4.61383100	-1.69705900
H	-7.03074700	-6.18658400	-1.94981400
H	-9.18852400	-4.10895600	1.12699000
H	-7.30444200	-2.53850700	1.38699400
C	1.09621300	-3.14225400	-0.01818800
C	5.25200600	1.08079800	-0.51438600
H	-8.34037800	7.87833300	-0.69689300
H	-8.87091200	7.06213100	-2.16652900
H	-9.16792900	-7.19193900	-0.05049800
H	-9.57570400	-6.49969500	-1.61953500
H	-10.31755400	-5.85475800	-0.14610700
H	-9.62358900	6.66799900	-0.61247800
C	-2.01742100	-1.10692200	4.18113500
C	-2.18739900	0.17198700	4.71666300
H	-2.70178100	0.21507000	5.67422000
H	-2.41440500	-1.92470900	4.77734900
C	0.21500100	2.50012100	0.34083100
Pd	2.99838500	0.82256100	1.53008500
Cl	2.38836600	2.23637600	3.32011300
Cl	3.35498100	-1.04058100	2.93407300
H	0.98032200	-0.09389000	-0.74796700
Pd	-2.43385900	-0.77139700	-1.39912200
Cl	-2.53747500	1.04171500	-2.88931900
Cl	-1.03744000	-1.97099100	-2.85950200
H	-2.12391800	1.72018500	-0.65811500
H	2.50051900	-1.98350500	1.10320700