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Supporting Information

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Supporting Information

for

N-Confused and N-Fused *meso*-Aryl Sapphyrins

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Table of Contents……S1

Synthesis of N-confused sapphyrin (**1**) and N-fused sapphyrin (**2**) via [5+0] route……S2

Synthesis of N-confused sapphyrin (**1**) via [3+2] route ……S3

Synthesis of normal sapphyrin via [3+2] route ……S4

Synthesis of bromo-derivatives of **1** ……S5

Synthesis of Re complexes of N-fused sapphyrins (**6**, **7**)……S6

Figure S1. ^{1}H NMR spectrum of N-confused sapphyrin (**1**) in $CDCl_3$ at 25 °C……S7

Figure S2. ^{1}H NMR spectrum of N-confused sapphyrin (**1**) (Neutral) in CD_2Cl_2 at –90 °C……S8

Figure S3. ^{1}H NMR spectrum of N-confused sapphyrin (**1**) (0.5 eq. TFA) in CD_2Cl_2 at –90 °C……S8

Figure S4. ^{1}H NMR spectrum of N-confused sapphyrin (**1**) (1 eq. TFA) in CD_2Cl_2 at –90 °C……S9

Figure S5. ^{1}H NMR spectrum of N-confused sapphyrin (**1**) (2 eq. TFA) in CD_2Cl_2 at –90 °C……S9

Figure S6. ^{1}H NMR spectrum of N-confused sapphyrin (**1**) (5 eq. TFA) in CD_2Cl_2 at –90 °C……S10

Figure S7. MALDI-TOF-MS spectrum of N-confused sapphyrin (**1**)……S11

Figure S8. MALDI-TOF-MS spectrum of N-fused sapphyrin (**2**)……S11

Figure S9. ^{1}H NMR spectrum of N-fused sapphyrin (**2**) in $CDCl_3$……S12

Figure S10. MALDI-TOF-MS spectrum of dibromo derivative of **1**……S12

Figure S11. MALDI-TOF-MS spectrum of Re complex of N-fused sapphyrin (**6**)……S13

Figure S12. MALDI-TOF-MS spectrum of Re complex of domino-fused sapphyrin (**7**)……S13

Figure S13. ^{1}H NMR spectrum of Re complex of N-fused sapphyrin (**6**)……S14

Figure S14. ^{1}H NMR spectrum of Re complex of domino-fused sapphyrin (**7**)……S14

Figure S15. UV-Vis-NIR spectra of **2**, **6**, and **7** in CH_2Cl_2……S15

Figure S16. X-ray crystal structure and packing diagram of **[1$^-$•Bu$_4$N$^+$]**……S16

Table S1. Selected bond distances (Å) and bond angles (deg) of **1** in **[1$^-$•Bu$_4$N$^+$]**……S16

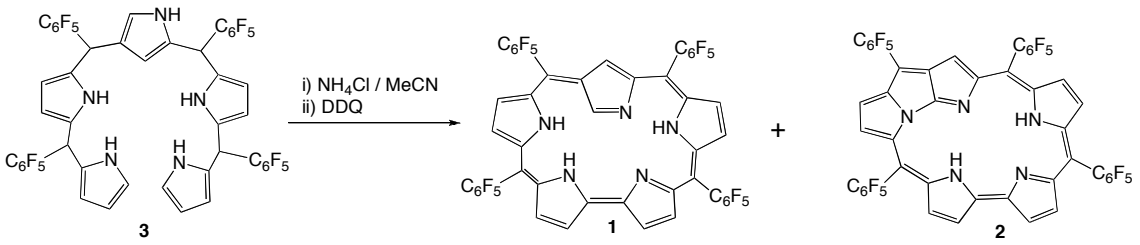
Figure S17. Schematic representation of given compounds showing the selected non-bonded distances (Å) between neighboring nitrogen atoms……S17

Figure S18. The most stable inverted tautomers of *meso*-tetraphenyl N-confused sapphyrin in various ionic states……S19

Total and relative energies of normal and N-confused sapphyrin tautomers ……S20–31

Cartesian coordinates for the optimized structures of normal and N-confused sapphyrin tautomers……S32–231

Synthesis of N-confused sapphyrin (1) and N-fused sapphyrin (2) via [5+0] route



Scheme S1 Synthesis of NC-sapphyrin from [5+0] route.

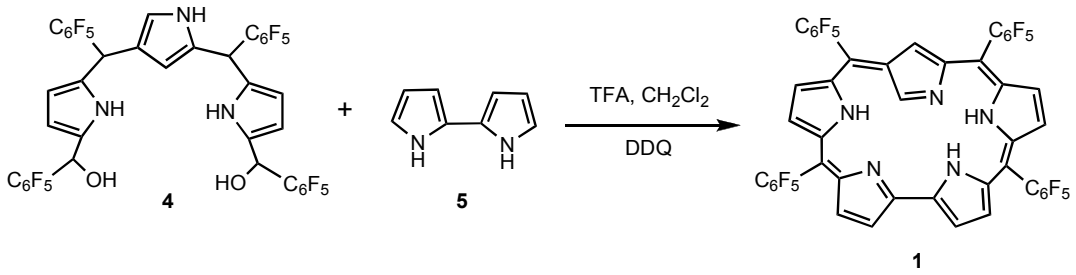
[5+0] route for N-confused sapphyrin (1) and N-fused sapphyrin (2)

5,10,15,20-Tetrakis(pentafluorophenyl) N-confused pentapyrrane* (**3**, 234 mg, 0.223 mmol) and NH_4Cl (119.5 mg, 2.234 mmol) were dissolved in acetonitrile (110 mL) under argon, the mixture was stirred at room temperature for 3 h. Then, DDQ (151.3 mg, 0.669 mmol) was added and the reaction mixture was stirred further for 2 h. After removal of the solvent, the crude mixture was dissolved in a small amount of dichloromethane and passed through a short alumina column using dichloromethane. The reaction mixture was further purified by silica gel [60N, particle size 63-210 μm] column chromatography. The first red colored band was collected in dichloromethane/hexane (10:90) mixture and the solvent was evaporated under reduced pressure to give **2** in < 2% yield (4.0 mg). The second brownish-green band was collected in dichloromethane/hexane (35:65) mixture, and evaporation of the solvent under reduced pressure afforded **1** in 6% yield (13.2 mg).

1: green solid. mp > 300 ^{o}C (dec). ^{1}H NMR (300 MHz, $CDCl_3$, δ in ppm): 1.08 (s, 1H, inner CH), 8.43 (d, J = 4.2 Hz, 1H), 8.62 (d, J = 4.8 Hz, 1H), 8.68 (m, 2H), 8.77 (d, J = 5.4 Hz, 1H), 8.82 (d, J = 4.8 Hz, 1H), 9.77 (d, J = 4.8 Hz, 1H), 9.89 (d, J = 5.4 Hz, 1H), 10.07 (s, 1H). ^{1}H NMR (300 MHz, CD_2Cl_2, δ in ppm at 183 K): –2.48 (s, 1H, NH), –0.92 (s, 1H, NH), 0.78 (s, 1H, NH), 1.64 (s, 1H, inner CH), 8.55 (m, 1H), 8.76 (m, 3H), 8.93 (m, 2H), 9.88 (m, 1H), 10.00 (m, 1H), 10.23 (d, J = 5.4 Hz, 1H). MALDI-TOF-MS: $C_{48}H_{13}N_5F_{20}$, calcd 1039.1, obsd m/z 1039.5 (M^+). HRMS (ESI+) m/z; found: 1040.07969, calcd for $C_{48}H_{14}F_{20}N_5$ (MH^+): 1040.09298. UV-Vis λ_{max}/nm (ε/mol^{-1} dm^3 cm^{-1}) in toluene: 395.3 (42909), 497.7 (Soret, 112000), 625.9 (7400), 679.9 (6200), 750.9 (5400), 819.6 (10500, sh), 871.6 (13300).

2: red solid. mp > 300 ^{o}C (dec). ^{1}H NMR (300 MHz, $CDCl_3$, δ in ppm): 5.56 (br s, 1H, NH), 7.51 (br s, 2H), 7.61 (s, 1H), 7.95 (d, J = 4.5 Hz, 1H), 8.30 (br s, 1H, NH), 8.39 (d, J = 4.5 Hz, 1H), 8.51 (m 3H), 8.71 (m, 1H). MALDI-TOF-MS: $C_{48}H_{11}N_5F_{20}$, calcd 1037.1, obsd m/z 1037.6 (M^+). HRMS (ESI–) m/z; found: 1036.06466, calcd for $C_{48}H_{10}F_{20}N_5$ ($[M–H]^–$): 1036.06168. UV-Vis λ_{max}/nm (ε/mol^{-1} dm^3 cm^{-1}) in toluene: 368.1 (11900), 417.1 (hump, 8200), 506.5 (Soret, 23600), 601.2 (sh, 1600), 657.2 (1200), 721.9 (550), 851.3 (590), 963.4 (830).

Synthesis of N-confused sapphyrin (1) via [3+2] route

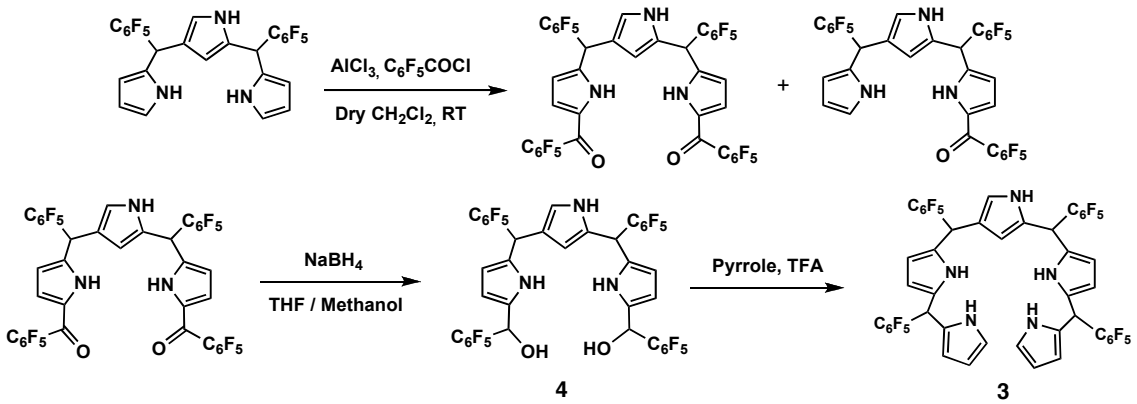


Scheme S2. Synthetic scheme for preparation of N-confused sapphyrin via [3+2] route.

[3+2] route for N-confused sapphyrin (1)

2,2'-Bipyrrole (14 mg, 0.106 mmol) and bis-carbinol derivative of N-confused pentafluorophenyl tripyrrane** (**4**, 100 mg, 0.106 mmol) were dissolved in dry CH_2Cl_2 (50 mL) under argon atmosphere. After few minutes TFA (0.106 mmol, 8.3 μL) was added and the mixture was stirred at room temperature for 3h. After this period DDQ (0.318 mmol, 71.9 mg) was added and the solution was stirred further 2h. Solvent was removed under vacuo and the crude mixture was subjected to a short alumina column using dichloromethane to remove polymeric side products. The crude compound was further purified by silica gel [KANTO Silica Gel 60N, particle size 63-210 μm] column chromatography. N-confused sapphyrin (**1**) was collected as brownish-green band in dichloromethane/hexane (35:65) mixture. Removal of solvent under reduced pressure afforded desired compound in 6.4% yield (7.1 mg).

***,** Syntheses of tripyrrane and pentapyrrane derivatives (3, 4)**:



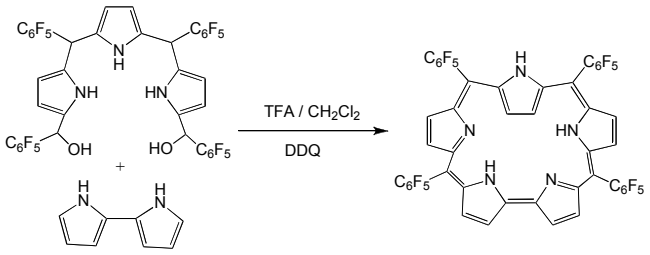
Aluminum chloride (1.72 g, 12.92 mmol) and pentafluorobenzoyl chloride (2.98 g, 12.92 mmol) were taken in three necked round bottom flask and CH_2Cl_2 (200 mL) was added, the solution was stirred at room temperature under N_2 atm. After 1 h, a solution of N-confused tripyrrane (3.0 g, 5.38 mmol) in 100 mL of CH_2Cl_2 was added dropwise at room temperature. After stirring for 12 h, water and aqueous NaOH solution were added. The aqueous layer was extracted with CH_2Cl_2 and the combined extracts were washed with brine, dried over anhydrous Na_2SO_4. After evaporation, the products were separated by silica gel column chromatography (eluted with 90% CH_2Cl_2/n-hexane). Bis(benzoylpentafluorophenyl)tripyrrane was obtained in

25% yield (1.29 g). Brown solid. ^{1}H NMR (300 MHz, $CDCl_3$, δ in ppm) 5.89 (s, 2H, *meso*-H). 6.08 (m, 2H, βH), 6.14 (m, 2H, βH), 6.64 (m, 2H, βH and αH), 8.27 (s, br, 1H, NH), 9.62 (s, br, 2H, NH). MALDI-TOF-MS: $C_{40}H_{11}N_3F_{20}O_2$; calcd 945.502, obsd *m*/*z* 1037.6 (M^+): 944.5.

To a solution of bis-pentafluorobenzoyl derivative of NC-tripyrrane (0.68 g, 0.72 mmol) was taken in 10 mL of THF/MeOH (4:1, v/v), $NaBH_4$ (1.36 g, 36.0 mmol) was added at 0 °C and the reaction solution was stirred overnight at room temperature. After the starting material was disappeared on TLC, water was added, and the aqueous layer was extracted with dichloromethane and the combined extracts were washed with brine, dried over anhydrous Na_2SO_4. After evaporation, the bis-carbinol derivative of NC-tripyrrane was obtained. The crude bis-carbinol derivative of NC-tripyrrane (**4**) being unstable was not purified further and directly used for the next step.

The crude **4** (0.68 g, 0.72 mmol) was dissolved into pyrrole (2 mL, 28.80 mmol) and trifluoroacetic acid (23 μL, 0.22 mmol) was added. After stirring at room temperature for 2 h, the reaction was quenched with aqueous NaOH solution. The reaction mixture was partitioned between dichloromethane and water, the organic phase was washed with water, dried over Na_2SO_4, and evaporated in vacuo. Excess pyrrole was removed by vacuum distillation then crude compound was purified by silica gel column chromatography (eluted with 70% CH_2Cl_2/hexane) affording N-confused pentapyrrane (**3**) in 71% yield (0.54 g). Brown flaky solid. ^{1}H NMR (300 MHz, $CDCl_3$, δ in ppm) 5.63 (s, 1H, *meso*-H), 5.73 (s, 1H, *meso*-H), 5.82 (m, 4H, βH + *meso*-H), 5.90-5.97 (m, 5H, βH), 6.12 (m, 2H), 6.48 (s, 1H), 6.71 (m, 2H), 8.08 (m, 5H, NH).

Synthesis of normal sapphyrin via [3+2] route



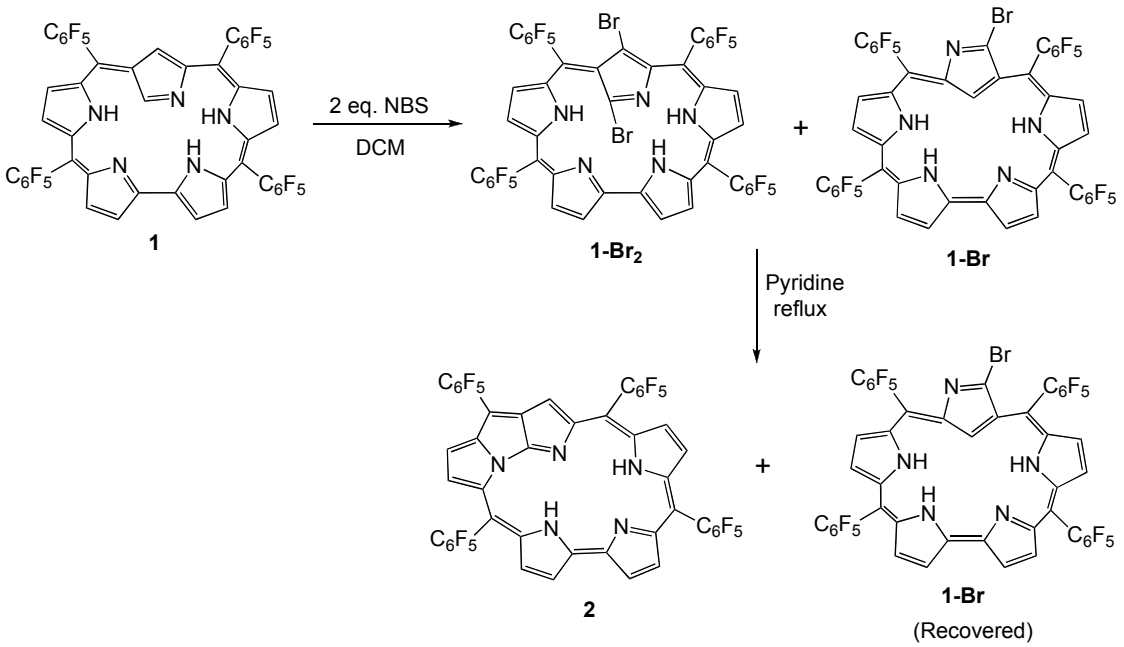
Scheme S3. Synthetic scheme for preparation of normal sapphyrin via [3+2] route.

[3+2] route for normal sapphyrin

2,2'-Bipyrrole (17 mg, 0.128 mmol) and bis-carbinol derivative of pentafluorophenyl tripyrrane (120 mg, 0.170 mmol) were dissolved in dry CH_2Cl_2 (60 mL) under argon atmosphere. After few minutes TFA (0.128 mmol, 10 μL) was added and the mixture was stirred at room temp for 3 h. After this period DDQ (0.384 mmol, 86.4 mg) was added and the solution was stirred further 2 h. Solvent was removed under vacuo and the crude mixture was subjected to a short alumina column using dichloromethane to remove polymeric side products. The crude compound was further purified by silica gel [KANTO Silica Gel 60N, particle size 63-210 μm] column chromatography. Normal sapphyrin, *meso*-tetrakis(pentafluorophenyl)sapphyrin, was collected as bright green band in dichloromethane. Removal of solvent under reduced pressure afforded desired compound in 4% yield (7.9 mg).

^{1}H NMR (300 MHz, CD_2Cl_2, δ in ppm): –1.39 (s, 2H, inner β-CH), 8.96 (m, 2H), 9.16 (s, 1H), 9.47 (s, 1H), 9.59 (s, 1H), 9.75 (s, 1H), 10.26 (s, 1H), 10.62 (s, 1H); ^{1}H NMR (300 MHz, CD_2Cl_2 , δ in ppm at 203 K): –2.98 (br s, 2H, inner NH), –1.59 (s, 2H, inner β-CH), 11.78 (br s, 1H, outer NH). MALDI-TOF-MS: $C_{48}H_{13}N_5F_{20}$, calcd 1039.1, obsd *m*/*z* 1039.2 (M^+). UV-Vis λ_{max}/nm (toluene, ε/mol^{-1} dm^3 cm^{-1}) in toluene: 387.2 (6100), 489.4 (Soret, 53900), 622.8 (4000), 678.9 (4600), 712.6 (3200), 790.6 (900).

Synthesis of bromo-derivatives of 1

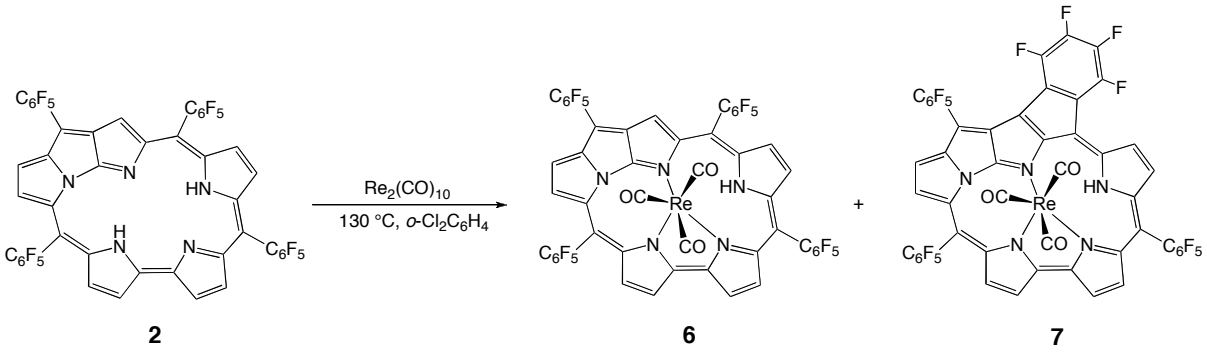


Scheme S5. Synthetic scheme for preparation of bromo-substituted N-confused sapphyrin and N-fused sapphyrin.

Bromination of N-confused sapphyrin (1)

N-confused sapphyrin (**1**, 2 mg, 0.002 mmol) was taken in dry CH_2Cl_2 (3 mL), to this added dropwise NBS (N-bromosuccinimide, 0.68 mg solution in 2 mL dry CH_2Cl_2). Progress of the reaction was judged by TLC and also by the appearance of M^+ ion peaks in MALDI-TOF-MS corresponding to the brominated products. The reaction mixture was stirred for few minutes then solvent was evaporated on a rotary evaporator. Attempts to separate the mixture of dibromo and monobromo derivatives, **1-Br$_2$** and **1-Br**, respectively, were unsuccessful due to the unstable nature of **1-Br$_2$**. Thus the crude mixture of **1-Br$_2$** and **1-Br** was refluxed in pyridine for 1 h, then a new red spot corresponding to **2** was observed on TLC along with unreacted **1-Br**. The reaction mixture was separated by silica gel column chromatography and formation of **2** and **1-Br** was confirmed by MALDI-TOF-MS spectrometry.

Synthesis of Re complexes of N-fused sapphyrins (6, 7)



2 **6** **7**

Scheme S6. Synthetic scheme for preparation of Re complexes of N-fused sapphyrin.

Re complexes of N-fused sapphyrin (6, 7)

To a solution of N-fused sapphyrin (**2**, 21 mg, 0.020 mmol) in *o*-dichlorobenzene (20 mL) added $Re_2(CO)_{10}$ (13.2 mg, 0.020 mmol), and the resulting solution was reflux at 130 °C for 12 h under argon. After this period two new spots were developed on the TLC along with the very faint spot of the starting material. Solvent was removed under vacuo and the residues were subjected to silica gel column chromatography. After collecting the trace amount of starting material in dichloromethane/hexane (10:90) mixture, the second violet color band was collected in dichloromethane/hexane (25:75) mixture. Removal of the solvent under reduced pressure afforded Re complex of *domino-fused* sapphyrin (**7**) in 55% yield (15 mg). The third reddish pink color band was eluted in dichloromethane/hexane (30:70) mixture and the evaporation of solvent under vacuo gave Re complex of N-fused sapphyrin (**6**) in 7% yield (2.2 mg).

6: reddish pink, solid. m.p. > 250 °C. ^{1}H NMR (300 MHz, CD_2Cl_2, δ in ppm): 5.99 (br s, 1H, NH), 7.20 (d, J = 4.2 Hz, 1H), 7.27 (br s, 1H), 7.35 (br s, 1H), 7.84 (d, J = 5.1 Hz, 1H), 7.88 (d, J = 4.2 Hz, 1H), 8.01 (d, J = 4.8 Hz, 1H), 8.37 (s, 1H), 8.50 (m, 1H), 8.57 (m, 1H). MALDI-TOF-MS: $C_{51}H_{10}N_5F_{20}ReO_3$, calcd 1307.0, obsd m/z 1305.8 (M^+). UV-Vis: λ_{max}/nm (ε/mol^{-1} dm^3 cm^{-1}) in toluene: 408.6 (34000), 519.7 (Soret, 56800), 734.3 (3900), 796.5 (sh, 2200), 906 (sh, 1900), 982.7 (1970).

7: violet, solid. m.p. > 250 °C. ^{1}H NMR (500 MHz, CD_2Cl_2, δ in ppm): 7.74 (s, 1H), 7.92 (s, 1H), 8.28 (s, 1H), 8.45 (s, 1H), 8.52 (s, 1H), 8.86 (s, 1H), 8.96 (s, 2H). MALDI-TOF-MS: $C_{51}H_8N_5F_{19}ReO_3$, calcd 1287.0, obsd m/z 1286.2 (M^+). HRMS (ESI–) m/z: calcd for $C_{51}H_9F_{19}N_5O_3{}^{185}Re$ (M^-): 1284.99316, found: 1285.00225. UV-Vis: λ_{max}/nm (ε/mol^{-1} dm^3 cm^{-1}) in toluene: 403.2 (23000), 484.8 (33000), 564.1 (Soret, 37100), 734.3 (3900), 831 (sh, 1900), 1058.7 (2000), 1180.6 (1800).

Figure S1. ^{1}H NMR spectrum of N-confused sapphyrin (**1**) in $CDCl_3$ at 25 °C.

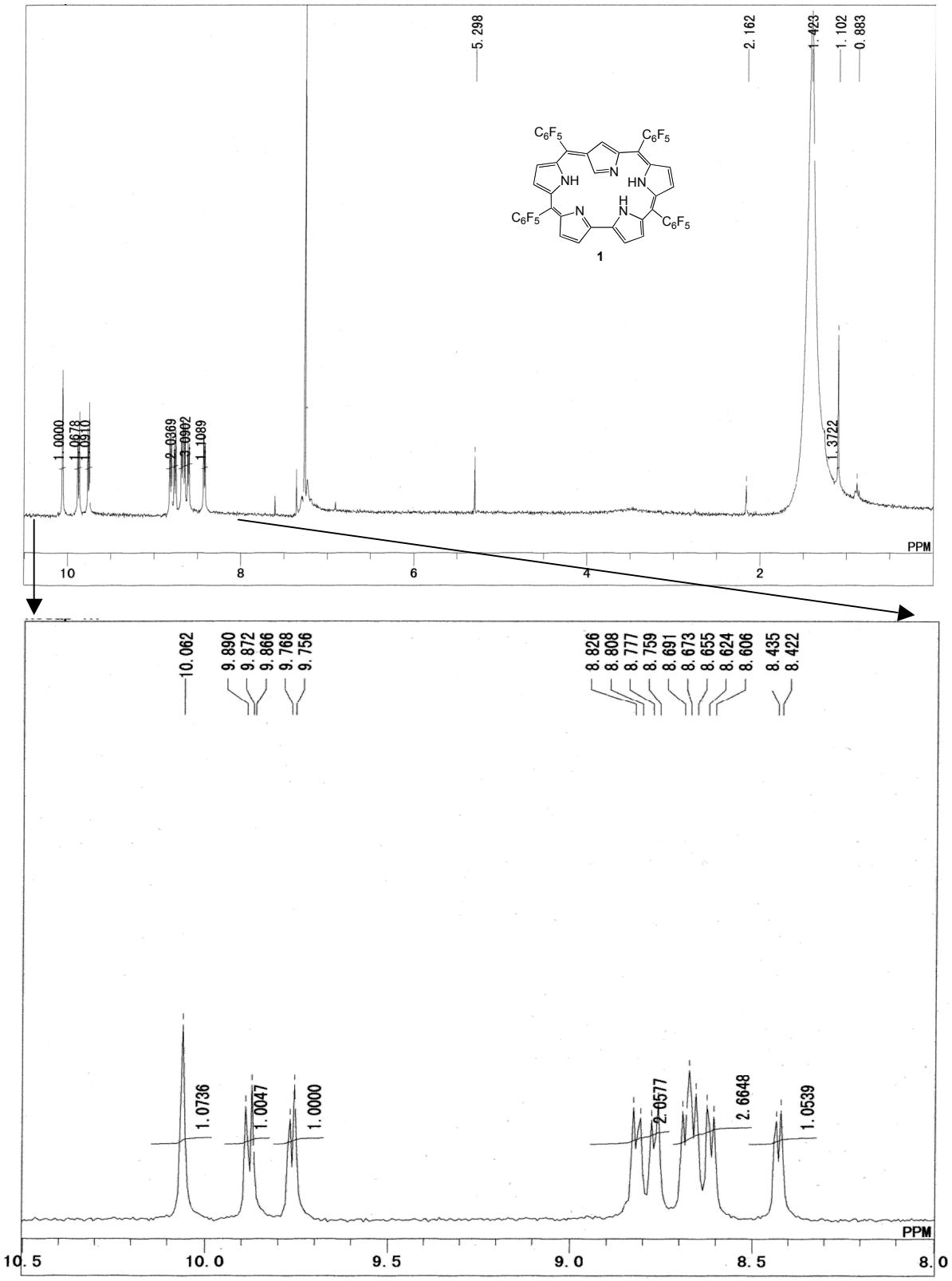


Figure S2. ^{1}H NMR spectrum of N-confused sapphyrin (**1**) (Neutral) in CD_2Cl_2 at –90 °C.

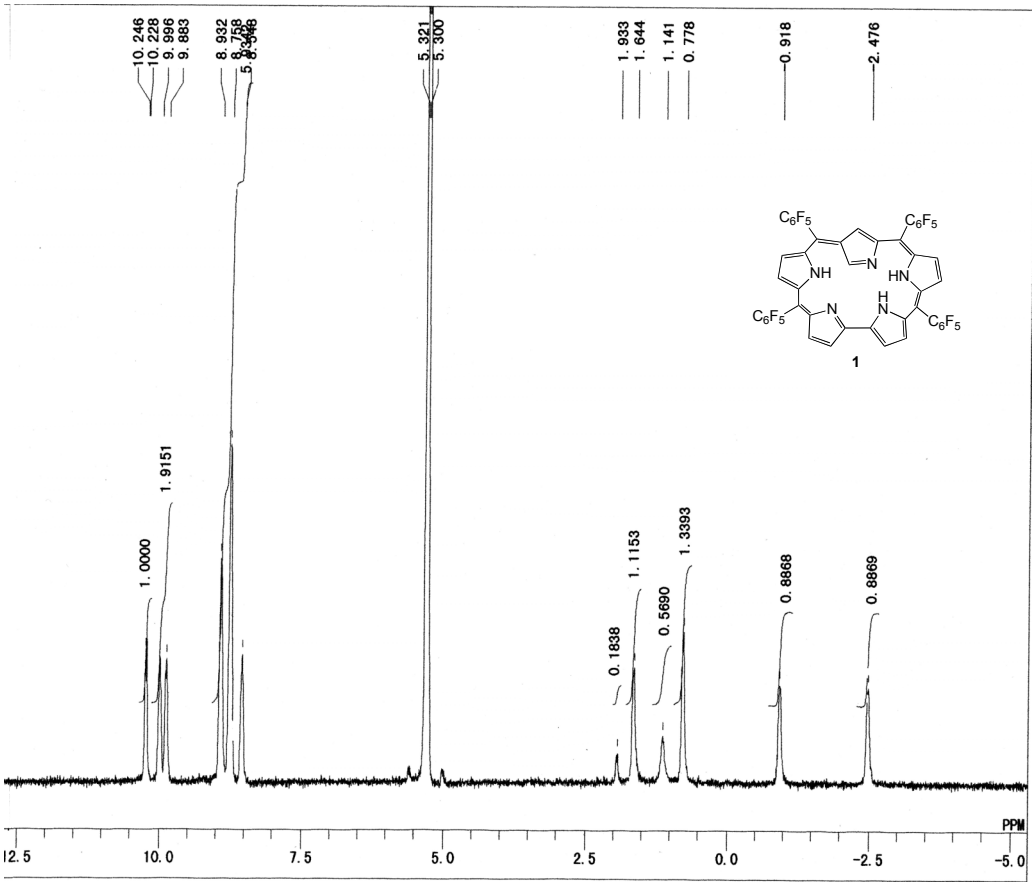


Figure S3. ^{1}H NMR spectrum of N-confused sapphyrin (**1**) (0.5 eq. TFA) in CD_2Cl_2 at –90 °C.

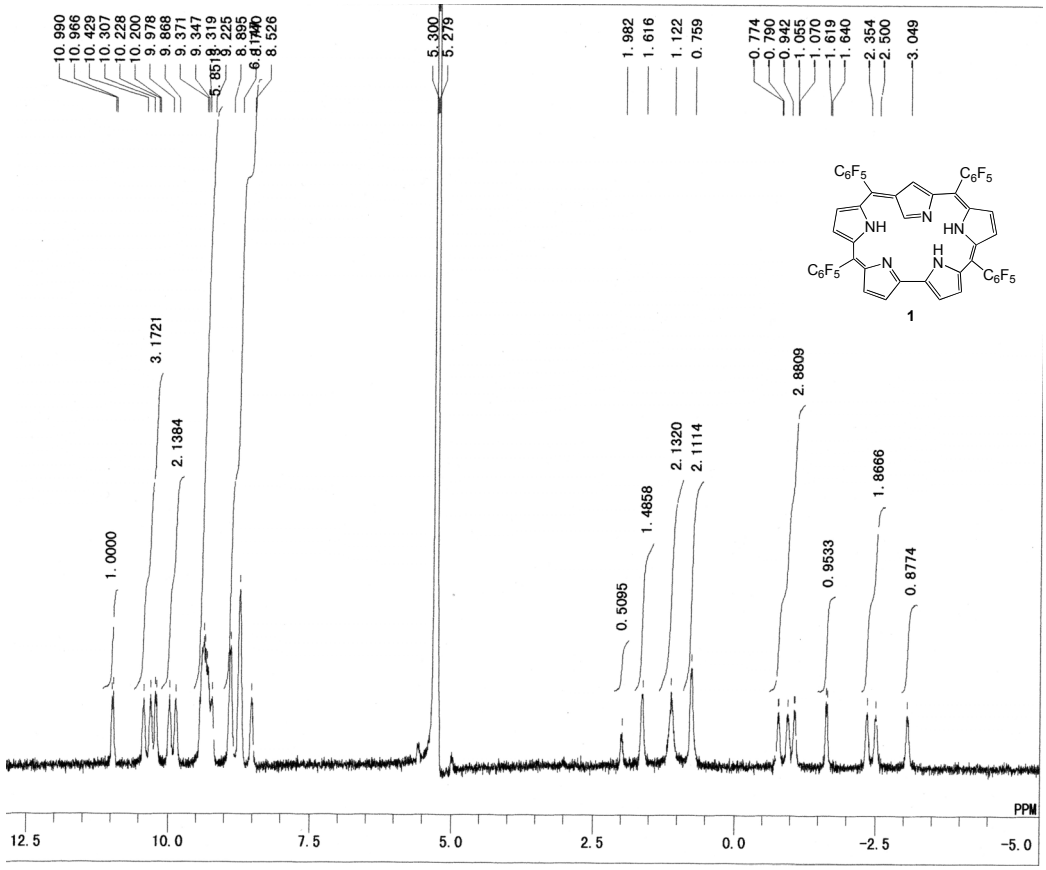


Figure S4. ^{1}H NMR spectrum of N-confused sapphyrin (**1**) (1 eq. TFA) in CD_2Cl_2 at –90 °C.

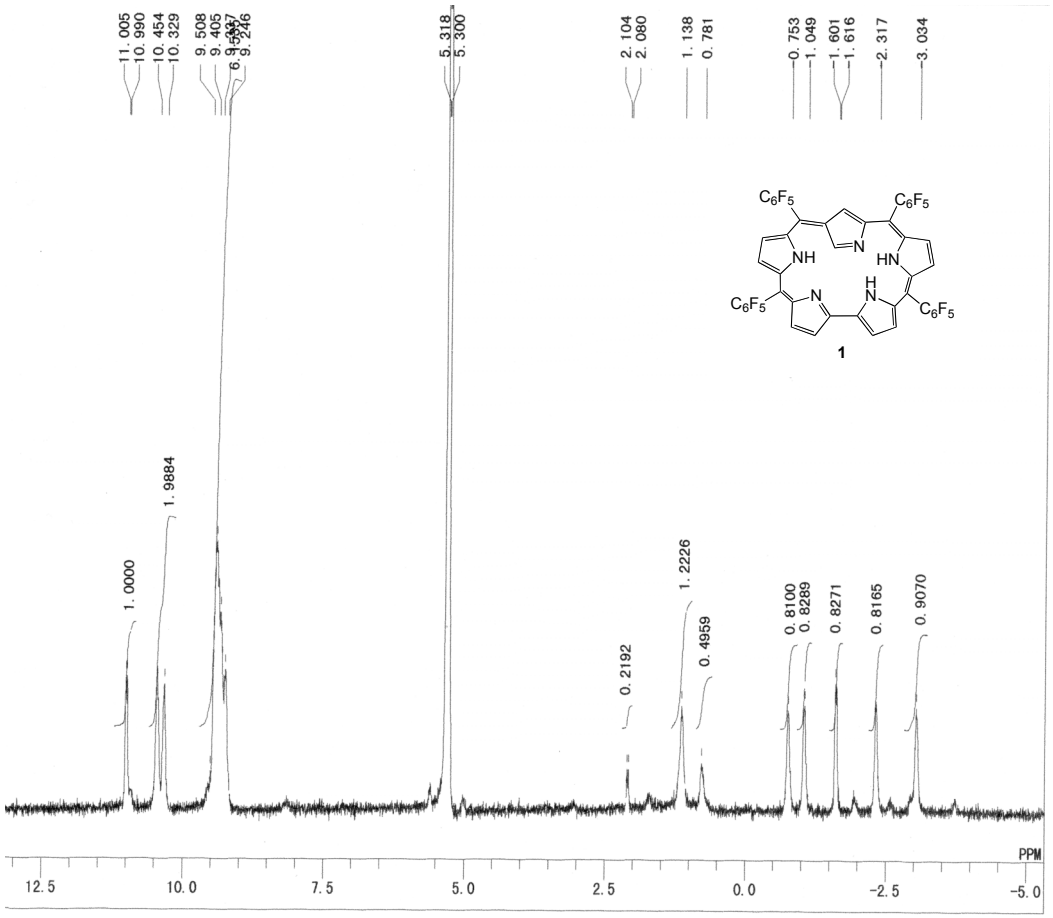


Figure S5. ^{1}H NMR spectrum of N-confused sapphyrin (**1**) (2 eq. TFA) in CD_2Cl_2 at –90 °C.

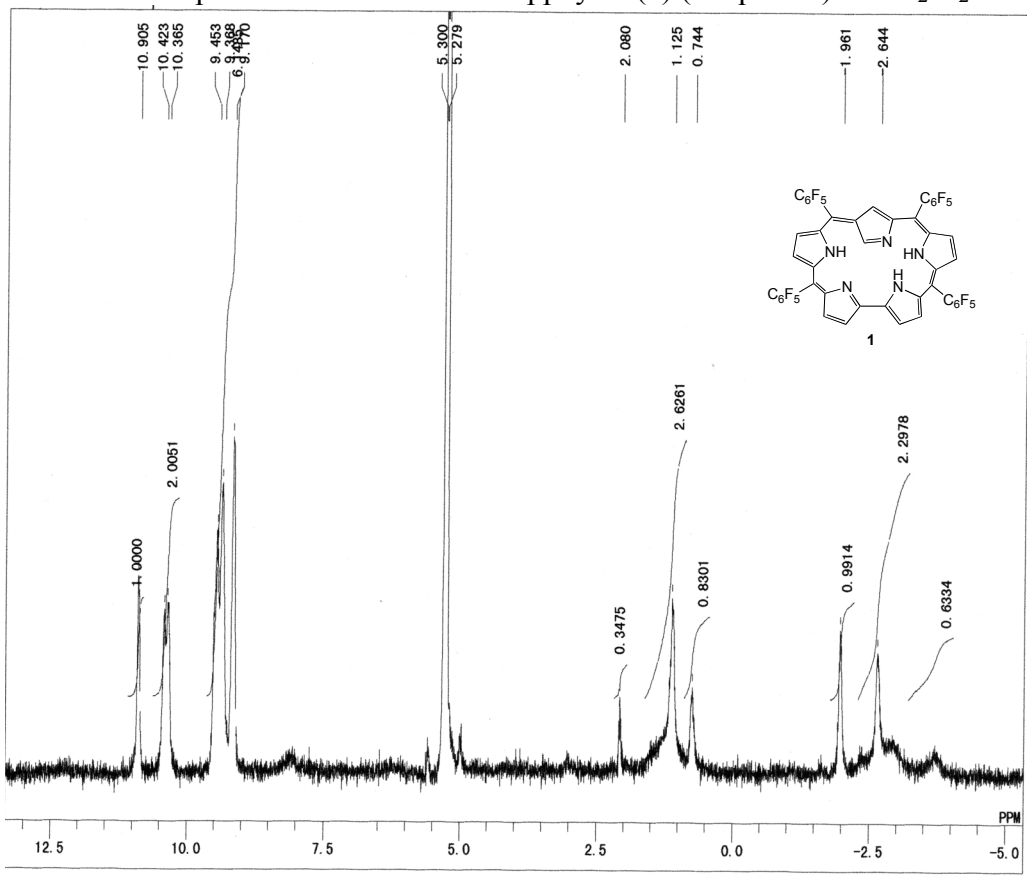


Figure S6. ^{1}H NMR spectrum of N-confused sapphyrin (**1**) (5 eq. TFA) in CD_2Cl_2 at –90 °C.

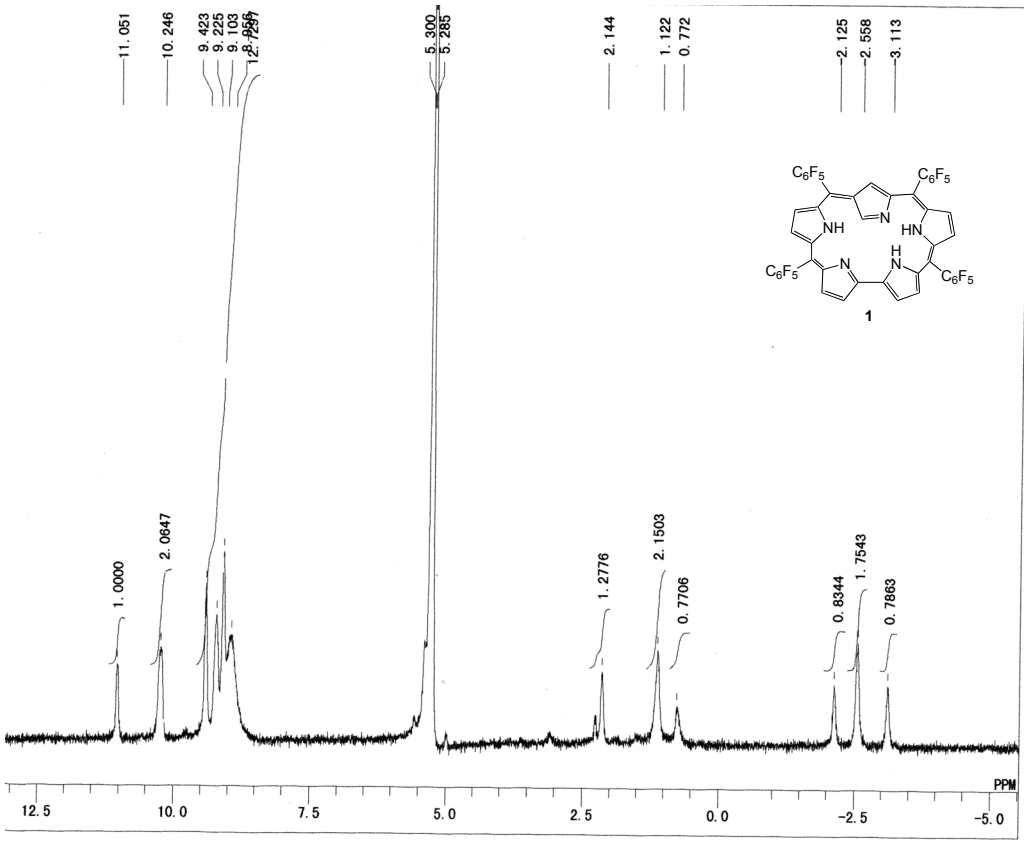


Figure S7. MALDI-TOF-MS spectrum of N-confused sapphyrin (**1**).

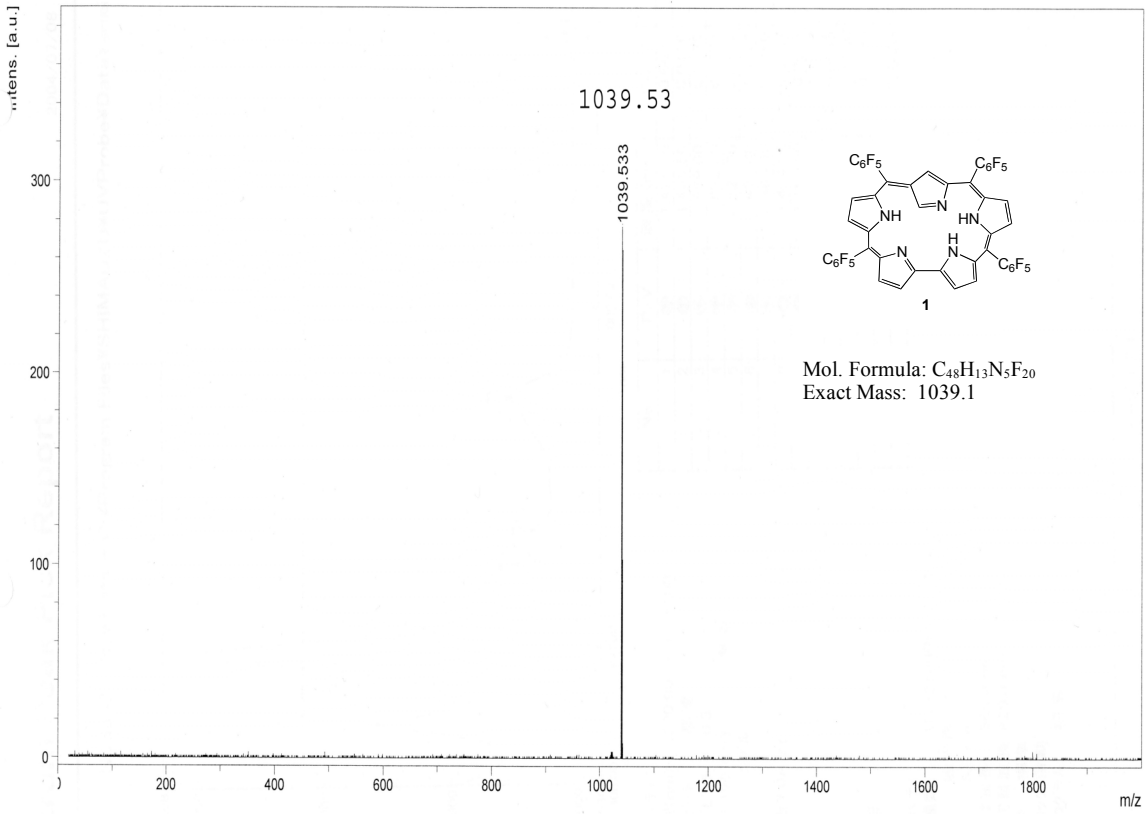


Figure S8. MALDI-MS spectrum of N-fused sapphyrin (**2**).

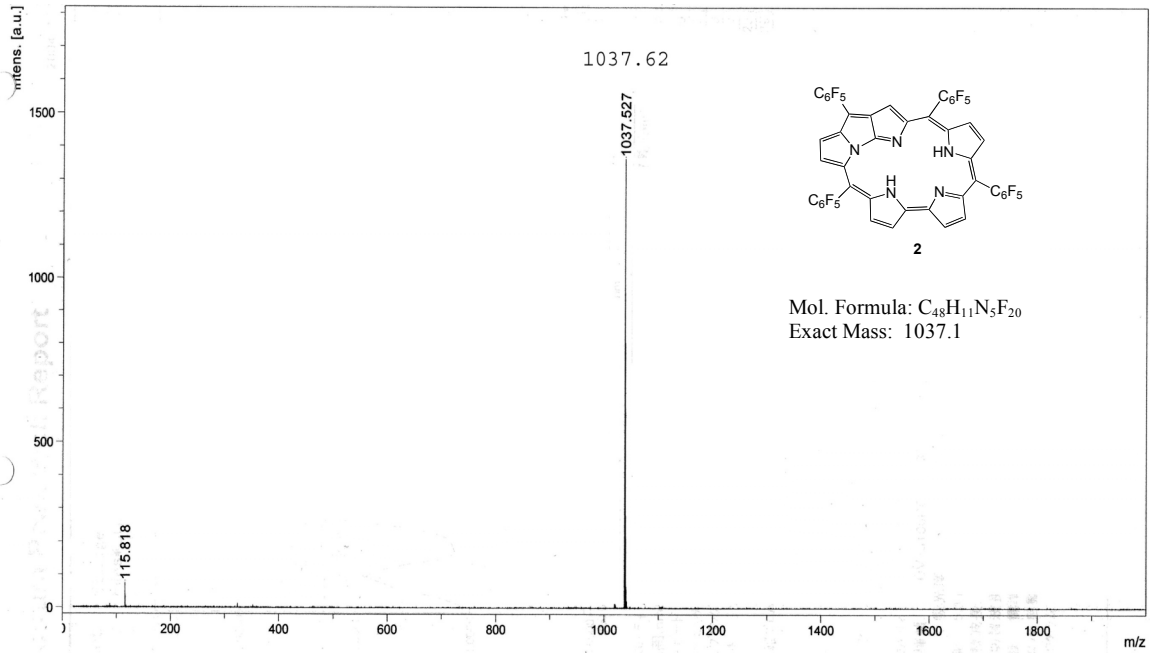


Figure S9. ^{1}H NMR spectrum of N-fused sapphyrin (**2**) in $CDCl_3$.

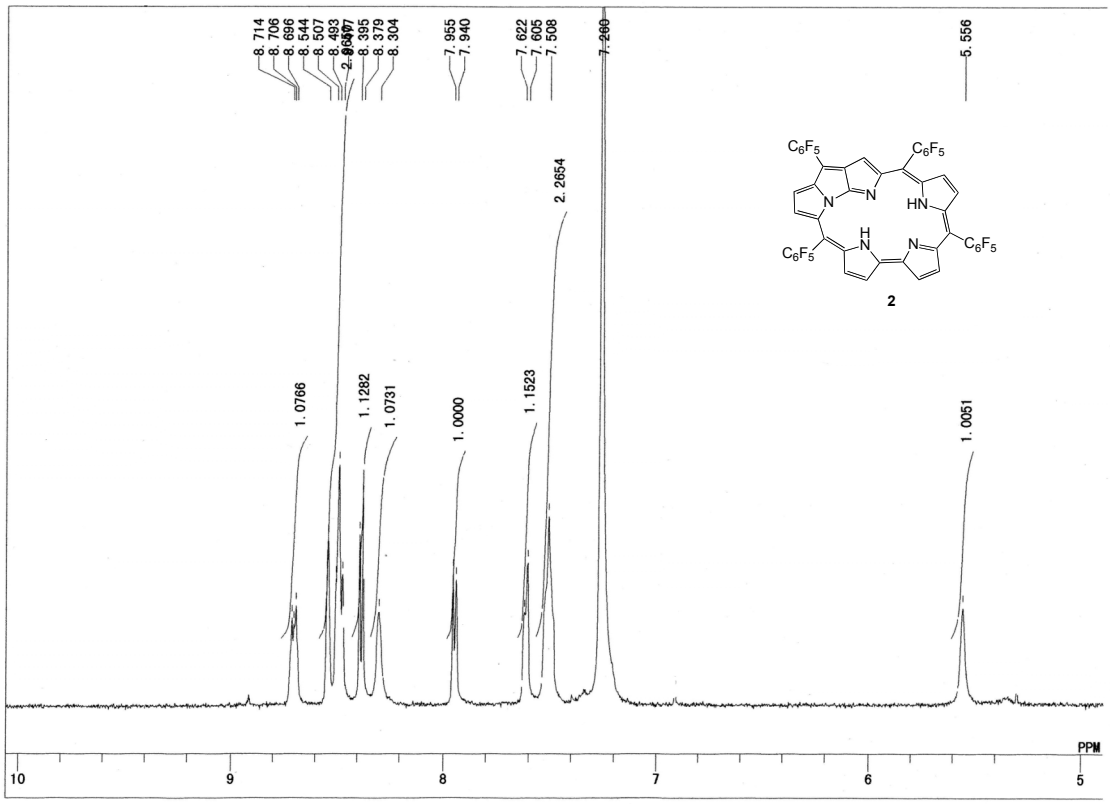


Figure S10. MALDI-MS spectrum of dibromo derivative of **1**

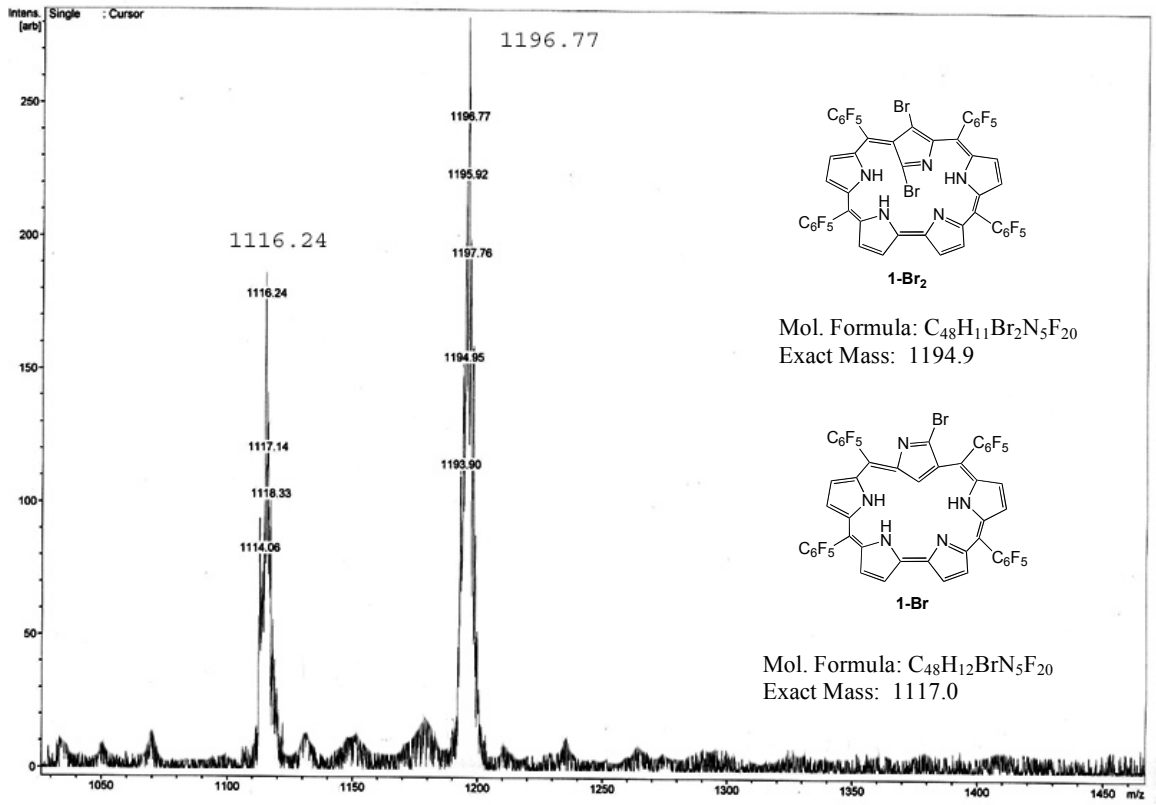


Figure S11. MALDI-TOF-MS spectrum of Re complex of N-fused sapphyrin (**6**).

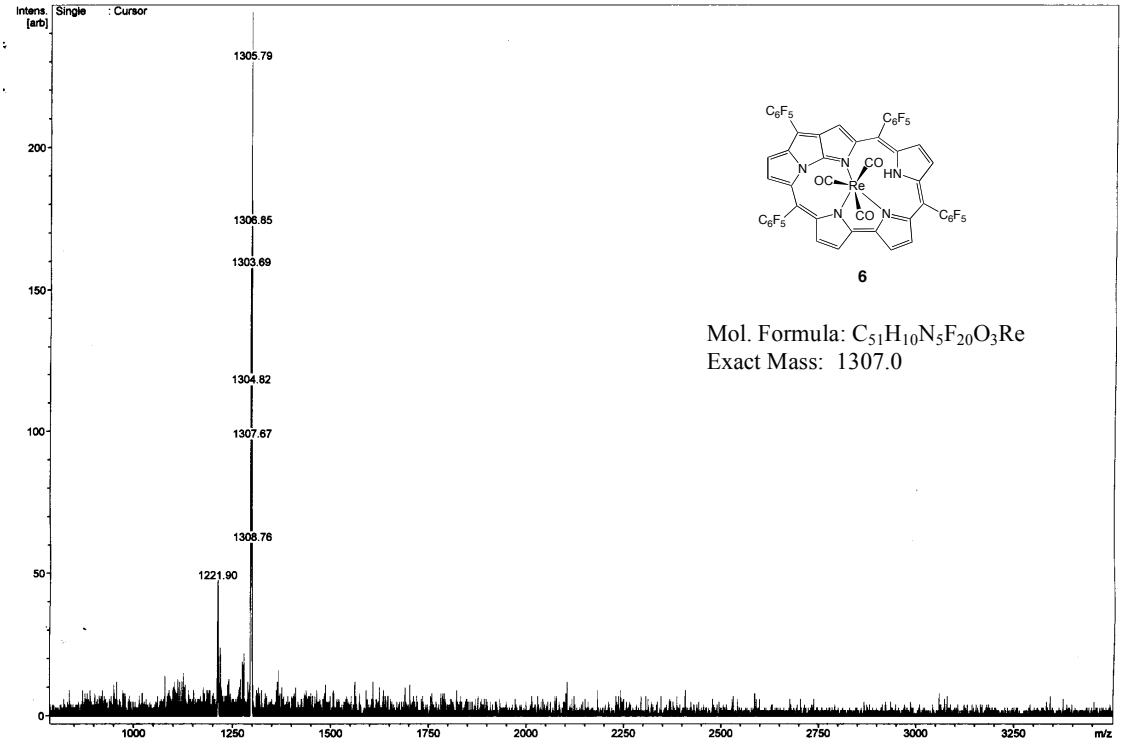


Figure S12. MALDI-TOF-MS spectrum of Re complex of *domino-fused* sapphyrin (**7**).

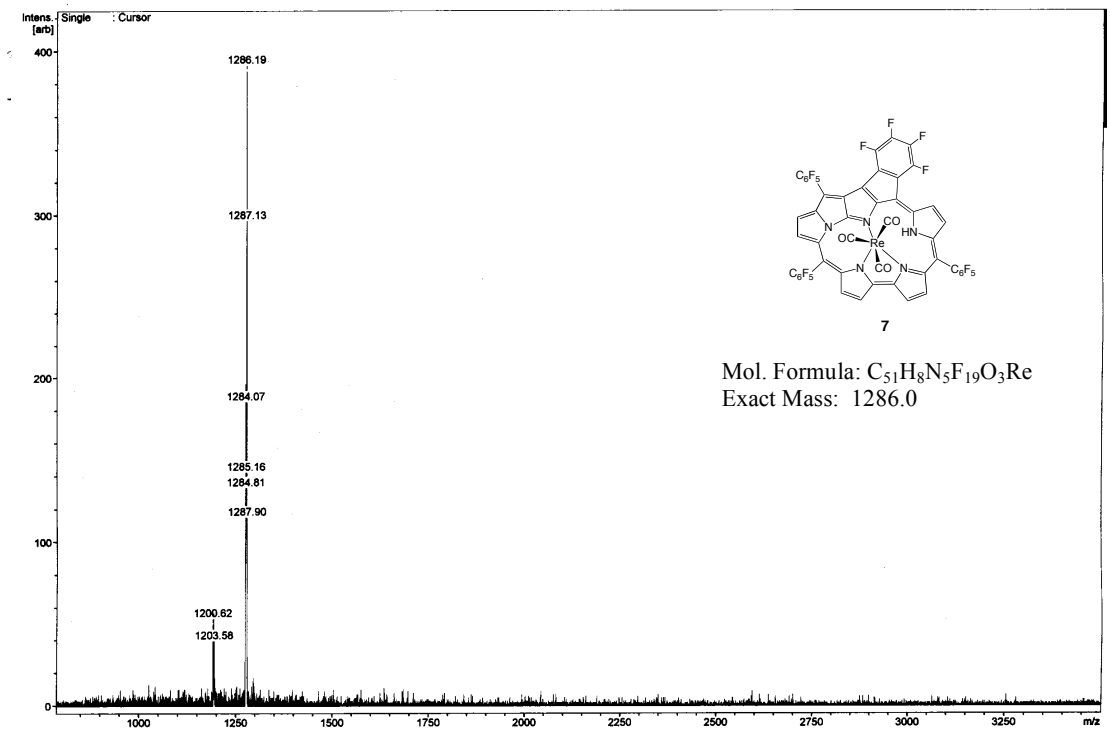


Figure S13. ^{1}H NMR spectrum of Re complex of N-fused sapphyrin (**6**) in CD_2Cl_2.

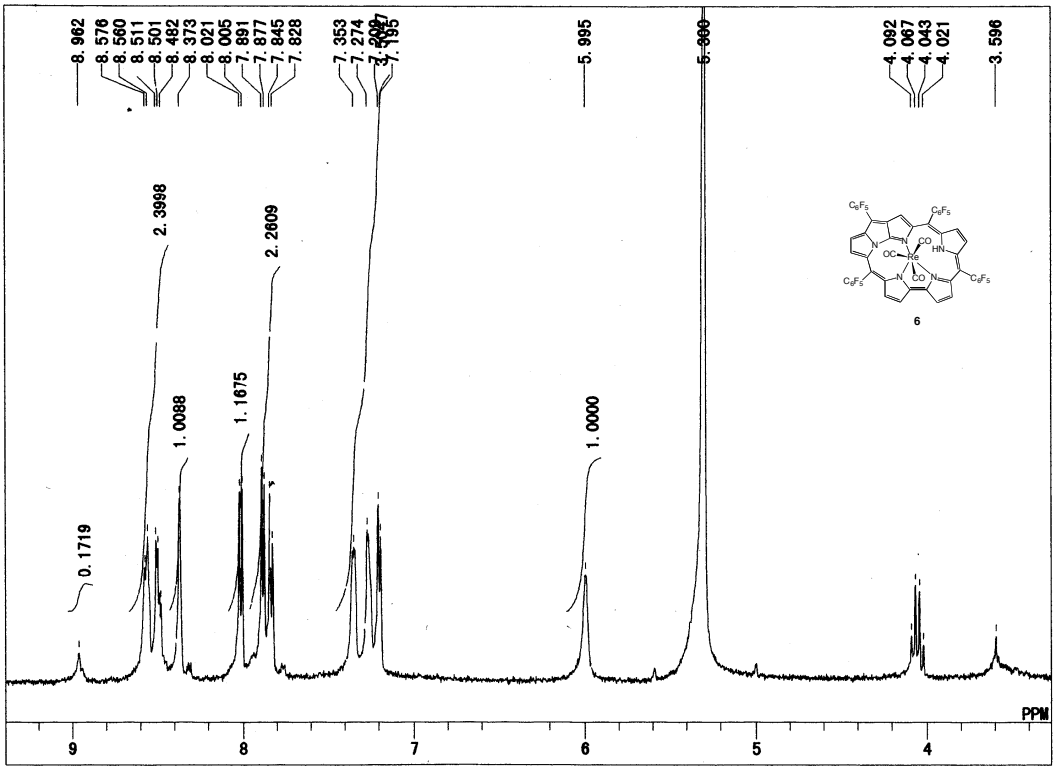


Figure S14. ^{1}H NMR spectrum of Re complex of domino-fused sapphyrin (**7**) in CD_2Cl_2.

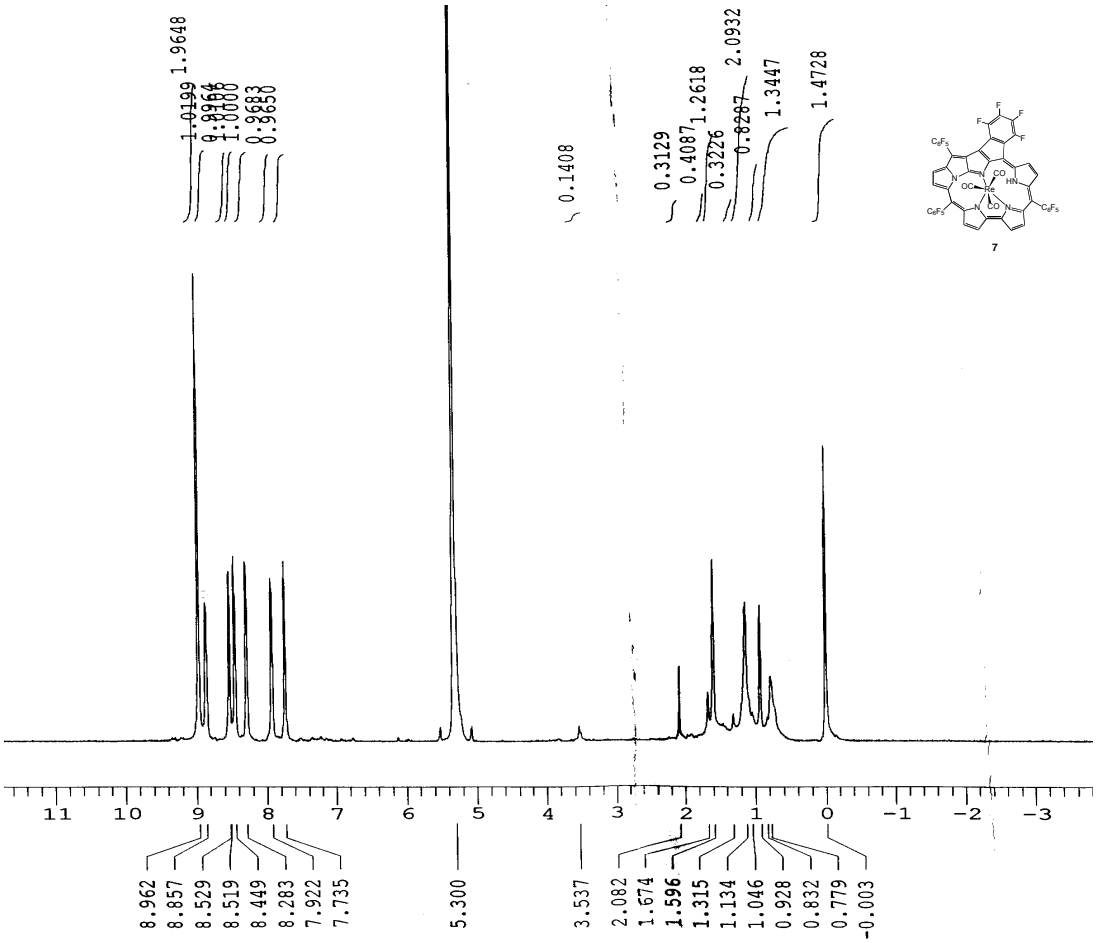


Figure S15. UV-Vis-NIR spectra of **2**, **6**, and **7** in CH_2Cl_2.

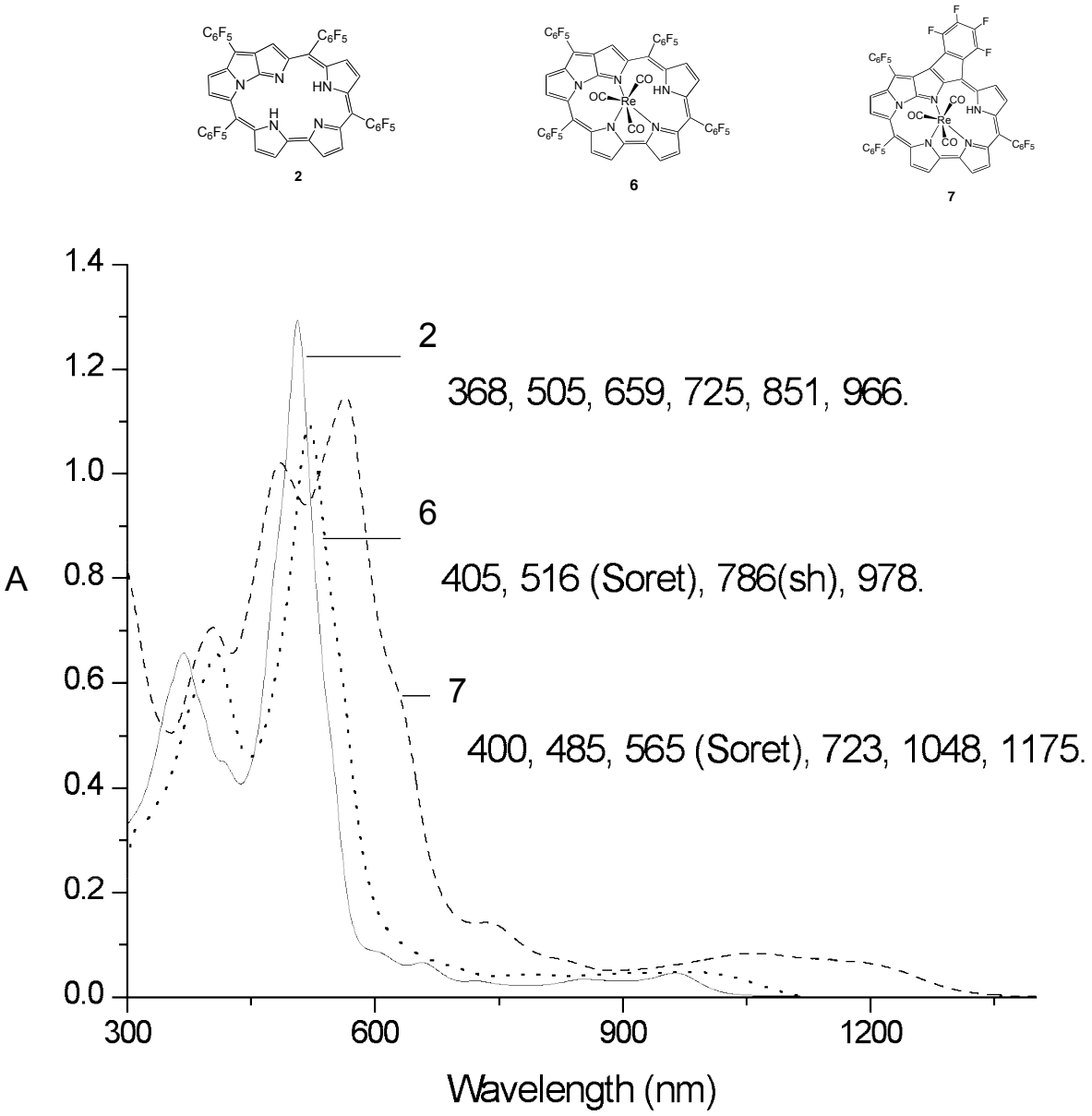
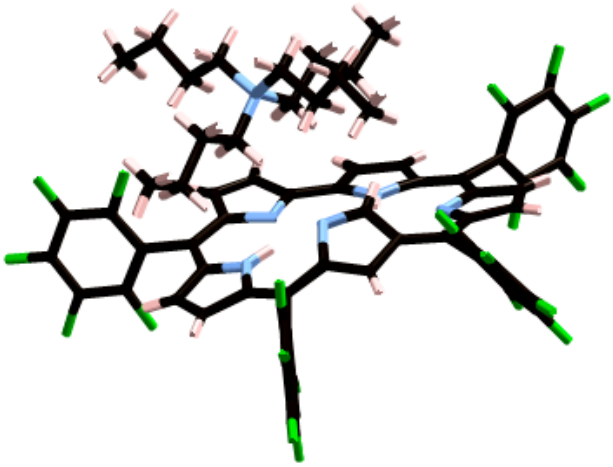
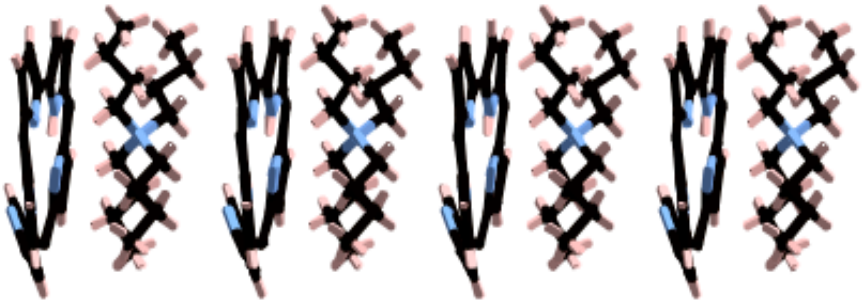


Figure S16. X-ray crystal structure and packing diagram of [**1**$^{-}$•**Bu**$_4$**N**$^{+}$]



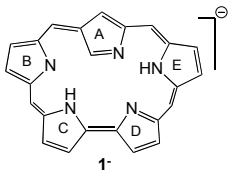
Solid state structure of [**1**$^{-}$•**Bu**$_4$**N**$^{+}$] complex



Packing diagram of [**1**$^{-}$•**Bu**$_4$**N**$^{+}$] complex. Meso-aryl groups are omitted for clarity.

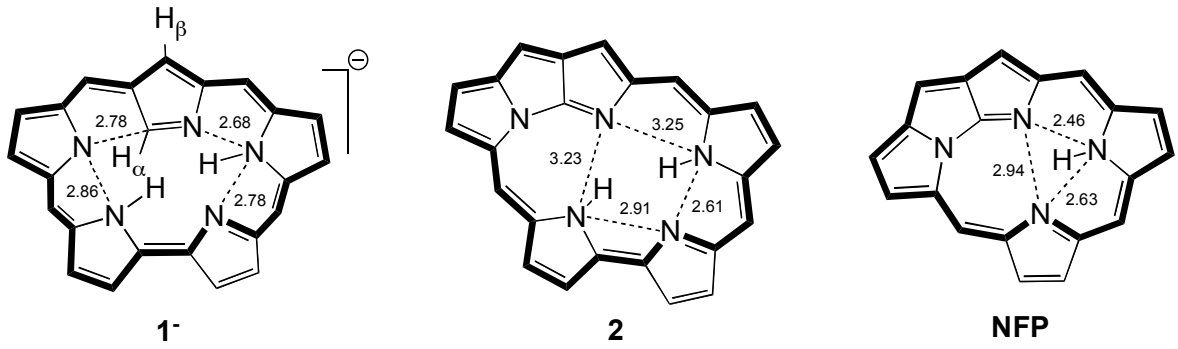
Table S1. Selected bond distances (Å) and bond angles (deg) of **1**$^{-}$.

Ring	C_α-X	C_α-C_β	C_β-C_β	C_α-N-C_α	
Compound **1**$^{-}$					
Pyrrole A	1.299(5), 1.431(5)	1.441(6), 1.397(6)	1.394(6)	105.6(3)	
Pyrrole B	1.374 (5), 1.353(5)	1.447(6), 1.444(6)	1.364(6)	106.7(3)	
Pyrrole C	1.383(5), 1.361(5)	1.414(5), 1.416(5)	1.359(5)	110.7(3)	
Pyrrole D	1.361(5), 1.380(4)	1.429(4), 1.437(5)	1.341(5)	105.5(3)	
Pyrrole E	1.363(5), 1.371(5)	1.427(6), 1.417(6)	1.346(6)	110.2(3)	
(Free pyrrole	1.370	1.382	1.417	-)	



1^{-}

Figure S17. Schematic representation of given compounds showing the selected non-bonded distances (Å) between neighboring nitrogen atoms.



1⁻ **2** **NFP**

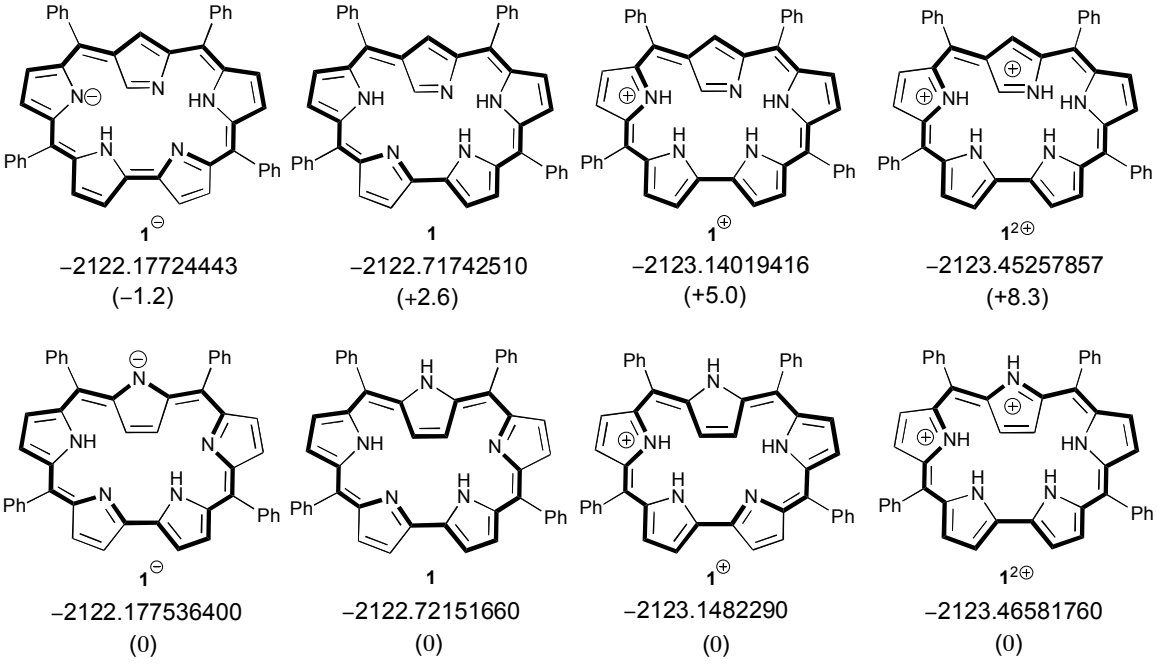
1⁻: from X-ray data (see text)
2: from the DFT Calculation (B3LYP/6-31G(d)) below
3: From X-ray data (ref [6a])

Cartesian coordinates for the optimized structure of N-fused tetraphenylsapphyrin (2)

```
 Stoichiometry    C48H31N5
Framework group  C1[X(C48H31N5)]
Deg. of freedom   246
Full point group                 C1
Largest Abelian subgroup         C1      NOp   1
Largest concise Abelian subgroup C1      NOp   1
                         Standard orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
   1          7              0       -0.488312    0.521093    0.076820
   2          7              0       -2.855053   -0.407159   -0.162490
   3          7              0        2.758580    0.740120    0.106867
   4          6              0       -0.168235    1.938725    0.098249
   5          6              0       -1.351119    2.734854   -0.089567
   6          6              0       -1.792075    0.526049   -0.075155
   7          6              0       -2.394111    1.856540   -0.200703
   8          6              0       -3.797701    1.744035   -0.363128
   9          6              0       -4.044691    0.374193   -0.286602
  10          6              0       -5.155783   -0.474271   -0.123098
  11          6              0       -4.682129   -1.733653    0.120959
  12          6              0       -3.237879   -1.768326    0.074225
  13          6              0       -2.569987   -2.988860    0.139352
  14          6              0       -1.218896   -3.408070   -0.068078
  15          6              0       -0.837270   -4.774361   -0.183690
  16          6              0        0.522088   -4.829679   -0.425869
  17          6              0        1.004393   -3.510131   -0.439408
  18          6              0        2.356700   -3.090005   -0.527482
  19          6              0        3.520248   -3.958714   -0.653524
  20          6              0        4.606437   -3.142083   -0.570975
  21          6              0        4.091622   -1.788694   -0.403103
  22          6              0        4.804202   -0.615583   -0.155063
  23          6              0        4.126266    0.615368    0.104333
  24          6              0        4.658526    1.910275    0.344114
  25          6              0        3.594450    2.781384    0.483896
  26          6              0        2.388659    2.038542    0.313451
  27          6              0        1.067386    2.564352    0.276726
```

28	1	0	-1.375602	3.810489	-0.148108
29	1	0	-6.189873	-0.161536	-0.147105
30	1	0	-5.288094	-2.607972	0.292400
31	1	0	-1.511158	-5.611974	-0.107663
32	1	0	1.126351	-5.715363	-0.562893
33	1	0	3.509420	-5.035008	-0.766562
34	1	0	5.649424	-3.426022	-0.593693
35	1	0	5.709811	2.152806	0.391080
36	1	0	3.646337	3.842154	0.675480
37	7	0	2.712010	-1.815030	-0.402786
38	7	0	-0.068713	-2.665076	-0.236817
39	1	0	0.011444	-1.649703	-0.143953
40	1	0	2.167781	-0.078507	-0.072785
41	6	0	1.029499	4.064713	0.424090
42	6	0	0.665817	4.645564	1.646914
43	6	0	1.374209	4.901014	-0.646783
44	6	0	0.648062	6.033263	1.796191
45	1	0	0.397379	4.002977	2.480774
46	6	0	1.348031	6.289020	-0.500346
47	1	0	1.657181	4.458426	-1.597826
48	6	0	0.987020	6.858563	0.722243
49	1	0	0.368088	6.468646	2.751873
50	1	0	1.609810	6.924398	-1.342336
51	1	0	0.969712	7.939081	0.837153
52	6	0	6.291706	-0.627064	-0.146203
53	6	0	7.013769	-0.198713	0.981324
54	6	0	7.009398	-1.077256	-1.267559
55	6	0	8.407887	-0.223115	0.987184
56	1	0	6.473583	0.135134	1.862404
57	6	0	8.403978	-1.099317	-1.261040
58	1	0	6.464298	-1.394472	-2.151698
59	6	0	9.108442	-0.672532	-0.134055
60	1	0	8.947302	0.103285	1.872473
61	1	0	8.940090	-1.444683	-2.141109
62	1	0	10.194957	-0.689644	-0.129216
63	6	0	-3.475392	-4.166684	0.437743
64	6	0	-4.109844	-4.870576	-0.595465
65	6	0	-3.675411	-4.583015	1.760012
66	6	0	-4.930567	-5.963671	-0.312000
67	1	0	-3.957020	-4.554968	-1.624146
68	6	0	-4.497824	-5.674854	2.045539
69	1	0	-3.184225	-4.044717	2.566105
70	6	0	-5.127396	-6.368082	1.010258
71	1	0	-5.416096	-6.498423	-1.124208
72	1	0	-4.645157	-5.983230	3.077250
73	1	0	-5.767037	-7.218227	1.231790
74	6	0	-4.783828	2.812949	-0.514267
75	6	0	-5.985974	2.612614	-1.221001
76	6	0	-4.547638	4.085655	0.041259
77	6	0	-6.920182	3.637518	-1.350276
78	1	0	-6.168739	1.655580	-1.700690
79	6	0	-5.482142	5.109396	-0.092940
80	1	0	-3.635372	4.257915	0.603971
81	6	0	-6.675067	4.891578	-0.786257
82	1	0	-7.837714	3.459856	-1.905478
83	1	0	-5.279981	6.081023	0.350571
84	1	0	-7.402405	5.691909	-0.891541

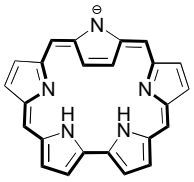
Figure S18. The structures and energies (B3LYP/6-31G(d) in hartree) of most stable inverted tautomers of *meso*-tetraphenyl N-confused and standard sapphyrin in various ionic states. The relative total energy (kcal/mol) to that of corresponding standard sapphyrin is shown in the parenthesis. (22 π aromatic circuits are shown in the bold line.)



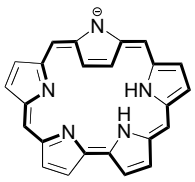
Total and relative energies of normal and N-confused sapphyrin tautomers

Deprotonated normal sapphyrins (monoanion)

$N_0SAP^{\ominus}$



$N_0SAP1^{\ominus}$
-1197.94601276
(+14.2)



$N_0SAP2^{\ominus}$
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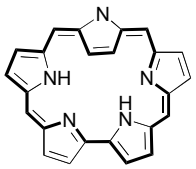
(+28.6)



$N_0SAP3^{\ominus}$
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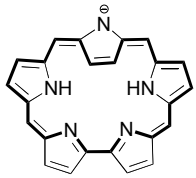
(+10.0)



$N_0SAP4^{\ominus}$
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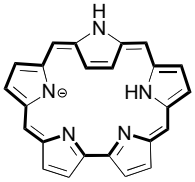

$N_0SAP5^{\ominus}$
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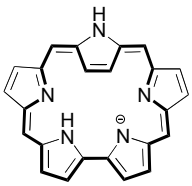

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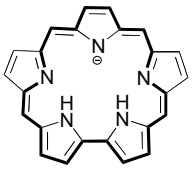

$N_0SAP7^{\ominus}$
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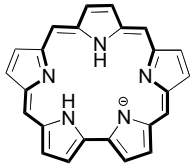

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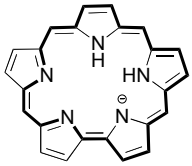

$N_0SAP9^{\ominus}$
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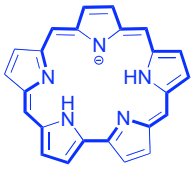
(+9.8)



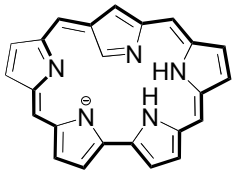
$N_0SAP10^{\ominus}$
-1197.96857602
(0)

Calculation level: B3LYP/6-31G(d); [upper: total energy (hartree); lower: relative energy (kcal/mol)]

Total and relative energies of normal and N-confused sapphyrin tautomers

Deprotonated N-confused sapphyrins (monoanion)

$N_1SAP^{\ominus}$



$N_1SAP1^{\ominus}$
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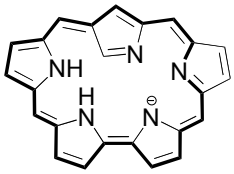
(+19.4)



$N_1SAP2^{\ominus}$
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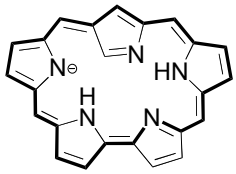
(+34.9)



$N_1SAP3^{\ominus}$
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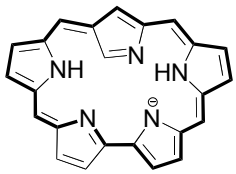
(+7.7)



$N_1SAP4^{\ominus}$
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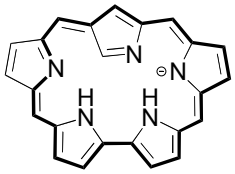
(+11.3)



$N_1SAP5^{\ominus}$
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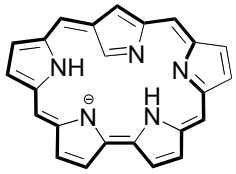
(+17.2)



$N_1SAP6^{\ominus}$
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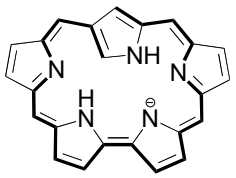
(+14.6)



$N_1SAP7^{\ominus}$
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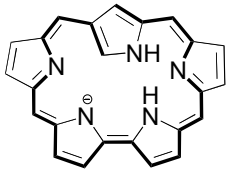
(+18.5)



$N_1SAP8^{\ominus}$
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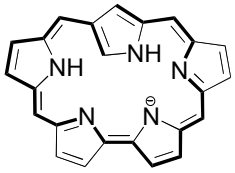
(+21.3)



$N_1SAP9^{\ominus}$
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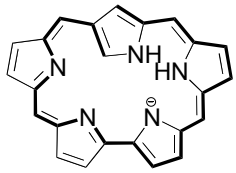

$N_1SAP10^{\ominus}$
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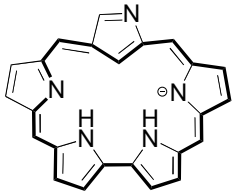
(+31.0)



$N_1SAP11^{\ominus}$
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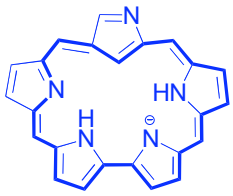
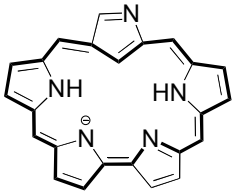
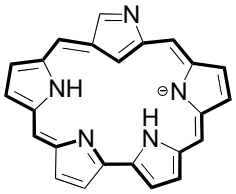


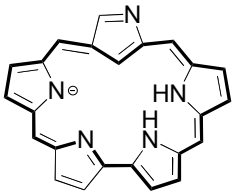
$N_1SAP12^{\ominus}$
-1197.97173491
(-2.0)



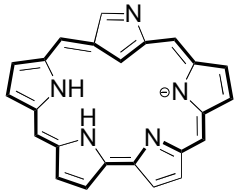
$N_1SAP13^{\ominus}$
-1197.96844045
(-0.09)



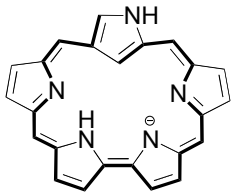
$N_1SAP14^{\ominus}$
-1197.97166172
(-1.9)



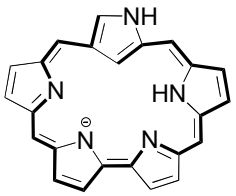
$N_1SAP15^{\ominus}$
-1197.94534451
(+14.6)



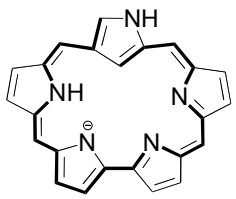
$N_1SAP16^{\ominus}$
-1197.94537558
(+14.6)



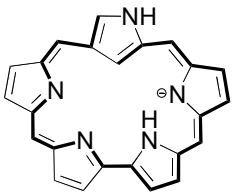
$N_1SAP17^{\ominus}$
-1197.94584085
(+14.3)



$N_1SAP18^{\ominus}$
-1197.92338643
(+28.4)



$N_1SAP19^{\ominus}$
-1197.92222698
(+29.1)

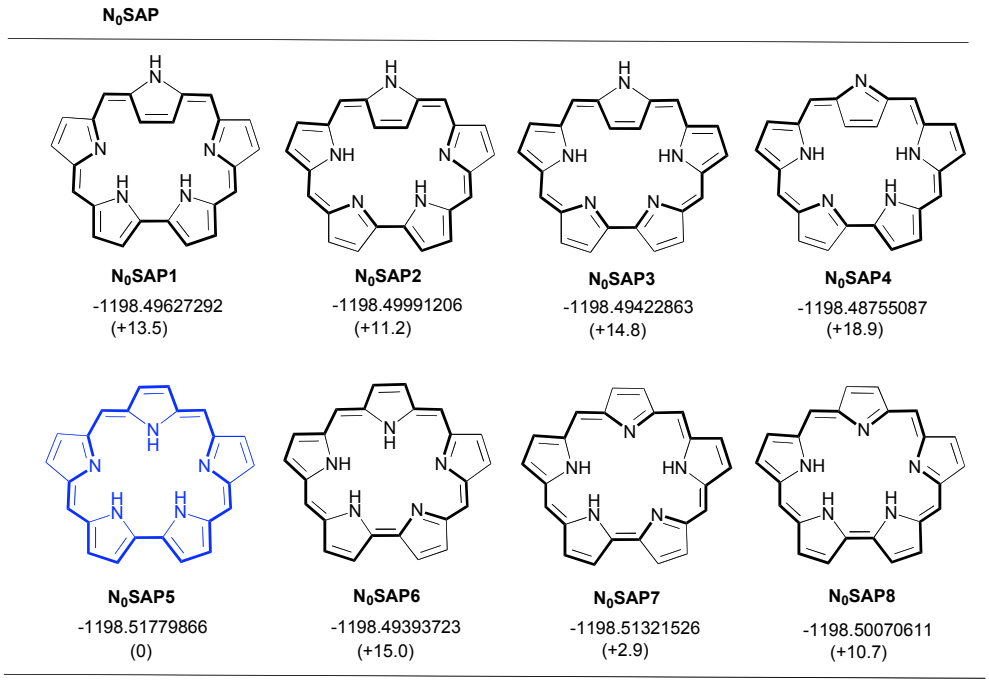


$N_1SAP20^{\ominus}$
-1197.93059533
(+23.8)

Calculation level: B3LYP/6-31G(d); [upper: total energy (hartree); lower: relative energy (kcal/mol)]

Total and relative energies of normal and N-confused sapphyrin tautomers

Normal sapphyrins (neutral)

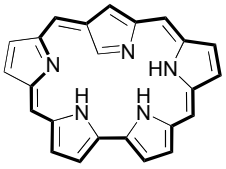


Calculation level: B3LYP/6-31G(d); [upper: total energy (hartree); lower: relative energy (kcal/mol)]

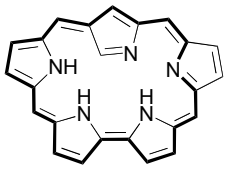
Total and relative energies of normal and N-confused sapphyrin tautomers

N-confused sapphyrins (neutral)

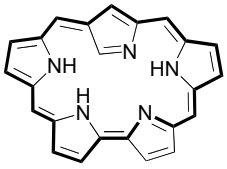
N_1SAP



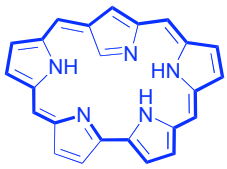
N_1SAP1
-1198.49635445
(+13.5)



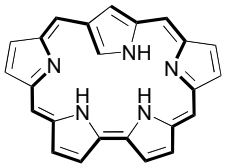
N_1SAP2
-1198.47727029
(+25.4)



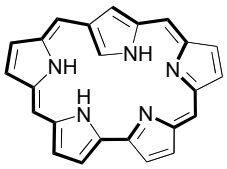
N_1SAP3
-1198.49348361
(+15.3)



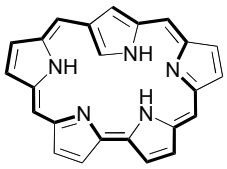
N_1SAP4
-1198.50175515
(+10.1)



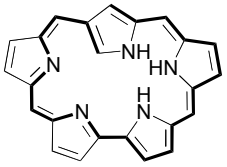
N_1SAP5
-1198.49318193
(+15.5)



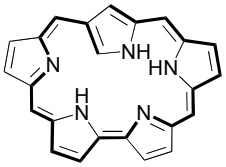
N_1SAP6
-1198.47564864
(+26.5)



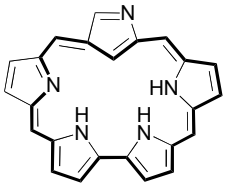
N_1SAP7
-1198.49707010
(+13.0)



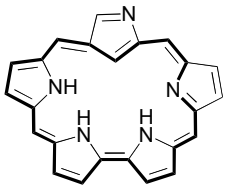
N_1SAP8
-1198.46454306
(+33.4)



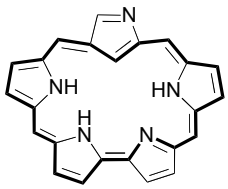
N_1SAP9
-1198.49127934
(+16.6)



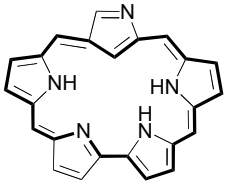
N_1SAP10
-1198.49013286
(+17.4)



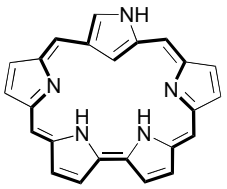
N_1SAP11
-1198.49027632
(+17.3)



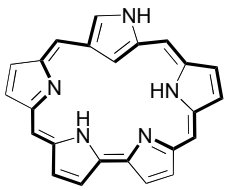
N_1SAP12
-1198.50073164
(+10.7)



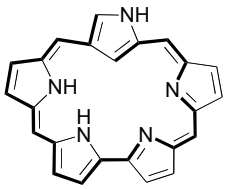
N_1SAP13
-1198.50032119
(+11.0)



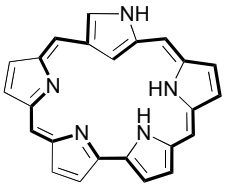
N_1SAP14
-1198.49574122
(+13.8)



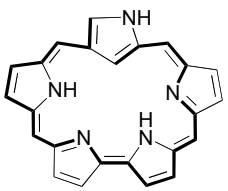
N_1SAP15
-1198.50004057
(+11.1)



N_1SAP16
-1198.47496624
(+26.9)



N_1SAP17
-1198.47530040
(+26.7)



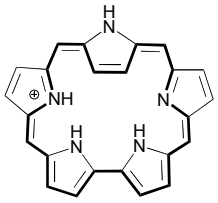
N_1SAP18
-1198.50018236
(+11.1)

Calculation level: B3LYP/6-31G(d); [upper: total energy (hartree); lower: relative energy (kcal/mol)]

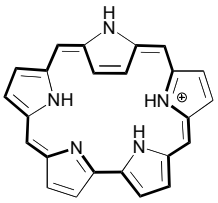
Total and relative energies of normal and N-confused sapphyrin tautomers

Monoprotonated normal sapphyrins (monocation)

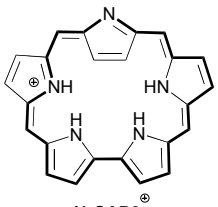
$N_0SAP^{\oplus}$



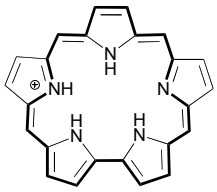
$N_0SAP1^{\oplus}$
-1198.91180770
(+11.4)



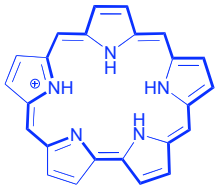
$N_0SAP2^{\oplus}$
-1198.91709215
(+8.1)



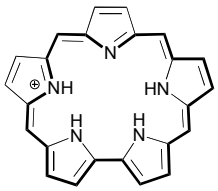
$N_0SAP3^{\oplus}$
-1198.89074073
(+24.6)



$N_0SAP4^{\oplus}$
-1198.92680723
(+2.0)



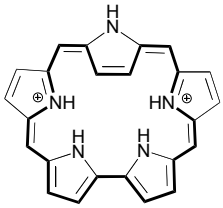
$N_0SAP5^{\oplus}$
-1198.92999927
(0)



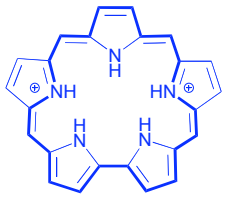
$N_0SAP6^{\oplus}$
-1198.92131162
(+5.5)

Diprotonated normal sapphyrins

$N_0SAP^{2\oplus}$



$N_0SAP1^{2\oplus}$
-1199.20775230
(+7.0)



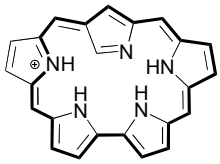
$N_0SAP2^{2\oplus}$
-1199.21894025
(0)

Calculation level: B3LYP/6-31G(d); [upper: total energy (hartree); lower: relative energy (kcal/mol)]

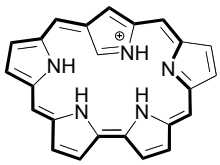
Total and relative energies of normal and N-confused sapphyrin tautomers

Monoprotonated N-confused sapphyrins (monocation)

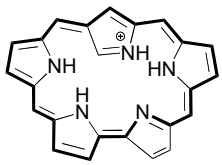
$N_1SAP^{\oplus}$



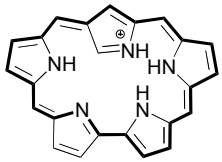
$N_1SAP1^{\oplus}$
-1198.91151773
(+11.6)



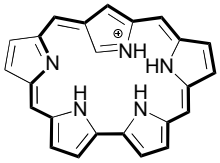
$N_1SAP2^{\oplus}$
-1198.90822543
(+13.7)



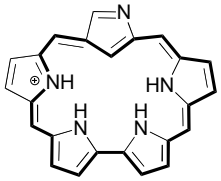
$N_1SAP3^{\oplus}$
-1198.90754616
(+14.1)



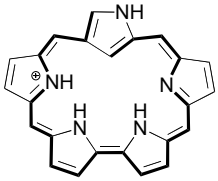
$N_1SAP4^{\oplus}$
-1198.90629443
(+14.9)



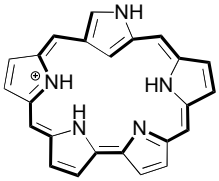
$N_1SAP5^{\oplus}$
-1198.90193045
(+17.6)



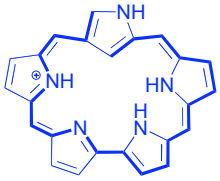
$N_1SAP6^{\oplus}$
-1198.90564310
(+15.3)



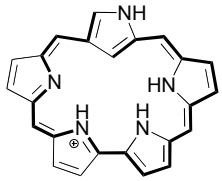
$N_1SAP7^{\oplus}$
-1198.91760453
(+7.8)



$N_1SAP8^{\oplus}$
-1198.91914304
(+6.8)



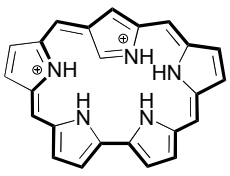
$N_1SAP9^{\oplus}$
-1198.92247979
(+4.7)



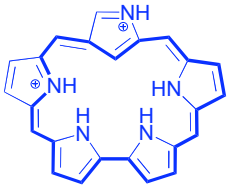
$N_1SAP10^{\oplus}$
-1198.91718048
(+8.0)

Diprotonated N-confused sapphyrins (dication)

$N_1SAP^{2\oplus}$



$N_1SAP1^{2\oplus}$
-1199.19808533
(+13.1)



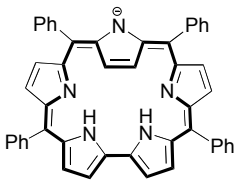
$N_1SAP2^{2\oplus}$
-1199.22031598
(-0.86)

Calculation level: B3LYP/6-31G(d); [upper: total energy (hartree); lower: relative energy (kcal/mol)]

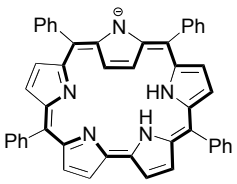
Total and relative energies of normal and N-confused sapphyrin tautomers

Deprotonated normal *meso*-tetraphenyl-sapphyrins (monoanion)

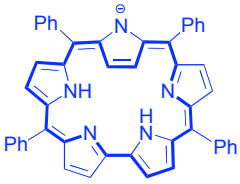
N_0SAPPh$^{\ominus}$



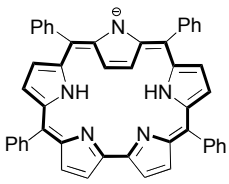
N_0SAPPh1$^{\ominus}$
-2122.16998297
(+3.4)



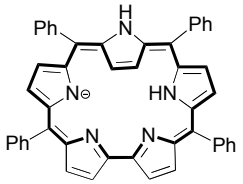
N_0SAPPh2$^{\ominus}$
-2122.14158179
(+22.0)



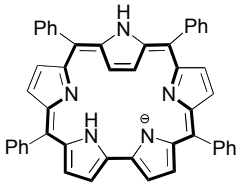
N_0SAPPh3$^{\ominus}$
-2122.17536400
(0)



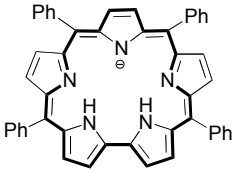
N_0SAPPh4$^{\ominus}$
-2122.17270659
(+1.7)



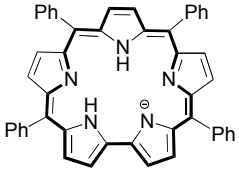
N_0SAPPh5$^{\ominus}$
-2122.14778131
(+17.3)



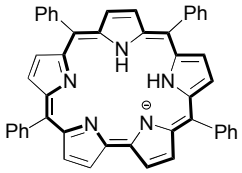
N_0SAPPh6$^{\ominus}$
-2122.15524133
(+12.6)



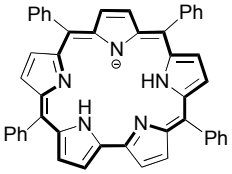
N_0SAPPh7$^{\ominus}$
-2122.14803314
(+17.2)



N_0SAPPh8$^{\ominus}$
-2122.15024969
(+15.8)



N_0SAPPh9$^{\ominus}$
-2122.14095269
(+21.6)



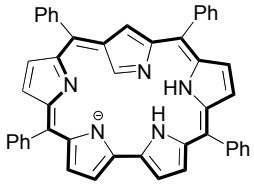
N_0SAPPh10$^{\ominus}$
-2122.15368106
(+13.6)

Calculation level: B3LYP/6-31G(d); [upper: total energy (hartree); lower: relative energy (kcal/mol)]

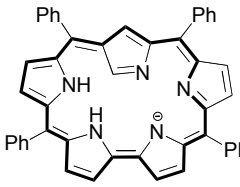
Total and relative energies of normal and N-confused sapphyrin tautomers

Deprotonated N-confused *meso*-tetraphenyl-sapphyrins (monoanion)

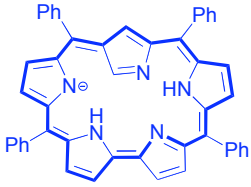
$N_1SAPPh^{\ominus}$



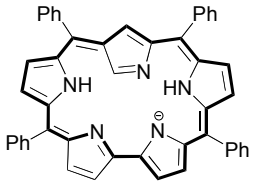
$N_1SAPPh1^{\ominus}$
-2122.15711058
(+11.5)



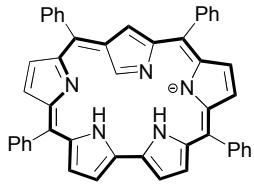
$N_1SAPPh2^{\ominus}$
-2122.13095762
(+27.9)



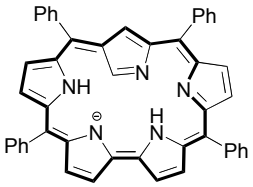
$N_1SAPPh3^{\ominus}$
-2122.17724443
(-1.2)



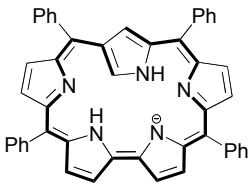
$N_1SAPPh4^{\ominus}$
-2122.17216974
(+2.0)



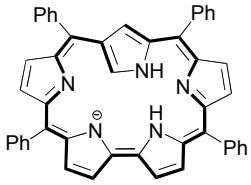
$N_1SAPPh5^{\ominus}$
-2122.16498082
(+6.5)



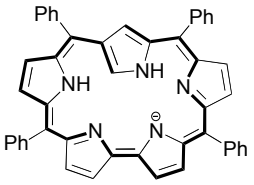
$N_1SAPPh6^{\ominus}$
-2122.16819736
(+4.5)



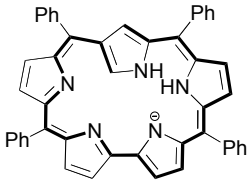
$N_1SAPPh7^{\ominus}$
-2122.16001744
(+9.6)



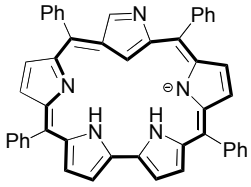
$N_1SAPPh8^{\ominus}$
-2122.15698081
(+11.5)



$N_1SAPPh9^{\ominus}$
-2122.15448281
(+13.1)



$N_1SAPPh10^{\ominus}$
-2122.14480364
(+19.2)



$N_1SAPPh11^{\ominus}$
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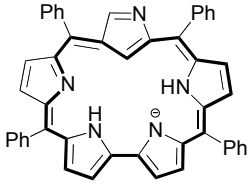
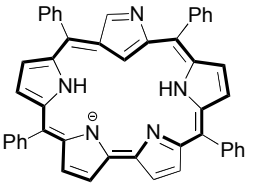
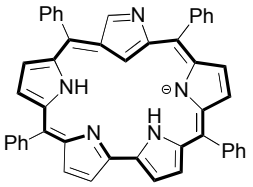
(+10.3)



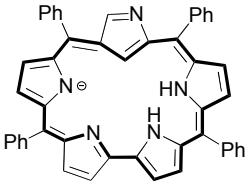
$N_1SAPPh12^{\ominus}$
-2122.16485672
(+6.6)



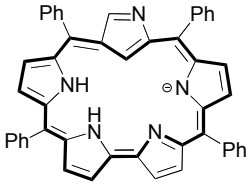
$N_1SAPPh13^{\ominus}$
-2122.16396866
(+7.2)



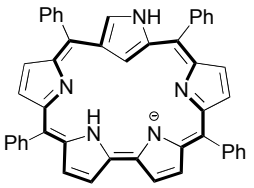
$N_1SAPPh14^{\ominus}$
-2122.16529917
(+6.3)



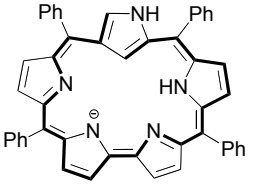
$N_1SAPPh15^{\ominus}$
-2122.14111156
(+21.5)



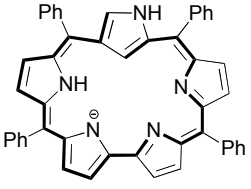
$N_1SAPPh16^{\ominus}$
-2122.14245935
(+20.7)



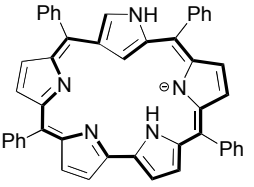
$N_1SAPPh17^{\ominus}$
-2122.12942358
(+28.8)



$N_1SAPPh18^{\ominus}$
-2122.12557907
(+31.2)



$N_1SAPPh19^{\ominus}$
-2122.12942358
(+32.4)



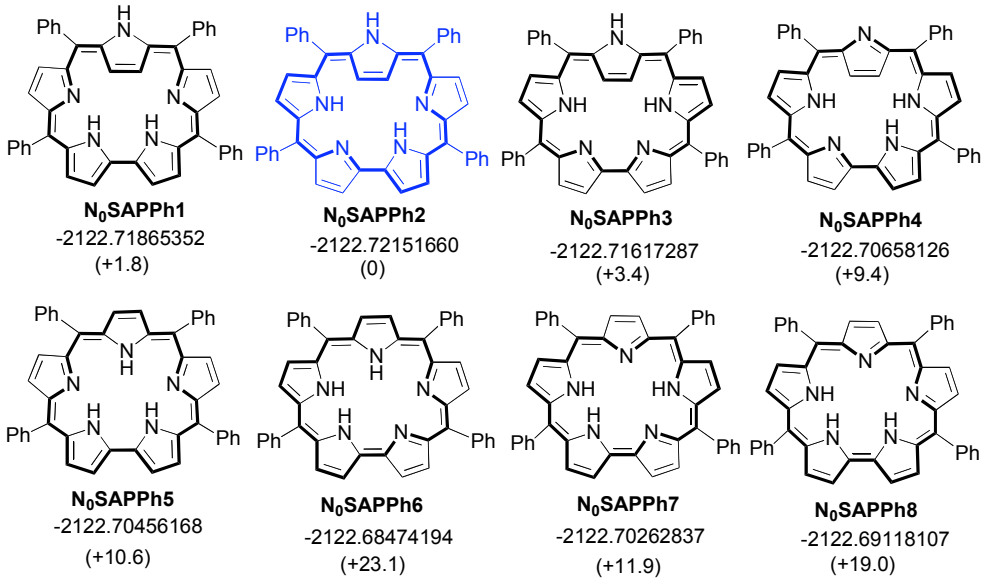
$N_1SAPPh20^{\ominus}$
-2122.13056960
(+28.1)

Calculation level: B3LYP/6-31G(d); [upper: total energy (hartree); lower: relative energy (kcal/mol)]

Total and relative energies of normal and N-confused sapphyrin tautomers

Normal *meso*-tetraphenyl-sapphyrins (neutral)

N_0SAPPh



N_0SAPPh1
-2122.71865352
(+1.8)

N_0SAPPh2
-2122.72151660
(0)

N_0SAPPh3
-2122.71617287
(+3.4)

N_0SAPPh4
-2122.70658126
(+9.4)

N_0SAPPh5
-2122.70456168
(+10.6)

N_0SAPPh6
-2122.68474194
(+23.1)

N_0SAPPh7
-2122.70262837
(+11.9)

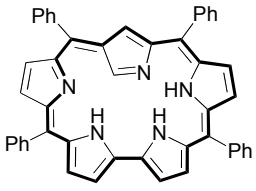
N_0SAPPh8
-2122.69118107
(+19.0)

Calculation level: B3LYP/6-31G(d); [upper: total energy (hartree); lower: relative energy (kcal/mol)]

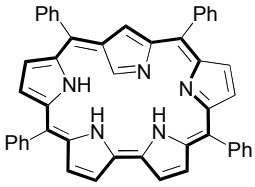
Total and relative energies of normal and N-confused sapphyrin tautomers

N-confused *meso*-tetraphenyl-sapphyrins (neutral)

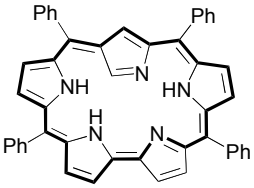
N_1SAPPh



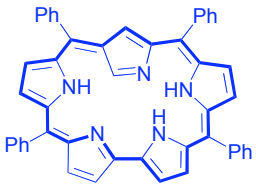
N_1SAPPh1
-2122.71279475
(+5.5)



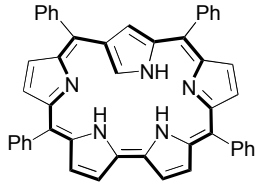
N_1SAPPh2
-2122.69832692
(+14.6)



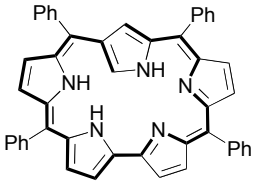
N_1SAPPh3
-2122.71064662
(+6.8)



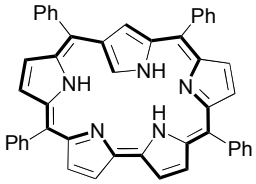
N_1SAPPh4
-2122.71742510
(+2.6)



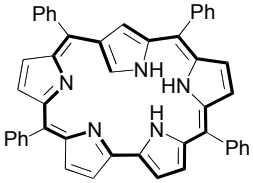
N_1SAPPh5
-2122.71135401
(+6.4)



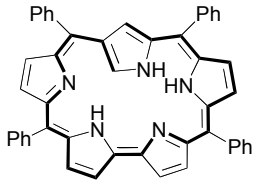
N_1SAPPh6
-2122.69176454
(+18.7)



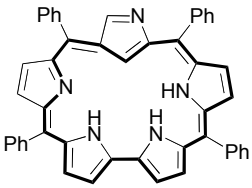
N_1SAPPh7
-2122.71461042
(+4.3)



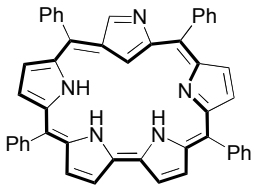
N_1SAPPh8
-2122.67727262
(+27.8)



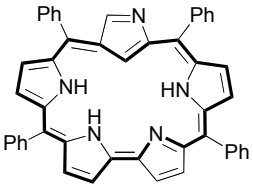
N_1SAPPh9
-2122.70923914
(+7.7)



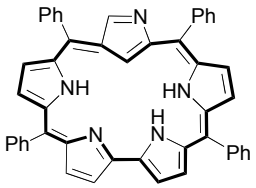
N_1SAPPh10
-2122.69108579
(+19.1)



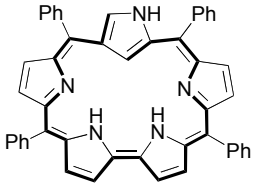
N_1SAPPh11
-2122.69377701
(+17.4)



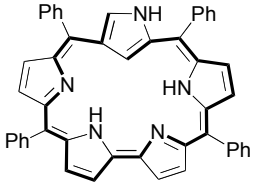
N_1SAPPh12
-2122.69300356
(+17.9)



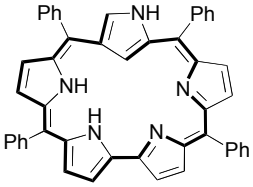
N_1SAPPh13
-2122.70046900
(+13.2)



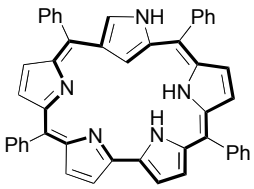
N_1SAPPh14
-2122.69404851
(+17.2)



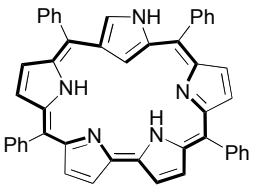
N_1SAPPh15
-2122.69808205
(+14.7)



N_1SAPPh16
-2122.67550363
(+28.9)



N_1SAPPh17
-2122.67611625
(+28.5)

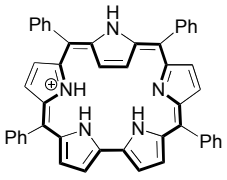
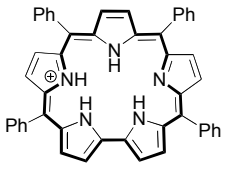
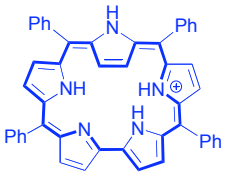
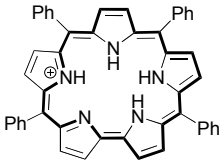
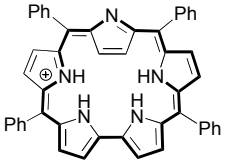
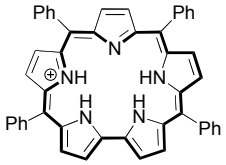


N_1SAPPh18
-2122.69815924
(+14.7)

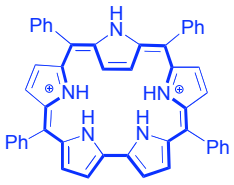
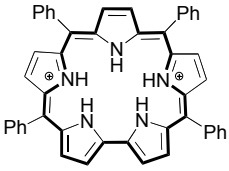
Calculation level: B3LYP/6-31G(d); [upper: total energy (hartree); lower: relative energy (kcal/mol)]

Total and relative energies of normal and N-confused sapphyrin tautomers

Monoprotonated normal *meso*-tetraphenyl-sapphyrins (monocation)

$N_0SAPPh^{\oplus}$			
			
$N_0SAPPh1^{\oplus}$	$N_0SAPPh2^{\oplus}$	$N_0SAPPh3^{\oplus}$	$N_0SAPPh4^{\oplus}$
-2123.14412552	-2123.13443276	-2123.1482290	-2123.14006537
(+2.6)	(+8.7)	(0)	(+5.1)
			
$N_0SAPPh5^{\oplus}$	$N_0SAPPh6^{\oplus}$		
-2123.11956034	-2123.11941782		
(+18.0)	(+18.1)		

Diprotonated normal *meso*-tetraphenyl-sapphyrins

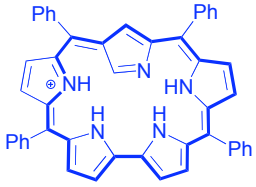
$N_0SAPPh^{2\oplus}$	
	
$N_0SAPPh1^{2\oplus}$	$N_0SAPPh2^{2\oplus}$
-2123.46581760	-2123.44806048
(0)	(+11.1)

Calculation level: B3LYP/6-31G(d); [upper: total energy (hartree); lower: relative energy (kcal/mol)]

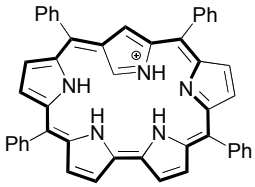
Total and relative energies of normal and N-confused sapphyrin tautomers

Monoprotonated N-confused *meso*-tetraphenyl-sapphyrins (monocation)

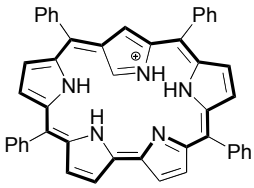
N_1SAPPh$^{\oplus}$



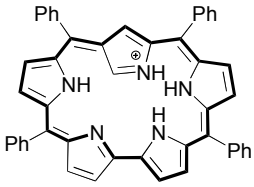
N_1SAPPh1$^{\oplus}$
-2123.14019416
(+5.0)



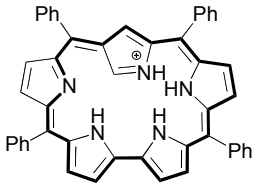
N_1SAPPh2$^{\oplus}$
-2123.13858153
(+6.1)



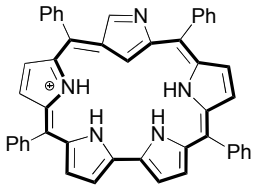
N_1SAPPh3$^{\oplus}$
-2123.13693333
(+7.1)



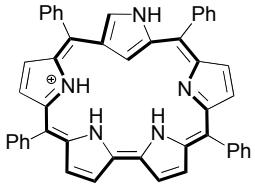
N_1SAPPh4$^{\oplus}$
-2123.13265940
(+9.8)



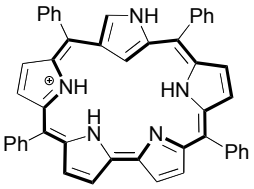
N_1SAPPh5$^{\oplus}$
-2123.12980006
(+11.6)



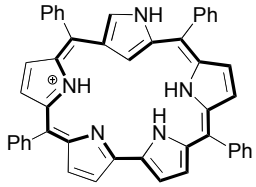
N_1SAPPh6$^{\oplus}$
-2123.11217758
(+22.6)



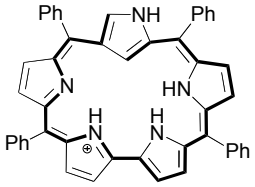
N_1SAPPh7$^{\oplus}$
-2123.13051234
(+11.1)



N_1SAPPh8$^{\oplus}$
-2123.13611503
(+7.6)



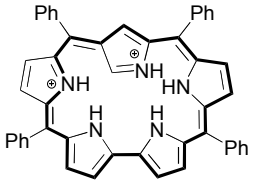
N_1SAPPh9$^{\oplus}$
-2123.13612733
(+7.6)



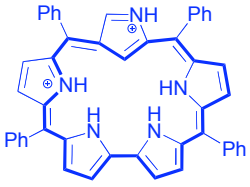
N_1SAPPh10$^{\oplus}$
-2123.13035388
(+11.2)

Diprotonated N-confused *meso*-tetraphenyl-sapphyrins (dication)

N_1SAPPh$^{2\oplus}$



N_1SAPPh1$^{2\oplus}$
-2123.45257857
(+8.3)

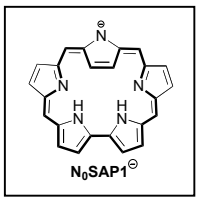


N_1SAPPh2$^{2\oplus}$
-2123.45566447
(+6.4)

Calculation level: B3LYP/6-31G(d); [upper: total energy (hartree); lower: relative energy (kcal/mol)]

Cartesian coordinates for the optimized structures of normal sapphyrins (monoanion)

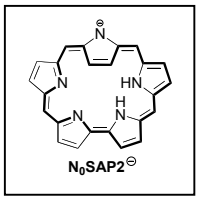
$N_0SAP1^{\ominus}$ (Energy = −1197.94601276)



Stoichiometry C24H16N5(1-)
Framework group C1[X(C24H16N5)]
Deg. of freedom 129
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.599909	1.697151	0.014028
2	7	0	-1.599899	1.697156	0.014027
3	7	0	-2.952576	-0.781412	-0.052559
4	7	0	2.952572	-0.781418	-0.052559
5	6	0	2.390112	-3.145800	-0.140067
6	6	0	-3.315060	-2.086457	-0.201174
7	6	0	-4.061888	1.359317	-0.135422
8	6	0	0.711298	2.755517	0.063569
9	6	0	-5.234204	-0.902169	-0.412848
10	6	0	-2.390126	-3.145796	-0.140064
11	6	0	-4.747865	-2.177300	-0.459082
12	6	0	-2.911167	2.157568	-0.031086
13	6	0	-4.083730	-0.039339	-0.174179
14	6	0	-0.711285	2.755519	0.063568
15	6	0	1.506383	3.937574	0.070789
16	6	0	3.315050	-2.086465	-0.201176
17	6	0	-2.836920	3.575336	0.011162
18	6	0	5.234199	-0.902186	-0.412849
19	6	0	4.747854	-2.177314	-0.459084
20	6	0	2.911178	2.157561	-0.031084
21	6	0	-1.506367	3.937579	0.070785
22	6	0	4.061896	1.359305	-0.135420
23	6	0	2.836935	3.575329	0.011166
24	6	0	4.083730	-0.039351	-0.174178
25	1	0	-1.426754	0.690343	-0.009539
26	1	0	-6.259656	-0.574109	-0.548193
27	1	0	-5.303049	-3.095681	-0.617660
28	1	0	1.112642	4.943705	0.106444
29	1	0	-3.695801	4.234546	-0.006215
30	1	0	6.259652	-0.574130	-0.548194
31	1	0	5.303033	-3.095698	-0.617664
32	1	0	-1.112623	4.943709	0.106439
33	1	0	3.695817	4.234536	-0.006209
34	1	0	1.426764	0.690338	-0.009539
35	6	0	-0.675628	-1.867186	1.216578
36	6	0	0.675619	-1.867186	1.216576
37	6	0	1.078473	-2.954341	0.319278
38	6	0	-1.078485	-2.954339	0.319279
39	7	0	-0.000007	-3.668810	-0.112578
40	1	0	1.354288	-1.233565	1.767123
41	1	0	-1.354296	-1.233564	1.767127
42	1	0	-2.659132	-4.105700	-0.576753
43	1	0	2.659115	-4.105704	-0.576758
44	1	0	5.004548	1.895018	-0.216577
45	1	0	-5.004538	1.895035	-0.216580

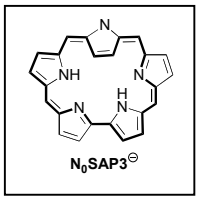
$N_0SAP2^{\ominus}$ (Energy = −1197.92293846)



Stoichiometry C24H16N5(1-)
Framework group C1[X(C24H16N5)]
Deg. of freedom 129
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.562453	1.795258	0.026532
2	7	0	-1.283169	2.000696	-0.029410
3	7	0	-2.940367	-0.772244	-0.003256
4	7	0	2.794577	-1.011866	-0.047317
5	6	0	2.164232	-3.333776	-0.226498
6	6	0	-3.411835	-2.076247	-0.139366
7	6	0	-3.765508	1.549914	-0.272111
8	6	0	0.958997	2.989327	0.115301
9	6	0	-5.099642	-0.591842	-0.560579
10	6	0	-2.614826	-3.202702	0.006595
11	6	0	-4.794986	-1.929467	-0.507006
12	6	0	-2.619206	2.370847	-0.107874
13	6	0	-3.914368	0.171825	-0.262140
14	6	0	-0.466396	3.107061	0.095127
15	6	0	1.911381	4.083661	0.171989
16	6	0	3.137786	-2.304898	-0.274544
17	6	0	-2.625367	3.782931	0.000317
18	6	0	5.050292	-1.136839	-0.529692
19	6	0	4.551245	-2.408616	-0.609133
20	6	0	2.914197	2.057679	0.006753
21	6	0	-1.311148	4.230985	0.129701
22	6	0	3.955741	1.131575	-0.123912
23	6	0	3.141641	3.493400	0.096911
24	6	0	3.918506	-0.276045	-0.198949
25	1	0	-6.055227	-0.147156	-0.811025
26	1	0	-5.465234	-2.760685	-0.687564
27	1	0	1.680308	5.140315	0.245698
28	1	0	-3.524976	4.386044	-0.004587
29	1	0	6.069725	-0.810576	-0.711290
30	1	0	5.089779	-3.321980	-0.839620
31	1	0	-0.977623	5.254867	0.235292
32	1	0	4.112454	3.978272	0.104615
33	6	0	-0.781344	-2.066752	1.365186
34	6	0	0.573635	-2.082196	1.281178
35	6	0	0.899866	-3.133092	0.327315
36	6	0	-1.258168	-3.097305	0.440003
37	7	0	-0.235877	-3.800681	-0.087767
38	1	0	1.291019	-1.465537	1.798712
39	1	0	-1.396145	-1.477733	2.036252
40	1	0	-1.975495	-0.586325	0.222777
41	1	0	-0.861700	1.093275	-0.182152
42	1	0	-2.986151	-4.147715	-0.381104
43	1	0	2.361409	-4.271617	-0.744030
44	1	0	4.949538	1.574318	-0.202024
45	1	0	-4.683351	2.107523	-0.438854

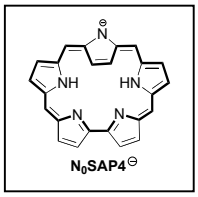
$N_0SAP3^{\ominus}$ (Energy = −1197.95264239)



Stoichiometry C24H16N5(1-)
Framework group C1[X(C24H16N5)]
Deg. of freedom 129
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.560485	1.735450	0.025481
2	7	0	-1.538228	1.692477	-0.002543
3	7	0	-2.974059	-0.806703	-0.053115
4	7	0	2.930960	-0.789411	-0.063845
5	6	0	2.392993	-3.156431	-0.188470
6	6	0	-3.313674	-2.141367	-0.176478
7	6	0	-3.993885	1.403393	-0.171828
8	6	0	0.692365	2.803267	0.077508
9	6	0	-5.190188	-0.857215	-0.394818
10	6	0	-2.393488	-3.195273	-0.108768
11	6	0	-4.728327	-2.157378	-0.409061
12	6	0	-2.824527	2.179155	-0.064138
13	6	0	-4.071699	0.011491	-0.191209
14	6	0	-0.734170	2.784000	0.058958
15	6	0	1.504714	3.973964	0.108131
16	6	0	3.310339	-2.085353	-0.232262
17	6	0	-2.823358	3.624774	-0.029468
18	6	0	5.216106	-0.877777	-0.416292
19	6	0	4.744226	-2.157736	-0.486927
20	6	0	2.879413	2.169592	-0.001172
21	6	0	-1.514940	4.007392	0.053081
22	6	0	4.024030	1.364765	-0.108263
23	6	0	2.829662	3.589798	0.058126
24	6	0	4.055191	-0.032968	-0.167495
25	1	0	-6.212272	-0.522375	-0.524409
26	1	0	-5.313554	-3.060342	-0.531680
27	1	0	1.124487	4.984776	0.154643
28	1	0	-3.703061	4.258463	-0.063272
29	1	0	6.238154	-0.535650	-0.542485
30	1	0	5.310204	-3.067094	-0.658765
31	1	0	-1.126462	5.017392	0.093412
32	1	0	3.701742	4.232043	0.058722
33	1	0	1.332054	0.744226	-0.019888
34	6	0	-0.656428	-1.931239	1.239438
35	6	0	0.695340	-1.923375	1.217948
36	6	0	1.089553	-2.987151	0.293389
37	6	0	-1.068369	-3.003197	0.326976
38	7	0	0.003747	-3.696648	-0.140224
39	1	0	1.376239	-1.293883	1.769719
40	1	0	-1.314421	-1.316150	1.838866
41	1	0	-2.037148	-0.407348	-0.020731
42	1	0	-2.680667	-4.152912	-0.535635
43	1	0	2.663458	-4.101626	-0.655345
44	1	0	4.968335	1.900322	-0.174778
45	1	0	-4.932688	1.943211	-0.270087

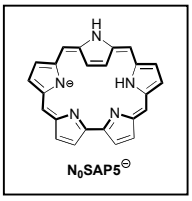
$N_0SAP4^{\ominus}$ (Energy = −1197.94983557)



Stoichiometry C24H16N5(1-)
Framework group C1[X(C24H16N5)]
Deg. of freedom 129
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.551056	1.666960	0.009488
2	7	0	-1.551204	1.666926	0.009319
3	7	0	-2.986625	-0.785062	-0.065503
4	7	0	2.986659	-0.784998	-0.065294
5	6	0	2.397750	-3.170100	-0.158139
6	6	0	-3.325009	-2.117312	-0.204713
7	6	0	-4.004856	1.424900	-0.136443
8	6	0	0.717961	2.732936	0.066245
9	6	0	-5.206374	-0.835757	-0.380385
10	6	0	-2.397581	-3.170175	-0.157749
11	6	0	-4.740059	-2.136107	-0.421016
12	6	0	-2.828053	2.181526	-0.033610
13	6	0	-4.088496	0.029624	-0.176291
14	6	0	-0.718146	2.732921	0.066140
15	6	0	1.481726	3.977436	0.078865
16	6	0	3.325104	-2.117183	-0.205013
17	6	0	-2.797697	3.629162	0.011485
18	6	0	5.206361	-0.835481	-0.380608
19	6	0	4.740128	-2.135848	-0.421496
20	6	0	2.827894	2.181608	-0.033234
21	6	0	-1.481952	3.977399	0.078591
22	6	0	4.004733	1.425046	-0.136108
23	6	0	2.797489	3.629241	0.011939
24	6	0	4.088449	0.029784	-0.176192
25	1	0	-6.230964	-0.502342	-0.492485
26	1	0	-5.324305	-3.038903	-0.549379
27	1	0	1.074084	4.978958	0.122824
28	1	0	-3.663846	4.282104	-0.005871
29	1	0	6.230913	-0.501972	-0.492781
30	1	0	5.324414	-3.038577	-0.550156
31	1	0	-1.074346	4.978935	0.122566
32	1	0	3.663620	4.282210	-0.005285
33	6	0	-0.675855	-1.929722	1.222504
34	6	0	0.676252	-1.929593	1.222254
35	6	0	1.080091	-2.986270	0.292501
36	6	0	-1.079847	-2.986280	0.292671
37	7	0	0.000090	-3.676935	-0.171412
38	1	0	1.336129	-1.311757	1.815847
39	1	0	-1.335618	-1.312011	1.816347
40	1	0	-2.052430	-0.370875	-0.041980
41	1	0	2.052443	-0.370866	-0.041351
42	1	0	-2.677813	-4.118965	-0.608562
43	1	0	2.677957	-4.118822	-0.609113
44	1	0	4.941230	1.972162	-0.214842
45	1	0	-4.941388	1.971956	-0.215162

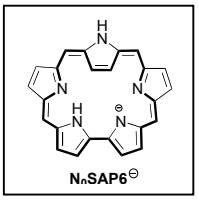
$N_0SAP5^{\ominus}$ (Energy = −1197.92214209)



Stoichiometry C24H16N5(1-)
Framework group C1[X(C24H16N5)]
Deg. of freedom 129
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.299135	1.801415	0.041202
2	7	0	-1.726652	1.621203	0.029977
3	7	0	-2.906973	-0.951713	-0.073538
4	7	0	3.031933	-0.651831	-0.066261
5	6	0	2.759015	-3.027267	-0.135126
6	6	0	-3.122545	-2.306218	-0.200667
7	6	0	-4.137080	1.159660	-0.134185
8	6	0	0.450922	2.840113	0.076592
9	6	0	-5.112008	-1.204632	-0.381751
10	6	0	-2.100500	-3.287260	-0.147145
11	6	0	-4.523473	-2.462341	-0.407570
12	6	0	-3.046194	2.024946	-0.024378
13	6	0	-4.086010	-0.242733	-0.183608
14	6	0	-0.989125	2.748298	0.076458
15	6	0	1.168406	4.116068	0.058156
16	6	0	3.591726	-1.871773	-0.203984
17	6	0	-3.135593	3.471584	0.007823
18	6	0	5.296383	-0.406199	-0.397050
19	6	0	5.022731	-1.750541	-0.440762
20	6	0	2.563013	2.342105	-0.021187
21	6	0	-1.851479	3.926635	0.072594
22	6	0	3.779235	1.650287	-0.129474
23	6	0	2.491949	3.798284	-0.005312
24	6	0	4.020302	0.263624	-0.170908
25	1	0	-6.163706	-0.971666	-0.496386
26	1	0	-5.021685	-3.416671	-0.526341
27	1	0	0.730619	5.107068	0.079800
28	1	0	-4.051912	4.051832	-0.020524
29	1	0	6.259224	0.075970	-0.536715
30	1	0	5.725435	-2.564851	-0.586803
31	1	0	-1.521272	4.957277	0.107539
32	1	0	3.340006	4.474893	-0.043268
33	6	0	-0.418201	-1.915155	1.160281
34	6	0	0.945290	-1.846411	1.163865
35	6	0	1.461446	-2.896161	0.339845
36	6	0	-0.823141	-3.001312	0.321947
37	7	0	0.350237	-3.684455	-0.022069
38	1	0	1.560162	-1.127379	1.676696
39	1	0	-1.094637	-1.274627	1.706361
40	1	0	-2.018331	-0.444385	-0.045415
41	1	0	0.378798	-4.215758	-0.881591
42	1	0	-2.320677	-4.263629	-0.572969
43	1	0	3.096354	-3.967350	-0.570250
44	1	0	4.662050	2.286106	-0.209529
45	1	0	-5.124589	1.609224	-0.212503

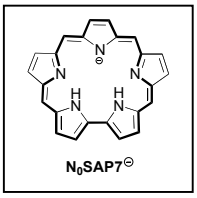
$N_0SAP6^{\ominus}$ (Energy = −1197.93027545)



Stoichiometry C24H16N5(1-)
Framework group C1[X(C24H16N5)]
Deg. of freedom 129
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.661941	1.747904	0.026210
2	7	0	-1.327711	1.836713	0.021424
3	7	0	-2.980910	-0.722283	-0.053892
4	7	0	2.857447	-0.924397	-0.038158
5	6	0	2.190505	-3.270026	-0.149175
6	6	0	-3.508686	-1.954188	-0.194312
7	6	0	-3.804016	1.558647	-0.149742
8	6	0	0.890005	2.882906	0.079400
9	6	0	-5.249707	-0.535797	-0.419180
10	6	0	-2.659687	-3.100695	-0.121001
11	6	0	-4.940043	-1.871266	-0.451001
12	6	0	-2.618604	2.308653	-0.040475
13	6	0	-3.994570	0.168426	-0.180569
14	6	0	-0.542141	2.925904	0.068976
15	6	0	1.788094	3.981539	0.098145
16	6	0	3.162458	-2.230656	-0.208009
17	6	0	-2.622040	3.762954	-0.016946
18	6	0	5.130297	-1.135965	-0.432305
19	6	0	4.585484	-2.388915	-0.481660
20	6	0	3.011083	2.067754	-0.012467
21	6	0	-1.315796	4.156485	0.055847
22	6	0	4.087205	1.165865	-0.124677
23	6	0	3.081011	3.484529	0.039289
24	6	0	4.026200	-0.225925	-0.169623
25	1	0	-6.222460	-0.078705	-0.573347
26	1	0	-5.617517	-2.705502	-0.603659
27	1	0	1.488903	5.019974	0.142882
28	1	0	-3.504929	4.393223	-0.053776
29	1	0	6.166603	-0.853238	-0.586052
30	1	0	5.096541	-3.330039	-0.656554
31	1	0	-0.927058	5.167878	0.085630
32	1	0	4.003842	4.051739	0.030052
33	6	0	-0.865214	-1.905352	1.192134
34	6	0	0.496783	-1.951718	1.181378
35	6	0	0.914129	-3.030633	0.337654
36	6	0	-1.368440	-2.960561	0.361742
37	7	0	-0.250279	-3.740441	0.006991
38	1	0	1.185548	-1.297444	1.690278
39	1	0	-1.494833	-1.196607	1.702338
40	1	0	-0.274222	-4.271023	-0.853430
41	1	0	1.324033	0.790086	-0.024610
42	1	0	-2.983623	-4.039680	-0.568469
43	1	0	2.432376	-4.231914	-0.598712
44	1	0	5.068267	1.628583	-0.211433
45	1	0	-4.710764	2.158415	-0.239694

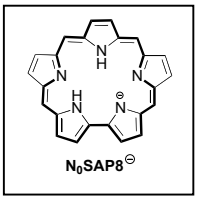
$N_0SAP7^{\ominus}$ (Energy = −1197.95597650)



Stoichiometry C24H16N5(1-)
Framework group C1[X(C24H16N5)]
Deg. of freedom 129
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.562477	-1.995636	-0.000349
2	7	0	-1.562459	-1.995646	-0.000350
3	7	0	-2.812056	0.557655	-0.000310
4	7	0	2.812052	0.557672	-0.000311
5	6	0	2.451933	3.034536	0.000009
6	6	0	-3.214125	1.855589	-0.000066
7	6	0	1.082269	3.338905	0.000069
8	6	0	-3.992305	-1.580884	-0.000203
9	6	0	0.707234	-3.075814	0.000149
10	6	0	-5.141802	0.663665	-0.000073
11	6	0	-2.451957	3.034521	0.000012
12	6	0	0.675969	4.750272	0.000324
13	6	0	-4.676607	1.939517	0.000053
14	6	0	-0.676004	4.750268	0.000324
15	6	0	-2.878582	-2.426402	-0.000204
16	6	0	-3.959722	-0.185599	-0.000155
17	6	0	-0.707210	-3.075819	0.000149
18	6	0	1.522849	-4.241642	0.000441
19	6	0	3.214109	1.855610	-0.000068
20	6	0	-1.082296	3.338899	0.000071
21	6	0	-2.845468	-3.845841	0.000176
22	6	0	5.141796	0.663702	-0.000073
23	6	0	4.676591	1.939550	0.000051
24	6	0	2.878602	-2.426384	-0.000202
25	6	0	-1.522818	-4.241652	0.000439
26	6	0	3.992319	-1.580857	-0.000200
27	6	0	2.845497	-3.845823	0.000180
28	6	0	3.959724	-0.185573	-0.000155
29	1	0	-1.364646	-0.990406	-0.000213
30	1	0	-6.169663	0.317029	0.000086
31	1	0	1.354174	5.597224	0.000457
32	1	0	-5.246463	2.862688	0.000298
33	1	0	-1.354214	5.597216	0.000459
34	1	0	1.147203	-5.255559	0.000784
35	1	0	-3.722683	-4.480461	0.000286
36	1	0	6.169660	0.317074	0.000086
37	1	0	5.246438	2.862726	0.000295
38	1	0	-1.147165	-5.255567	0.000780
39	1	0	3.722716	-4.480438	0.000290
40	7	0	-0.000011	2.513059	-0.000037
41	1	0	1.364659	-0.990397	-0.000214
42	1	0	-3.075764	3.928531	0.000141
43	1	0	3.075733	3.928551	0.000138
44	1	0	4.964571	-2.067186	-0.000232
45	1	0	-4.964553	-2.067221	-0.000235

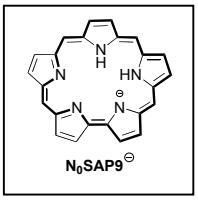
$N_0SAP8^{\ominus}$ (Energy = −1197.96361182)



Stoichiometry C24H16N5(1-)
Framework group C1[X(C24H16N5)]
Deg. of freedom 129
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.419765	-1.199171	0.000035
2	7	0	0.137454	-2.451728	-0.000001
3	7	0	2.772439	-0.600603	-0.000120
4	7	0	-2.113900	1.738143	0.000063
5	6	0	-0.622169	3.761053	0.000319
6	6	0	3.871399	0.191804	-0.000012
7	6	0	0.736417	3.450971	0.000033
8	6	0	2.528078	-3.084133	-0.000302
9	6	0	-2.268375	-2.558609	0.000133
10	6	0	4.708961	-1.890593	0.000141
11	6	0	3.865528	1.599259	-0.000045
12	6	0	1.728999	4.493071	-0.000003
13	6	0	5.101385	-0.587749	0.000083
14	6	0	2.969577	3.922828	-0.000103
15	6	0	1.158072	-3.361288	-0.000160
16	6	0	3.250260	-1.881325	-0.000141
17	6	0	-0.991483	-3.180423	0.000105
18	6	0	-3.570450	-3.120454	0.000060
19	6	0	-1.851653	3.068288	0.000157
20	6	0	2.810441	2.499561	-0.000084
21	6	0	0.631821	-4.719564	0.000146
22	6	0	-4.109469	2.951598	-0.000115
23	6	0	-3.089859	3.847461	0.000149
24	6	0	-3.753041	-0.855428	-0.000125
25	6	0	-0.729373	-4.607021	0.000231
26	6	0	-4.232906	0.459734	-0.000193
27	6	0	-4.482824	-2.075216	-0.000154
28	6	0	-3.487767	1.637601	-0.000100
29	1	0	5.329723	-2.780542	0.000332
30	1	0	1.481875	5.547391	-0.000039
31	1	0	6.108458	-0.184233	0.000271
32	1	0	3.931956	4.419418	-0.000195
33	1	0	-3.785670	-4.180815	0.000198
34	1	0	1.226275	-5.627329	0.000186
35	1	0	-5.177392	3.141167	-0.000282
36	1	0	-3.144587	4.930836	0.000282
37	1	0	-1.467655	-5.400775	0.000462
38	1	0	-5.563697	-2.143875	-0.000295
39	7	0	1.440630	2.256558	-0.000040
40	1	0	-1.666202	-0.516010	-0.000002
41	1	0	1.055304	1.317173	-0.000215
42	1	0	-0.765468	4.840160	0.000452
43	1	0	4.845434	2.072848	-0.000047
44	1	0	3.159409	-3.973322	-0.000382
45	1	0	-5.315197	0.566947	-0.000397

$N_0SAP9^{\ominus}$ (Energy = −1197.95296246)

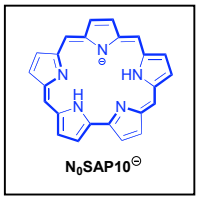


Stoichiometry C24H16N5(1-)
Framework group C1[X(C24H16N5)]
Deg. of freedom 129
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.193560	-2.352050	-0.000163
2	7	0	2.439392	-1.100655	0.000214
3	7	0	2.270514	1.667272	-0.000353
4	7	0	-2.841753	-0.567086	-0.000186
5	6	0	-3.934065	1.620865	-0.000133
6	6	0	1.887951	2.990093	0.000165
7	6	0	-2.851421	2.489239	0.000033
8	6	0	4.369483	0.358837	-0.000419
9	6	0	0.955710	-3.045017	0.000155
10	6	0	4.171241	2.886249	0.000008
11	6	0	0.635521	3.630980	0.000178
12	6	0	-2.947476	3.913981	0.000079
13	6	0	3.102272	3.752558	0.000379
14	6	0	-1.680884	4.427053	0.000114
15	6	0	3.797214	-0.912598	-0.000231
16	6	0	3.656460	1.561897	-0.000353
17	6	0	2.244806	-2.430917	0.000080
18	6	0	0.722667	-4.487168	0.000344
19	6	0	-3.950154	0.216065	-0.000206
20	6	0	-0.733437	3.343922	0.000133
21	6	0	4.491600	-2.185204	-0.000252
22	6	0	-4.762112	-1.874684	-0.000262
23	6	0	-5.170190	-0.575331	-0.000195
24	6	0	-1.188705	-3.289397	0.000197
25	6	0	3.515643	-3.141980	0.000087
26	6	0	-2.561629	-3.044498	0.000114
27	6	0	-0.630416	-4.639208	0.000288
28	6	0	-3.303943	-1.850209	-0.000087
29	1	0	5.225583	3.133672	-0.000023
30	1	0	-3.885266	4.455434	0.000133
31	1	0	3.128638	4.835197	0.000634
32	1	0	-1.387546	5.469430	0.000204
33	1	0	1.479695	-5.262819	0.000487
34	1	0	5.567357	-2.325009	-0.000507
35	1	0	-5.373422	-2.771155	-0.000349
36	1	0	-6.181990	-0.183863	-0.000267
37	1	0	3.644533	-4.217761	0.000188
38	1	0	-1.202285	-5.561577	0.000450
39	7	0	-1.491651	2.181207	0.000189
40	1	0	-1.183149	1.211048	-0.000045
41	1	0	1.717823	0.803510	0.000057
42	1	0	0.780310	4.708969	0.000350
43	1	0	-4.903804	2.114510	-0.000158
44	1	0	-3.177718	-3.944353	0.000178
45	1	0	5.453824	0.440771	-0.000527

$N_0SAP10^{\ominus}$ (Energy = −1197.96857602)

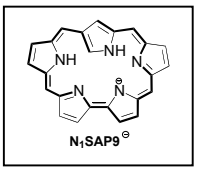


Stoichiometry C24H16N5(1-)
Framework group C1[X(C24H16N5)]
Deg. of freedom 129
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.958976	-1.725390	0.000017
2	7	0	-0.963229	-2.269160	-0.000030
3	7	0	-2.880991	0.089876	-0.000138
4	7	0	2.581580	1.084876	-0.000145
5	6	0	1.698044	3.434027	-0.000151
6	6	0	-3.591725	1.272295	0.000082
7	6	0	0.297935	3.486044	0.000061
8	6	0	-3.418239	-2.346659	-0.000269
9	6	0	1.384178	-2.968950	0.000182
10	6	0	-5.069803	-0.457863	-0.000072
11	6	0	-3.129644	2.588319	0.000249
12	6	0	-0.336499	4.809942	0.000204
13	6	0	-4.978345	0.911097	-0.000069
14	6	0	-1.672250	4.595852	0.000413
15	6	0	-2.153384	-2.945001	-0.000194
16	6	0	-3.745285	-0.993793	-0.000203
17	6	0	-0.009578	-3.227447	0.000064
18	6	0	2.447585	-3.914487	0.000249
19	6	0	2.692263	2.437025	-0.000258
20	6	0	-1.841587	3.142533	0.000245
21	6	0	-1.937776	-4.377898	-0.000205
22	6	0	4.833451	1.696452	-0.000411
23	6	0	4.100903	2.839879	-0.000411
24	6	0	3.336077	-1.827217	0.000220
25	6	0	-0.583791	-4.558443	-0.000011
26	6	0	4.215911	-0.741607	0.000134
27	6	0	3.640902	-3.216879	0.000520
28	6	0	3.865907	0.610065	-0.000092
29	1	0	-5.967030	-1.064562	-0.000086
30	1	0	0.196546	5.754817	0.000250
31	1	0	-5.786803	1.631581	-0.000065
32	1	0	-2.477571	5.322751	0.000644
33	1	0	2.316684	-4.988132	0.000256
34	1	0	-2.714227	-5.135357	-0.000335
35	1	0	5.912183	1.582359	-0.000564
36	1	0	4.455058	3.865356	-0.000569
37	1	0	-0.037436	-5.493996	0.000031
38	1	0	4.644230	-3.624542	0.000753
39	7	0	-0.644794	2.496032	0.000040
40	1	0	-1.867647	0.005635	-0.000141
41	1	0	1.488837	-0.819619	-0.000097
42	1	0	-3.935021	3.320286	0.000368
43	1	0	2.136039	4.432262	-0.000217
44	1	0	5.275769	-0.984994	0.000255
45	1	0	-4.271901	-3.021211	-0.000343

Cartesian coordinates for the optimized structures of N-confused sapphyrins (monoanion)

$N_1SAP1^{\ominus}$ (Energy = –1197.93772367)

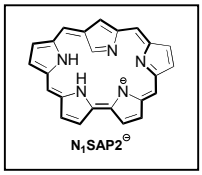


Stoichiometry C24H16N5(1-)
Framework group C1[X(C24H16N5)]
Deg. of freedom 129
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.693959	-1.852139	0.833020
2	7	0	2.941231	-0.873586	-0.155028
3	7	0	-2.994150	-0.885680	0.075901
4	6	0	-1.102212	-3.090946	0.263492
5	6	0	0.026108	-3.890458	0.010534
6	6	0	0.607197	-1.851068	0.838601
7	6	0	1.165471	-3.080861	0.279393
8	6	0	2.527718	-3.243981	-0.011984
9	6	0	3.410998	-2.148488	-0.129500
10	6	0	4.865185	-2.152157	-0.220047
11	6	0	5.243256	-0.836834	-0.248259
12	6	0	4.009337	-0.055290	-0.201181
13	6	0	3.914864	1.354373	-0.197246
14	6	0	2.788718	2.179869	-0.108740
15	6	0	2.893030	3.634498	-0.078047
16	6	0	1.621835	4.118376	0.016793
17	6	0	0.761777	2.943514	0.037036
18	6	0	-0.665195	2.984718	0.090786
19	6	0	-1.530128	4.096010	0.163015
20	6	0	-2.838995	3.627516	0.133651
21	6	0	-2.815343	2.211709	0.043765
22	6	0	-3.952483	1.374167	-0.065332
23	6	0	-4.037039	-0.012798	-0.115772
24	6	0	-5.168211	-0.836064	-0.460949
25	6	0	-4.761489	-2.151540	-0.487561
26	6	0	-3.369800	-2.201936	-0.137600
27	6	0	-2.469464	-3.265458	-0.060954
28	1	0	0.025610	-4.866808	-0.460772
29	1	0	1.176403	-1.020487	1.226961
30	1	0	5.506457	-3.027674	-0.224864
31	1	0	6.251528	-0.437907	-0.302164
32	1	0	3.818343	4.199745	-0.122155
33	1	0	1.303348	5.153573	0.060977
34	1	0	-1.207698	5.126681	0.228408
35	1	0	-3.747326	4.215984	0.173804
36	1	0	-6.150331	-0.450062	-0.706550
37	1	0	-5.363640	-3.015286	-0.742687
38	1	0	2.915516	-4.241603	-0.221327
39	1	0	-2.824591	-4.249336	-0.357209
40	1	0	-4.892994	1.909516	-0.164252
41	1	0	4.865561	1.886078	-0.247524
42	7	0	-1.470680	1.862340	0.037287
43	7	0	1.464694	1.802397	-0.033614
44	1	0	-2.084720	-0.738318	0.528600
45	1	0	-1.072224	0.941361	-0.095570

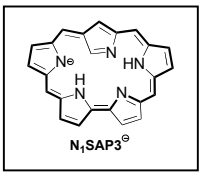
$N_1SAP2^{\ominus}$ (Energy = −1197.91289108)



Stoichiometry C24H16N5(1-)
Framework group C1[X(C24H16N5)]
Deg. of freedom 129
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.584968	-2.279684	1.219634
2	7	0	2.937468	-0.768660	-0.021748
3	7	0	-2.785799	-1.000193	-0.035006
4	6	0	-0.941508	-3.257797	0.274120
5	6	0	0.225461	-3.917080	-0.226843
6	6	0	0.718662	-2.244786	1.203271
7	6	0	1.318734	-3.197637	0.266104
8	6	0	2.705230	-3.213048	-0.083129
9	6	0	3.461609	-2.057006	-0.147628
10	6	0	4.868760	-1.863550	-0.377221
11	6	0	5.136721	-0.519631	-0.372444
12	6	0	3.907311	0.207878	-0.169974
13	6	0	3.750540	1.582956	-0.161762
14	6	0	2.603642	2.415260	-0.059411
15	6	0	2.621930	3.830209	-0.015213
16	6	0	1.308216	4.296010	0.059636
17	6	0	0.457132	3.178569	0.058069
18	6	0	-0.968503	3.056269	0.069710
19	6	0	-1.933378	4.141068	0.112116
20	6	0	-3.156243	3.533998	0.066301
21	6	0	-2.910744	2.098796	0.003086
22	6	0	-3.940002	1.159495	-0.082036
23	6	0	-3.905525	-0.251729	-0.134265
24	6	0	-5.076035	-1.094637	-0.372624
25	6	0	-4.608669	-2.375510	-0.453090
26	6	0	-3.173982	-2.290801	-0.207391
27	6	0	-2.247740	-3.356360	-0.209277
28	1	0	0.244164	-4.667558	-1.009938
29	1	0	1.273883	-1.636903	1.915142
30	1	0	5.577682	-2.672560	-0.503648
31	1	0	6.098801	-0.042014	-0.513600
32	1	0	3.527243	4.424419	-0.035069
33	1	0	0.981311	5.326533	0.103954
34	1	0	-1.713892	5.201416	0.165257
35	1	0	-4.133397	4.005845	0.077025
36	1	0	-6.098835	-0.749201	-0.488126
37	1	0	-5.176704	-3.284569	-0.622837
38	1	0	3.183161	-4.137155	-0.402492
39	1	0	-2.541805	-4.279523	-0.710513
40	1	0	-4.940283	1.592263	-0.130581
41	1	0	4.678062	2.139739	-0.266913
42	7	0	-1.555268	1.854980	0.009095
43	7	0	1.264987	2.061746	-0.002949
44	1	0	0.831280	1.148504	-0.050611
45	1	0	1.944661	-0.612192	0.049125

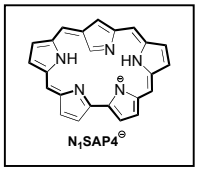
$N_1SAP3^{\ominus}$ (Energy = −1197.95624460)



Stoichiometry C24H16N5(1-)
Framework group C1[X(C24H16N5)]
Deg. of freedom 129
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.712047	-1.905657	0.947687
2	7	0	2.945720	-0.788728	-0.098320
3	7	0	-3.001720	-0.820206	0.035486
4	6	0	-1.116209	-3.080949	0.259338
5	6	0	0.014643	-3.859889	-0.082067
6	6	0	0.586061	-1.913969	0.934779
7	6	0	1.144999	-3.076126	0.239866
8	6	0	2.508159	-3.192938	-0.081662
9	6	0	3.371404	-2.085155	-0.154890
10	6	0	4.820997	-2.129225	-0.303728
11	6	0	5.251835	-0.834247	-0.287344
12	6	0	4.055357	-0.010261	-0.162328
13	6	0	4.012226	1.390721	-0.137259
14	6	0	2.870240	2.199205	-0.051593
15	6	0	2.828862	3.621757	0.004765
16	6	0	1.507435	4.014740	0.068794
17	6	0	0.687531	2.849784	0.050883
18	6	0	-0.735732	2.827305	0.064634
19	6	0	-1.528616	4.047302	0.063652
20	6	0	-2.832087	3.649381	0.017623
21	6	0	-2.816997	2.198342	-0.002588
22	6	0	-3.981416	1.417596	-0.091200
23	6	0	-4.069870	0.022486	-0.121967
24	6	0	-5.203926	-0.814914	-0.378125
25	6	0	-4.772376	-2.125854	-0.396307
26	6	0	-3.366531	-2.139220	-0.120377
27	6	0	-2.469269	-3.218936	-0.082098
28	1	0	0.007171	-4.777858	-0.658867
29	1	0	1.169387	-1.153927	1.436243
30	1	0	5.421277	-3.030116	-0.376660
31	1	0	6.270469	-0.468145	-0.364566
32	1	0	3.705611	4.257602	0.000748
33	1	0	1.133591	5.027743	0.123540
34	1	0	-1.148857	5.061548	0.080607
35	1	0	-3.719932	4.272436	-0.003598
36	1	0	-6.208533	-0.450781	-0.556234
37	1	0	-5.369383	-3.011441	-0.577328
38	1	0	2.911835	-4.164412	-0.366897
39	1	0	-2.837488	-4.180081	-0.433843
40	1	0	-4.921596	1.956961	-0.182519
41	1	0	4.958225	1.925239	-0.185296
42	7	0	-1.526402	1.728139	0.035093
43	7	0	1.549436	1.775282	-0.013835
44	1	0	-2.059625	-0.519170	0.285663
45	1	0	1.302620	0.790983	-0.068578

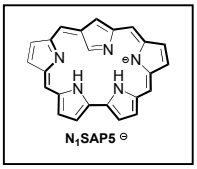
$N_1SAP4^{\ominus}$ (Energy = −1197.95063283)



Stoichiometry C24H16N5(1-)
Framework group C1[X(C24H16N5)]
Deg. of freedom 129
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.497142	1.710029	0.044988
2	7	0	-1.603494	1.662219	-0.012931
3	7	0	-2.998353	-0.810118	-0.093847
4	7	0	3.039432	-0.748106	0.024629
5	6	0	2.558979	-3.157095	-0.108784
6	6	0	-3.330187	-2.152629	-0.140988
7	6	0	-4.054604	1.382661	-0.145320
8	6	0	0.650143	2.763403	0.069817
9	6	0	-5.235715	-0.896412	-0.265350
10	6	0	-2.424625	-3.215671	-0.073526
11	6	0	-4.758930	-2.190181	-0.267816
12	6	0	-2.884264	2.158469	-0.062125
13	6	0	-4.116877	-0.010678	-0.162798
14	6	0	-0.783240	2.742947	0.047850
15	6	0	1.396312	4.024508	0.072728
16	6	0	3.434791	-2.057619	-0.134018
17	6	0	-2.875913	3.605908	-0.024333
18	6	0	5.244387	-0.691154	-0.366365
19	6	0	4.841294	-2.012518	-0.396651
20	6	0	2.764935	2.240961	0.010903
21	6	0	-1.565019	3.974137	0.048163
22	6	0	3.957277	1.511580	-0.076600
23	6	0	2.714808	3.693899	0.031763
24	6	0	4.089670	0.116415	-0.116714
25	1	0	-6.268747	-0.576908	-0.330244
26	1	0	-5.339344	-3.103476	-0.316831
27	1	0	0.973517	5.020672	0.090086
28	1	0	-3.751761	4.245713	-0.046623
29	1	0	6.242702	-0.304260	-0.530980
30	1	0	5.459881	-2.883815	-0.574490
31	1	0	-1.172877	4.981806	0.093497
32	1	0	3.572782	4.357730	0.014241
33	6	0	-0.502363	-1.913216	0.946224
34	6	0	1.207404	-3.049057	0.244788
35	6	0	-1.054485	-3.063326	0.226416
36	1	0	-1.068987	-1.162433	1.485846
37	1	0	0.091511	-4.725718	-0.725429
38	7	0	0.795907	-1.900385	0.963842
39	6	0	0.079923	-3.825459	-0.121543
40	1	0	2.088974	-0.449911	0.250467
41	1	0	-2.075301	-0.373376	-0.115437
42	1	0	-2.809157	-4.196155	-0.348989
43	1	0	2.942103	-4.103613	-0.483733
44	1	0	4.878740	2.083715	-0.158101
45	1	0	-5.000683	1.915321	-0.204362

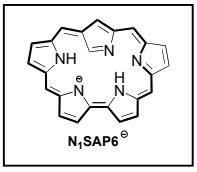
$N_1SAP5^{\ominus}$ (Energy = −1197.94123752)



Stoichiometry C24H16N5(1-)
Framework group C1[X(C24H16N5)]
Deg. of freedom 129
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.623565	-1.880602	1.046011
2	7	0	2.993340	-0.731628	-0.097184
3	7	0	-2.971506	-0.792508	-0.059837
4	6	0	-1.040704	-3.000815	0.278399
5	6	0	0.081953	-3.772385	-0.120184
6	6	0	0.673858	-1.899130	1.004320
7	6	0	1.218520	-3.017449	0.223013
8	6	0	2.576099	-3.133170	-0.129178
9	6	0	3.431706	-2.023752	-0.188912
10	6	0	4.879849	-2.047187	-0.352421
11	6	0	5.297107	-0.748542	-0.307268
12	6	0	4.093028	0.059638	-0.153568
13	6	0	4.022186	1.458767	-0.102346
14	6	0	2.849924	2.222031	-0.011760
15	6	0	2.742433	3.638574	0.054320
16	6	0	1.405025	3.969671	0.101656
17	6	0	0.634665	2.770943	0.063955
18	6	0	-0.784832	2.744849	0.049983
19	6	0	-1.592268	3.922293	0.013779
20	6	0	-2.915710	3.546303	-0.045347
21	6	0	-2.975126	2.125183	-0.045673
22	6	0	-4.118329	1.320125	-0.124351
23	6	0	-4.122569	-0.081399	-0.141594
24	6	0	-5.268417	-0.970135	-0.287446
25	6	0	-4.757514	-2.236605	-0.309606
26	6	0	-3.314516	-2.104352	-0.137230
27	6	0	-2.380058	-3.155799	-0.092126
28	1	0	0.055354	-4.650373	-0.756410
29	1	0	1.275479	-1.193762	1.564200
30	1	0	5.489155	-2.939416	-0.451817
31	1	0	6.311237	-0.369969	-0.383780
32	1	0	3.587177	4.315898	0.065581
33	1	0	0.989444	4.965909	0.159445
34	1	0	-1.207371	4.932334	0.012071
35	1	0	-3.781239	4.195210	-0.095138
36	1	0	-6.306866	-0.666869	-0.371862
37	1	0	-5.300472	-3.171651	-0.401355
38	1	0	2.973708	-4.098644	-0.441842
39	1	0	-2.705479	-4.133256	-0.447611
40	1	0	-5.067888	1.845871	-0.190299
41	1	0	4.951198	2.022091	-0.141850
42	7	0	-1.659929	1.676223	0.018855
43	7	0	1.549082	1.732316	0.007687
44	1	0	1.391355	0.726527	-0.050199
45	1	0	-1.484604	0.667559	0.079664

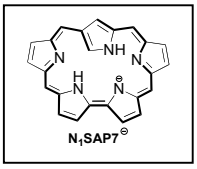
$N_1SAP6^{\ominus}$ (Energy = −1197.94537558)



Stoichiometry C24H16N5(1-)
Framework group C1[X(C24H16N5)]
Deg. of freedom 129
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.711147	-1.955912	1.080443
2	7	0	3.009459	-0.782483	-0.074574
3	7	0	-2.965482	-0.762452	-0.074409
4	6	0	-1.126701	-3.031782	0.257987
5	6	0	-0.002900	-3.789979	-0.169774
6	6	0	0.587056	-1.974824	1.043983
7	6	0	1.132868	-3.061511	0.220251
8	6	0	2.500709	-3.194752	-0.109547
9	6	0	3.380395	-2.114120	-0.161212
10	6	0	4.808328	-2.104826	-0.313872
11	6	0	5.244943	-0.799238	-0.290350
12	6	0	4.101199	0.053138	-0.151912
13	6	0	4.006887	1.440497	-0.123136
14	6	0	2.822045	2.200676	-0.037877
15	6	0	2.804699	3.645203	0.005232
16	6	0	1.490734	4.012402	0.065484
17	6	0	0.723138	2.781234	0.053260
18	6	0	-0.701598	2.793823	0.057081
19	6	0	-1.505817	3.975433	0.046559
20	6	0	-2.830533	3.603244	0.001033
21	6	0	-2.892280	2.180380	-0.016056
22	6	0	-4.044919	1.391697	-0.095974
23	6	0	-4.090552	-0.008988	-0.134631
24	6	0	-5.270131	-0.851056	-0.288077
25	6	0	-4.807473	-2.135201	-0.338142
26	6	0	-3.360240	-2.058168	-0.170990
27	6	0	-2.460570	-3.142259	-0.143343
28	1	0	-0.026492	-4.633320	-0.851232
29	1	0	1.173304	-1.296113	1.656670
30	1	0	5.414806	-2.998742	-0.394254
31	1	0	6.266230	-0.446305	-0.367779
32	1	0	3.677909	4.288624	-0.006979
33	1	0	1.092253	5.018140	0.109858
34	1	0	-1.116132	4.983340	0.058540
35	1	0	-3.697324	4.252080	-0.027166
36	1	0	-6.296867	-0.507102	-0.359394
37	1	0	-5.385530	-3.047695	-0.441365
38	1	0	2.893544	-4.161234	-0.420289
39	1	0	-2.805241	-4.096682	-0.540959
40	1	0	-4.984779	1.937120	-0.145495
41	1	0	4.941221	1.993215	-0.183748
42	7	0	-1.577298	1.732538	0.027297
43	7	0	1.543790	1.697533	-0.002031
44	1	0	2.069476	-0.389957	-0.077406
45	1	0	-1.367356	0.733919	0.058046

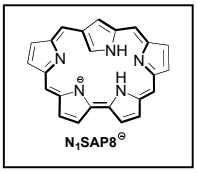
N_1SAP7$^{\ominus}$ (Energy = −1197.93912237)



Stoichiometry C24H16N5(1-)
Framework group C1[X(C24H16N5)]
Deg. of freedom 129
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.360599	1.770900	0.079777
2	7	0	-1.685837	1.719423	-0.052404
3	7	0	-2.915971	-0.903270	-0.097885
4	7	0	3.064833	-0.733288	0.091727
5	6	0	2.725920	-3.111777	-0.119393
6	6	0	-3.257752	-2.232704	-0.082502
7	6	0	-4.118785	1.204827	-0.181383
8	6	0	0.551726	2.852721	0.071089
9	6	0	-5.215802	-1.102886	-0.228822
10	6	0	-2.340589	-3.279267	0.036526
11	6	0	-4.708445	-2.366974	-0.191341
12	6	0	-3.022376	2.079694	-0.103769
13	6	0	-4.069419	-0.197577	-0.167310
14	6	0	-0.870273	2.832461	0.025183
15	6	0	1.316440	4.096273	0.071712
16	6	0	3.565519	-1.983655	-0.133689
17	6	0	-3.045728	3.503715	-0.046452
18	6	0	5.298941	-0.548948	-0.361505
19	6	0	4.987425	-1.881920	-0.423103
20	6	0	2.646808	2.263939	0.061422
21	6	0	-1.741980	3.956561	0.033988
22	6	0	3.854343	1.552404	-0.008731
23	6	0	2.624335	3.723825	0.062604
24	6	0	4.058318	0.157654	-0.058166
25	1	0	-1.394398	0.752222	-0.146788
26	1	0	-6.256399	-0.804297	-0.303958
27	1	0	-5.255298	-3.304088	-0.206209
28	1	0	0.912508	5.101568	0.062386
29	1	0	-3.949685	4.100168	-0.053436
30	1	0	6.264412	-0.088365	-0.543436
31	1	0	5.654939	-2.707584	-0.646178
32	1	0	-1.415910	4.985594	0.101768
33	1	0	3.499902	4.364652	0.049449
34	1	0	4.749691	2.168587	-0.083124
35	1	0	-5.096254	1.677939	-0.234032
36	1	0	-2.705868	-4.293809	-0.114648
37	1	0	3.133537	-4.078223	-0.404617
38	6	0	-0.455574	-1.823550	0.746408
39	6	0	1.343100	-3.019207	0.163797
40	6	0	-0.947940	-3.067211	0.249539
41	1	0	1.519771	-0.990057	0.701416
42	1	0	-1.025236	-0.995664	1.130869
43	1	0	0.231220	-4.832931	-0.472208
44	7	0	0.860004	-1.809127	0.687164
45	6	0	0.213071	-3.836425	-0.048757

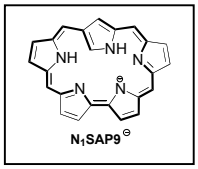
$N_1SAP8^{\ominus}$ (Energy = −1197.93462515)



Stoichiometry C24H16N5(1-)
Framework group C1[X(C24H16N5)]
Deg. of freedom 129
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.643974	1.767581	0.022581
2	7	0	-1.353229	1.810632	-0.036665
3	7	0	-3.012623	-0.754225	-0.172313
4	7	0	2.887802	-0.923544	0.017565
5	6	0	2.323091	-3.307183	-0.150934
6	6	0	-3.557589	-2.004997	-0.092155
7	6	0	-3.835041	1.529580	-0.186815
8	6	0	0.847412	2.895795	0.063617
9	6	0	-5.306798	-0.578275	-0.147210
10	6	0	-2.741185	-3.132902	0.046271
11	6	0	-5.014319	-1.912748	-0.114363
12	6	0	-2.650164	2.271310	-0.122315
13	6	0	-4.022193	0.127087	-0.172769
14	6	0	-0.575613	2.909025	0.004456
15	6	0	1.731852	3.998863	0.163237
16	6	0	3.233714	-2.242404	-0.172372
17	6	0	-2.661319	3.732510	-0.125802
18	6	0	5.165200	-1.068590	-0.315421
19	6	0	4.669280	-2.337099	-0.394069
20	6	0	2.987434	2.099429	0.067045
21	6	0	-1.364614	4.135800	-0.044058
22	6	0	4.076348	1.208508	-0.005610
23	6	0	3.032383	3.518133	0.166013
24	6	0	4.028663	-0.188024	-0.073789
25	1	0	-6.289285	-0.116581	-0.163479
26	1	0	-5.710467	-2.743886	-0.067558
27	1	0	1.420518	5.032519	0.235372
28	1	0	-3.549560	4.353009	-0.185633
29	1	0	6.194140	-0.748048	-0.440453
30	1	0	5.218069	-3.255391	-0.574467
31	1	0	-0.981704	5.149547	-0.029798
32	1	0	3.945772	4.095831	0.236243
33	1	0	5.057226	1.676330	-0.040679
34	1	0	-4.746646	2.125846	-0.225225
35	1	0	-3.183147	-4.121991	-0.067819
36	1	0	2.681003	-4.298445	-0.415281
37	6	0	-0.760396	-1.804367	0.752517
38	6	0	0.946457	-3.138056	0.138892
39	6	0	-1.339473	-3.011845	0.255487
40	1	0	1.271096	-1.173109	0.797250
41	1	0	-1.251284	-0.913804	1.106764
42	1	0	-0.297908	-4.852676	-0.502447
43	7	0	0.554712	-1.905765	0.684913
44	6	0	-0.236059	-3.865786	-0.061605
45	1	0	1.315310	0.825522	-0.144842

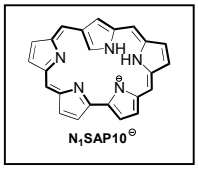
$N_1SAP9^{\ominus}$ (Energy = −1197.93308621)



Stoichiometry C24H16N5(1-)
Framework group C1[X(C24H16N5)]
Deg. of freedom 129
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.370424	1.701325	0.116152
2	7	0	-1.724127	1.578176	-0.025370
3	7	0	-3.016466	-0.898639	-0.141288
4	7	0	3.132888	-0.687410	0.098746
5	6	0	2.781218	-3.051330	-0.121668
6	6	0	-3.261025	-2.259489	-0.073923
7	6	0	-4.172398	1.224005	-0.183946
8	6	0	0.505724	2.736319	0.090414
9	6	0	-5.250770	-1.123602	-0.175026
10	6	0	-2.295930	-3.248898	0.052749
11	6	0	-4.699225	-2.381535	-0.119211
12	6	0	-3.014299	2.038779	-0.107483
13	6	0	-4.180874	-0.163985	-0.178735
14	6	0	-0.926579	2.685309	0.033533
15	6	0	1.225126	4.020167	0.075617
16	6	0	3.634394	-1.936255	-0.129643
17	6	0	-3.042119	3.482326	-0.095222
18	6	0	5.361003	-0.490351	-0.353697
19	6	0	5.057314	-1.826063	-0.416314
20	6	0	2.633937	2.254105	0.086230
21	6	0	-1.739254	3.888021	-0.005288
22	6	0	3.869613	1.600178	0.009821
23	6	0	2.545623	3.714433	0.071228
24	6	0	4.114650	0.207943	-0.048021
25	1	0	-6.304130	-0.871534	-0.198777
26	1	0	-5.227688	-3.326297	-0.075550
27	1	0	0.780770	5.006990	0.054232
28	1	0	-3.932687	4.099935	-0.146076
29	1	0	6.324890	-0.025978	-0.534171
30	1	0	5.731717	-2.645952	-0.640013
31	1	0	-1.376864	4.907252	0.031100
32	1	0	3.390806	4.394730	0.048287
33	1	0	4.740151	2.250505	-0.066079
34	1	0	-5.133160	1.730146	-0.235256
35	1	0	-2.629141	-4.279458	-0.044649
36	1	0	3.175837	-4.026593	-0.395367
37	6	0	-0.406001	-1.722559	0.683054
38	6	0	1.393285	-2.936617	0.145881
39	6	0	-0.901015	-2.980152	0.224968
40	1	0	1.565552	-0.892630	0.634723
41	1	0	-0.921977	-0.856644	1.066854
42	1	0	0.275392	-4.763208	-0.450441
43	7	0	0.911175	-1.717091	0.629450
44	6	0	0.260267	-3.753709	-0.058641
45	1	0	-2.132717	-0.398032	-0.232713

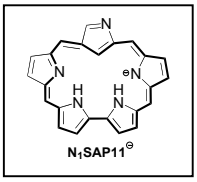
N_1SAP10$^{\ominus}$ (Energy = −1197.91922745)



Stoichiometry C24H16N5(1-)
Framework group C1[X(C24H16N5)]
Deg. of freedom 129
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.742229	1.585659	0.015987
2	7	0	-1.322039	1.749167	0.024010
3	7	0	-3.089684	-0.664170	-0.201137
4	7	0	2.954007	-0.924217	-0.115096
5	6	0	2.201895	-3.280911	-0.135417
6	6	0	-3.670733	-1.901948	-0.142312
7	6	0	-3.811898	1.641723	-0.130329
8	6	0	0.971955	2.710395	0.056290
9	6	0	-5.373207	-0.419612	-0.128394
10	6	0	-2.869391	-3.035973	-0.016553
11	6	0	-5.124505	-1.763770	-0.141322
12	6	0	-2.584402	2.301199	-0.058006
13	6	0	-4.065484	0.245693	-0.154203
14	6	0	-0.461805	2.780676	0.033436
15	6	0	1.809079	3.892381	0.093036
16	6	0	3.178891	-2.293933	-0.184704
17	6	0	-2.495526	3.762914	-0.076258
18	6	0	5.188153	-1.193408	-0.181431
19	6	0	4.610411	-2.441272	-0.235402
20	6	0	3.046211	2.017833	0.015084
21	6	0	-1.175476	4.067458	-0.021179
22	6	0	4.178709	1.170460	-0.052571
23	6	0	3.107587	3.457115	0.069118
24	6	0	4.144796	-0.214296	-0.112959
25	1	0	-6.341109	0.072256	-0.115534
26	1	0	-5.847400	-2.572131	-0.103316
27	1	0	1.465806	4.918266	0.136923
28	1	0	-3.338376	4.443985	-0.136205
29	1	0	6.246953	-0.963834	-0.176056
30	1	0	5.118753	-3.397495	-0.264547
31	1	0	-0.726983	5.053072	-0.029937
32	1	0	4.013491	4.054097	0.082714
33	1	0	5.156853	1.645200	-0.065131
34	1	0	-4.688669	2.288596	-0.155626
35	1	0	-3.310307	-4.024675	-0.135752
36	1	0	2.511559	-4.302695	-0.333031
37	6	0	-0.904035	-1.735339	0.774941
38	6	0	0.826264	-3.040597	0.127116
39	6	0	-1.466216	-2.910074	0.212907
40	1	0	1.046401	-1.121193	1.082602
41	1	0	-1.389076	-0.862904	1.176840
42	1	0	-0.405160	-4.699808	-0.637759
43	7	0	0.422507	-1.829113	0.719253
44	6	0	-0.354429	-3.743121	-0.133537
45	1	0	2.097057	-0.393585	-0.291395

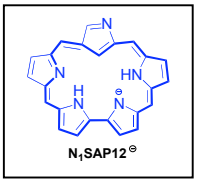
N_1SAP11$^{\ominus}$ (Energy = −1197.96451796)



Stoichiometry C24H16N5(1-)
Framework group C1[X(C24H16N5)]
Deg. of freedom 129
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.596432	1.957620	0.000056
2	7	0	1.532462	1.996033	0.000052
3	7	0	2.846906	-0.574630	-0.000023
4	7	0	-2.838443	-0.640530	-0.000031
5	6	0	-2.470123	-3.101699	-0.000011
6	6	0	3.299911	-1.862977	-0.000009
7	6	0	-1.081293	-3.295889	-0.000006
8	6	0	3.966205	1.608807	0.000007
9	6	0	-0.750374	3.048831	0.000015
10	6	0	5.175257	-0.600536	-0.000019
11	6	0	2.552805	-3.050803	-0.000004
12	6	0	-0.512957	-4.648432	0.000045
13	6	0	4.756847	-1.895119	-0.000007
14	6	0	2.845730	2.439191	0.000009
15	6	0	3.967184	0.207678	0.000000
16	6	0	0.660770	3.065696	0.000017
17	6	0	-1.584741	4.203086	-0.000028
18	6	0	-3.254585	-1.942978	-0.000014
19	6	0	1.177478	-3.294838	0.000003
20	6	0	2.792626	3.860572	-0.000002
21	6	0	-5.165099	-0.734046	-0.000020
22	6	0	-4.711439	-2.015635	0.000003
23	6	0	-2.919234	2.368741	0.000006
24	6	0	1.467211	4.240551	-0.000026
25	6	0	-4.018942	1.509747	0.000005
26	6	0	-2.900987	3.791154	-0.000017
27	6	0	-3.979077	0.109184	0.000000
28	1	0	6.190096	-0.217695	-0.000028
29	1	0	-1.103832	-5.564933	0.000053
30	1	0	5.358564	-2.797385	-0.000003
31	1	0	-1.222976	5.222117	-0.000062
32	1	0	3.661785	4.506095	-0.000019
33	1	0	-6.190260	-0.379581	-0.000018
34	1	0	-5.289344	-2.933635	0.000027
35	1	0	1.080464	5.250319	-0.000062
36	1	0	-3.785457	4.415492	-0.000043
37	1	0	-4.996702	1.984571	-0.000009
38	1	0	4.930791	2.110160	-0.000005
39	1	0	3.146149	-3.963205	-0.000005
40	1	0	-3.052829	-4.024132	-0.000002
41	1	0	-1.388706	0.958339	0.000100
42	7	0	0.785699	-4.672174	-0.000029
43	6	0	0.045193	-2.451900	0.000014
44	1	0	0.052182	-1.373439	0.000024
45	1	0	1.348527	0.992362	0.000097

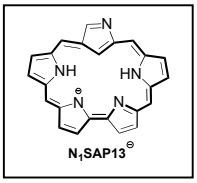
N_1SAP12$^{\ominus}$ (Energy = −1197.97173491)



Stoichiometry C24H16N5(1-)
Framework group C1[X(C24H16N5)]
Deg. of freedom 129
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.556878	1.995635	-0.000165
2	7	0	1.471869	1.970308	-0.000144
3	7	0	2.892276	-0.604302	-0.000027
4	7	0	-2.826092	-0.645817	0.000200
5	6	0	-2.488582	-3.107661	-0.000020
6	6	0	3.303279	-1.925346	0.000041
7	6	0	-1.103478	-3.309061	-0.000095
8	6	0	3.914958	1.638962	0.000102
9	6	0	-0.727137	3.090867	-0.000053
10	6	0	5.145327	-0.578631	0.000152
11	6	0	2.539599	-3.091997	0.000014
12	6	0	-0.540429	-4.660719	-0.000259
13	6	0	4.735276	-1.890312	0.000142
14	6	0	2.761986	2.436623	0.000016
15	6	0	3.980214	0.248183	0.000083
16	6	0	0.688934	3.078811	-0.000044
17	6	0	-1.573462	4.237838	-0.000056
18	6	0	-3.262642	-1.938831	0.000062
19	6	0	1.156270	-3.313789	-0.000075
20	6	0	2.787802	3.884590	0.000051
21	6	0	-5.154337	-0.703646	0.000173
22	6	0	-4.720259	-1.992476	0.000226
23	6	0	-2.883954	2.384506	-0.000031
24	6	0	1.484863	4.290841	-0.000074
25	6	0	-3.980241	1.522046	0.000019
26	6	0	-2.884715	3.809201	-0.000057
27	6	0	-3.955349	0.121195	0.000073
28	1	0	6.160174	-0.200758	0.000222
29	1	0	-1.132833	-5.575871	-0.000271
30	1	0	5.355046	-2.778244	0.000201
31	1	0	-1.221755	5.260300	-0.000047
32	1	0	3.680722	4.500129	0.000138
33	1	0	-6.174114	-0.333960	0.000195
34	1	0	-5.311991	-2.901649	0.000285
35	1	0	1.107222	5.305926	-0.000097
36	1	0	-3.778824	4.420067	-0.000041
37	1	0	-4.956911	2.000085	0.000046
38	1	0	4.870882	2.157102	0.000197
39	1	0	3.124812	-4.007977	0.000078
40	1	0	-3.078044	-4.025674	-0.000021
41	1	0	-1.294649	1.013211	-0.000276
42	7	0	0.758921	-4.688033	-0.000071
43	6	0	0.028776	-2.466307	-0.000192
44	1	0	0.006165	-1.385795	-0.000228
45	1	0	1.947228	-0.230764	-0.000115

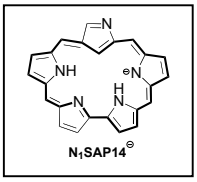
N_1SAP13$^{\ominus}$ (Energy = −1197.96844045)



Stoichiometry C24H16N5(1-)
Framework group C1[X(C24H16N5)]
Deg. of freedom 129
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.547083	1.898096	-0.000509
2	7	0	-1.506572	1.922069	-0.000443
3	7	0	-2.920488	-0.577693	0.000260
4	7	0	2.917358	-0.624576	0.000322
5	6	0	2.493300	-3.095186	-0.000078
6	6	0	-3.318701	-1.900494	0.000007
7	6	0	1.100534	-3.271982	0.000001
8	6	0	-3.947446	1.656172	0.000155
9	6	0	0.741151	2.986969	-0.000145
10	6	0	-5.173572	-0.572256	0.000075
11	6	0	-2.542864	-3.062360	-0.000089
12	6	0	0.535916	-4.622238	-0.000241
13	6	0	-4.749717	-1.881724	-0.000066
14	6	0	-2.782638	2.428306	0.000040
15	6	0	-4.016536	0.261618	0.000109
16	6	0	-0.684361	2.997018	-0.000126
17	6	0	1.528504	4.214362	-0.000021
18	6	0	3.293616	-1.953896	0.000030
19	6	0	-1.161452	-3.279057	-0.000011
20	6	0	-2.766138	3.878849	0.000043
21	6	0	5.171412	-0.657117	0.000098
22	6	0	4.727459	-1.957940	-0.000059
23	6	0	2.829502	2.384020	0.000038
24	6	0	-1.453045	4.238316	0.000006
25	6	0	3.983198	1.590577	0.000178
26	6	0	2.836765	3.833358	-0.000057
27	6	0	4.027367	0.197833	0.000141
28	1	0	-6.192158	-0.204645	0.000073
29	1	0	1.129606	-5.536449	-0.000416
30	1	0	-5.360626	-2.775779	-0.000187
31	1	0	1.139548	5.224409	0.000084
32	1	0	-3.639430	4.522111	0.000178
33	1	0	6.195883	-0.306012	0.000088
34	1	0	5.325040	-2.861215	-0.000199
35	1	0	-1.047343	5.241719	0.000099
36	1	0	3.720100	4.462805	0.000032
37	1	0	4.942739	2.101866	0.000238
38	1	0	-4.898325	2.183344	0.000233
39	1	0	-3.121850	-3.982266	-0.000264
40	1	0	3.070728	-4.019027	-0.000297
41	7	0	-0.763291	-4.649850	-0.000058
42	6	0	-0.030338	-2.428341	0.000261
43	1	0	-0.036874	-1.345544	0.000495
44	1	0	-1.981950	-0.178661	0.000504
45	1	0	1.984786	-0.211822	0.000605

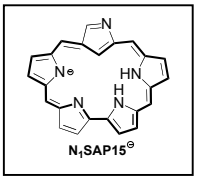
N_1SAP14$^{\ominus}$ (Energy = −1197.97166172)



Stoichiometry C24H16N5(1-)
Framework group C1[X(C24H16N5)]
Deg. of freedom 129
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.527789	1.939112	-0.000449
2	7	0	-1.496467	2.033575	-0.000116
3	7	0	-2.831725	-0.584342	-0.000039
4	7	0	2.881891	-0.670799	0.000133
5	6	0	2.464649	-3.142584	0.000032
6	6	0	-3.301571	-1.863816	0.000002
7	6	0	1.068897	-3.317096	-0.000053
8	6	0	-3.930372	1.613182	0.000103
9	6	0	0.771444	3.067168	-0.000137
10	6	0	-5.160766	-0.580400	0.000096
11	6	0	-2.563146	-3.060096	-0.000024
12	6	0	0.494786	-4.666464	-0.000390
13	6	0	-4.758903	-1.880545	0.000087
14	6	0	-2.815767	2.450618	0.000061
15	6	0	-3.942112	0.212285	0.000053
16	6	0	-0.644298	3.110225	-0.000039
17	6	0	1.595573	4.258213	-0.000128
18	6	0	3.260771	-2.001681	0.000094
19	6	0	-1.191662	-3.310985	-0.000094
20	6	0	-2.785869	3.874796	0.000143
21	6	0	5.136153	-0.700641	0.000228
22	6	0	4.695909	-2.000527	0.000144
23	6	0	2.827536	2.373984	-0.000007
24	6	0	-1.466064	4.275540	0.000119
25	6	0	3.961742	1.545600	0.000165
26	6	0	2.889267	3.819663	-0.000202
27	6	0	3.990544	0.156265	0.000152
28	1	0	-6.170738	-0.184931	0.000159
29	1	0	1.083612	-5.584140	-0.000413
30	1	0	-5.371878	-2.775193	0.000134
31	1	0	1.243226	5.282378	-0.000028
32	1	0	-3.666864	4.504446	0.000253
33	1	0	6.159758	-0.346976	0.000293
34	1	0	5.295460	-2.902469	0.000136
35	1	0	-1.092102	5.290022	0.000192
36	1	0	3.796888	4.413320	-0.000163
37	1	0	4.930400	2.039538	0.000257
38	1	0	-4.895341	2.114668	0.000207
39	1	0	-3.162466	-3.968505	0.000043
40	1	0	3.042731	-4.066052	0.000007
41	7	0	-0.804221	-4.685972	0.000147
42	6	0	-0.053329	-2.469045	-0.000158
43	1	0	-0.085380	-1.388768	-0.000174
44	1	0	-1.253985	1.046367	-0.000249
45	1	0	1.945338	-0.276685	0.000150

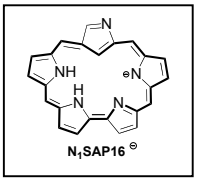
$N_1SAP15^{\ominus}$ (Energy = −1197.94534451)



Stoichiometry C24H16N5(1-)
Framework group C1[X(C24H16N5)]
Deg. of freedom 129
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.179628	2.260223	-0.000054
2	7	0	-1.576487	2.118810	-0.000006
3	7	0	-2.699077	-0.964116	-0.000007
4	7	0	2.785487	-0.528582	-0.000087
5	6	0	2.808906	-2.991579	0.000059
6	6	0	-3.043634	-2.314660	-0.000048
7	6	0	1.457855	-3.339412	0.000064
8	6	0	-3.924879	1.232564	-0.000008
9	6	0	0.471165	3.400402	0.000009
10	6	0	-4.945263	-1.055623	-0.000132
11	6	0	-2.203357	-3.414703	-0.000020
12	6	0	1.010637	-4.728712	0.000102
13	6	0	-4.476698	-2.342106	-0.000122
14	6	0	-2.949494	2.254052	0.000031
15	6	0	-3.827682	-0.151153	-0.000041
16	6	0	-0.951533	3.345973	0.000044
17	6	0	1.317869	4.577310	0.000052
18	6	0	3.427503	-1.728574	0.000020
19	6	0	-0.794550	-3.522802	0.000026
20	6	0	-3.191946	3.652212	0.000107
21	6	0	5.088220	-0.211820	-0.000026
22	6	0	4.874196	-1.556395	-0.000029
23	6	0	2.497549	2.641703	-0.000056
24	6	0	-1.967003	4.319274	0.000136
25	6	0	3.618590	1.813394	-0.000083
26	6	0	2.596343	4.096505	-0.000037
27	6	0	3.767046	0.409818	-0.000086
28	1	0	-5.977283	-0.727536	-0.000198
29	1	0	1.672289	-5.594713	0.000123
30	1	0	-5.056859	-3.256292	-0.000179
31	1	0	0.989069	5.610217	0.000116
32	1	0	-4.179711	4.096068	0.000152
33	1	0	6.034693	0.318938	0.000002
34	1	0	5.607562	-2.355962	-0.000007
35	1	0	-1.804868	5.389111	0.000205
36	1	0	3.520903	4.664201	-0.000049
37	1	0	4.566140	2.353166	-0.000086
38	1	0	-4.946675	1.602285	-0.000017
39	1	0	-2.713297	-4.374514	-0.000030
40	1	0	3.502451	-3.834337	0.000072
41	7	0	-0.285231	-4.858067	0.000119
42	6	0	0.253197	-2.588677	0.000047
43	1	0	0.222004	-1.507068	0.000013
44	1	0	-1.742785	-0.650246	0.000170
45	1	0	-1.002099	1.286855	-0.000106

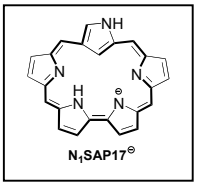
N_1SAP16$^{\ominus}$ (Energy = −1197.94537558)



Stoichiometry C24H16N5(1-)
Framework group C1[X(C24H16N5)]
Deg. of freedom 129
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.716257	2.017759	-0.000045
2	7	0	-1.022309	2.331923	0.000175
3	7	0	-2.804509	-0.356316	0.000057
4	7	0	2.636250	-1.133614	0.000022
5	6	0	1.983321	-3.541627	0.000172
6	6	0	-3.523009	-1.509885	0.000090
7	6	0	0.565879	-3.547635	-0.000432
8	6	0	-3.484902	2.035626	0.000868
9	6	0	1.172630	3.282221	-0.000461
10	6	0	-5.081556	0.111800	0.000606
11	6	0	-2.995171	-2.817243	-0.000299
12	6	0	-0.171820	-4.812879	-0.001140
13	6	0	-4.954589	-1.244324	0.000490
14	6	0	-2.314879	2.794060	0.000558
15	6	0	-3.724083	0.645851	0.000683
16	6	0	-0.245753	3.426343	-0.000144
17	6	0	2.247784	4.187728	-0.001233
18	6	0	2.895086	-2.503112	0.000510
19	6	0	-1.678350	-3.265546	-0.000623
20	6	0	-2.323935	4.250850	0.000346
21	6	0	4.873345	-1.367799	0.001470
22	6	0	4.325715	-2.620988	0.001444
23	6	0	3.095070	2.064166	-0.000306
24	6	0	-1.017623	4.652288	-0.000315
25	6	0	4.001988	0.979503	0.000140
26	6	0	3.427931	3.442004	-0.001149
27	6	0	3.814947	-0.392767	0.000453
28	1	0	-5.991635	0.702744	0.000808
29	1	0	0.297159	-5.797192	-0.001346
30	1	0	-5.736940	-1.995721	0.000543
31	1	0	2.155387	5.265816	-0.001819
32	1	0	-3.211757	4.874471	0.000536
33	1	0	5.924101	-1.105673	0.002214
34	1	0	4.848195	-3.569505	0.002164
35	1	0	-0.626069	5.663058	-0.000697
36	1	0	4.442313	3.821237	-0.001664
37	1	0	5.045679	1.282295	0.000309
38	1	0	-4.396564	2.634226	0.001125
39	1	0	-3.729795	-3.620916	-0.000399
40	1	0	2.448613	-4.526572	0.000426
41	7	0	-1.466439	-4.671598	-0.001248
42	6	0	-0.438551	-2.568604	-0.000659
43	1	0	-0.369472	-1.488350	-0.000287
44	1	0	1.700534	-0.762289	-0.002101
45	1	0	1.088643	1.225109	0.001032

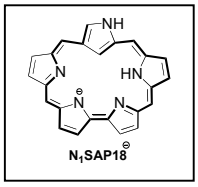
$N_1SAP17^{\ominus}$ (Energy = −1197.94584085)



Stoichiometry C24H16N5(1-)
Framework group C1[X(C24H16N5)]
Deg. of freedom 129
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.716257	2.017759	-0.000045
2	7	0	-1.022309	2.331923	0.000175
3	7	0	-2.804509	-0.356316	0.000057
4	7	0	2.636250	-1.133614	0.000022
5	6	0	1.983321	-3.541627	0.000172
6	6	0	-3.523009	-1.509885	0.000090
7	6	0	0.565879	-3.547635	-0.000432
8	6	0	-3.484902	2.035626	0.000868
9	6	0	1.172630	3.282221	-0.000461
10	6	0	-5.081556	0.111800	0.000606
11	6	0	-2.995171	-2.817243	-0.000299
12	6	0	-0.171820	-4.812879	-0.001140
13	6	0	-4.954589	-1.244324	0.000490
14	6	0	-2.314879	2.794060	0.000558
15	6	0	-3.724083	0.645851	0.000682
16	6	0	-0.245753	3.426343	-0.000144
17	6	0	2.247784	4.187728	-0.001233
18	6	0	2.895086	-2.503112	0.000510
19	6	0	-1.678350	-3.265546	-0.000623
20	6	0	-2.323935	4.250850	0.000346
21	6	0	4.873345	-1.367799	0.001470
22	6	0	4.325715	-2.620988	0.001444
23	6	0	3.095070	2.064166	-0.000306
24	6	0	-1.017623	4.652288	-0.000315
25	6	0	4.001988	0.979503	0.000140
26	6	0	3.427931	3.442004	-0.001149
27	6	0	3.814947	-0.392767	0.000453
28	1	0	-5.991635	0.702744	0.000808
29	1	0	0.297159	-5.797192	-0.001346
30	1	0	-5.736940	-1.995721	0.000543
31	1	0	2.155387	5.265816	-0.001819
32	1	0	-3.211757	4.874471	0.000536
33	1	0	5.924101	-1.105673	0.002214
34	1	0	4.848195	-3.569505	0.002163
35	1	0	-0.626069	5.663058	-0.000697
36	1	0	4.442313	3.821237	-0.001664
37	1	0	5.045679	1.282295	0.000309
38	1	0	-4.396564	2.634226	0.001125
39	1	0	-3.729795	-3.620916	-0.000399
40	1	0	2.448613	-4.526572	0.000426
41	7	0	-1.466439	-4.671598	-0.001248
42	6	0	-0.438551	-2.568604	-0.000659
43	1	0	-0.369472	-1.488350	-0.000287
44	1	0	1.700534	-0.762289	-0.002101
45	1	0	1.088643	1.225109	0.001032

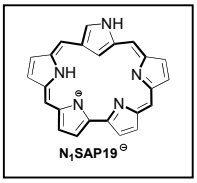
N_1SAP18$^{\ominus}$ (Energy = −1197.92338643)



Stoichiometry C24H16N5(1-)
Framework group C1[X(C24H16N5)]
Deg. of freedom 129
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.756245	2.250098	-0.000020
2	7	0	2.110795	1.525434	-0.000051
3	7	0	2.603765	-1.254601	-0.000041
4	7	0	-2.957224	0.056282	0.000007
5	6	0	-3.496487	-2.318811	0.000016
6	6	0	2.552137	-2.634968	0.000034
7	6	0	-2.183664	-2.883681	-0.000040
8	6	0	4.325692	0.513663	0.000026
9	6	0	0.248903	3.135122	-0.000018
10	6	0	4.746589	-1.983650	0.000099
11	6	0	1.480801	-3.510259	0.000032
12	6	0	-2.006351	-4.274718	-0.000043
13	6	0	3.929768	-3.078852	0.000101
14	6	0	3.468215	1.636024	-0.000014
15	6	0	3.922665	-0.809516	0.000034
16	6	0	1.632540	2.795824	-0.000027
17	6	0	-0.249296	4.522078	0.000033
18	6	0	-3.852731	-0.986510	0.000022
19	6	0	0.064514	-3.341328	-0.000034
20	6	0	3.878326	3.021777	-0.000062
21	6	0	-5.132826	0.863492	0.000093
22	6	0	-5.230602	-0.489900	0.000048
23	6	0	-1.909652	2.989837	0.000008
24	6	0	2.719138	3.754190	-0.000008
25	6	0	-3.212127	2.510695	0.000027
26	6	0	-1.600725	4.427757	-0.000031
27	6	0	-3.694349	1.175195	0.000026
28	1	0	5.829749	-1.965205	0.000149
29	1	0	-2.745354	-5.065078	-0.000012
30	1	0	4.220328	-4.122624	0.000150
31	1	0	0.355289	5.421324	0.000062
32	1	0	4.900479	3.386014	-0.000082
33	1	0	-5.935889	1.593742	0.000140
34	1	0	-6.126881	-1.101588	0.000059
35	1	0	2.622156	4.833421	0.000011
36	1	0	-2.331183	5.230435	-0.000049
37	1	0	-3.988814	3.275335	0.000046
38	1	0	5.398474	0.692837	0.000061
39	1	0	1.798464	-4.552862	0.000096
40	1	0	-4.314804	-3.039233	0.000056
41	7	0	-0.682916	-4.535841	-0.000066
42	6	0	-0.869526	-2.302975	-0.000166
43	1	0	-0.677287	-1.238676	-0.000255
44	1	0	1.847490	-0.566699	-0.000127
45	1	0	-0.265154	-5.453672	-0.000054

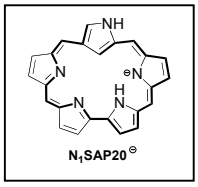
N_1SAP19$^{\ominus}$ (Energy = −1197.92222698)



Stoichiometry C24H16N5(1-)
Framework group C1[X(C24H16N5)]
Deg. of freedom 129
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.095639	1.534222	-0.000094
2	7	0	-0.775476	2.252047	-0.000058
3	7	0	-2.945684	0.050763	-0.000013
4	7	0	2.616354	-1.253637	0.000048
5	6	0	1.531741	-3.532471	0.000004
6	6	0	-3.823936	-0.997617	0.000018
7	6	0	0.102333	-3.404242	-0.000028
8	6	0	-3.231491	2.500203	0.000045
9	6	0	1.611206	2.803902	-0.000020
10	6	0	-5.131557	0.832204	0.000040
11	6	0	-3.445142	-2.329076	0.000011
12	6	0	-0.674180	-4.580168	-0.000071
13	6	0	-5.209604	-0.523262	0.000051
14	6	0	-1.927778	2.987280	0.000019
15	6	0	-3.698338	1.164446	0.000032
16	6	0	0.229900	3.140920	-0.000008
17	6	0	2.695504	3.767528	-0.000020
18	6	0	2.582992	-2.639033	0.000027
19	6	0	-2.126547	-2.853165	-0.000024
20	6	0	-1.624241	4.425910	-0.000002
21	6	0	4.769031	-1.954883	0.000050
22	6	0	3.969587	-3.060424	0.000057
23	6	0	3.451004	1.650976	0.000009
24	6	0	-0.272480	4.525281	0.000000
25	6	0	4.317716	0.535803	0.000046
26	6	0	3.856182	3.040394	-0.000055
27	6	0	3.926503	-0.791275	0.000047
28	1	0	-5.945454	1.550268	0.000053
29	1	0	-0.348852	-5.612225	-0.000084
30	1	0	-6.097339	-1.147586	0.000071
31	1	0	2.593587	4.846241	-0.000009
32	1	0	-2.357179	5.226410	0.000004
33	1	0	5.851769	-1.919013	0.000056
34	1	0	4.275059	-4.099880	0.000067
35	1	0	0.328436	5.426993	0.000005
36	1	0	4.877141	3.407908	-0.000070
37	1	0	5.388803	0.724180	0.000057
38	1	0	-4.012998	3.259852	0.000072
39	1	0	-4.249878	-3.065556	0.000034
40	1	0	1.870120	-4.567761	0.000007
41	7	0	-1.980619	-4.246929	-0.000042
42	6	0	-0.829747	-2.318860	-0.000074
43	1	0	-0.633280	-1.255084	-0.000092
44	1	0	1.850298	-0.577691	0.000062
45	1	0	-2.753670	-4.894529	-0.000037

N_1SAP20$^{\ominus}$ (Energy = −1197.93059533)

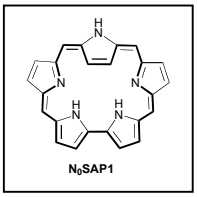


Stoichiometry C24H16N5(1-)
Framework group C1[X(C24H16N5)]
Deg. of freedom 129
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.800599	2.293593	-0.000207
2	7	0	2.045638	1.677071	-0.000212
3	7	0	2.546950	-1.211296	0.000045
4	7	0	-2.919625	-0.035756	0.000125
5	6	0	-3.387593	-2.433046	0.000033
6	6	0	2.627725	-2.577590	0.000057
7	6	0	-2.064887	-2.970435	-0.000128
8	6	0	4.247360	0.570665	0.000130
9	6	0	0.146490	3.245564	-0.000081
10	6	0	4.780983	-1.883259	0.000239
11	6	0	1.605311	-3.517063	-0.000002
12	6	0	-1.861427	-4.361559	-0.000247
13	6	0	4.030487	-3.010405	0.000222
14	6	0	3.420947	1.703744	0.000035
15	6	0	3.835777	-0.765563	0.000105
16	6	0	1.531170	2.953632	-0.000053
17	6	0	-0.424050	4.591056	-0.000096
18	6	0	-3.777645	-1.107608	0.000107
19	6	0	0.189599	-3.390534	-0.000144
20	6	0	3.796960	3.078820	0.000112
21	6	0	-5.124287	0.695716	0.000245
22	6	0	-5.172403	-0.660009	0.000373
23	6	0	-1.996692	2.960929	-0.000009
24	6	0	2.639435	3.839611	-0.000066
25	6	0	-3.275058	2.409866	0.000098
26	6	0	-1.771031	4.409583	-0.000217
27	6	0	-3.698976	1.059042	0.000143
28	1	0	5.862084	-1.791580	0.000338
29	1	0	-2.588029	-5.163714	-0.000244
30	1	0	4.365490	-4.042753	0.000299
31	1	0	0.125765	5.525189	-0.000085
32	1	0	4.819997	3.434211	0.000244
33	1	0	-5.952928	1.396813	0.000293
34	1	0	-6.045599	-1.304312	0.000522
35	1	0	2.565523	4.919309	-0.000089
36	1	0	-2.547629	5.167490	-0.000296
37	1	0	-4.086054	3.138053	0.000127
38	1	0	5.317595	0.761309	0.000269
39	1	0	1.956276	-4.550313	0.000080
40	1	0	-4.190859	-3.170241	0.000129
41	7	0	-0.536750	-4.600571	-0.000227
42	6	0	-0.763518	-2.369717	-0.000377
43	1	0	-0.569471	-1.308179	-0.000507
44	1	0	1.513187	0.809852	-0.000394
45	1	0	-0.102698	-5.511056	-0.000217

Cartesian coordinates for the optimized structures of normal sapphyrins (neutral)

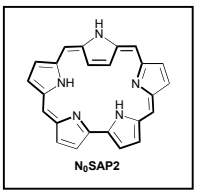
N_0SAP1 (Energy = –1198.49627292)



Stoichiometry C24H17N5
Framework group C1[X(C24H17N5)]
Deg. of freedom 132
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.591864	1.720359	0.001491
2	7	0	-1.591866	1.720358	0.001491
3	7	0	-2.957666	-0.768494	-0.051832
4	7	0	2.957668	-0.768493	-0.051823
5	6	0	2.427664	-3.133019	-0.147680
6	6	0	-3.345466	-2.058592	-0.198207
7	6	0	-4.052826	1.380937	-0.127060
8	6	0	0.711782	2.779378	0.051849
9	6	0	-5.250768	-0.859670	-0.387944
10	6	0	-2.427662	-3.133019	-0.147683
11	6	0	-4.782631	-2.138054	-0.439376
12	6	0	-2.901085	2.179799	-0.032379
13	6	0	-4.086256	-0.011460	-0.162128
14	6	0	-0.711784	2.779377	0.051851
15	6	0	1.506250	3.962027	0.068484
16	6	0	3.345467	-2.058591	-0.198203
17	6	0	-2.834234	3.596640	0.013959
18	6	0	5.250769	-0.859667	-0.387943
19	6	0	4.782633	-2.138052	-0.439373
20	6	0	2.901083	2.179801	-0.032384
21	6	0	-1.506253	3.962026	0.068492
22	6	0	4.052825	1.380939	-0.127064
23	6	0	2.834231	3.596642	0.013949
24	6	0	4.086256	-0.011458	-0.162126
25	1	0	-1.415012	0.716273	-0.035149
26	1	0	-6.271280	-0.517272	-0.512818
27	1	0	-5.348437	-3.049695	-0.590451
28	1	0	1.115486	4.968219	0.108624
29	1	0	-3.694574	4.252597	0.005108
30	1	0	6.271280	-0.517268	-0.512818
31	1	0	5.348440	-3.049693	-0.590448
32	1	0	-1.115490	4.968218	0.108638
33	1	0	3.694571	4.252600	0.005092
34	1	0	4.993798	1.919334	-0.198537
35	1	0	-4.993800	1.919331	-0.198529
36	1	0	-2.712232	-4.090550	-0.577857
37	1	0	2.712236	-4.090549	-0.577854
38	1	0	1.415011	0.716274	-0.035141
39	6	0	-0.682922	-1.892179	1.203199
40	6	0	0.682922	-1.892180	1.203202
41	6	0	1.136824	-2.930916	0.326834
42	6	0	-1.136822	-2.930916	0.326832
43	7	0	0.000001	-3.637825	-0.056669
44	1	0	1.348163	-1.260856	1.770212
45	1	0	-1.348163	-1.260854	1.770208
46	1	0	0.000002	-4.236196	-0.871495

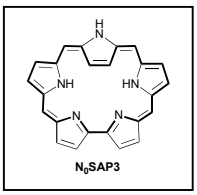
N_0SAP2 (Energy = −1198.49991206)



Stoichiometry C24H17N5
Framework group C1[X(C24H17N5)]
Deg. of freedom 132
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.556548	1.686029	-0.002756
2	7	0	-1.537878	1.753747	0.016413
3	7	0	-2.952855	-0.754990	-0.062929
4	7	0	2.987744	-0.800935	-0.055166
5	6	0	2.392847	-3.180349	-0.122324
6	6	0	-3.368621	-2.034983	-0.227228
7	6	0	-4.005155	1.417961	-0.105651
8	6	0	0.763508	2.779524	0.051553
9	6	0	-5.246745	-0.794333	-0.399403
10	6	0	-2.468276	-3.124107	-0.184393
11	6	0	-4.806125	-2.081963	-0.470843
12	6	0	-2.848591	2.205146	-0.004002
13	6	0	-4.063987	0.025091	-0.161084
14	6	0	-0.663032	2.811086	0.070550
15	6	0	1.548904	4.006428	0.043317
16	6	0	3.328332	-2.129488	-0.174725
17	6	0	-2.786462	3.624861	0.059816
18	6	0	5.208204	-0.859721	-0.372585
19	6	0	4.741470	-2.159399	-0.387758
20	6	0	2.846979	2.172942	-0.062941
21	6	0	-1.460138	3.993568	0.107965
22	6	0	4.011323	1.402710	-0.161812
23	6	0	2.850875	3.622044	-0.033967
24	6	0	4.091437	0.008004	-0.182067
25	1	0	-1.319561	0.762291	-0.041793
26	1	0	-6.259634	-0.428389	-0.519961
27	1	0	-5.391463	-2.978862	-0.635150
28	1	0	1.162394	5.015921	0.079343
29	1	0	-3.651012	4.275578	0.066625
30	1	0	6.232154	-0.530229	-0.491599
31	1	0	5.323818	-3.064163	-0.502233
32	1	0	-1.070227	4.999432	0.159854
33	1	0	3.732579	4.250544	-0.068566
34	1	0	4.950243	1.942381	-0.248635
35	1	0	-4.940062	1.968737	-0.165489
36	1	0	-2.760170	-4.071818	-0.631223
37	1	0	2.678375	-4.140879	-0.542303
38	6	0	-0.730404	-1.926320	1.206681
39	6	0	0.636957	-1.937853	1.224324
40	6	0	1.094571	-2.964228	0.336989
41	6	0	-1.180745	-2.943905	0.309010
42	7	0	-0.042100	-3.649403	-0.079171
43	1	0	1.284403	-1.325146	1.834835
44	1	0	-1.394017	-1.296543	1.776669
45	1	0	-0.035989	-4.227390	-0.908434
46	1	0	2.055190	-0.388890	-0.033202

N_0SAP3 (Energy = −1198.49422863)

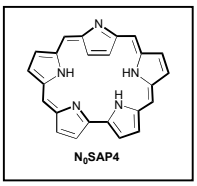


Stoichiometry C24H17N5
Framework group C1[X(C24H17N5)]
Deg. of freedom 132
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.552872	1.662324	0.012048
2	7	0	-1.552860	1.662328	0.012060
3	7	0	-3.011865	-0.759549	-0.067444
4	7	0	3.011861	-0.759555	-0.067483
5	6	0	2.434455	-3.139924	-0.160554
6	6	0	-3.364361	-2.083449	-0.201603
7	6	0	-4.009111	1.452881	-0.133663
8	6	0	0.718517	2.722628	0.064504
9	6	0	-5.235309	-0.797361	-0.368135
10	6	0	-2.434471	-3.139917	-0.160571
11	6	0	-4.778503	-2.101054	-0.405261
12	6	0	-2.827303	2.190994	-0.033411
13	6	0	-4.109633	0.056984	-0.173615
14	6	0	-0.718501	2.722630	0.064503
15	6	0	1.474119	3.977893	0.073220
16	6	0	3.364351	-2.083461	-0.201598
17	6	0	-2.787234	3.641138	0.007171
18	6	0	5.235309	-0.797384	-0.368124
19	6	0	4.778496	-2.101076	-0.405237
20	6	0	2.827317	2.190985	-0.033425
21	6	0	-1.474099	3.977897	0.073199
22	6	0	4.009122	1.452868	-0.133683
23	6	0	2.787253	3.641129	0.007183
24	6	0	4.109636	0.056970	-0.173632
25	1	0	-6.257473	-0.458359	-0.474919
26	1	0	-5.368939	-2.999657	-0.526762
27	1	0	1.059781	4.975212	0.115069
28	1	0	-3.648656	4.297860	-0.012967
29	1	0	6.257477	-0.458391	-0.474897
30	1	0	5.368929	-2.999684	-0.526714
31	1	0	-1.059756	4.975216	0.115020
32	1	0	3.648678	4.297849	-0.012942
33	6	0	-0.684090	-1.924565	1.213464
34	6	0	0.684063	-1.924571	1.213475
35	6	0	1.138856	-2.935429	0.311003
36	6	0	-1.138876	-2.935428	0.310996
37	7	0	-0.000009	-3.620388	-0.105837
38	1	0	1.330166	-1.307703	1.820463
39	1	0	-1.330198	-1.307692	1.820442
40	1	0	-0.000007	-4.185602	-0.943688
41	1	0	2.077380	-0.343345	-0.049793
42	1	0	-2.077384	-0.343342	-0.049712
43	1	0	-2.721505	-4.094285	-0.593451
44	1	0	2.721487	-4.094298	-0.593422
45	1	0	4.938388	2.010903	-0.206192
46	1	0	-4.938373	2.010921	-0.206185

N_0SAP4 (Energy = −1198.48755087)

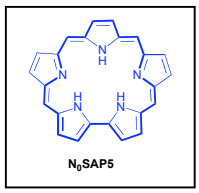


Stoichiometry C24H17N5
Framework group C1[X(C24H17N5)]
Deg. of freedom 132
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.757859	1.600208	0.086634
2	7	0	-1.236584	1.903988	0.041887
3	7	0	-3.049002	-0.646175	-0.111810
4	7	0	2.869467	-1.034213	-0.054405
5	6	0	1.994401	-3.315914	-0.300636
6	6	0	-3.607688	-1.920407	-0.158078
7	6	0	-3.756179	1.704472	-0.156181
8	6	0	1.097590	2.777951	0.092082
9	6	0	-5.267714	-0.356522	-0.206447
10	6	0	-2.804389	-3.054260	-0.121328
11	6	0	-5.025183	-1.709970	-0.233174
12	6	0	-2.530972	2.400259	-0.090383
13	6	0	-4.010967	0.340106	-0.156269
14	6	0	-0.313800	2.933792	0.026321
15	6	0	2.014970	3.908277	0.121132
16	6	0	3.047055	-2.384457	-0.273156
17	6	0	-2.391880	3.809765	-0.200798
18	6	0	5.072981	-1.346725	-0.336329
19	6	0	4.450016	-2.571809	-0.468272
20	6	0	3.098049	1.932451	0.087678
21	6	0	-1.049749	4.132941	-0.127801
22	6	0	4.160175	1.031159	-0.003101
23	6	0	3.265681	3.375162	0.122405
24	6	0	4.064201	-0.363836	-0.102403
25	1	0	-6.233677	0.131841	-0.201774
26	1	0	-5.761201	-2.503026	-0.242135
27	1	0	1.739661	4.954628	0.139731
28	1	0	-3.221903	4.488794	-0.344716
29	1	0	6.132459	-1.138359	-0.407650
30	1	0	4.919174	-3.530642	-0.645049
31	1	0	-0.615327	5.119429	-0.205020
32	1	0	4.214569	3.897507	0.136550
33	6	0	-0.952053	-1.925295	1.207222
34	6	0	0.400784	-1.986596	1.158854
35	6	0	0.716762	-3.032615	0.185633
36	6	0	-1.438729	-2.934852	0.254896
37	7	0	-0.421708	-3.646059	-0.270268
38	1	0	1.109341	-1.452767	1.777702
39	1	0	-1.567626	-1.339469	1.877210
40	1	0	1.992594	-0.516619	-0.024685
41	1	0	-2.089131	-0.506429	-0.383009
42	1	0	-0.963270	0.966224	0.300666
43	1	0	2.165831	-4.265870	-0.799060
44	1	0	-3.195632	-4.003991	-0.472669
45	1	0	5.161645	1.450222	-0.040266
46	1	0	-4.627900	2.345839	-0.241280

N_0SAP5 (Energy = –1198.51779866)

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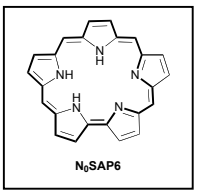
Stoichiometry    C24H17N5
Framework group  C1[X(C24H17N5)]
Deg. of freedom   132
Full point group                 C1
Largest Abelian subgroup         C1      NOp   1
Largest concise Abelian subgroup C1      NOp   1
                         Standard orientation:
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.529991	-2.064097	0.000055
2	7	0	1.529953	-2.064119	0.000056
3	7	0	2.752343	0.589580	-0.000063
4	7	0	-2.752334	0.589620	-0.000109
5	6	0	-2.484531	3.076031	0.000093
6	6	0	3.207121	1.869794	-0.000084
7	6	0	-1.137606	3.413463	0.000080
8	6	0	3.934886	-1.579105	0.000003
9	6	0	-0.705633	-3.162631	0.000031
10	6	0	5.091455	0.630105	-0.000101
11	6	0	2.484588	3.075995	-0.000058
12	6	0	-0.681814	4.774956	0.000129
13	6	0	4.667718	1.916421	-0.000100
14	6	0	0.681894	4.774947	0.000072
15	6	0	2.852187	-2.460416	0.000044
16	6	0	3.888660	-0.187480	-0.000043
17	6	0	0.705578	-3.162642	0.000063
18	6	0	-1.546221	-4.309758	-0.000013
19	6	0	-3.207088	1.869843	0.000012
20	6	0	1.137668	3.413448	0.000000
21	6	0	2.857239	-3.880405	0.000103
22	6	0	-5.091445	0.630189	-0.000100
23	6	0	-4.667684	1.916497	0.000006
24	6	0	-2.852232	-2.460373	-0.000041
25	6	0	1.546149	-4.309781	0.000094
26	6	0	-3.934917	-1.579044	-0.000062
27	6	0	-2.857305	-3.880363	-0.000057
28	6	0	-3.888666	-0.187419	-0.000052
29	1	0	1.303076	-1.071435	0.000082
30	1	0	6.106101	0.250854	-0.000116
31	1	0	-1.346988	5.628312	0.000196
32	1	0	5.261147	2.822787	-0.000117
33	1	0	1.347079	5.628294	0.000088
34	1	0	-1.194707	-5.331717	-0.000027
35	1	0	3.749208	-4.492406	0.000129
36	1	0	-6.106099	0.250957	-0.000142
37	1	0	-5.261096	2.822874	0.000057
38	1	0	1.194620	-5.331735	0.000118
39	1	0	-3.749283	-4.492351	-0.000109
40	1	0	-4.919086	-2.038610	-0.000101
41	1	0	4.919047	-2.038688	0.000003
42	1	0	3.121910	3.956723	-0.000063
43	1	0	-3.121839	3.956770	0.000167
44	7	0	0.000026	2.623738	0.000007
45	1	0	0.000021	1.614101	-0.000048
46	1	0	-1.303101	-1.071414	0.000144

N_0SAP6 (Energy = −1198.49393723)

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Stoichiometry    C24H17N5
Framework group  C1[X(C24H17N5)]
Deg. of freedom   132
Full point group                 C1
Largest Abelian subgroup         C1      NOp   1
Largest concise Abelian subgroup C1      NOp   1
                       Standard orientation:
```
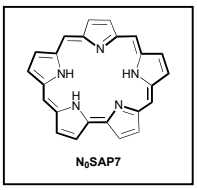

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.636597	-0.728915	-0.019637
2	7	0	-0.496345	-2.439813	0.067510
3	7	0	2.534989	-1.152434	0.061562
4	7	0	-1.631175	2.214913	0.014000
5	6	0	0.303884	3.846752	0.030826
6	6	0	3.802440	-0.654470	-0.008694
7	6	0	1.557023	3.226462	-0.091923
8	6	0	1.725340	-3.519016	0.213927
9	6	0	-2.843489	-2.079898	-0.134772
10	6	0	4.113591	-2.864259	0.183225
11	6	0	4.148220	0.694039	-0.140886
12	6	0	2.748602	4.010589	-0.225475
13	6	0	4.807847	-1.706919	0.063942
14	6	0	3.826503	3.168358	-0.284987
15	6	0	0.335084	-3.521773	0.141058
16	6	0	2.696250	-2.499936	0.168888
17	6	0	-1.733477	-2.954583	-0.048635
18	6	0	-4.232151	-2.273642	-0.318376
19	6	0	-1.031757	3.467221	0.123732
20	6	0	3.347408	1.830538	-0.182435
21	6	0	-0.434518	-4.764616	0.081639
22	6	0	-3.284253	3.724333	0.352284
23	6	0	-2.091862	4.398050	0.363516
24	6	0	-3.829740	-0.041195	-0.089793
25	6	0	-1.740405	-4.406754	-0.050202
26	6	0	-3.987400	1.346493	0.016486
27	6	0	-4.837028	-1.025722	-0.289578
28	6	0	-3.026010	2.342261	0.109803
29	1	0	4.496361	-3.874852	0.262972
30	1	0	2.749380	5.091591	-0.270532
31	1	0	5.880513	-1.558973	0.028732
32	1	0	4.870997	3.432517	-0.383891
33	1	0	-4.713882	-3.230295	-0.466291
34	1	0	-0.017018	-5.763815	0.120982
35	1	0	-4.272086	4.130412	0.526455
36	1	0	-1.933684	5.453262	0.543145
37	1	0	-2.609084	-5.048004	-0.131349
38	1	0	-5.888913	-0.804982	-0.415295
39	7	0	1.963267	1.903703	-0.086933
40	1	0	1.416072	1.059968	0.055872
41	1	0	-1.730605	-0.394109	0.279525
42	1	0	-1.193393	1.458994	-0.494688
43	1	0	0.408831	4.927201	0.075579
44	1	0	5.212885	0.903116	-0.208698
45	1	0	2.158460	-4.515870	0.281069
46	1	0	-5.014410	1.697779	0.039477

N_0SAP7 (Energy = –1198.51321526)

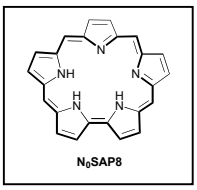


Stoichiometry C24H17N5
Framework group C1[X(C24H17N5)]
Deg. of freedom 132
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.006765	-2.526380	-0.000303
2	7	0	2.426043	-1.043897	0.000229
3	7	0	2.057853	1.887341	0.000033
4	7	0	-2.783368	-0.740910	-0.000756
5	6	0	-3.916017	1.460580	-0.000693
6	6	0	1.661760	3.205597	0.000176
7	6	0	-2.863148	2.388127	-0.000477
8	6	0	4.203918	0.634078	0.000158
9	6	0	1.234957	-3.140886	-0.000325
10	6	0	3.937991	3.136376	0.000509
11	6	0	0.393158	3.799691	0.000039
12	6	0	-3.159929	3.817251	-0.000130
13	6	0	2.862393	3.987272	0.000396
14	6	0	-1.963760	4.443390	0.000052
15	6	0	3.748121	-0.680922	0.000007
16	6	0	3.438231	1.801618	0.000228
17	6	0	2.432930	-2.392948	-0.000235
18	6	0	0.999804	-4.536883	-0.000146
19	6	0	-3.898761	0.073029	-0.000504
20	6	0	-0.944250	3.391062	-0.000050
21	6	0	4.607080	-1.853244	-0.000374
22	6	0	-4.593567	-2.083454	0.000838
23	6	0	-5.039766	-0.790501	0.000357
24	6	0	-1.009099	-3.458946	0.000363
25	6	0	3.778515	-2.934476	-0.000525
26	6	0	-2.390552	-3.235571	0.000546
27	6	0	-0.369074	-4.731614	0.000251
28	6	0	-3.158530	-2.077752	0.000261
29	1	0	4.989087	3.393058	0.000753
30	1	0	-4.153395	4.248993	-0.000035
31	1	0	2.874087	5.069187	0.000491
32	1	0	-1.756649	5.506786	0.000291
33	1	0	1.769541	-5.295921	-0.000306
34	1	0	5.690282	-1.840735	-0.000604
35	1	0	-5.186610	-2.988655	0.001478
36	1	0	-6.063864	-0.441758	0.000463
37	1	0	4.046909	-3.983208	-0.000844
38	1	0	-0.898345	-5.675368	0.000359
39	7	0	-1.519410	2.145992	-0.000260
40	1	0	-0.063446	-1.519847	0.001198
41	1	0	-1.858829	-0.327367	-0.000467
42	1	0	1.469047	1.061258	-0.000282
43	1	0	0.485286	4.883200	0.000091
44	1	0	-4.912842	1.892707	-0.000714
45	1	0	-2.979745	-4.147741	0.001000
46	1	0	5.279881	0.785150	0.000203

N_0SAP8 (Energy = −1198.50070611)



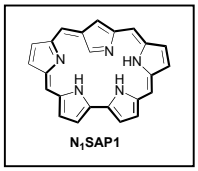
Stoichiometry C24H17N5
Framework group C1[X(C24H17N5)]
Deg. of freedom 132
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.166424	-2.431448	0.004366
2	7	0	-2.500556	-1.100653	-0.066042
3	7	0	-2.186028	1.658325	-0.002514
4	7	0	2.875141	-0.573974	-0.039944
5	6	0	3.899841	1.666413	-0.109810
6	6	0	-1.848217	2.968887	0.082764
7	6	0	2.777378	2.504736	-0.011050
8	6	0	-4.340297	0.487686	-0.152470
9	6	0	-1.048956	-3.088815	0.068348
10	6	0	-4.111183	2.984737	-0.034895
11	6	0	-0.595331	3.612770	0.156769
12	6	0	2.939956	3.952787	0.053163
13	6	0	-3.045976	3.814491	0.070852
14	6	0	1.690575	4.454501	0.148777
15	6	0	-3.848371	-0.818576	-0.143299
16	6	0	-3.559247	1.641401	-0.073684
17	6	0	-2.304337	-2.455021	-0.017161
18	6	0	-0.765649	-4.460457	0.254119
19	6	0	3.955958	0.282420	-0.131074
20	6	0	0.770967	3.309096	0.125073
21	6	0	-4.532670	-2.064852	-0.163392
22	6	0	4.736336	-1.843535	-0.155427
23	6	0	5.127916	-0.534915	-0.217243
24	6	0	1.209399	-3.339046	0.107027
25	6	0	-3.587257	-3.067916	-0.081583
26	6	0	2.583672	-3.074860	0.052296
27	6	0	0.608851	-4.613102	0.277813
28	6	0	3.305642	-1.892861	-0.036104
29	1	0	-5.164369	3.234162	-0.078292
30	1	0	3.886246	4.479456	0.030189
31	1	0	-3.040446	4.896345	0.129050
32	1	0	1.383462	5.491219	0.216196
33	1	0	-1.510968	-5.232893	0.382360
34	1	0	-5.606360	-2.179459	-0.229535
35	1	0	5.362734	-2.725016	-0.197308
36	1	0	6.133310	-0.147028	-0.313008
37	1	0	-3.762679	-4.134791	-0.082164
38	1	0	1.163122	-5.530917	0.421546
39	7	0	1.467730	2.130039	0.037247
40	1	0	0.266876	-1.479140	-0.316005
41	1	0	1.951437	-0.185807	0.126663
42	1	0	-1.844251	-0.314763	0.014691
43	1	0	-0.737596	4.689268	0.230621
44	1	0	4.862799	2.166176	-0.164495
45	1	0	3.201978	-3.966908	0.082849
46	1	0	-5.418248	0.608255	-0.204003

Cartesian coordinates for the optimized structures of confused sapphyrins (neutral)

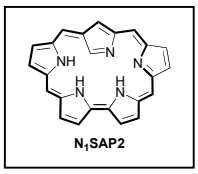
N_1SAP1 (Energy = –1198.49635445)



Stoichiometry C24H17N5
Framework group C1[X(C24H17N5)]
Deg. of freedom 132
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.822912	-1.782392	0.895856
2	7	0	2.933879	-0.863530	-0.081785
3	7	0	-3.099873	-0.763834	0.113686
4	6	0	-1.254972	-2.985166	0.263008
5	6	0	-0.142581	-3.803496	-0.016380
6	6	0	0.477020	-1.833577	0.925489
7	6	0	1.004231	-3.044128	0.303272
8	6	0	2.362755	-3.235986	0.003909
9	6	0	3.286420	-2.185415	-0.094949
10	6	0	4.729438	-2.321301	-0.243508
11	6	0	5.234738	-1.056856	-0.276235
12	6	0	4.088691	-0.161593	-0.180125
13	6	0	4.123685	1.243071	-0.207252
14	6	0	3.021358	2.094144	-0.138370
15	6	0	3.014096	3.520258	-0.108868
16	6	0	1.710385	3.942541	-0.017290
17	6	0	0.861067	2.791452	0.004602
18	6	0	-0.548760	2.839651	0.072138
19	6	0	-1.330442	4.021359	0.186931
20	6	0	-2.661485	3.668299	0.184027
21	6	0	-2.761207	2.252820	0.070068
22	6	0	-3.953911	1.518398	-0.031067
23	6	0	-4.110719	0.132917	-0.102886
24	6	0	-5.246345	-0.643715	-0.516933
25	6	0	-4.869007	-1.968674	-0.566337
26	6	0	-3.498911	-2.058829	-0.159072
27	6	0	-2.606601	-3.132343	-0.101192
28	1	0	-0.164914	-4.759293	-0.524811
29	1	0	1.072025	-1.075487	1.415947
30	1	0	5.272464	-3.257947	-0.286028
31	1	0	6.270862	-0.752942	-0.366796
32	1	0	3.901807	4.137580	-0.146842
33	1	0	1.361406	4.964468	0.022006
34	1	0	-0.928230	5.020750	0.271056
35	1	0	-3.513383	4.330353	0.263222
36	1	0	-6.205263	-0.227012	-0.796476
37	1	0	-5.477438	-2.807722	-0.878110
38	1	0	2.716039	-4.237371	-0.236098
39	1	0	-2.956298	-4.100830	-0.446703
40	1	0	-4.855806	2.116519	-0.112809
41	1	0	5.093885	1.726676	-0.276556
42	7	0	-1.448982	1.783691	0.029164
43	7	0	1.692633	1.694620	-0.070591
44	1	0	-1.194304	0.829236	-0.183739
45	1	0	1.477798	0.697805	-0.079025
46	1	0	-2.227518	-0.647658	0.639566

N_1SAP2 (Energy = −1198.47727029)

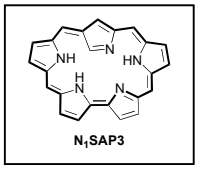


Stoichiometry C24H17N5
Framework group C1[X(C24H17N5)]
Deg. of freedom 132
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.384871	-1.914409	0.932492
2	7	0	3.113053	-0.600811	-0.135632
3	7	0	-2.872133	-0.988856	-0.081134
4	6	0	-0.706512	-3.011834	0.098261
5	6	0	0.478492	-3.714410	-0.280531
6	6	0	0.913401	-1.895576	0.984020
7	6	0	1.551932	-2.956417	0.185979
8	6	0	2.958809	-3.022814	-0.031031
9	6	0	3.712886	-1.862894	-0.071469
10	6	0	5.125352	-1.610993	-0.018753
11	6	0	5.330690	-0.253287	-0.032336
12	6	0	4.056766	0.409232	-0.124390
13	6	0	3.768146	1.762845	-0.169008
14	6	0	2.516022	2.418125	-0.151413
15	6	0	2.321323	3.809794	-0.316692
16	6	0	0.967593	4.084188	-0.229947
17	6	0	0.278352	2.871350	-0.010398
18	6	0	-1.130586	2.729740	0.098338
19	6	0	-2.047468	3.822473	0.163708
20	6	0	-3.324974	3.310329	0.200549
21	6	0	-3.232733	1.891956	0.152188
22	6	0	-4.273131	0.959755	0.074953
23	6	0	-4.109119	-0.422526	-0.057041
24	6	0	-5.145614	-1.430810	-0.231829
25	6	0	-4.488896	-2.615040	-0.384538
26	6	0	-3.065827	-2.315647	-0.255220
27	6	0	-2.011934	-3.253794	-0.314104
28	1	0	0.522616	-4.575829	-0.936002
29	1	0	1.442079	-1.225328	1.656195
30	1	0	5.878560	-2.381375	0.083713
31	1	0	6.278798	0.262941	0.046908
32	1	0	3.119060	4.515207	-0.507239
33	1	0	0.496265	5.049031	-0.351199
34	1	0	-1.763268	4.864746	0.188270
35	1	0	-4.252707	3.865175	0.247055
36	1	0	-6.214078	-1.251528	-0.244562
37	1	0	-4.915802	-3.599495	-0.535306
38	1	0	3.454194	-3.972209	-0.216457
39	1	0	-2.235107	-4.228537	-0.744421
40	1	0	-5.281614	1.363770	0.091117
41	1	0	4.621630	2.430635	-0.230577
42	7	0	-1.880016	1.580959	0.113263
43	7	0	1.242314	1.868035	0.011671
44	1	0	-1.607829	0.591694	0.068526
45	1	0	1.063475	0.947519	0.391019
46	1	0	2.207483	-0.493295	-0.567436

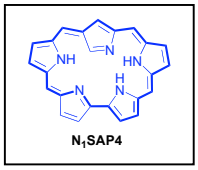
N_1SAP3 (Energy = −1198.49348361)



Stoichiometry C24H17N5
Framework group C1[X(C24H17N5)]
Deg. of freedom 132
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.488770	-1.961284	0.869400
2	7	0	3.055331	-0.665507	-0.153868
3	7	0	-2.904523	-1.029380	0.046772
4	6	0	-0.803875	-3.115069	0.115088
5	6	0	0.385402	-3.821319	-0.227537
6	6	0	0.809543	-1.926714	0.930199
7	6	0	1.452955	-3.026628	0.202103
8	6	0	2.860771	-3.092256	-0.007498
9	6	0	3.626497	-1.939675	-0.071072
10	6	0	5.044461	-1.718821	-0.024512
11	6	0	5.280473	-0.366857	-0.058640
12	6	0	4.022531	0.324162	-0.154541
13	6	0	3.778889	1.687219	-0.197907
14	6	0	2.559261	2.400213	-0.160449
15	6	0	2.440084	3.810547	-0.269554
16	6	0	1.102574	4.153031	-0.172943
17	6	0	0.354373	2.965215	-0.007313
18	6	0	-1.056394	2.821882	0.099305
19	6	0	-1.969424	3.960731	0.141466
20	6	0	-3.218859	3.431578	0.183823
21	6	0	-3.053939	1.983646	0.158695
22	6	0	-4.121684	1.093714	0.086634
23	6	0	-4.059079	-0.306840	-0.029228
24	6	0	-5.104888	-1.233881	-0.330192
25	6	0	-4.535338	-2.484304	-0.463067
26	6	0	-3.134968	-2.360607	-0.208967
27	6	0	-2.126030	-3.340290	-0.262005
28	1	0	0.442053	-4.720268	-0.828849
29	1	0	1.323949	-1.196588	1.546430
30	1	0	5.779576	-2.504986	0.088713
31	1	0	6.240089	0.128955	0.012128
32	1	0	3.278418	4.478395	-0.417455
33	1	0	0.681094	5.146278	-0.235300
34	1	0	-1.689816	5.006253	0.137110
35	1	0	-4.166439	3.955686	0.216621
36	1	0	-6.145733	-0.968097	-0.460104
37	1	0	-5.036720	-3.412227	-0.705229
38	1	0	3.354302	-4.046389	-0.172222
39	1	0	-2.399718	-4.305141	-0.680711
40	1	0	-5.117846	1.526810	0.057935
41	1	0	4.659844	2.318834	-0.258357
42	7	0	-1.715257	1.649093	0.126193
43	7	0	1.262599	1.921915	-0.013687
44	1	0	0.978327	0.981917	0.223572
45	1	0	2.149021	-0.542161	-0.578945
46	1	0	-1.996080	-0.643193	0.299660

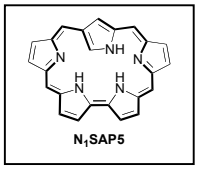
N_1SAP4 (Energy = −1198.50175515)



Stoichiometry C24H17N5
Framework group C1[X(C24H17N5)]
Deg. of freedom 132
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.859786	-1.829814	0.936459
2	7	0	2.964028	-0.894288	-0.106379
3	7	0	-3.089514	-0.746386	0.104380
4	6	0	-1.294234	-3.008613	0.271260
5	6	0	-0.183962	-3.820094	-0.037546
6	6	0	0.440544	-1.877393	0.954009
7	6	0	0.965277	-3.072687	0.299928
8	6	0	2.327477	-3.276299	0.006905
9	6	0	3.262895	-2.245944	-0.100500
10	6	0	4.689100	-2.328583	-0.225164
11	6	0	5.198388	-1.051237	-0.272678
12	6	0	4.099865	-0.134854	-0.206578
13	6	0	4.083344	1.262680	-0.234551
14	6	0	2.952032	2.083659	-0.149786
15	6	0	3.025243	3.535288	-0.113667
16	6	0	1.748039	3.981916	0.002771
17	6	0	0.904819	2.793272	0.021353
18	6	0	-0.506838	2.875087	0.093613
19	6	0	-1.291698	4.057328	0.198315
20	6	0	-2.620698	3.698918	0.181885
21	6	0	-2.711395	2.279868	0.070479
22	6	0	-3.906660	1.551753	-0.039657
23	6	0	-4.082860	0.168809	-0.112857
24	6	0	-5.232917	-0.585872	-0.528109
25	6	0	-4.881168	-1.917259	-0.576892
26	6	0	-3.513504	-2.033568	-0.165705
27	6	0	-2.646377	-3.127642	-0.105311
28	1	0	-0.207858	-4.758159	-0.577689
29	1	0	1.015538	-1.123414	1.479726
30	1	0	5.244906	-3.257116	-0.238165
31	1	0	6.238097	-0.760550	-0.346207
32	1	0	3.936214	4.119515	-0.161673
33	1	0	1.408941	5.007730	0.059712
34	1	0	-0.892001	5.057974	0.277847
35	1	0	-3.478454	4.355210	0.247110
36	1	0	-6.183314	-0.150415	-0.808184
37	1	0	-5.504876	-2.745266	-0.887903
38	1	0	2.680797	-4.278217	-0.225460
39	1	0	-3.012405	-4.084277	-0.466466
40	1	0	-4.803205	2.157608	-0.125676
41	1	0	5.046692	1.757686	-0.313728
42	7	0	-1.398598	1.820129	0.041799
43	7	0	1.644959	1.659671	-0.069175
44	1	0	2.052177	-0.444912	-0.146302
45	1	0	-2.216121	-0.640434	0.628767
46	1	0	-1.101035	0.870667	-0.134405

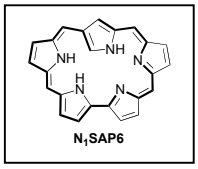
N_1SAP5 (Energy = −1198.49318193)



Stoichiometry C24H17N5
Framework group C1[X(C24H17N5)]
Deg. of freedom 132
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.573138	1.739002	0.024891
2	7	0	-1.598212	1.733451	-0.076013
3	7	0	-2.961465	-0.776694	-0.049891
4	7	0	2.965246	-0.777182	0.024350
5	6	0	2.509726	-3.161568	-0.222072
6	6	0	-3.384765	-2.091107	-0.071993
7	6	0	-4.048451	1.388734	-0.171925
8	6	0	0.686583	2.803432	0.031291
9	6	0	-5.270280	-0.857088	-0.228053
10	6	0	-2.527676	-3.175053	0.022481
11	6	0	-4.836979	-2.144837	-0.210441
12	6	0	-2.910171	2.185458	-0.129122
13	6	0	-4.073251	-0.021726	-0.136479
14	6	0	-0.717210	2.798910	-0.029578
15	6	0	1.490400	3.985381	0.130936
16	6	0	3.376472	-2.073857	-0.219920
17	6	0	-2.843160	3.615189	-0.117154
18	6	0	5.245415	-0.812322	-0.350456
19	6	0	4.808995	-2.096614	-0.472116
20	6	0	2.884956	2.191947	0.082571
21	6	0	-1.526110	3.983918	-0.052152
22	6	0	4.031917	1.403725	0.026959
23	6	0	2.810531	3.618079	0.162205
24	6	0	4.067913	-0.001194	-0.064076
25	1	0	-1.420504	0.731265	-0.107980
26	1	0	-6.287952	-0.495106	-0.315752
27	1	0	-5.430246	-3.050327	-0.256078
28	1	0	1.099509	4.991351	0.182517
29	1	0	-3.706670	4.266289	-0.146537
30	1	0	6.254024	-0.436850	-0.475679
31	1	0	5.394184	-2.981083	-0.693599
32	1	0	-1.138018	4.991943	-0.027255
33	1	0	3.670882	4.269680	0.237231
34	1	0	1.391206	0.753661	-0.139731
35	6	0	-0.599246	-1.904770	0.964464
36	6	0	1.145352	-3.058539	0.145440
37	6	0	-1.131330	-3.024929	0.275839
38	1	0	1.404943	-1.218099	1.123890
39	1	0	-1.128168	-1.142982	1.513819
40	1	0	-0.043878	-4.684912	-0.761800
41	7	0	0.727559	-1.944121	0.883352
42	6	0	-0.011766	-3.780725	-0.169013
43	1	0	-2.927559	-4.166772	-0.176425
44	1	0	2.877964	-4.122919	-0.567854
45	1	0	4.976878	1.938252	0.009752
46	1	0	-4.997639	1.912748	-0.231165

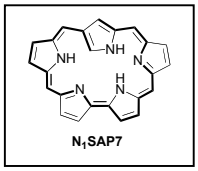
N_1SAP6 (Energy = −1198.47564864)



Stoichiometry C24H17N5
Framework group C1[X(C24H17N5)]
Deg. of freedom 132
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.479731	1.759346	0.176873
2	7	0	-1.456368	1.873891	-0.038484
3	7	0	-2.974847	-0.835093	-0.132659
4	7	0	2.971870	-0.903939	0.120945
5	6	0	2.482168	-3.225265	-0.292694
6	6	0	-3.429969	-2.162472	-0.016426
7	6	0	-3.934650	1.427405	-0.269468
8	6	0	0.791510	2.905470	0.129339
9	6	0	-5.231864	-0.755467	-0.086572
10	6	0	-2.583636	-3.237615	0.099381
11	6	0	-4.869862	-2.070520	0.009332
12	6	0	-2.776812	2.251782	-0.219951
13	6	0	-4.042363	0.055767	-0.193146
14	6	0	-0.626877	2.979369	-0.008445
15	6	0	1.661283	4.083446	0.179225
16	6	0	3.386219	-2.166847	-0.237855
17	6	0	-2.763159	3.663424	-0.322862
18	6	0	5.201271	-0.842361	-0.420811
19	6	0	4.798852	-2.135964	-0.585391
20	6	0	2.814129	2.134682	0.221566
21	6	0	-1.452138	4.106413	-0.189059
22	6	0	3.937231	1.325343	0.143386
23	6	0	2.923437	3.597065	0.244002
24	6	0	4.018561	-0.088515	-0.004117
25	1	0	-1.099241	0.950676	0.155485
26	1	0	-6.236346	-0.352925	-0.051812
27	1	0	-5.529068	-2.918281	0.145304
28	1	0	1.342920	5.117911	0.160567
29	1	0	-3.644984	4.269123	-0.484473
30	1	0	6.185168	-0.426325	-0.602398
31	1	0	5.393700	-2.981434	-0.909293
32	1	0	-1.105485	5.129405	-0.232967
33	1	0	3.852687	4.152910	0.284617
34	6	0	-0.600001	-1.917749	0.885282
35	6	0	1.120967	-3.088702	0.082374
36	6	0	-1.157574	-3.059112	0.250277
37	1	0	1.412313	-1.172300	0.870740
38	1	0	-1.100678	-1.142655	1.445859
39	1	0	-0.090168	-4.752784	-0.747988
40	7	0	0.724037	-1.949606	0.777891
41	6	0	-0.049636	-3.818877	-0.203109
42	1	0	-2.118154	-0.659487	-0.639203
43	1	0	-3.005465	-4.236488	0.037738
44	1	0	2.809994	-4.181397	-0.690981
45	1	0	4.888194	1.853833	0.115742
46	1	0	-4.868853	1.973836	-0.354444

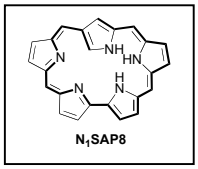
N_1SAP7 (Energy = −1198.49707010)



Stoichiometry C24H17N5
Framework group C1[X(C24H17N5)]
Deg. of freedom 132
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.530691	1.758820	0.047128
2	7	0	-1.558461	1.684572	-0.071350
3	7	0	-3.005236	-0.798655	-0.070624
4	7	0	2.970411	-0.770600	0.021584
5	6	0	2.538680	-3.151907	-0.245163
6	6	0	-3.374065	-2.138639	-0.049671
7	6	0	-4.017215	1.403421	-0.234104
8	6	0	0.650256	2.820234	0.069840
9	6	0	-5.251227	-0.847325	-0.228218
10	6	0	-2.505201	-3.201596	0.069819
11	6	0	-4.814779	-2.141755	-0.163150
12	6	0	-2.833895	2.169825	-0.167790
13	6	0	-4.099880	0.019435	-0.180565
14	6	0	-0.755858	2.789622	-0.010344
15	6	0	1.457262	4.002280	0.185537
16	6	0	3.396296	-2.058078	-0.245263
17	6	0	-2.840790	3.623254	-0.172446
18	6	0	5.242483	-0.766167	-0.392085
19	6	0	4.824801	-2.055950	-0.522729
20	6	0	2.844289	2.202426	0.106617
21	6	0	-1.544420	4.013311	-0.064111
22	6	0	3.996522	1.427169	0.033533
23	6	0	2.774872	3.631228	0.208169
24	6	0	4.056059	0.022009	-0.075694
25	1	0	-6.273732	-0.501200	-0.305522
26	1	0	-5.418999	-3.039759	-0.161262
27	1	0	1.066636	5.007281	0.251312
28	1	0	-3.723537	4.247304	-0.241674
29	1	0	6.242450	-0.372936	-0.531284
30	1	0	5.420294	-2.927646	-0.766138
31	1	0	-1.160943	5.024414	-0.039104
32	1	0	3.639563	4.276483	0.290532
33	6	0	-0.558776	-1.919296	0.993589
34	6	0	1.177389	-3.057004	0.144313
35	6	0	-1.099150	-3.027107	0.293540
36	1	0	1.443167	-1.220201	1.118598
37	1	0	-1.060155	-1.159438	1.575038
38	1	0	-0.021781	-4.665964	-0.785266
39	7	0	0.769851	-1.959592	0.902912
40	6	0	0.016444	-3.771427	-0.178486
41	1	0	-2.072037	-0.399629	-0.140544
42	1	0	1.304600	0.786203	-0.122899
43	1	0	-2.905031	-4.199362	-0.087007
44	1	0	2.905665	-4.107372	-0.608227
45	1	0	4.934638	1.974150	0.018140
46	1	0	-4.952183	1.948081	-0.323072

N_1SAP8 (Energy = −1198.46454306)

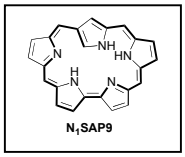


N_1SAP8

Stoichiometry C24H17N5
Framework group C1[X(C24H17N5)]
Deg. of freedom 132
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.427956	1.936655	0.001484
2	7	0	-1.458035	1.832102	0.087389
3	7	0	-2.905485	-0.886274	-0.047495
4	7	0	2.906931	-0.839797	-0.075584
5	6	0	2.548536	-3.270235	-0.096165
6	6	0	-3.381516	-2.171120	-0.211673
7	6	0	-3.898930	1.339886	0.004126
8	6	0	0.629979	3.062101	0.020114
9	6	0	-5.202486	-0.849957	-0.286565
10	6	0	-2.524679	-3.258529	-0.184025
11	6	0	-4.829802	-2.153944	-0.395137
12	6	0	-2.800708	2.177897	0.080132
13	6	0	-3.966042	-0.082966	-0.082435
14	6	0	-0.795502	2.990137	0.078493
15	6	0	1.488159	4.172016	-0.074130
16	6	0	3.379039	-2.174698	-0.123383
17	6	0	-2.941448	3.637944	0.096623
18	6	0	5.173271	-0.760881	-0.146660
19	6	0	4.814762	-2.080855	-0.151092
20	6	0	2.764132	2.282619	-0.102195
21	6	0	-1.687054	4.150997	0.090990
22	6	0	3.899211	1.427414	-0.157453
23	6	0	2.794223	3.695758	-0.151931
24	6	0	3.986423	0.054764	-0.138803
25	1	0	-6.201042	-0.435303	-0.366109
26	1	0	-5.463176	-3.019448	-0.549107
27	1	0	1.169989	5.205074	-0.095013
28	1	0	-3.882763	4.174775	0.098907
29	1	0	6.179299	-0.361004	-0.126889
30	1	0	5.478426	-2.935733	-0.127797
31	1	0	-1.388180	5.191621	0.089991
32	1	0	3.699478	4.281380	-0.243346
33	6	0	-0.667805	-2.062102	0.964091
34	6	0	1.139911	-3.160507	0.156993
35	6	0	-1.146543	-3.119885	0.165482
36	1	0	1.282156	-1.492567	1.477936
37	1	0	-1.222273	-1.321108	1.514797
38	1	0	0.012720	-4.683734	-0.958300
39	7	0	0.670124	-2.093877	0.943755
40	6	0	0.009248	-3.837686	-0.284114
41	1	0	1.019223	1.020318	0.111723
42	1	0	2.063381	-0.633478	-0.596477
43	1	0	-2.901265	-4.234410	-0.484031
44	1	0	2.973329	-4.248582	-0.295371
45	1	0	4.846054	1.954453	-0.227526
46	1	0	-4.862077	1.847083	-0.017929

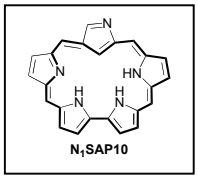
N_1SAP9 (Energy = −1198.49127934)



Stoichiometry C24H17N5
Framework group C1[X(C24H17N5)]
Deg. of freedom 132
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.542097	1.692446	-0.015771
2	7	0	-1.560699	1.749458	-0.014377
3	7	0	-2.964456	-0.766787	-0.065036
4	7	0	2.992563	-0.774970	-0.049403
5	6	0	2.502772	-3.187351	-0.133297
6	6	0	-3.401941	-2.072848	-0.168240
7	6	0	-4.019196	1.414213	-0.084526
8	6	0	0.725498	2.789843	0.021334
9	6	0	-5.270706	-0.811771	-0.276945
10	6	0	-2.549492	-3.160127	-0.105320
11	6	0	-4.852063	-2.103527	-0.332959
12	6	0	-2.874965	2.195960	-0.021799
13	6	0	-4.064510	0.002075	-0.121964
14	6	0	-0.683575	2.809780	0.027301
15	6	0	1.503379	4.019486	0.030261
16	6	0	3.367520	-2.111612	-0.169753
17	6	0	-2.810874	3.628078	0.036218
18	6	0	5.239721	-0.805770	-0.249201
19	6	0	4.803830	-2.102726	-0.295511
20	6	0	2.814691	2.192403	-0.042112
21	6	0	-1.494691	3.997154	0.068112
22	6	0	4.005564	1.434473	-0.105189
23	6	0	2.808624	3.643006	-0.013365
24	6	0	4.092297	0.052851	-0.122899
25	1	0	-6.283020	-0.433289	-0.357484
26	1	0	-5.454579	-2.997668	-0.439575
27	1	0	1.111083	5.027001	0.058790
28	1	0	-3.678170	4.274861	0.055190
29	1	0	6.262277	-0.455065	-0.301798
30	1	0	5.408993	-2.996613	-0.374585
31	1	0	-1.105686	5.003547	0.116544
32	1	0	3.687315	4.276464	-0.025222
33	6	0	-0.669171	-1.966274	1.011040
34	6	0	1.118433	-3.065723	0.178148
35	6	0	-1.164675	-3.019545	0.215560
36	1	0	1.280905	-1.396234	1.508463
37	1	0	-1.214551	-1.250657	1.604057
38	1	0	-0.031784	-4.581835	-0.925568
39	7	0	0.669064	-1.997443	0.973085
40	6	0	-0.024009	-3.741360	-0.244805
41	1	0	2.066926	-0.366640	-0.176581
42	1	0	-2.937320	-4.142206	-0.366282
43	1	0	2.889911	-4.164020	-0.404225
44	1	0	4.938829	1.986680	-0.160094
45	1	0	-4.962577	1.951674	-0.112253
46	1	0	-1.343306	0.760950	-0.099394

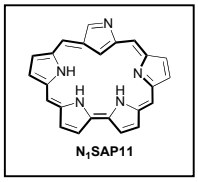
N_1SAP10 (Energy = −1198.49013286)



Stoichiometry C24H17N5
Framework group C1[X(C24H17N5)]
Deg. of freedom 132
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.067205	1.652016	0.000103
2	7	0	0.877737	2.317202	0.000055
3	7	0	2.999041	-0.098768	-0.000107
4	7	0	-2.585526	-1.185147	0.000127
5	6	0	-1.657242	-3.510431	-0.000203
6	6	0	3.765490	-1.252900	0.000170
7	6	0	-0.263430	-3.441961	-0.000225
8	6	0	3.387556	2.367762	-0.000012
9	6	0	-1.525619	2.915971	-0.000023
10	6	0	5.142940	0.558385	0.000546
11	6	0	3.283467	-2.555156	0.000053
12	6	0	0.543875	-4.669961	-0.000441
13	6	0	5.126408	-0.813758	0.000567
14	6	0	2.112142	2.951061	-0.000160
15	6	0	3.790523	1.035927	0.000128
16	6	0	-0.154679	3.238221	-0.000159
17	6	0	-2.617413	3.831833	0.000008
18	6	0	-2.680803	-2.546211	-0.000021
19	6	0	1.961064	-3.029099	-0.000111
20	6	0	1.823551	4.343487	-0.000510
21	6	0	-4.826839	-1.841409	0.000211
22	6	0	-4.077340	-2.971627	0.000035
23	6	0	-3.447909	1.722104	0.000207
24	6	0	0.452647	4.516928	-0.000514
25	6	0	-4.279287	0.604907	0.000272
26	6	0	-3.787733	3.104650	0.000161
27	6	0	-3.880665	-0.737477	0.000211
28	1	0	6.009067	1.206837	0.000822
29	1	0	0.134105	-5.677989	-0.000630
30	1	0	5.976746	-1.482554	0.000863
31	1	0	-2.516704	4.908204	-0.000054
32	1	0	2.579405	5.117287	-0.000754
33	1	0	-5.905658	-1.743933	0.000297
34	1	0	-4.412616	-4.001818	-0.000045
35	1	0	-0.083830	5.455289	-0.000770
36	1	0	-4.798777	3.489343	0.000225
37	1	0	-5.347150	0.803118	0.000335
38	1	0	4.202221	3.085150	0.000016
39	1	0	4.037062	-3.336666	0.000117
40	1	0	-2.041729	-4.529982	-0.000341
41	1	0	-1.629005	0.729684	0.000031
42	7	0	1.821163	-4.449437	-0.000354
43	6	0	0.694704	-2.406337	-0.000026
44	1	0	0.446386	-1.353442	0.000264
45	1	0	1.996078	-0.132537	-0.000745
46	1	0	0.725488	1.323484	0.000592

N_1SAP11 (Energy = −1198.49027632)

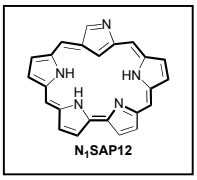


Stoichiometry C24H17N5
Framework group C1[X(C24H17N5)]
Deg. of freedom 132
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.909685	2.311498	0.000081
2	7	0	-2.041262	1.680576	0.000138
3	7	0	-2.589037	-1.154379	0.000091
4	7	0	3.002077	-0.134915	-0.000122
5	6	0	3.257318	-2.588574	0.000043
6	6	0	-2.700884	-2.511496	-0.000040
7	6	0	1.920251	-3.034731	-0.000132
8	6	0	-4.263791	0.654358	0.000314
9	6	0	-0.110858	3.245428	-0.000161
10	6	0	-4.839249	-1.783329	0.000195
11	6	0	-1.692985	-3.497510	-0.000219
12	6	0	1.614364	-4.472866	-0.000351
13	6	0	-4.101656	-2.921710	0.000017
14	6	0	-3.421332	1.764870	0.000251
15	6	0	-3.881531	-0.690580	0.000224
16	6	0	-1.487595	2.938308	0.000008
17	6	0	0.510808	4.515044	-0.000609
18	6	0	3.758148	-1.296804	0.000174
19	6	0	-0.302362	-3.464899	-0.000251
20	6	0	-3.747291	3.149024	0.000211
21	6	0	5.154071	0.500577	0.000616
22	6	0	5.125238	-0.869228	0.000635
23	6	0	2.151015	2.930178	-0.000179
24	6	0	-2.568520	3.864923	0.000046
25	6	0	3.420369	2.327616	-0.000013
26	6	0	1.881316	4.324248	-0.000610
27	6	0	3.804458	0.993047	0.000139
28	1	0	-5.916894	-1.673913	0.000281
29	1	0	2.366245	-5.259763	-0.000445
30	1	0	-4.445919	-3.948669	-0.000066
31	1	0	-0.013864	5.460049	-0.000926
32	1	0	-4.754281	3.544160	0.000275
33	1	0	6.026029	1.141252	0.000940
34	1	0	5.970183	-1.545043	0.000977
35	1	0	-2.456641	4.940159	-0.000023
36	1	0	2.646630	5.088676	-0.000922
37	1	0	4.244481	3.034163	0.000013
38	1	0	-5.329539	0.864191	0.000389
39	1	0	-2.074682	-4.515734	-0.000340
40	1	0	4.016222	-3.367593	0.000139
41	1	0	0.745628	1.319512	0.000778
42	7	0	0.345590	-4.735963	-0.000441
43	6	0	0.655582	-2.420834	-0.000082
44	1	0	0.391750	-1.371469	0.000153
45	1	0	-1.612671	0.753772	0.000081
46	1	0	1.998629	-0.161808	-0.000893

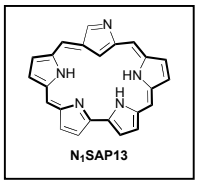
N_1SAP12 (Energy = −1198.50073164)



Framework group C1[X(C24H17N5)]
Deg. of freedom 132
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.022559	2.307065	-0.000023
2	7	0	1.824527	1.776333	-0.000033
3	7	0	2.697866	-1.079415	-0.000009
4	7	0	-2.961136	-0.274024	0.000067
5	6	0	-3.084465	-2.746139	-0.000030
6	6	0	2.857353	-2.451496	0.000052
7	6	0	-1.732404	-3.140063	-0.000019
8	6	0	4.138954	0.930961	-0.000051
9	6	0	-0.072144	3.302266	-0.000013
10	6	0	4.915517	-1.476446	0.000020
11	6	0	1.898871	-3.473120	0.000059
12	6	0	-1.371427	-4.563391	-0.000048
13	6	0	4.266621	-2.688361	0.000076
14	6	0	3.189482	1.948726	-0.000068
15	6	0	3.925836	-0.451779	-0.000004
16	6	0	1.314731	3.028259	-0.000045
17	6	0	-0.771788	4.532629	0.000083
18	6	0	-3.646674	-1.478313	-0.000013
19	6	0	0.505943	-3.485375	0.000019
20	6	0	3.531288	3.362423	-0.000063
21	6	0	-5.148412	0.232165	-0.000083
22	6	0	-5.036956	-1.133553	-0.000074
23	6	0	-2.299699	2.837429	0.000053
24	6	0	2.353941	4.042628	-0.000067
25	6	0	-3.528833	2.158807	0.000052
26	6	0	-2.125906	4.250636	0.000111
27	6	0	-3.831628	0.803298	0.000024
28	1	0	5.982144	-1.295493	0.000020
29	1	0	-2.091433	-5.379368	-0.000090
30	1	0	4.708403	-3.675935	0.000121
31	1	0	-0.308996	5.509553	0.000119
32	1	0	4.536977	3.764848	-0.000075
33	1	0	-6.057300	0.819324	-0.000137
34	1	0	-5.839102	-1.859665	-0.000126
35	1	0	2.200489	5.114030	-0.000087
36	1	0	-2.943096	4.959743	0.000173
37	1	0	-4.395792	2.812228	0.000064
38	1	0	5.181268	1.237522	-0.000056
39	1	0	2.328418	-4.471029	0.000085
40	1	0	-3.810314	-3.556080	-0.000076
41	1	0	-0.739667	1.340640	-0.000081
42	7	0	-0.092612	-4.777769	0.000007
43	6	0	-0.491273	-2.477336	0.000015
44	1	0	-0.299756	-1.411186	0.000032
45	1	0	-1.957950	-0.227391	0.000166
46	1	0	1.841533	-0.536210	-0.000036

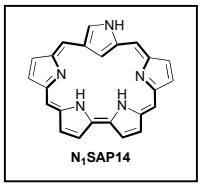
N_1SAP13 (Energy = −1198.50032119)



Stoichiometry C24H17N5
Framework group C1[X(C24H17N5)]
Deg. of freedom 132
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.852118	1.750389	-0.000001
2	7	0	0.988298	2.317704	0.000019
3	7	0	2.958155	-0.234462	0.000082
4	7	0	-2.691426	-1.116978	-0.000398
5	6	0	-1.860631	-3.493363	0.000270
6	6	0	3.655488	-1.431144	-0.000264
7	6	0	-0.463569	-3.468364	0.000389
8	6	0	3.495912	2.204544	-0.000090
9	6	0	-1.356705	3.010253	0.000170
10	6	0	5.138566	0.295185	-0.000942
11	6	0	3.113398	-2.710922	-0.000016
12	6	0	0.299336	-4.722946	0.001187
13	6	0	5.040166	-1.073400	-0.000900
14	6	0	2.259301	2.864281	0.000176
15	6	0	3.817539	0.850845	-0.000282
16	6	0	0.025052	3.300215	0.000310
17	6	0	-2.408335	4.010915	0.000305
18	6	0	-2.835556	-2.491377	-0.000100
19	6	0	1.775703	-3.135647	0.000273
20	6	0	2.066120	4.276754	0.000539
21	6	0	-4.905107	-1.539753	-0.000707
22	6	0	-4.244312	-2.743301	-0.000170
23	6	0	-3.217032	1.906347	-0.000226
24	6	0	0.710023	4.540801	0.000772
25	6	0	-4.155948	0.875801	-0.000451
26	6	0	-3.577013	3.315462	-0.000044
27	6	0	-3.926030	-0.502128	-0.000453
28	1	0	6.041642	0.891155	-0.001407
29	1	0	-0.147031	-5.715378	0.001549
30	1	0	5.848456	-1.792466	-0.001329
31	1	0	-2.268686	5.084221	0.000517
32	1	0	2.874228	4.996214	0.000725
33	1	0	-5.973659	-1.370245	-0.000985
34	1	0	-4.677198	-3.735014	0.000003
35	1	0	0.234260	5.511474	0.001147
36	1	0	-4.587811	3.704923	-0.000134
37	1	0	-5.201718	1.170289	-0.000578
38	1	0	4.353992	2.869526	-0.000212
39	1	0	3.834991	-3.522072	-0.000100
40	1	0	-2.293568	-4.491983	0.000560
41	7	0	1.583797	-4.548236	0.000501
42	6	0	0.532084	-2.466887	0.000112
43	1	0	0.352344	-1.398915	-0.000460
44	1	0	-1.839925	-0.566330	-0.000376
45	1	0	1.954867	-0.195307	0.001091
46	1	0	0.717172	1.347960	-0.000584

N_1SAP14 (Energy = −1198.49574122)

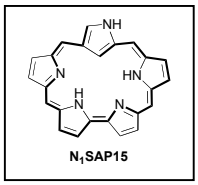


Stoichiometry C24H17N5
Framework group C1[X(C24H17N5)]
Deg. of freedom 132
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.543464	1.997281	0.000154
2	7	0	1.569991	1.987147	0.000015
3	7	0	2.834184	-0.590697	0.000023
4	7	0	-2.849411	-0.579450	-0.000128
5	6	0	-2.580142	-3.046535	-0.000073
6	6	0	3.274063	-1.892232	0.000052
7	6	0	-1.174505	-3.279573	-0.000035
8	6	0	3.990680	1.571098	-0.000086
9	6	0	-0.683147	3.074463	0.000043
10	6	0	5.165355	-0.660472	0.000018
11	6	0	2.516010	-3.049406	0.000072
12	6	0	-0.687308	-4.604351	-0.000022
13	6	0	4.736847	-1.944458	0.000072
14	6	0	2.885254	2.411061	-0.000087
15	6	0	3.960225	0.165810	-0.000019
16	6	0	0.716531	3.070597	-0.000016
17	6	0	-1.503742	4.250067	0.000060
18	6	0	-3.314053	-1.877861	-0.000080
19	6	0	1.113639	-3.241549	0.000042
20	6	0	2.855976	3.841292	-0.000146
21	6	0	-5.181032	-0.608596	-0.000051
22	6	0	-4.777484	-1.900245	-0.000134
23	6	0	-2.857250	2.430250	0.000106
24	6	0	1.544702	4.239725	-0.000121
25	6	0	-3.968922	1.603031	0.000093
26	6	0	-2.816887	3.861225	0.000127
27	6	0	-3.959910	0.194077	0.000007
28	1	0	6.182501	-0.287382	0.000004
29	1	0	-1.238495	-5.535095	-0.000040
30	1	0	5.328833	-2.852237	0.000110
31	1	0	-1.125601	5.262382	0.000033
32	1	0	3.735647	4.470947	-0.000218
33	1	0	-6.190614	-0.215382	-0.000013
34	1	0	-5.386264	-2.796731	-0.000174
35	1	0	1.174329	5.254936	-0.000170
36	1	0	-3.692226	4.496912	0.000153
37	1	0	-4.936211	2.096189	0.000126
38	1	0	4.963676	2.052698	-0.000138
39	1	0	3.099486	-3.969506	0.000114
40	1	0	-3.181571	-3.954276	-0.000101
41	1	0	-1.347914	0.997047	0.000183
42	7	0	0.651559	-4.571812	0.000067
43	6	0	-0.026184	-2.435301	0.000006
44	1	0	-0.025120	-1.358552	0.000010
45	1	0	1.369250	0.987411	0.000127
46	1	0	1.258005	-5.379340	0.000116

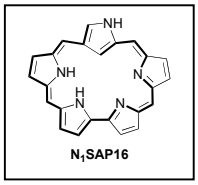
N_1SAP15 (Energy = −1198.50004057)



Stoichiometry C24H17N5
Framework group C1[X(C24H17N5)]
Deg. of freedom 132
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.455453	2.058068	0.000039
2	7	0	-1.562873	1.927906	0.000027
3	7	0	-2.865826	-0.668525	-0.000038
4	7	0	2.852146	-0.530079	-0.000154
5	6	0	2.669916	-3.000542	0.000045
6	6	0	-3.223095	-2.003943	-0.000012
7	6	0	1.271883	-3.270207	0.000043
8	6	0	-3.988343	1.517680	-0.000049
9	6	0	0.588778	3.121681	0.000028
10	6	0	-5.126945	-0.745243	-0.000057
11	6	0	-2.428544	-3.130485	0.000017
12	6	0	0.816663	-4.602984	0.000095
13	6	0	-4.667620	-2.029341	-0.000025
14	6	0	-2.856385	2.355276	-0.000029
15	6	0	-3.990182	0.134783	-0.000046
16	6	0	-0.813659	3.067271	0.000018
17	6	0	1.398237	4.308623	0.000058
18	6	0	3.367071	-1.809522	-0.000021
19	6	0	-1.017627	-3.281657	0.000025
20	6	0	-2.934840	3.805709	-0.000017
21	6	0	5.182795	-0.471538	-0.000156
22	6	0	4.829637	-1.778288	-0.000030
23	6	0	2.765686	2.497028	0.000037
24	6	0	-1.651399	4.255239	0.000045
25	6	0	3.891800	1.694149	0.000022
26	6	0	2.713360	3.931551	0.000066
27	6	0	3.930787	0.282985	-0.000015
28	1	0	-6.155366	-0.408610	-0.000076
29	1	0	1.387229	-5.521716	0.000137
30	1	0	-5.250829	-2.941234	-0.000018
31	1	0	1.007893	5.316150	0.000075
32	1	0	-3.848570	4.387633	-0.000025
33	1	0	6.176584	-0.039948	-0.000272
34	1	0	5.472449	-2.650659	-0.000053
35	1	0	-1.309292	5.281710	0.000088
36	1	0	3.585360	4.572185	0.000088
37	1	0	4.846126	2.212695	0.000025
38	1	0	-4.961259	2.000156	-0.000061
39	1	0	-2.992169	-4.061008	0.000037
40	1	0	3.296396	-3.891204	0.000105
41	1	0	1.225634	1.068965	0.000041
42	7	0	-0.524682	-4.599012	0.000071
43	6	0	0.103111	-2.449176	0.000005
44	1	0	0.106694	-1.370351	-0.000025
45	1	0	-1.940174	-0.247707	-0.000045
46	1	0	-1.112751	-5.419864	0.000093

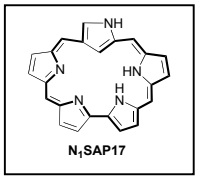
N_1SAP16 (Energy = −1198.47496624)



Stoichiometry C24H17N5
Framework group C1[X(C24H17N5)]
Deg. of freedom 132
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.816033	1.941533	0.006383
2	7	0	0.906994	2.376967	-0.001642
3	7	0	2.818514	-0.195237	-0.005271
4	7	0	-2.594987	-1.222402	-0.004209
5	6	0	-1.860264	-3.604633	-0.006736
6	6	0	3.607824	-1.322673	0.003027
7	6	0	-0.425897	-3.567238	0.001762
8	6	0	3.376214	2.225604	-0.015633
9	6	0	-1.324862	3.226631	0.011572
10	6	0	5.074968	0.376301	-0.013203
11	6	0	3.150707	-2.626249	0.010083
12	6	0	0.302503	-4.775015	0.016983
13	6	0	5.028920	-0.976514	0.000492
14	6	0	2.175116	2.909104	-0.009540
15	6	0	3.678367	0.835050	-0.012978
16	6	0	0.080992	3.428222	0.004728
17	6	0	-2.434392	4.092872	0.019481
18	6	0	-2.794492	-2.601284	-0.009763
19	6	0	1.820369	-3.110260	0.009259
20	6	0	2.107301	4.376341	-0.007837
21	6	0	-4.824934	-1.560442	-0.020426
22	6	0	-4.227800	-2.782363	-0.020729
23	6	0	-3.190396	1.939111	0.007510
24	6	0	0.791353	4.704341	0.002800
25	6	0	-4.055773	0.819336	-0.000144
26	6	0	-3.580720	3.303780	0.015901
27	6	0	-3.805747	-0.537136	-0.006953
28	1	0	5.946984	1.019861	-0.021603
29	1	0	-0.064863	-5.792102	0.025186
30	1	0	5.851989	-1.681447	0.004876
31	1	0	-2.383735	5.173028	0.029254
32	1	0	2.961687	5.042886	-0.012358
33	1	0	-5.885253	-1.343914	-0.029383
34	1	0	-4.707717	-3.752320	-0.030650
35	1	0	0.344278	5.690479	0.008204
36	1	0	-4.608736	3.641397	0.022927
37	1	0	-5.110077	1.078916	-0.002585
38	1	0	4.257789	2.864475	-0.021609
39	1	0	3.924277	-3.393822	0.017286
40	1	0	-2.289012	-4.603722	-0.010567
41	7	0	1.616886	-4.495331	0.021467
42	6	0	0.548756	-2.525982	-0.002516
43	1	0	0.414673	-1.453782	-0.016746
44	1	0	2.360507	-5.178363	0.031872
45	1	0	-1.680722	-0.804727	0.029070
46	1	0	-1.160367	1.173033	-0.003104

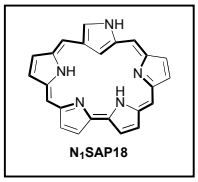
N_1SAP17 (Energy = –1198.47530040)



Stoichiometry C24H17N5
Framework group C1[X(C24H17N5)]
Deg. of freedom 132
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.910977	2.371912	-0.000049
2	7	0	1.812066	1.951108	0.000001
3	7	0	2.590574	-1.204344	-0.000016
4	7	0	-2.828885	-0.213859	-0.000253
5	6	0	-3.173763	-2.646095	0.000237
6	6	0	2.787325	-2.579748	-0.000155
7	6	0	-1.842680	-3.155264	0.000223
8	6	0	4.054683	0.834742	-0.000019
9	6	0	-0.092957	3.427101	0.000068
10	6	0	4.820047	-1.546645	-0.000388
11	6	0	1.844197	-3.578541	-0.000075
12	6	0	-1.600737	-4.538860	0.000385
13	6	0	4.218599	-2.767594	-0.000399
14	6	0	3.187015	1.953780	0.000096
15	6	0	3.805191	-0.520580	-0.000118
16	6	0	1.316672	3.233244	0.000138
17	6	0	-0.809912	4.699438	0.000076
18	6	0	-3.623664	-1.343772	0.000029
19	6	0	0.418809	-3.512778	0.000068
20	6	0	3.571904	3.318311	0.000317
21	6	0	-5.083496	0.362937	-0.000409
22	6	0	-5.042586	-0.989914	-0.000033
23	6	0	-2.184653	2.897372	-0.000111
24	6	0	2.421283	4.103718	0.000329
25	6	0	-3.380768	2.209551	-0.000167
26	6	0	-2.124207	4.364566	0.000002
27	6	0	-3.685351	0.815933	-0.000155
28	1	0	5.881165	-1.334048	-0.000564
29	1	0	-2.302714	-5.361334	0.000555
30	1	0	4.695757	-3.738934	-0.000586
31	1	0	-0.366893	5.687414	0.000147
32	1	0	4.598134	3.661366	0.000460
33	1	0	-5.952938	1.010103	-0.000656
34	1	0	-5.868104	-1.691852	0.000039
35	1	0	2.367912	5.183722	0.000487
36	1	0	-2.982678	5.025803	-0.000001
37	1	0	-4.263793	2.846638	-0.000188
38	1	0	5.108838	1.095095	-0.000052
39	1	0	2.263291	-4.582156	-0.000144
40	1	0	-3.952450	-3.407762	0.000398
41	7	0	-0.270501	-4.737800	0.000311
42	6	0	-0.560439	-2.519855	0.000015
43	1	0	-0.432990	-1.446989	-0.000199
44	1	0	1.676114	-0.785323	0.000479
45	1	0	0.185071	-5.638786	0.000421
46	1	0	1.157263	1.181650	-0.000269

N_1SAP18 (Energy = −1198.50018236)

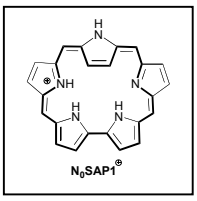


Stoichiometry C24H17N5
Framework group C1[X(C24H17N5)]
Deg. of freedom 132
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.551172	1.928807	-0.000413
2	7	0	-1.469193	2.055388	-0.000134
3	7	0	-2.840491	-0.527898	0.000095
4	7	0	2.877880	-0.669111	0.000124
5	6	0	2.472302	-3.139449	0.000019
6	6	0	-3.339725	-1.807546	0.000023
7	6	0	1.057107	-3.325052	-0.000027
8	6	0	-3.903659	1.684077	0.000077
9	6	0	0.799985	3.065582	-0.000105
10	6	0	-5.172306	-0.493723	0.000214
11	6	0	-2.626346	-2.993177	-0.000041
12	6	0	0.532640	-4.635380	-0.000146
13	6	0	-4.802977	-1.796196	-0.000038
14	6	0	-2.778115	2.493246	0.000041
15	6	0	-3.929926	0.276717	0.000041
16	6	0	-0.602640	3.120351	-0.000026
17	6	0	1.635544	4.257257	-0.000220
18	6	0	3.250047	-2.004739	0.000077
19	6	0	-1.231807	-3.228990	-0.000055
20	6	0	-2.728446	3.926467	0.000140
21	6	0	5.139312	-0.722386	0.000284
22	6	0	4.695525	-2.011116	0.000022
23	6	0	2.844651	2.359322	-0.000032
24	6	0	-1.412521	4.305336	0.000040
25	6	0	3.979189	1.529286	0.000115
26	6	0	2.919075	3.811642	-0.000049
27	6	0	3.991161	0.144102	0.000105
28	1	0	-6.171523	-0.074991	0.000338
29	1	0	1.058985	-5.580204	-0.000200
30	1	0	-5.435343	-2.676299	-0.000122
31	1	0	1.290045	5.282555	-0.000245
32	1	0	-3.600989	4.566320	0.000255
33	1	0	6.163269	-0.372396	0.000418
34	1	0	5.289185	-2.916210	-0.000052
35	1	0	-1.024066	5.313616	0.000060
36	1	0	3.831559	4.395491	0.000064
37	1	0	4.949333	2.017181	0.000239
38	1	0	-4.860763	2.197273	0.000182
39	1	0	-3.240730	-3.892917	-0.000094
40	1	0	3.049321	-4.061142	-0.000024
41	7	0	-0.805894	-4.567354	-0.000118
42	6	0	-0.070037	-2.451034	-0.000036
43	1	0	-0.075194	-1.372052	0.000002
44	1	0	-1.433006	-5.358953	-0.000147
45	1	0	-1.240273	1.065710	-0.000275
46	1	0	1.947697	-0.259408	0.000188

Cartesian coordinates for the optimized structures of normal sapphyrins (monocation)

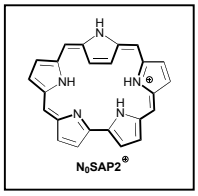
N_0SAP1$^{\oplus}$ (Energy = −1198.91180770)



Stoichiometry C24H18N5(1+)
Framework group C1[X(C24H18N5)]
Deg. of freedom 135
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.724351	1.699112	-0.029927
2	7	0	-1.372398	1.855053	-0.108217
3	7	0	-3.044345	-0.679916	-0.001547
4	7	0	2.865492	-0.898409	-0.059003
5	6	0	2.192355	-3.229137	-0.175339
6	6	0	-3.492205	-1.981464	-0.148647
7	6	0	-3.869909	1.613152	-0.262105
8	6	0	0.938337	2.821820	0.055654
9	6	0	-5.196148	-0.542389	-0.625545
10	6	0	-2.668659	-3.095243	-0.002931
11	6	0	-4.863134	-1.872246	-0.567267
12	6	0	-2.682483	2.347439	-0.082703
13	6	0	-4.036217	0.234643	-0.280997
14	6	0	-0.473355	2.900874	0.077666
15	6	0	1.822430	3.946521	0.078663
16	6	0	3.162889	-2.218867	-0.237694
17	6	0	-2.581408	3.734783	0.187107
18	6	0	5.140924	-1.160686	-0.460953
19	6	0	4.583335	-2.397861	-0.523715
20	6	0	3.064100	2.055174	-0.065006
21	6	0	-1.244881	4.068238	0.294643
22	6	0	4.132860	1.163826	-0.160557
23	6	0	3.111290	3.480247	-0.002342
24	6	0	4.041799	-0.235373	-0.195772
25	1	0	-1.121720	1.026907	-0.632950
26	1	0	-6.148377	-0.119790	-0.917354
27	1	0	-5.503135	-2.716362	-0.786333
28	1	0	1.506504	4.978866	0.122595
29	1	0	-3.428498	4.393074	0.324951
30	1	0	6.178593	-0.886795	-0.604499
31	1	0	5.075544	-3.344977	-0.705009
32	1	0	-0.842293	5.041712	0.535368
33	1	0	4.020207	4.066229	-0.020315
34	1	0	5.120136	1.610261	-0.232478
35	1	0	-4.768573	2.208553	-0.385992
36	1	0	-3.020117	-4.047761	-0.387836
37	1	0	2.421737	-4.200457	-0.607372
38	1	0	1.475715	0.709435	-0.015621
39	6	0	-0.832014	-1.980004	1.380133
40	6	0	0.541921	-1.993005	1.301779
41	6	0	0.920939	-2.984861	0.353682
42	6	0	-1.344985	-2.950896	0.466341
43	7	0	-0.249647	-3.623992	-0.035201
44	1	0	1.246359	-1.418231	1.882738
45	1	0	-1.435231	-1.424258	2.086663
46	1	0	-0.301131	-4.239178	-0.837063
47	1	0	-2.146574	-0.448274	0.393196

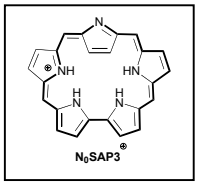
$N_0SAP2^{\oplus}$ (Energy = −1198.91709215)



Stoichiometry C24H18N5(1+)
Framework group C1[X(C24H18N5)]
Deg. of freedom 135
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.654676	1.678398	-0.031467
2	7	0	-1.335821	1.890647	-0.070398
3	7	0	-3.035352	-0.680652	0.009686
4	7	0	2.900786	-0.925060	-0.073021
5	6	0	2.187894	-3.272581	-0.158677
6	6	0	-3.495002	-1.975421	-0.155912
7	6	0	-3.831907	1.624943	-0.260751
8	6	0	0.959297	2.831366	0.086066
9	6	0	-5.178960	-0.513609	-0.630152
10	6	0	-2.681010	-3.098758	-0.022883
11	6	0	-4.861991	-1.848150	-0.580012
12	6	0	-2.646794	2.360462	-0.084022
13	6	0	-4.012002	0.246864	-0.275005
14	6	0	-0.453023	2.939334	0.107276
15	6	0	1.839453	3.996592	0.134431
16	6	0	3.159379	-2.272858	-0.235123
17	6	0	-2.565359	3.762871	0.143043
18	6	0	5.105079	-1.120774	-0.482349
19	6	0	4.563164	-2.383278	-0.509094
20	6	0	2.976824	2.063875	-0.078936
21	6	0	-1.237103	4.111975	0.268879
22	6	0	4.073274	1.209413	-0.204806
23	6	0	3.099944	3.513644	0.016301
24	6	0	4.043345	-0.189859	-0.237295
25	1	0	-1.019192	1.014327	-0.461536
26	1	0	-6.124364	-0.077359	-0.923989
27	1	0	-5.510279	-2.683312	-0.808612
28	1	0	1.530047	5.028962	0.224236
29	1	0	-3.423970	4.414843	0.231463
30	1	0	6.140741	-0.847570	-0.633367
31	1	0	5.083655	-3.318535	-0.665833
32	1	0	-0.844430	5.098182	0.469892
33	1	0	4.030331	4.066850	0.001875
34	1	0	5.051361	1.671686	-0.296072
35	1	0	-4.727115	2.223124	-0.396684
36	1	0	-3.036651	-4.041840	-0.426593
37	1	0	2.426192	-4.246393	-0.577438
38	6	0	-0.848311	-2.024387	1.391734
39	6	0	0.527764	-2.044858	1.324015
40	6	0	0.909433	-3.020644	0.361295
41	6	0	-1.359582	-2.971416	0.456503
42	7	0	-0.261991	-3.638553	-0.054406
43	1	0	1.218651	-1.492914	1.945687
44	1	0	-1.451723	-1.475986	2.103498
45	1	0	-0.311044	-4.231902	-0.872604
46	1	0	-2.127730	-0.463743	0.388800
47	1	0	1.996588	-0.460355	-0.012634

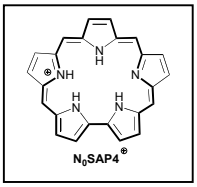
$N_0SAP3^{\oplus}$ (Energy = −1198.89074073)



Stoichiometry C24H18N5(1+)
Framework group C1[X(C24H18N5)]
Deg. of freedom 135
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.528628	1.814728	-0.125482
2	7	0	-1.529257	1.814437	-0.125573
3	7	0	-2.961748	-0.841288	0.001223
4	7	0	2.962014	-0.840881	0.001454
5	6	0	2.370618	-3.216356	-0.058072
6	6	0	-3.287270	-2.176044	-0.196988
7	6	0	-3.986946	1.378873	-0.252339
8	6	0	0.702771	2.919916	0.049416
9	6	0	-5.097896	-0.881769	-0.686268
10	6	0	-2.369713	-3.216683	-0.057786
11	6	0	-4.642431	-2.178984	-0.660362
12	6	0	-2.871366	2.207368	-0.092402
13	6	0	-4.025044	-0.018128	-0.287440
14	6	0	-0.703625	2.919788	0.049333
15	6	0	1.559261	4.035816	0.257380
16	6	0	3.287882	-2.175478	-0.197228
17	6	0	-2.865913	3.608449	0.159029
18	6	0	5.098035	-0.880567	-0.686468
19	6	0	4.642979	-2.177929	-0.660779
20	6	0	2.870666	2.207904	-0.092143
21	6	0	-1.560346	4.035542	0.257155
22	6	0	3.986444	1.379675	-0.252135
23	6	0	2.864917	3.608969	0.159374
24	6	0	4.024953	-0.017316	-0.287387
25	1	0	-1.236089	0.976249	-0.608317
26	1	0	-6.075816	-0.537884	-0.995605
27	1	0	-5.192812	-3.070360	-0.929961
28	1	0	1.224066	5.040395	0.473565
29	1	0	-3.757254	4.207046	0.289854
30	1	0	6.075802	-0.536318	-0.995882
31	1	0	5.193593	-3.069083	-0.930637
32	1	0	-1.225360	5.040191	0.473336
33	1	0	3.756132	4.207731	0.290297
34	1	0	4.937717	1.889758	-0.363082
35	1	0	-4.938364	1.888695	-0.363250
36	1	0	-2.610398	-4.172368	-0.513839
37	1	0	2.611430	-4.171948	-0.514257
38	1	0	1.235663	0.976575	-0.608409
39	6	0	-0.679058	-2.011973	1.451932
40	6	0	0.680028	-2.011647	1.451600
41	6	0	1.078407	-3.031287	0.474902
42	6	0	-1.077449	-3.031405	0.475016
43	7	0	0.000490	-3.696084	-0.010792
44	1	0	1.334717	-1.492838	2.143107
45	1	0	-1.333659	-1.493483	2.143760
46	1	0	-2.111154	-0.549575	0.459453
47	1	0	2.111466	-0.549568	0.460028

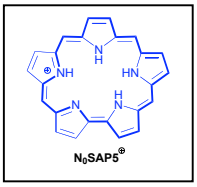
$N_0SAP4^{\oplus}$ (Energy = −1198.92680723)



Stoichiometry C24H18N5(1+)
Framework group C1[X(C24H18N5)]
Deg. of freedom 135
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.308927	-2.182744	0.090148
2	7	0	-1.655496	-1.985251	-0.094903
3	7	0	-2.655826	0.774714	-0.072160
4	7	0	2.807924	0.449852	-0.084540
5	6	0	2.679049	2.955577	-0.192675
6	6	0	-3.040317	2.070512	0.094722
7	6	0	1.363818	3.351750	0.065488
8	6	0	-3.981236	-1.289426	-0.406720
9	6	0	0.436401	-3.245886	0.256322
10	6	0	-4.982938	0.985923	-0.257715
11	6	0	-2.252952	3.211388	0.326411
12	6	0	1.013502	4.709359	0.356639
13	6	0	-4.491059	2.220051	-0.005888
14	6	0	-0.339209	4.778588	0.536082
15	6	0	-2.990657	-2.262915	-0.302037
16	6	0	-3.832459	0.093095	-0.274190
17	6	0	-0.955527	-3.154683	0.068082
18	6	0	1.208831	-4.370210	0.630079
19	6	0	3.319467	1.726424	-0.318554
20	6	0	-0.888999	3.471999	0.338441
21	6	0	-3.126176	-3.681178	-0.303369
22	6	0	5.014268	0.232511	-0.580507
23	6	0	4.693418	1.562964	-0.671073
24	6	0	2.618627	-2.626498	0.263677
25	6	0	-1.884613	-4.226290	-0.063035
26	6	0	3.763423	-1.850791	0.057981
27	6	0	2.539530	-3.992728	0.633601
28	6	0	3.850584	-0.486611	-0.181349
29	1	0	-1.362819	-1.023390	0.065152
30	1	0	-6.012346	0.682950	-0.400078
31	1	0	1.733739	5.512658	0.433361
32	1	0	-5.029289	3.154079	0.093830
33	1	0	-0.930173	5.651609	0.778063
34	1	0	0.807139	-5.337457	0.897786
35	1	0	-4.055135	-4.210869	-0.464951
36	1	0	5.968136	-0.229224	-0.798262
37	1	0	5.342470	2.375698	-0.968551
38	1	0	-1.627509	-5.275218	-0.017351
39	1	0	3.390124	-4.606890	0.896732
40	1	0	4.706094	-2.388349	0.068067
41	1	0	-4.991427	-1.657671	-0.557746
42	1	0	-2.839324	4.110083	0.497718
43	1	0	3.356612	3.798045	-0.293090
44	7	0	0.184091	2.623034	0.097293
45	1	0	0.050717	1.687812	-0.261179
46	1	0	1.097587	-1.408797	-0.527242
47	1	0	2.059402	0.310134	0.584415

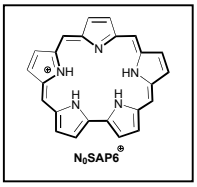
N_0SAP5$^{\oplus}$ (Energy = −1198.92999927)



Stoichiometry C24H18N5(1+)
Framework group C1[X(C24H18N5)]
Deg. of freedom 135
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.929146	-2.353569	0.077573
2	7	0	-1.886994	-1.703562	-0.034546
3	7	0	-2.595393	1.133225	-0.124868
4	7	0	2.853083	0.077138	-0.084456
5	6	0	3.147770	2.567554	-0.042213
6	6	0	-2.695727	2.506332	-0.040421
7	6	0	1.896649	3.136507	0.192107
8	6	0	-4.137994	-0.783709	-0.347416
9	6	0	-0.067635	-3.279835	0.275814
10	6	0	-4.773820	1.659767	-0.423225
11	6	0	-1.728889	3.490965	0.200569
12	6	0	1.703045	4.506339	0.546310
13	6	0	-4.078035	2.826722	-0.237162
14	6	0	0.359153	4.748339	0.621814
15	6	0	-3.247913	-1.837820	-0.170516
16	6	0	-3.846065	0.582369	-0.327816
17	6	0	-1.438503	-2.961618	0.162000
18	6	0	0.562061	-4.524713	0.537015
19	6	0	3.579022	1.257552	-0.246221
20	6	0	-0.343520	3.543002	0.307505
21	6	0	-3.651973	-3.232784	-0.059916
22	6	0	4.980863	-0.486639	-0.638451
23	6	0	4.900047	0.883813	-0.630320
24	6	0	2.169483	-2.968578	0.131966
25	6	0	-2.516202	-3.939941	0.168087
26	6	0	3.406701	-2.361476	-0.094352
27	6	0	1.925844	-4.336626	0.443896
28	6	0	3.714025	-1.017142	-0.262218
29	1	0	-5.834319	1.541823	-0.599605
30	1	0	2.510391	5.201071	0.734734
31	1	0	-4.468061	3.835675	-0.241620
32	1	0	-0.128659	5.678479	0.880982
33	1	0	0.045965	-5.443771	0.775884
34	1	0	-4.667107	-3.601202	-0.134899
35	1	0	5.836879	-1.092016	-0.905411
36	1	0	5.679443	1.589088	-0.885914
37	1	0	-2.409830	-5.007831	0.303873
38	1	0	2.701501	-5.074467	0.599067
39	1	0	4.252609	-3.039254	-0.151207
40	1	0	-5.186386	-1.036433	-0.474220
41	1	0	-2.177732	4.472680	0.320701
42	1	0	3.952118	3.296422	-0.066412
43	7	0	0.629122	2.560335	0.107774
44	1	0	0.455335	1.727015	-0.438050
45	1	0	0.734020	-1.467094	-0.365276
46	1	0	-1.805267	0.523581	0.068135
47	1	0	2.096038	0.030982	0.587878

$N_0SAP6^{\oplus}$ (Energy = −1198.92131162)

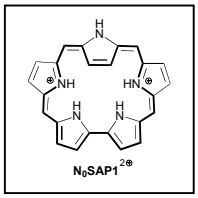


Stoichiometry C24H18N5(1+)
Framework group C1[X(C24H18N5)]
Deg. of freedom 135
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.435505	-2.148603	0.122762
2	7	0	-1.434518	-2.149256	-0.122700
3	7	0	-2.722105	0.685771	0.018828
4	7	0	2.721814	0.686870	-0.018768
5	6	0	2.415048	3.138339	-0.392830
6	6	0	-3.159833	1.962777	0.319131
7	6	0	1.059933	3.435298	-0.198683
8	6	0	-3.825012	-1.541703	-0.340481
9	6	0	0.690501	-3.318809	0.133958
10	6	0	-4.975205	0.604600	0.217611
11	6	0	-2.416495	3.137381	0.392814
12	6	0	0.657967	4.842787	-0.140751
13	6	0	-4.579804	1.889183	0.476431
14	6	0	-0.660080	4.842520	0.140863
15	6	0	-2.764832	-2.446511	-0.401895
16	6	0	-3.813162	-0.175026	-0.079309
17	6	0	-0.688959	-3.319112	-0.134105
18	6	0	1.557803	-4.371835	0.504532
19	6	0	3.158893	1.964071	-0.319201
20	6	0	-1.061520	3.434887	0.198665
21	6	0	-2.820194	-3.838491	-0.678018
22	6	0	4.974949	0.606779	-0.217711
23	6	0	4.578913	1.891162	-0.476512
24	6	0	2.765943	-2.445323	0.401881
25	6	0	-1.555850	-4.372516	-0.504574
26	6	0	3.825752	-1.540075	0.340436
27	6	0	2.821862	-3.837231	0.678232
28	6	0	3.813289	-0.173411	0.079249
29	1	0	-1.180734	-1.375694	0.479380
30	1	0	-5.978214	0.201268	0.257217
31	1	0	1.322742	5.686609	-0.274771
32	1	0	-5.203199	2.729149	0.751527
33	1	0	-1.325187	5.686071	0.274944
34	1	0	1.254847	-5.396573	0.669706
35	1	0	-3.711665	-4.365435	-0.990578
36	1	0	5.978147	0.203927	-0.257395
37	1	0	5.201873	2.731420	-0.751703
38	1	0	-1.252479	-5.397114	-0.669851
39	1	0	3.713509	-4.363785	0.990951
40	1	0	4.813144	-1.973605	0.462687
41	1	0	-4.812217	-1.975660	-0.462731
42	1	0	-3.033469	4.008987	0.592557
43	1	0	3.031621	4.010229	-0.592568
44	7	0	-0.000607	2.593492	0.000029
45	1	0	1.181349	-1.375004	-0.479107
46	1	0	1.800222	0.534739	0.371076
47	1	0	-1.800352	0.534103	-0.370812

Cartesian coordinates for the optimized structures of normal sapphyrins (dication)

$N_0SAP1^{2\oplus}$ (Energy = −1199.20775230)

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 Stoichiometry    C24H19N5(2+)
 Framework group  C1[X(C24H19N5)]
 Deg. of freedom   138
 Full point group                 C1
 Largest Abelian subgroup         C1      NOp   1
 Largest concise Abelian subgroup C1      NOp   1
                       Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          7             0        1.527868    1.840843   -0.158435
    2          7             0       -1.527835    1.840866   -0.158414
    3          7             0       -2.975528   -0.814393   -0.001114
    4          7             0        2.975510   -0.814416   -0.001161
    5          6             0        2.433675   -3.206378   -0.051322
    6          6             0       -3.325498   -2.145389   -0.183103
    7          6             0       -3.987984    1.413600   -0.251265
    8          6             0        0.702996    2.944067    0.033437
    9          6             0       -5.127307   -0.835903   -0.663399
   10          6             0       -2.433730   -3.206363   -0.051301
   11          6             0       -4.690620   -2.136360   -0.630978
   12          6             0       -2.867495    2.237730   -0.099923
   13          6             0       -4.034903    0.016974   -0.284036
   14          6             0       -0.702949    2.944077    0.033432
   15          6             0        1.557032    4.058499    0.278462
   16          6             0        3.325460   -2.145417   -0.183126
   17          6             0       -2.862055    3.635538    0.181465
   18          6             0        5.127304   -0.835967   -0.663390
   19          6             0        4.690594   -2.136415   -0.630970
   20          6             0        2.867538    2.237702   -0.099917
   21          6             0       -1.556977    4.058533    0.278389
   22          6             0        3.988013    1.413559   -0.251274
   23          6             0        2.862109    3.635493    0.181537
   24          6             0        4.034904    0.016931   -0.284056
   25          1             0       -1.246023    1.029744   -0.692884
   26          1             0       -6.104227   -0.481899   -0.965035
   27          1             0       -5.256760   -3.022280   -0.886607
   28          1             0        1.221383    5.057515    0.519026
   29          1             0       -3.751518    4.231702    0.336259
   30          1             0        6.104241   -0.481980   -0.964992
   31          1             0        5.256729   -3.022348   -0.886565
   32          1             0       -1.221318    5.057560    0.518891
   33          1             0        3.751575    4.231639    0.336388
   34          1             0        4.939454    1.927089   -0.346710
   35          1             0       -4.939413    1.927150   -0.346722
   36          1             0       -2.726157   -4.166584   -0.467139
   37          1             0        2.726089   -4.166604   -0.467159
   38          6             0       -0.689553   -2.084432    1.445475
   39          6             0        0.689516   -2.084436    1.445468
   40          6             0        1.133922   -3.023746    0.468655
   41          6             0       -1.133973   -3.023743    0.468669
   42          7             0       -0.000030   -3.648879   -0.013392
   43          1             0        1.334638   -1.578456    2.152920
   44          1             0       -1.334664   -1.578453    2.152938
   45          1             0       -0.000036   -4.271478   -0.813317
   46          1             0       -2.128119   -0.519622    0.460004
   47          1             0        2.128041   -0.519610    0.459824
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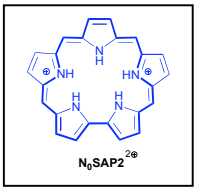
$N_0SAP2^{2\oplus}$ (Energy = −1199.21894025)

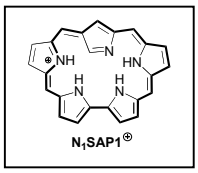


Stoichiometry C24H19N5(2+)
Framework group C1[X(C24H19N5)]
Deg. of freedom 138
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.463636	-2.131567	0.106312
2	7	0	-1.453703	-2.137633	-0.107295
3	7	0	-2.770667	0.639436	-0.074703
4	7	0	2.768034	0.650474	0.075842
5	6	0	2.476967	3.147671	-0.178733
6	6	0	-3.214082	1.941822	0.172817
7	6	0	1.128151	3.488684	-0.078697
8	6	0	-3.871117	-1.602415	-0.250394
9	6	0	0.700136	-3.290468	0.119651
10	6	0	-5.013474	0.557906	0.311130
11	6	0	-2.491519	3.137889	0.179443
12	6	0	0.669755	4.847382	-0.056269
13	6	0	-4.611091	1.863977	0.448666
14	6	0	-0.691336	4.844889	0.050887
15	6	0	-2.787067	-2.476424	-0.337611
16	6	0	-3.878059	-0.225513	-0.038346
17	6	0	-0.685372	-3.293295	-0.121211
18	6	0	1.557966	-4.368043	0.455059
19	6	0	3.205201	1.955032	-0.170919
20	6	0	-1.144258	3.484485	0.077816
21	6	0	-2.818426	-3.875196	-0.596042
22	6	0	5.011413	0.579852	-0.308468
23	6	0	4.602815	1.884016	-0.445734
24	6	0	2.798343	-2.464911	0.337105
25	6	0	-1.538827	-4.374342	-0.456670
26	6	0	3.878677	-1.586213	0.250995
27	6	0	2.835431	-3.863605	0.595076
28	6	0	3.879496	-0.209161	0.039794
29	1	0	-6.004958	0.157192	0.476574
30	1	0	1.325251	5.706477	-0.107110
31	1	0	-5.221488	2.708367	0.740669
32	1	0	-1.350271	5.701544	0.098304
33	1	0	1.241504	-5.389628	0.615638
34	1	0	-3.705120	-4.428718	-0.875607
35	1	0	6.004920	0.183969	-0.473406
36	1	0	5.209332	2.731454	-0.736988
37	1	0	-1.218155	-5.394554	-0.617625
38	1	0	3.724305	-4.413507	0.874862
39	1	0	4.860155	-2.046176	0.312517
40	1	0	-4.850590	-2.066684	-0.311562
41	1	0	-3.130206	4.006804	0.307304
42	1	0	3.111844	4.019314	-0.307002
43	7	0	-0.006544	2.692437	0.000243
44	1	0	-0.004617	1.685679	0.005875
45	1	0	1.227032	-1.355635	-0.500682
46	1	0	-2.033289	0.465899	-0.748522
47	1	0	2.030686	0.472658	0.748525
48	1	0	-1.219958	-1.360603	0.499368

Cartesian coordinates for the optimized structures of N-confused sapphyrins (monocation)

N_1SAP1$^{\oplus}$ (Energy = –1198.91151773)

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 Stoichiometry    C24H18N5(1+)
 Framework group  C1[X(C24H18N5)]
 Deg. of freedom   135
 Full point group                 C1
 Largest Abelian subgroup         C1      NOp   1
 Largest concise Abelian subgroup C1      NOp   1
                        Standard orientation:
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 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
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    1          7             0       -0.611733   -1.866940    0.809882
    2          7             0        3.037422   -0.756649   -0.146607
    3          7             0       -2.991846   -0.968349    0.109432
    4          6             0       -0.957860   -3.049310    0.100431
    5          6             0        0.208909   -3.803311   -0.183348
    6          6             0        0.685333   -1.871784    0.900617
    7          6             0        1.297845   -3.026313    0.235507
    8          6             0        2.698655   -3.165436    0.062459
    9          6             0        3.534094   -2.058327   -0.000161
   10          6             0        4.955780   -1.925752    0.101639
   11          6             0        5.277292   -0.591025    0.027284
   12          6             0        4.070293    0.162133   -0.153362
   13          6             0        3.905687    1.540140   -0.279169
   14          6             0        2.721726    2.291900   -0.278605
   15          6             0        2.627483    3.700641   -0.460839
   16          6             0        1.310656    4.079437   -0.321254
   17          6             0        0.536662    2.917854   -0.060939
   18          6             0       -0.857919    2.859842    0.115638
   19          6             0       -1.735646    3.963859    0.327934
   20          6             0       -3.018990    3.482372    0.414154
   21          6             0       -2.990255    2.063083    0.251062
   22          6             0       -4.095231    1.216275    0.163043
   23          6             0       -4.101785   -0.175536   -0.009481
   24          6             0       -5.161823   -1.024764   -0.465628
   25          6             0       -4.649692   -2.294046   -0.636822
   26          6             0       -3.271714   -2.268670   -0.258393
   27          6             0       -2.283773   -3.264259   -0.292023
   28          1             0        0.247018   -4.737695   -0.728160
   29          1             0        1.213133   -1.143768    1.507724
   30          1             0        5.635614   -2.748877    0.277499
   31          1             0        6.261390   -0.152072    0.124565
   32          1             0        3.468267    4.340975   -0.690859
   33          1             0        0.908676    5.076270   -0.436500
   34          1             0       -1.419118    4.992106    0.431314
   35          1             0       -3.920127    4.054819    0.588230
   36          1             0       -6.166382   -0.690274   -0.687481
   37          1             0       -5.175086   -3.164564   -1.006173
   38          1             0        3.142109   -4.148688   -0.068455
   39          1             0       -2.558079   -4.228860   -0.708254
   40          1             0       -5.061740    1.709630    0.163189
   41          1             0        4.817076    2.122416   -0.366218
   42          7             0       -1.642914    1.720588    0.117004
   43          7             0        1.415602    1.837117   -0.078798
   44          1             0       -1.335249    0.832393   -0.255129
   45          1             0        1.211270    0.970682    0.401963
   46          1             0       -2.134307   -0.801438    0.643960
   47          1             0        2.185454   -0.597446   -0.666069
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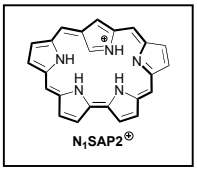
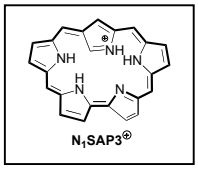
N_1SAP2$^{\oplus}$ (Energy = −1198.90822543)



Stoichiometry C24H18N5(1+)
Framework group C1[X(C24H18N5)]
Deg. of freedom 135
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.559318	-2.063610	0.868320
2	7	0	3.039982	-0.676290	-0.074626
3	7	0	-2.875459	-0.940377	0.027432
4	6	0	-0.887488	-3.087292	-0.021099
5	6	0	0.317739	-3.713459	-0.376018
6	6	0	0.763172	-1.993313	1.029135
7	6	0	1.375156	-2.992753	0.228163
8	6	0	2.808936	-3.097605	0.092958
9	6	0	3.588996	-1.971577	0.036229
10	6	0	5.015961	-1.787320	0.105805
11	6	0	5.289171	-0.449736	0.031346
12	6	0	4.049474	0.271346	-0.117992
13	6	0	3.854593	1.635918	-0.261332
14	6	0	2.642172	2.353529	-0.283181
15	6	0	2.500278	3.749871	-0.504629
16	6	0	1.168917	4.084018	-0.373072
17	6	0	0.436592	2.904776	-0.081150
18	6	0	-0.955345	2.811073	0.098076
19	6	0	-1.845380	3.925663	0.269899
20	6	0	-3.118754	3.442142	0.396350
21	6	0	-3.071051	2.012130	0.292923
22	6	0	-4.134320	1.127834	0.234265
23	6	0	-4.045671	-0.270133	0.023460
24	6	0	-5.154350	-1.144235	-0.336766
25	6	0	-4.608049	-2.362018	-0.602733
26	6	0	-3.181611	-2.235461	-0.350214
27	6	0	-2.224415	-3.237769	-0.456890
28	1	0	0.413936	-4.537432	-1.069712
29	1	0	1.220627	-1.328798	1.748337
30	1	0	5.726571	-2.590183	0.251953
31	1	0	6.261073	0.021754	0.095008
32	1	0	3.317630	4.413391	-0.751815
33	1	0	0.733046	5.062784	-0.515758
34	1	0	-1.532983	4.959177	0.314121
35	1	0	-4.024922	4.013593	0.545968
36	1	0	-6.193506	-0.849290	-0.409336
37	1	0	-5.114440	-3.266931	-0.913710
38	1	0	3.283018	-4.069856	-0.000910
39	1	0	-2.504617	-4.179149	-0.920137
40	1	0	-5.125966	1.566507	0.287849
41	1	0	4.748746	2.242196	-0.358998
42	7	0	-1.727034	1.675546	0.152285
43	7	0	1.358419	1.857325	-0.070750
44	1	0	-1.478643	0.717541	-0.082929
45	1	0	1.190555	0.988020	0.416696
46	1	0	2.193589	-0.552726	-0.615007
47	1	0	-1.278177	-1.432547	1.218546

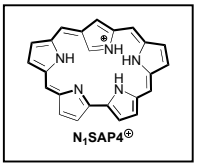
N_1SAP3$^{\oplus}$ (Energy = −1198.90754616)



Stoichiometry C24H18N5(1+)
Framework group C1[X(C24H18N5)]
Deg. of freedom 135
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.508493	-2.148398	0.947438
2	7	0	3.039018	-0.671522	-0.095602
3	7	0	-2.910565	-0.937436	-0.012232
4	6	0	-0.873045	-3.114223	-0.001021
5	6	0	0.316782	-3.679457	-0.470010
6	6	0	0.828647	-2.091260	1.060206
7	6	0	1.400634	-3.003295	0.147188
8	6	0	2.828490	-3.095062	-0.057175
9	6	0	3.601128	-1.963377	-0.071647
10	6	0	5.027919	-1.769369	-0.014894
11	6	0	5.284470	-0.426822	-0.004358
12	6	0	4.034770	0.288208	-0.091517
13	6	0	3.829897	1.657541	-0.150481
14	6	0	2.619083	2.376299	-0.150297
15	6	0	2.501243	3.789188	-0.301835
16	6	0	1.169428	4.128440	-0.231014
17	6	0	0.414728	2.937489	-0.040541
18	6	0	-0.984601	2.813959	0.062565
19	6	0	-1.869112	3.980616	0.107279
20	6	0	-3.126979	3.490570	0.180318
21	6	0	-3.003098	2.034173	0.161783
22	6	0	-4.108659	1.181804	0.124096
23	6	0	-4.070872	-0.210933	0.003671
24	6	0	-5.150630	-1.135482	-0.203214
25	6	0	-4.611270	-2.377793	-0.408742
26	6	0	-3.181251	-2.277954	-0.287002
27	6	0	-2.230993	-3.276674	-0.379386
28	1	0	0.385729	-4.424328	-1.250907
29	1	0	1.311851	-1.490893	1.817436
30	1	0	5.748720	-2.571974	0.068955
31	1	0	6.251676	0.051664	0.076767
32	1	0	3.339564	4.453478	-0.461759
33	1	0	0.748943	5.118660	-0.330601
34	1	0	-1.559530	5.016586	0.093659
35	1	0	-4.059011	4.039000	0.228620
36	1	0	-6.197818	-0.864625	-0.208804
37	1	0	-5.142353	-3.302631	-0.591265
38	1	0	3.299090	-4.059809	-0.219435
39	1	0	-2.538116	-4.233420	-0.789300
40	1	0	-5.091600	1.641347	0.135013
41	1	0	4.723112	2.270652	-0.206678
42	7	0	-1.683167	1.651864	0.110717
43	7	0	1.326975	1.894444	-0.014100
44	1	0	1.066277	0.969621	0.293173
45	1	0	2.172325	-0.526570	-0.595112
46	1	0	-1.164357	-1.704296	1.577575
47	1	0	-2.021132	-0.444638	-0.094727

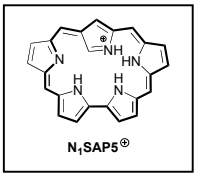
N_1SAP4$^{\oplus}$ (Energy = −1198.90629443)



Stoichiometry C24H18N5(1+)
Framework group C1[X(C24H18N5)]
Deg. of freedom 135
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.926568	-2.118810	1.226682
2	7	0	2.895382	-0.960246	-0.081522
3	7	0	-3.030471	-0.633530	-0.036852
4	6	0	-1.439235	-3.067962	0.321653
5	6	0	-0.346122	-3.705383	-0.244226
6	6	0	0.426814	-2.149491	1.217294
7	6	0	0.840796	-3.094881	0.266689
8	6	0	2.205418	-3.320145	-0.118246
9	6	0	3.148106	-2.325579	-0.203612
10	6	0	4.571435	-2.446220	-0.416806
11	6	0	5.117556	-1.194639	-0.394486
12	6	0	4.048200	-0.245685	-0.210381
13	6	0	4.113425	1.152957	-0.186352
14	6	0	3.029040	2.023291	-0.082805
15	6	0	3.178341	3.476247	0.016338
16	6	0	1.929592	3.980097	0.128689
17	6	0	1.024993	2.827251	0.069094
18	6	0	-0.375528	2.961954	0.088868
19	6	0	-1.141240	4.141912	0.280631
20	6	0	-2.475900	3.815345	0.167006
21	6	0	-2.580009	2.419430	-0.089893
22	6	0	-3.780582	1.701960	-0.261400
23	6	0	-3.983408	0.330958	-0.269691
24	6	0	-5.211266	-0.385350	-0.530839
25	6	0	-4.959718	-1.725067	-0.468667
26	6	0	-3.565494	-1.918670	-0.143920
27	6	0	-2.834845	-3.075192	-0.016742
28	1	0	-0.392822	-4.435211	-1.040824
29	1	0	1.011762	-1.578536	1.924545
30	1	0	5.088778	-3.389140	-0.534823
31	1	0	6.159251	-0.927010	-0.509632
32	1	0	4.119789	4.010524	0.009906
33	1	0	1.636290	5.017058	0.219723
34	1	0	-0.732459	5.117092	0.503539
35	1	0	-3.323651	4.476725	0.283862
36	1	0	-6.152923	0.095081	-0.760815
37	1	0	-5.661718	-2.532496	-0.628759
38	1	0	2.510481	-4.323707	-0.401392
39	1	0	-3.304286	-4.014996	-0.286886
40	1	0	-4.669900	2.313430	-0.370807
41	1	0	5.103013	1.592713	-0.254360
42	7	0	-1.282426	1.924945	-0.099111
43	7	0	1.703698	1.660736	-0.048592
44	1	0	1.995442	-0.484506	-0.058663
45	1	0	-1.475006	-1.733209	1.986311
46	1	0	-2.081259	-0.452232	0.245170
47	1	0	-0.990279	1.073917	-0.559510

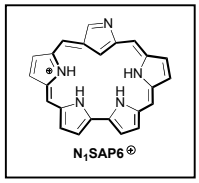
N_1SAP5$^{\oplus}$ (Energy = −1198.90193045)



Stoichiometry C24H18N5(1+)
Framework group C1[X(C24H18N5)]
Deg. of freedom 135
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.903826	-2.068144	1.203428
2	7	0	2.857265	-0.939873	-0.053192
3	7	0	-3.040473	-0.630110	-0.043140
4	6	0	-1.430071	-3.055341	0.340852
5	6	0	-0.343441	-3.714340	-0.212606
6	6	0	0.447303	-2.097601	1.172104
7	6	0	0.848399	-3.075189	0.248787
8	6	0	2.201294	-3.286113	-0.162537
9	6	0	3.147937	-2.285067	-0.220646
10	6	0	4.576038	-2.470759	-0.458374
11	6	0	5.138500	-1.238738	-0.381134
12	6	0	4.037022	-0.305570	-0.151843
13	6	0	4.165268	1.108135	-0.103638
14	6	0	3.126159	2.013938	-0.043373
15	6	0	3.198449	3.446393	0.031904
16	6	0	1.924665	3.936224	0.083768
17	6	0	1.010983	2.824376	0.029616
18	6	0	-0.389733	2.931818	0.035528
19	6	0	-1.143296	4.106609	0.272532
20	6	0	-2.485132	3.793217	0.185236
21	6	0	-2.609122	2.410029	-0.100091
22	6	0	-3.812229	1.695769	-0.263788
23	6	0	-4.006531	0.322735	-0.267837
24	6	0	-5.231120	-0.406544	-0.505029
25	6	0	-4.966231	-1.743643	-0.429872
26	6	0	-3.567190	-1.921506	-0.121493
27	6	0	-2.825904	-3.070990	0.014636
28	1	0	-0.400853	-4.476255	-0.978144
29	1	0	1.054068	-1.493055	1.828734
30	1	0	5.065958	-3.422165	-0.622581
31	1	0	6.181212	-0.969612	-0.494157
32	1	0	4.120440	4.011949	0.043289
33	1	0	1.626775	4.973822	0.130088
34	1	0	-0.724767	5.070953	0.524066
35	1	0	-3.320860	4.460333	0.346666
36	1	0	-6.180319	0.062506	-0.727156
37	1	0	-5.663644	-2.558773	-0.570074
38	1	0	2.492851	-4.283454	-0.483558
39	1	0	-3.293182	-4.016999	-0.237763
40	1	0	-4.704402	2.305508	-0.357337
41	1	0	5.168000	1.523350	-0.130339
42	7	0	-1.311311	1.892394	-0.149660
43	7	0	1.773500	1.688202	-0.047679
44	1	0	-1.438877	-1.669671	1.966237
45	1	0	-2.093328	-0.433352	0.236986
46	1	0	-1.088944	1.105330	-0.747106
47	1	0	1.501677	0.705242	-0.052356

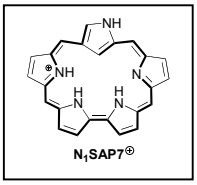
N_1SAP6$^{\oplus}$ (Energy = −1198.90564310)



Stoichiometry C24H18N5(1+)
Framework group C1[X(C24H18N5)]
Deg. of freedom 135
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.493961	2.050126	0.097204
2	7	0	1.462054	2.070025	-0.102816
3	7	0	2.843065	-0.668668	-0.039384
4	7	0	-2.841252	-0.707088	0.036645
5	6	0	-2.487499	-3.164412	-0.213886
6	6	0	3.285042	-1.968362	0.192405
7	6	0	-1.103203	-3.347760	-0.099593
8	6	0	3.896903	1.581281	-0.243911
9	6	0	-0.716118	3.204346	0.105756
10	6	0	5.083868	-0.579566	0.266977
11	6	0	2.523627	-3.136615	0.207265
12	6	0	-0.533701	-4.709323	-0.065998
13	6	0	4.690962	-1.888890	0.412760
14	6	0	2.795090	2.431626	-0.318155
15	6	0	3.932185	0.202230	-0.038208
16	6	0	0.669638	3.213020	-0.116186
17	6	0	-1.571413	4.287731	0.423007
18	6	0	-3.269502	-2.013475	-0.189081
19	6	0	1.148793	-3.354208	0.089644
20	6	0	2.800369	3.832319	-0.563304
21	6	0	-5.087195	-0.647592	-0.243933
22	6	0	-4.680791	-1.950471	-0.393279
23	6	0	-2.829798	2.394448	0.317752
24	6	0	1.511764	4.307986	-0.432640
25	6	0	-3.922063	1.528667	0.249987
26	6	0	-2.853375	3.794664	0.560758
27	6	0	-3.940363	0.150394	0.047211
28	1	0	6.078761	-0.173859	0.392694
29	1	0	-1.118912	-5.623808	-0.122143
30	1	0	5.311702	-2.735936	0.672252
31	1	0	-1.246910	5.307592	0.577168
32	1	0	3.680609	4.402214	-0.828925
33	1	0	-6.088258	-0.253772	-0.358063
34	1	0	-5.295463	-2.804314	-0.645359
35	1	0	1.173873	5.323032	-0.589557
36	1	0	-3.740122	4.353080	0.828911
37	1	0	-4.895795	2.001627	0.325819
38	1	0	4.865054	2.066350	-0.315552
39	1	0	3.097891	-4.050741	0.326245
40	1	0	-3.065538	-4.076540	-0.343197
41	1	0	-1.255146	1.266058	-0.498341
42	7	0	0.752721	-4.722581	0.056545
43	6	0	0.019517	-2.503118	0.002279
44	1	0	0.025426	-1.420435	0.015881
45	1	0	1.231086	1.283861	0.492979
46	1	0	-2.007641	-0.517380	0.577437
47	1	0	2.014569	-0.489243	-0.591369

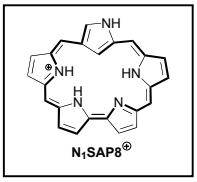
N_1SAP7$^{\oplus}$ (Energy = −1198.91760453)



Stoichiometry C24H18N5(1+)
Framework group C1[X(C24H18N5)]
Deg. of freedom 135
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.206439	-2.183350	0.026647
2	7	0	-1.804920	-1.855664	-0.104741
3	7	0	-2.711133	0.878045	-0.049024
4	7	0	2.928553	0.343995	-0.056581
5	6	0	2.948402	2.828498	-0.123179
6	6	0	-2.997110	2.218221	0.071760
7	6	0	1.574606	3.179091	0.044994
8	6	0	-4.131592	-1.114839	-0.273059
9	6	0	0.261170	-3.199023	0.146823
10	6	0	-5.017280	1.239386	-0.135721
11	6	0	-2.114043	3.277788	0.208128
12	6	0	1.211047	4.532535	0.249316
13	6	0	-4.440039	2.452184	0.027168
14	6	0	-3.163255	-2.098409	-0.227220
15	6	0	-3.920603	0.278244	-0.169064
16	6	0	-1.124960	-3.039231	0.010049
17	6	0	0.966405	-4.385069	0.466935
18	6	0	3.543701	1.595423	-0.204105
19	6	0	-0.704431	3.343705	0.199389
20	6	0	-3.329720	-3.522508	-0.225346
21	6	0	5.145089	-0.013269	-0.402125
22	6	0	4.935740	1.334105	-0.453349
23	6	0	2.480768	-2.714999	0.189849
24	6	0	-2.095927	-4.093624	-0.068933
25	6	0	3.690965	-2.019173	0.049520
26	6	0	2.314630	-4.091160	0.496741
27	6	0	3.893685	-0.659188	-0.119140
28	1	0	-6.069095	0.996758	-0.217504
29	1	0	1.847185	5.403462	0.331543
30	1	0	-4.918257	3.420849	0.102036
31	1	0	0.506459	-5.337574	0.690358
32	1	0	-4.280256	-4.028344	-0.327760
33	1	0	6.074336	-0.542364	-0.566178
34	1	0	5.665311	2.104040	-0.667507
35	1	0	-1.861341	-5.148155	-0.038105
36	1	0	3.125059	-4.766441	0.734780
37	1	0	4.585947	-2.631861	0.069467
38	1	0	-5.159385	-1.453121	-0.360303
39	1	0	-2.604094	4.243943	0.318088
40	1	0	3.636647	3.665915	-0.199366
41	1	0	1.047467	-1.364158	-0.546732
42	7	0	-0.117005	4.613706	0.343691
43	6	0	0.354722	2.446529	0.023087
44	1	0	0.214624	1.393825	-0.166762
45	1	0	-1.481235	-0.895656	0.011710
46	1	0	2.104090	0.243199	0.522546
47	1	0	-0.638794	5.467275	0.494655

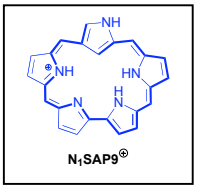
N_1SAP8$^{\oplus}$ (Energy = −1198.91914304)



Stoichiometry C24H18N5(1+)
Framework group C1[X(C24H18N5)]
Deg. of freedom 135
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.982313	2.333424	-0.000080
2	7	0	-1.855479	1.761276	-0.001547
3	7	0	-2.688442	-1.085095	-0.000501
4	7	0	2.964586	-0.202703	0.000164
5	6	0	3.162185	-2.670839	-0.000351
6	6	0	-2.832209	-2.462789	0.000082
7	6	0	1.806673	-3.115334	0.000044
8	6	0	-4.159542	0.896733	-0.000373
9	6	0	0.014989	3.313977	0.000546
10	6	0	-4.907935	-1.520006	0.000091
11	6	0	-1.880002	-3.465178	0.000545
12	6	0	1.523515	-4.501489	0.000502
13	6	0	-4.251304	-2.716507	0.000126
14	6	0	-3.214566	1.923375	-0.000678
15	6	0	-3.922607	-0.477594	-0.000385
16	6	0	-1.358269	3.023910	-0.000084
17	6	0	0.697305	4.562642	0.001452
18	6	0	3.677415	-1.395662	-0.000509
19	6	0	-0.467121	-3.439861	0.000435
20	6	0	-3.577657	3.339886	0.000126
21	6	0	5.147461	0.343794	-0.000947
22	6	0	5.066783	-1.018459	-0.001449
23	6	0	2.244845	2.886257	0.000641
24	6	0	-2.413621	4.031454	-0.001064
25	6	0	3.486860	2.236773	0.000306
26	6	0	2.048736	4.303994	0.001738
27	6	0	3.813274	0.885756	-0.000148
28	1	0	-5.975937	-1.349741	0.000262
29	1	0	2.212158	-5.335485	0.000864
30	1	0	-4.684929	-3.707791	0.000386
31	1	0	0.219214	5.531916	0.002028
32	1	0	-4.588427	3.727539	0.000578
33	1	0	6.042686	0.950924	-0.001372
34	1	0	5.884961	-1.726214	-0.002318
35	1	0	-2.272136	5.103866	-0.001446
36	1	0	2.854771	5.025217	0.002575
37	1	0	4.340480	2.906509	0.000444
38	1	0	-5.204365	1.191135	0.000093
39	1	0	-2.315687	-4.461426	0.001104
40	1	0	3.910107	-3.458583	-0.000765
41	1	0	0.714620	1.363137	-0.001707
42	7	0	0.199981	-4.676733	0.001434
43	6	0	0.536760	-2.465652	-0.000551
44	1	0	0.339310	-1.403725	-0.001783
45	1	0	1.961697	-0.166487	0.002384
46	1	0	-0.267389	-5.574028	0.002384
47	1	0	-1.843652	-0.523038	-0.000570

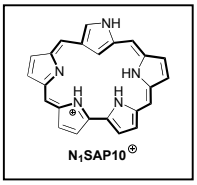
N_1SAP9$^{\oplus}$ (Energy = −1198.92247979)



Stoichiometry C24H18N5(1+)
Framework group C1[X(C24H18N5)]
Deg. of freedom 135
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.759147	1.801443	-0.079044
2	7	0	-1.147566	2.232283	0.029086
3	7	0	-2.914943	-0.303647	-0.049826
4	7	0	2.756958	-0.949983	-0.091681
5	6	0	2.085617	-3.353158	0.175241
6	6	0	-3.549646	-1.541902	-0.178672
7	6	0	0.666141	-3.406060	0.212224
8	6	0	-3.634335	2.077953	-0.031747
9	6	0	1.184685	3.015521	0.070306
10	6	0	-5.115695	0.087886	-0.449038
11	6	0	-2.972219	-2.784764	-0.064015
12	6	0	0.028230	-4.650979	0.419207
13	6	0	-4.931740	-1.264783	-0.459527
14	6	0	-2.419284	2.765309	0.124097
15	6	0	-3.858653	0.719205	-0.161540
16	6	0	-0.201847	3.229074	0.178149
17	6	0	2.170785	4.096821	0.072976
18	6	0	2.980639	-2.316231	0.012997
19	6	0	-1.604878	-3.127007	0.099576
20	6	0	-2.257840	4.152059	0.400688
21	6	0	4.990543	-1.271386	-0.239275
22	6	0	4.406979	-2.496173	-0.084693
23	6	0	3.104152	2.061221	-0.175587
24	6	0	-0.907525	4.433506	0.433642
25	6	0	4.106629	1.103829	-0.275961
26	6	0	3.370937	3.497847	-0.100059
27	6	0	3.948632	-0.286213	-0.224219
28	1	0	-6.031831	0.628620	-0.645866
29	1	0	0.468821	-5.620286	0.608908
30	1	0	-5.671447	-2.026531	-0.667681
31	1	0	1.959074	5.152727	0.173763
32	1	0	-3.075525	4.838595	0.573259
33	1	0	6.042812	-1.045659	-0.345602
34	1	0	4.895301	-3.460986	-0.047828
35	1	0	-0.448565	5.390180	0.639078
36	1	0	4.349355	3.957360	-0.158052
37	1	0	5.128627	1.459594	-0.358706
38	1	0	-4.520197	2.704019	-0.055251
39	1	0	-3.668302	-3.617337	-0.123387
40	1	0	2.571555	-4.320367	0.275671
41	7	0	-1.293608	-4.474588	0.347131
42	6	0	-0.382158	-2.454735	0.023674
43	1	0	-0.260573	-1.414696	-0.241668
44	1	0	1.889305	-0.429171	0.001685
45	1	0	-1.985356	-5.200769	0.480498
46	1	0	-2.096105	-0.205794	0.537551
47	1	0	-0.915764	1.350910	-0.406692

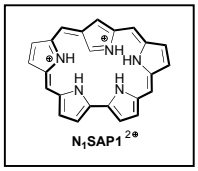
N_1SAP10$^{\oplus}$ (Energy = −1198.91718048)



Stoichiometry C24H18N5(1+)
Framework group C1[X(C24H18N5)]
Deg. of freedom 135
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.816945	-1.838381	-0.107561
2	7	0	1.190828	-2.191710	0.036823
3	7	0	2.920068	0.318305	-0.057390
4	7	0	-2.713190	0.906581	-0.054389
5	6	0	-2.113099	3.303388	0.232314
6	6	0	3.535867	1.563211	-0.225296
7	6	0	-0.695086	3.381392	0.220992
8	6	0	3.676042	-2.045606	0.059613
9	6	0	-1.148399	-3.026511	0.011849
10	6	0	5.133048	-0.048238	-0.420841
11	6	0	2.940128	2.798445	-0.146027
12	6	0	-0.068890	4.640096	0.375466
13	6	0	4.924278	1.298852	-0.488024
14	6	0	2.459373	-2.733101	0.207976
15	6	0	3.884122	-0.690193	-0.119210
16	6	0	0.236950	-3.198019	0.160085
17	6	0	-2.125728	-4.073765	-0.078020
18	6	0	-2.997016	2.249333	0.081879
19	6	0	1.571238	3.127856	0.038034
20	6	0	2.281437	-4.103812	0.524335
21	6	0	-5.018073	1.273813	-0.140504
22	6	0	-4.439370	2.483907	0.038217
23	6	0	-3.177011	-2.070642	-0.244009
24	6	0	0.929390	-4.386793	0.491370
25	6	0	-4.137467	-1.081553	-0.294806
26	6	0	-3.353736	-3.493384	-0.246073
27	6	0	-3.922676	0.312482	-0.181538
28	1	0	6.060591	-0.579453	-0.587772
29	1	0	-0.516393	5.608358	0.554525
30	1	0	5.652518	2.064980	-0.719578
31	1	0	-1.898576	-5.129891	-0.046910
32	1	0	3.085019	-4.784623	0.769681
33	1	0	-6.069994	1.033112	-0.226994
34	1	0	-4.916197	3.452317	0.123574
35	1	0	0.460532	-5.333758	0.719777
36	1	0	-4.306862	-3.992106	-0.359037
37	1	0	-5.166412	-1.414292	-0.390978
38	1	0	4.566912	-2.664374	0.077775
39	1	0	3.623675	3.638462	-0.239378
40	1	0	-2.601703	4.267514	0.359669
41	7	0	1.251725	4.479952	0.260422
42	6	0	0.356530	2.439815	0.018250
43	1	0	0.213704	1.392332	-0.196211
44	1	0	1.937780	5.217979	0.350071
45	1	0	2.103051	0.228126	0.534534
46	1	0	1.040702	-1.372476	-0.538894
47	1	0	-1.486858	-0.881282	0.014626

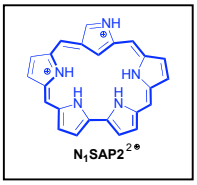
$N_1SAP1^{2\oplus}$ (Energy = −1199.19808533)



Stoichiometry C24H19N5(2+)
Framework group C1[X(C24H19N5)]
Deg. of freedom 138
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.668431	-2.258306	1.125099
2	7	0	2.963807	-0.798572	-0.085125
3	7	0	-2.955804	-0.867024	0.010327
4	6	0	-1.082857	-3.172933	0.132527
5	6	0	0.073118	-3.719486	-0.420464
6	6	0	0.681950	-2.232915	1.181691
7	6	0	1.194293	-3.085127	0.184954
8	6	0	2.605922	-3.214450	-0.087088
9	6	0	3.440630	-2.126343	-0.098149
10	6	0	4.876475	-2.035023	-0.085813
11	6	0	5.225022	-0.711664	-0.068060
12	6	0	4.024325	0.079854	-0.120293
13	6	0	3.931281	1.473577	-0.208346
14	6	0	2.794741	2.281191	-0.208504
15	6	0	2.774212	3.703801	-0.372797
16	6	0	1.480864	4.143619	-0.253075
17	6	0	0.642067	3.008946	-0.033979
18	6	0	-0.746171	2.986199	0.096214
19	6	0	-1.617387	4.080940	0.374701
20	6	0	-2.905584	3.608873	0.406068
21	6	0	-2.888079	2.203584	0.138728
22	6	0	-3.996032	1.370444	0.013165
23	6	0	-4.029116	-0.025886	-0.122786
24	6	0	-5.155006	-0.850244	-0.470931
25	6	0	-4.724827	-2.146315	-0.575708
26	6	0	-3.322362	-2.188732	-0.256482
27	6	0	-2.446617	-3.255740	-0.271333
28	1	0	0.100461	-4.409973	-1.252851
29	1	0	1.208476	-1.720834	1.975598
30	1	0	5.542774	-2.886516	-0.037131
31	1	0	6.224350	-0.299854	-0.016150
32	1	0	3.649638	4.304635	-0.580670
33	1	0	1.129929	5.160604	-0.363858
34	1	0	-1.294870	5.093496	0.576083
35	1	0	-3.800547	4.176046	0.625618
36	1	0	-6.153394	-0.474370	-0.650649
37	1	0	-5.315250	-3.012333	-0.844735
38	1	0	3.025093	-4.194167	-0.298863
39	1	0	-2.799724	-4.192435	-0.691819
40	1	0	-4.960148	1.868194	0.007192
41	1	0	4.874822	2.002501	-0.292131
42	7	0	-1.538991	1.834375	0.008541
43	7	0	1.465039	1.879896	-0.052414
44	1	0	-1.281590	1.117841	-0.661903
45	1	0	1.224775	1.061792	0.493491
46	1	0	2.083185	-0.582371	-0.532950
47	1	0	-1.257541	-2.012660	1.914554
48	1	0	-2.044945	-0.589185	0.340733

$N_1SAP2^{2\oplus}$ (Energy = −1199.22031598)

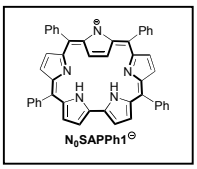


Stoichiometry C24H19N5(2+)
Framework group C1[X(C24H19N5)]
Deg. of freedom 138
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.506820	-2.059869	0.101030
2	7	0	-1.436776	-2.105282	-0.109436
3	7	0	-2.844095	0.616633	-0.050418
4	7	0	2.835217	0.705183	0.060076
5	6	0	2.497957	3.167640	-0.201173
6	6	0	-3.309799	1.914412	0.183421
7	6	0	1.096037	3.370524	-0.092605
8	6	0	-3.874866	-1.645164	-0.243861
9	6	0	0.743015	-3.224403	0.100071
10	6	0	-5.088334	0.497544	0.283894
11	6	0	-2.578857	3.086726	0.204582
12	6	0	0.580588	4.697458	-0.084039
13	6	0	-4.719618	1.809291	0.420791
14	6	0	-2.762905	-2.480804	-0.322746
15	6	0	-3.921765	-0.265689	-0.034227
16	6	0	-0.636351	-3.245746	-0.115852
17	6	0	1.613984	-4.307982	0.411882
18	6	0	3.263015	2.019339	-0.166931
19	6	0	-1.189266	3.309875	0.080649
20	6	0	-2.760139	-3.888050	-0.568015
21	6	0	5.083225	0.654007	-0.256215
22	6	0	4.677527	1.955518	-0.390551
23	6	0	2.844550	-2.394543	0.318712
24	6	0	-1.473805	-4.353554	-0.429894
25	6	0	3.929016	-1.526624	0.254087
26	6	0	2.883818	-3.803928	0.556840
27	6	0	3.936304	-0.142393	0.049102
28	1	0	-6.074627	0.074854	0.421512
29	1	0	1.116405	5.635656	-0.148162
30	1	0	-5.355356	2.642575	0.690247
31	1	0	1.301310	-5.333135	0.556645
32	1	0	-3.636251	-4.464060	-0.834779
33	1	0	6.082184	0.259876	-0.386891
34	1	0	5.290870	2.808293	-0.650866
35	1	0	-1.130454	-5.367983	-0.580713
36	1	0	3.776422	-4.353429	0.824970
37	1	0	4.906608	-1.991277	0.330990
38	1	0	-4.838225	-2.139924	-0.312100
39	1	0	-3.185321	3.977739	0.346142
40	1	0	3.081173	4.073477	-0.343654
41	7	0	-0.741221	4.645815	0.028048
42	6	0	-0.037793	2.516492	0.009548
43	1	0	-0.030393	1.437157	0.042146
44	1	0	2.027578	0.507679	0.637481
45	1	0	-1.351913	5.455172	0.047940
46	1	0	-2.040579	0.448697	-0.643355
47	1	0	-1.217981	-1.323990	0.498149
48	1	0	1.265685	-1.284410	-0.505619

Cartesian coordinates for the optimized structures of normal *meso*-tetraphenyl-sapphyrins (monoanion)

N_0SAPPh1$^{\ominus}$ (Energy = −2122.16998297)

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 Stoichiometry    C48H32N5(1-)
 Framework group  C1[X(C48H32N5)]
 Deg. of freedom   249
 Full point group                 C1
 Largest Abelian subgroup         C1      NOp   1
 Largest concise Abelian subgroup C1      NOp   1
                         Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          7             0        1.626284   -2.346830    0.036340
    2          7             0       -1.626301   -2.346779    0.036362
    3          7             0       -2.976530    0.071957   -0.213657
    4          7             0        2.976431    0.071829   -0.213756
    5          6             0        2.404380    2.443844   -0.378033
    6          6             0       -3.344523    1.383085   -0.266408
    7          6             0       -4.113589   -2.065542    0.000499
    8          6             0        0.712063   -3.383338    0.064125
    9          6             0       -5.282236    0.221110   -0.125203
   10          6             0       -2.404488    2.443941   -0.377954
   11          6             0       -4.795429    1.493160   -0.201581
   12          6             0       -2.928153   -2.839329    0.052873
   13          6             0       -4.121535   -0.658998   -0.131452
   14          6             0       -0.712113   -3.383325    0.064070
   15          6             0        1.478336   -4.583360    0.100382
   16          6             0        3.344388    1.382964   -0.266503
   17          6             0       -2.815703   -4.256725    0.089413
   18          6             0        5.282131    0.221051   -0.125288
   19          6             0        4.795285    1.493085   -0.201671
   20          6             0        2.928118   -2.839430    0.052892
   21          6             0       -1.478428   -4.583319    0.100258
   22          6             0        4.113552   -2.065641    0.000450
   23          6             0        2.815624   -4.256816    0.089616
   24          6             0        4.121469   -0.659103   -0.131561
   25          1             0       -1.480586   -1.336062   -0.029987
   26          1             0       -6.318552   -0.084027   -0.063574
   27          1             0       -5.363343    2.413159   -0.249516
   28          1             0        1.065116   -5.581023    0.124886
   29          1             0       -3.650113   -4.942391    0.090447
   30          1             0        6.318456   -0.084057   -0.063655
   31          1             0        5.363152    2.413113   -0.249600
   32          1             0       -1.065250   -5.581001    0.124729
   33          1             0        3.650009   -4.942514    0.090737
   34          1             0        1.480676   -1.336083   -0.029967
   35          6             0       -0.678216    0.985293   -1.585255
   36          6             0        0.678014    0.985264   -1.585269
   37          6             0        1.082459    2.149313   -0.798131
   38          6             0       -1.082599    2.149351   -0.798112
   39          7             0       -0.000050    2.877918   -0.414300
   40          1             0        1.349441    0.300314   -2.080806
   41          1             0       -1.349687    0.300369   -2.080769
   42          6             0        2.769823    3.817681    0.027956
   43          6             0        2.265753    4.933754   -0.669834
   44          6             0        3.628262    4.064774    1.117529
   45          6             0        2.622166    6.230101   -0.310517
   46          1             0        1.587495    4.765383   -1.498667
   47          6             0        3.986598    5.363927    1.476663
   48          1             0        3.994849    3.224789    1.698735
   49          6             0        3.489463    6.455014    0.762712
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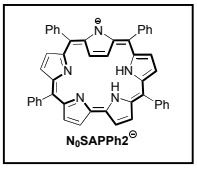
50	1	0	2.220554	7.071703	-0.870734
51	1	0	4.646019	5.522741	2.327383
52	1	0	3.764907	7.468945	1.044224
53	6	0	-2.769810	3.817802	0.028034
54	6	0	-2.265595	4.933807	-0.669756
55	6	0	-3.628101	4.065008	1.117700
56	6	0	-2.621811	6.230201	-0.310416
57	1	0	-1.587385	4.765348	-1.498610
58	6	0	-3.986255	5.364209	1.476844
59	1	0	-3.994725	3.225083	1.698964
60	6	0	-3.489036	6.455229	0.762847
61	1	0	-2.220100	7.071747	-0.870644
62	1	0	-4.645582	5.523112	2.327621
63	1	0	-3.764321	7.469197	1.044381
64	6	0	5.413573	-2.790263	0.084336
65	6	0	6.366942	-2.685105	-0.944797
66	6	0	5.735403	-3.592278	1.194339
67	6	0	7.590649	-3.350343	-0.866543
68	1	0	6.132468	-2.078897	-1.814901
69	6	0	6.956154	-4.262827	1.271786
70	1	0	5.018765	-3.674687	2.006466
71	6	0	7.891608	-4.144741	0.241594
72	1	0	8.307650	-3.253832	-1.678839
73	1	0	7.180717	-4.871481	2.144934
74	1	0	8.844399	-4.665380	0.302128
75	6	0	-5.413613	-2.790189	0.084336
76	6	0	-6.367038	-2.684854	-0.944727
77	6	0	-5.735386	-3.592389	1.194218
78	6	0	-7.590736	-3.350112	-0.866529
79	1	0	-6.132607	-2.078493	-1.814737
80	6	0	-6.956134	-4.262950	1.271618
81	1	0	-5.018696	-3.674949	2.006286
82	6	0	-7.891638	-4.144694	0.241493
83	1	0	-8.307777	-3.253462	-1.678773
84	1	0	-7.180649	-4.871750	2.144676
85	1	0	-8.844425	-4.665344	0.301990

N_0SAPPh2$^{\ominus}$ (Energy = −2122.14158179)



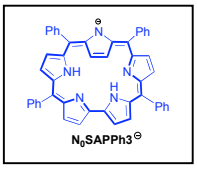
Stoichiometry C48H32N5(1-)
Framework group C1[X(C48H32N5)]
Deg. of freedom 249
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.665341	-2.443080	-0.008173
2	7	0	-1.291003	-2.653004	0.016026
3	7	0	-2.926855	-0.018704	-0.304271
4	7	0	2.885571	0.258398	-0.194778
5	6	0	2.224891	2.593242	-0.262311
6	6	0	-3.383122	1.299799	-0.324217
7	6	0	-3.815100	-2.310954	0.087879
8	6	0	1.005846	-3.598046	-0.167873
9	6	0	-5.111934	-0.109933	0.171371
10	6	0	-2.562593	2.409704	-0.558566
11	6	0	-4.782643	1.207743	-0.019514
12	6	0	-2.614886	-3.086727	-0.024585
13	6	0	-3.936736	-0.920386	-0.018106

14	6	0	-0.419303	-3.709766	-0.173609
15	6	0	1.903467	-4.727152	-0.337622
16	6	0	3.216092	1.573170	-0.128048
17	6	0	-2.547070	-4.479294	-0.272773
18	6	0	5.161556	0.465735	0.140645
19	6	0	4.646233	1.730097	0.092920
20	6	0	3.005806	-2.765465	-0.065434
21	6	0	-1.210915	-4.854884	-0.364772
22	6	0	4.094475	-1.868024	-0.011236
23	6	0	3.159867	-4.205629	-0.265624
24	6	0	4.031699	-0.443692	-0.038370
25	1	0	-6.084032	-0.500527	0.434547
26	1	0	-5.451914	2.054333	0.031555
27	1	0	1.622928	-5.761943	-0.494742
28	1	0	-3.409339	-5.115884	-0.407181
29	1	0	6.195065	0.187649	0.300920
30	1	0	5.188329	2.664705	0.163063
31	1	0	-0.828027	-5.845628	-0.567615
32	1	0	4.095310	-4.737324	-0.374994
33	6	0	-0.694054	1.091756	-1.769965
34	6	0	0.664023	1.127883	-1.658236
35	6	0	0.964683	2.269985	-0.811727
36	6	0	-1.196300	2.203487	-0.968961
37	7	0	-0.185222	2.944314	-0.475002
38	1	0	1.390329	0.465794	-2.102027
39	1	0	-1.282140	0.429752	-2.395940
40	1	0	-1.981802	-0.253541	-0.569495
41	1	0	-0.941576	-1.751243	0.311517
42	6	0	2.479989	3.955732	0.256633
43	6	0	1.978486	5.087819	-0.415172
44	6	0	3.228573	4.168910	1.430100
45	6	0	2.233541	6.373655	0.052782
46	1	0	1.382910	4.941392	-1.308904
47	6	0	3.482021	5.457213	1.900049
48	1	0	3.592491	3.310045	1.984238
49	6	0	2.990362	6.567303	1.211742
50	1	0	1.837449	7.230166	-0.488179
51	1	0	4.056887	5.591883	2.813750
52	1	0	3.186419	7.572539	1.578236
53	6	0	5.463777	-2.470124	0.060873
54	6	0	6.416352	-2.229990	-0.944230
55	6	0	5.838114	-3.288247	1.140497
56	6	0	7.692568	-2.789612	-0.875480
57	1	0	6.141266	-1.602415	-1.786777
58	6	0	7.115317	-3.845622	1.213563
59	1	0	5.114720	-3.477477	1.928096
60	6	0	8.048824	-3.599780	0.204833
61	1	0	8.409170	-2.594566	-1.670270
62	1	0	7.382116	-4.470403	2.063118
63	1	0	9.044216	-4.034562	0.260001
64	6	0	-5.072941	-3.088038	0.301895
65	6	0	-6.153565	-2.994678	-0.593395
66	6	0	-5.212492	-3.945463	1.408754
67	6	0	-7.330526	-3.714735	-0.383414
68	1	0	-6.057344	-2.354448	-1.465469
69	6	0	-6.385251	-4.669808	1.617687
70	1	0	-4.387297	-4.033191	2.109320
71	6	0	-7.452828	-4.556262	0.723472
72	1	0	-8.149159	-3.625875	-1.094099
73	1	0	-6.468522	-5.319492	2.486007
74	1	0	-8.368139	-5.120273	0.886398
75	6	0	-3.033204	3.777728	-0.254027
76	6	0	-2.663948	4.849775	-1.090838
77	6	0	-3.840675	4.072973	0.861381
78	6	0	-3.106355	6.145642	-0.842921

79	1	0	-2.021192	4.647261	-1.941272
80	6	0	-4.286973	5.371021	1.108469
81	1	0	-4.090725	3.278638	1.557532
82	6	0	-3.928131	6.415437	0.255341
83	1	0	-2.808422	6.951209	-1.510510
84	1	0	-4.903094	5.568307	1.983200
85	1	0	-4.271795	7.428658	0.450205

N_0SAPPh3$^{\ominus}$ (Energy = −2122.17536400)

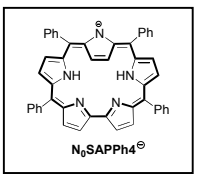


Stoichiometry C48H32N5(1-)
Framework group C1[X(C48H32N5)]
Deg. of freedom 249
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.595543	-2.371093	0.017889
2	7	0	-1.572800	-2.339945	0.028214
3	7	0	-2.997852	0.081922	-0.249950
4	7	0	2.956598	0.089378	-0.200739
5	6	0	2.402116	2.466790	-0.335098
6	6	0	-3.341694	1.419426	-0.320376
7	6	0	-4.051196	-2.119832	0.013458
8	6	0	0.698056	-3.416766	0.033486
9	6	0	-5.236479	0.161246	-0.142069
10	6	0	-2.408871	2.477274	-0.437079
11	6	0	-4.770519	1.453666	-0.251468
12	6	0	-2.846394	-2.867881	0.056164
13	6	0	-4.109894	-0.720223	-0.133747
14	6	0	-0.729771	-3.404193	0.041040
15	6	0	1.480552	-4.608194	0.044441
16	6	0	3.335858	1.396797	-0.230117
17	6	0	-2.792237	-4.315844	0.080394
18	6	0	5.263721	0.220147	-0.097032
19	6	0	4.786563	1.497101	-0.154013
20	6	0	2.904604	-2.841561	0.020907
21	6	0	-1.472143	-4.650913	0.071471
22	6	0	4.083479	-2.059553	-0.017527
23	6	0	2.812829	-4.263068	0.032717
24	6	0	4.096574	-0.650784	-0.124825
25	1	0	-6.267957	-0.153422	-0.073314
26	1	0	-5.362880	2.355269	-0.316859
27	1	0	1.078983	-5.610694	0.051621
28	1	0	-3.640579	-4.986368	0.080456
29	1	0	6.297397	-0.093547	-0.034315
30	1	0	5.361032	2.413901	-0.182990
31	1	0	-1.056230	-5.649574	0.078681
32	1	0	3.658166	-4.935164	0.016914
33	1	0	1.404399	-1.370186	-0.021397
34	6	0	-0.653266	1.037357	-1.632345
35	6	0	0.703363	1.038505	-1.604006
36	6	0	1.090195	2.186287	-0.788818
37	6	0	-1.074623	2.188320	-0.834892
38	7	0	-0.003089	2.906251	-0.411599
39	1	0	1.382795	0.359281	-2.095712
40	1	0	-1.300329	0.357812	-2.170570
41	1	0	-2.063861	-0.322894	-0.172203
42	6	0	2.765328	3.828113	0.111486

43	6	0	2.267306	4.964114	-0.558241
44	6	0	3.616673	4.043511	1.213476
45	6	0	2.622707	6.249332	-0.160249
46	1	0	1.594116	4.820202	-1.395709
47	6	0	3.973928	5.331603	1.611177
48	1	0	3.978796	3.187193	1.773155
49	6	0	3.482907	6.442972	0.924737
50	1	0	2.225897	7.106807	-0.699414
51	1	0	4.627863	5.465633	2.470335
52	1	0	3.757710	7.448233	1.236327
53	6	0	-2.798101	3.850842	-0.054219
54	6	0	-2.283729	4.960342	-0.755402
55	6	0	-3.683568	4.108680	1.010929
56	6	0	-2.655522	6.259264	-0.422645
57	1	0	-1.584216	4.784600	-1.564850
58	6	0	-4.058387	5.410459	1.342136
59	1	0	-4.057964	3.276473	1.598448
60	6	0	-3.550563	6.494692	0.625275
61	1	0	-2.244587	7.094964	-0.984850
62	1	0	-4.738396	5.576870	2.174980
63	1	0	-3.838614	7.510684	0.885473
64	6	0	5.387280	-2.781831	0.055790
65	6	0	6.331022	-2.674560	-0.981276
66	6	0	5.719158	-3.581227	1.164104
67	6	0	7.556910	-3.337099	-0.912636
68	1	0	6.088051	-2.068674	-1.849295
69	6	0	6.942675	-4.247890	1.232703
70	1	0	5.008006	-3.665888	1.980756
71	6	0	7.868908	-4.128700	0.194398
72	1	0	8.267034	-3.239907	-1.730834
73	1	0	7.176017	-4.855125	2.104485
74	1	0	8.823567	-4.646726	0.247772
75	6	0	-5.351558	-2.842394	0.135498
76	6	0	-6.315102	-2.782908	-0.886908
77	6	0	-5.657233	-3.597981	1.281357
78	6	0	-7.535701	-3.448671	-0.768433
79	1	0	-6.091290	-2.215172	-1.785590
80	6	0	-6.874974	-4.268002	1.399937
81	1	0	-4.927551	-3.648094	2.084203
82	6	0	-7.821826	-4.195603	0.375865
83	1	0	-8.260982	-3.390413	-1.577017
84	1	0	-7.087407	-4.842223	2.298987
85	1	0	-8.771973	-4.716406	0.468462

N_0SAPPh4$^{\ominus}$ (Energy = −2122.17270659)

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Stoichiometry    C48H32N5(1-)
Framework group  C1[X(C48H32N5)]
Deg. of freedom   249
Full point group                 C1
Largest Abelian subgroup         C1      NOp   1
Largest concise Abelian subgroup C1      NOp   1
                       Standard orientation:
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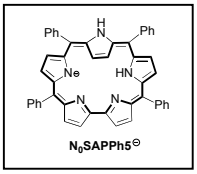
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.578361	-2.310953	0.014800
2	7	0	-1.579262	-2.310540	0.014869
3	7	0	-3.000311	0.089815	-0.230471
4	7	0	3.000315	0.089094	-0.230949
5	6	0	2.408665	2.486686	-0.388348
6	6	0	-3.343322	1.427724	-0.281638

7	6	0	-4.053034	-2.115309	-0.003530
8	6	0	0.717508	-3.358779	0.021473
9	6	0	-5.239209	0.169850	-0.126805
10	6	0	-2.407690	2.487237	-0.387508
11	6	0	-4.770721	1.464539	-0.214133
12	6	0	-2.846586	-2.853523	0.033947
13	6	0	-4.114020	-0.710520	-0.130019
14	6	0	-0.718680	-3.358586	0.021269
15	6	0	1.453831	-4.618445	0.037356
16	6	0	3.343891	1.426873	-0.282391
17	6	0	-2.777802	-4.303411	0.043896
18	6	0	5.239243	0.168221	-0.127225
19	6	0	4.771315	1.463082	-0.214884
20	6	0	2.845523	-2.854247	0.034366
21	6	0	-1.455331	-4.618070	0.036397
22	6	0	4.052182	-2.116393	-0.003293
23	6	0	2.776382	-4.304117	0.045020
24	6	0	4.113677	-0.711687	-0.130221
25	1	0	-6.271152	-0.144784	-0.064994
26	1	0	-5.361425	2.368100	-0.267016
27	1	0	1.029700	-5.612816	0.035248
28	1	0	-3.618234	-4.983938	0.032948
29	1	0	6.271047	-0.146850	-0.065291
30	1	0	5.362411	2.366375	-0.267952
31	1	0	-1.031450	-5.612546	0.033747
32	1	0	3.616650	-4.984855	0.034676
33	6	0	-0.678536	1.066536	-1.633423
34	6	0	0.678739	1.066280	-1.633504
35	6	0	1.083442	2.204136	-0.812942
36	6	0	-1.082701	2.204379	-0.812564
37	7	0	0.000533	2.913895	-0.398130
38	1	0	1.333837	0.389076	-2.164094
39	1	0	-1.333935	0.389575	-2.163940
40	1	0	-2.068650	-0.327086	-0.151752
41	1	0	2.068454	-0.327308	-0.152237
42	6	0	5.350872	-2.844102	0.101677
43	6	0	6.312733	-2.765434	-0.921028
44	6	0	5.656423	-3.623909	1.231097
45	6	0	7.531390	-3.437243	-0.818981
46	1	0	6.089051	-2.178444	-1.807294
47	6	0	6.872510	-4.299726	1.333178
48	1	0	4.928081	-3.688576	2.034060
49	6	0	7.817489	-4.208727	0.308973
50	1	0	8.255286	-3.364271	-1.627617
51	1	0	7.084851	-4.893367	2.219533
52	1	0	8.766281	-4.734122	0.388747
53	6	0	2.790693	3.851343	0.030806
54	6	0	2.277247	4.977037	-0.645005
55	6	0	3.670386	4.084225	1.106574
56	6	0	2.644411	6.267900	-0.277790
57	1	0	1.582144	4.820382	-1.462052
58	6	0	4.040155	5.378077	1.472433
59	1	0	4.044729	3.238243	1.674036
60	6	0	3.533367	6.478871	0.780493
61	1	0	2.234618	7.116558	-0.821085
62	1	0	4.715742	5.524957	2.312489
63	1	0	3.817757	7.488634	1.067557
64	6	0	-2.789191	3.851879	0.032157
65	6	0	-2.275780	4.977659	-0.643542
66	6	0	-3.668500	4.084660	1.108271
67	6	0	-2.642580	6.268492	-0.275864
68	1	0	-1.580969	4.821096	-1.460849
69	6	0	-4.037884	5.378486	1.474606
70	1	0	-4.042836	3.238606	1.675631
71	6	0	-3.531120	6.479366	0.782785

72	1	0	-2.232810	7.117207	-0.819087
73	1	0	-4.713155	5.525256	2.314934
74	1	0	-3.815226	7.489112	1.070190
75	6	0	-5.351923	-2.842639	0.101084
76	6	0	-6.313945	-2.762894	-0.921411
77	6	0	-5.657576	-3.623242	1.229942
78	6	0	-7.532790	-3.434397	-0.819695
79	1	0	-6.090225	-2.175322	-1.807279
80	6	0	-6.873850	-4.298767	1.331674
81	1	0	-4.929155	-3.688752	2.032765
82	6	0	-7.818966	-4.206684	0.307693
83	1	0	-8.256785	-3.360558	-1.628165
84	1	0	-7.086226	-4.893042	2.217597
85	1	0	-8.767907	-4.731847	0.387202

N_0SAPPh5$^{\ominus}$ (Energy = −2122.14778131)

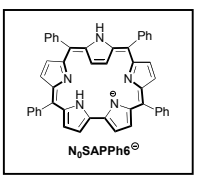


Stoichiometry C48H32N5(1-)
Framework group C1[X(C48H32N5)]
Deg. of freedom 249
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.340916	-2.433656	-0.006130
2	7	0	-1.748207	-2.291291	-0.016144
3	7	0	-2.969598	0.207993	-0.221270
4	7	0	2.997677	-0.019903	-0.242538
5	6	0	2.669407	2.361612	-0.417358
6	6	0	-3.212405	1.565007	-0.268217
7	6	0	-4.191695	-1.917546	0.011392
8	6	0	0.476944	-3.460817	-0.052461
9	6	0	-5.192281	0.454457	-0.060705
10	6	0	-2.208690	2.569580	-0.408078
11	6	0	-4.626197	1.713071	-0.166480
12	6	0	-3.051247	-2.747609	0.018798
13	6	0	-4.143841	-0.506706	-0.095286
14	6	0	-0.962594	-3.390204	-0.037625
15	6	0	1.179568	-4.743940	-0.105452
16	6	0	3.523188	1.225148	-0.246469
17	6	0	-3.078283	-4.199667	0.007844
18	6	0	5.281793	-0.158831	0.026267
19	6	0	4.967047	1.169718	-0.068036
20	6	0	2.600406	-2.990289	-0.011597
21	6	0	-1.777611	-4.599330	-0.028930
22	6	0	3.835969	-2.297635	0.005538
23	6	0	2.505467	-4.449339	-0.078333
24	6	0	4.020158	-0.889961	-0.087590
25	1	0	-6.243526	0.222177	0.032608
26	1	0	-5.148058	2.658959	-0.204902
27	1	0	0.734639	-5.728853	-0.167818
28	1	0	-3.962222	-4.823169	0.006338
29	1	0	6.264252	-0.586014	0.181816
30	1	0	5.650929	2.009796	-0.053770
31	1	0	-1.411662	-5.617174	-0.048359
32	1	0	3.332368	-5.144929	-0.127768
33	6	0	-0.513541	1.050041	-1.590502
34	6	0	0.857027	0.992453	-1.591512
35	6	0	1.360511	2.119127	-0.876604

36	6	0	-0.922943	2.205454	-0.859927
37	7	0	0.244275	2.889415	-0.548917
38	1	0	1.475564	0.228669	-2.029892
39	1	0	-1.184036	0.349198	-2.064600
40	1	0	-2.073817	-0.287032	-0.160113
41	1	0	0.274572	3.612215	0.155993
42	6	0	5.081623	-3.120410	0.122401
43	6	0	6.057219	-3.104319	-0.889278
44	6	0	5.319440	-3.922424	1.251831
45	6	0	7.223635	-3.862282	-0.778822
46	1	0	5.886161	-2.493906	-1.771164
47	6	0	6.486371	-4.678865	1.366108
48	1	0	4.577068	-3.941202	2.044223
49	6	0	7.444646	-4.652948	0.350663
50	1	0	7.959378	-3.837960	-1.579817
51	1	0	6.648352	-5.287453	2.253129
52	1	0	8.353893	-5.243376	0.438410
53	6	0	-5.542906	-2.540831	0.124635
54	6	0	-6.513762	-2.359820	-0.876204
55	6	0	-5.887456	-3.324793	1.239687
56	6	0	-7.778586	-2.938580	-0.767320
57	1	0	-6.261056	-1.767442	-1.750905
58	6	0	-7.150660	-3.906770	1.348813
59	1	0	-5.151573	-3.467817	2.025337
60	6	0	-8.103657	-3.715716	0.346226
61	1	0	-8.508837	-2.788213	-1.559388
62	1	0	-7.392510	-4.506021	2.223758
63	1	0	-9.088857	-4.168236	0.431394
64	6	0	-2.491790	3.960128	0.005677
65	6	0	-1.971939	5.053231	-0.722176
66	6	0	-3.275828	4.256892	1.141138
67	6	0	-2.226125	6.367925	-0.338486
68	1	0	-1.374544	4.856758	-1.607685
69	6	0	-3.537589	5.572696	1.517434
70	1	0	-3.666530	3.437930	1.736656
71	6	0	-3.014621	6.639324	0.782646
72	1	0	-1.814418	7.185823	-0.925764
73	1	0	-4.141943	5.765224	2.401293
74	1	0	-3.214496	7.665544	1.080877
75	6	0	3.084209	3.716247	-0.001979
76	6	0	2.665231	4.857425	-0.719679
77	6	0	3.906544	3.924835	1.125485
78	6	0	3.050357	6.138882	-0.332459
79	1	0	2.044417	4.723654	-1.600898
80	6	0	4.297679	5.206921	1.506145
81	1	0	4.220350	3.065593	1.709049
82	6	0	3.872420	6.323336	0.782130
83	1	0	2.714811	6.997343	-0.910163
84	1	0	4.927933	5.335344	2.383435
85	1	0	4.174267	7.323376	1.083910

N_0SAPPh6$^{\ominus}$ (Energy = −2122.15524133)



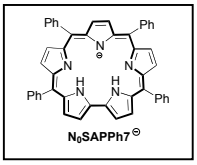
Stoichiometry C48H32N5(1-)
Framework group C1[X(C48H32N5)]
Deg. of freedom 249
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	7	0	1.690994	-2.404519	-0.005413
2	7	0	-1.383787	-2.466194	0.004918
3	7	0	-2.973982	0.019671	-0.258383
4	7	0	2.921584	0.164115	-0.235446
5	6	0	2.270592	2.525451	-0.397551
6	6	0	-3.472801	1.273653	-0.284776
7	6	0	-3.877499	-2.233671	0.013152
8	6	0	0.864212	-3.502992	-0.027183
9	6	0	-5.266101	-0.065735	-0.011584
10	6	0	-2.600285	2.399296	-0.457468
11	6	0	-4.919897	1.252884	-0.121858
12	6	0	-2.665216	-2.971813	0.009203
13	6	0	-4.020691	-0.826813	-0.101458
14	6	0	-0.567736	-3.533351	-0.029444
15	6	0	1.710818	-4.642334	-0.039756
16	6	0	3.239897	1.481263	-0.244857
17	6	0	-2.625365	-4.431146	-0.034117
18	6	0	5.214231	0.400964	-0.019851
19	6	0	4.678924	1.653805	-0.101284
20	6	0	3.025733	-2.789835	0.001072
21	6	0	-1.310505	-4.783764	-0.060252
22	6	0	4.156136	-1.929738	-0.003837
23	6	0	3.023720	-4.211915	-0.024159
24	6	0	4.095659	-0.526377	-0.105509
25	1	0	-6.259862	-0.468544	0.136362
26	1	0	-5.583633	2.109006	-0.126296
27	1	0	1.366062	-5.666321	-0.061263
28	1	0	-3.479432	-5.093874	-0.067738
29	1	0	6.256960	0.138733	0.101270
30	1	0	5.210008	2.597155	-0.099304
31	1	0	-0.899747	-5.785034	-0.104463
32	1	0	3.910408	-4.828523	-0.045288
33	6	0	-0.799121	0.998678	-1.612085
34	6	0	0.569702	1.034722	-1.594955
35	6	0	0.987977	2.191999	-0.869588
36	6	0	-1.294187	2.139843	-0.908055
37	7	0	-0.172346	2.903368	-0.587176
38	1	0	1.251154	0.320663	-2.027422
39	1	0	-1.428474	0.240992	-2.046480
40	1	0	-0.199411	3.630218	0.113941
41	1	0	1.414719	-1.424706	-0.018538
42	6	0	5.497627	-2.576364	0.101336
43	6	0	6.463920	-2.402947	-0.905276
44	6	0	5.840539	-3.370290	1.210219
45	6	0	7.723356	-2.995246	-0.806069
46	1	0	6.212150	-1.801235	-1.773615
47	6	0	7.098118	-3.965649	1.309818
48	1	0	5.109767	-3.508112	2.001831
49	6	0	8.046993	-3.780695	0.301872
50	1	0	8.450798	-2.847960	-1.601271
51	1	0	7.339509	-4.569666	2.181655
52	1	0	9.027793	-4.244056	0.379162
53	6	0	2.567814	3.905957	0.039641
54	6	0	2.096255	5.018993	-0.690448
55	6	0	3.321328	4.170664	1.203289
56	6	0	2.368760	6.323117	-0.283566
57	1	0	1.523485	4.846239	-1.597083
58	6	0	3.601867	5.475804	1.603487
59	1	0	3.672371	3.334920	1.800092
60	6	0	3.127487	6.562395	0.865152
61	1	0	1.994997	7.157472	-0.873151
62	1	0	4.182444	5.644420	2.507959
63	1	0	3.341457	7.580224	1.182122
64	6	0	-3.000187	3.759742	-0.045935

65	6	0	-2.565962	4.894534	-0.764980
66	6	0	-3.822250	3.981535	1.079394
67	6	0	-2.935605	6.181523	-0.381005
68	1	0	-1.944667	4.751481	-1.644387
69	6	0	-4.198207	5.269171	1.456625
70	1	0	-4.148436	3.127870	1.664393
71	6	0	-3.757628	6.378837	0.731424
72	1	0	-2.587842	7.034426	-0.959766
73	1	0	-4.828562	5.407103	2.332451
74	1	0	-4.047522	7.383214	1.030556
75	6	0	-5.148006	-3.017508	0.141645
76	6	0	-6.107399	-3.013956	-0.885094
77	6	0	-5.424352	-3.767676	1.297310
78	6	0	-7.296574	-3.734183	-0.763389
79	1	0	-5.906468	-2.442528	-1.786622
80	6	0	-6.613876	-4.486234	1.422892
81	1	0	-4.694336	-3.776194	2.101412
82	6	0	-7.556173	-4.473454	0.392307
83	1	0	-8.019946	-3.720394	-1.575797
84	1	0	-6.806127	-5.054621	2.330303
85	1	0	-8.483070	-5.034315	0.488788

N_0SAPPh7$^{\ominus}$ (Energy = −2122.14803314)



Stoichiometry C48H32N5(1-)
Framework group C1[X(C48H32N5)]
Deg. of freedom 249
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

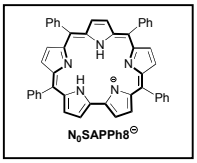
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.558163	-2.464867	-0.434508
2	7	0	-1.557982	-2.464886	-0.434713
3	7	0	-2.793721	-0.010635	0.018547
4	7	0	2.793654	-0.010644	0.018535
5	6	0	2.454281	2.464024	-0.000766
6	6	0	-3.151049	1.269179	0.319522
7	6	0	1.086355	2.672109	-0.331468
8	6	0	-3.961740	-2.171066	0.060553
9	6	0	0.707475	-3.463464	-0.849610
10	6	0	-4.929566	0.007467	0.940870
11	6	0	-2.454403	2.463989	-0.000026
12	6	0	0.675305	3.895852	-1.028795
13	6	0	-4.483678	1.289189	0.926961
14	6	0	-0.675780	3.895871	-1.028523
15	6	0	-2.860503	-2.932622	-0.387787
16	6	0	-3.874483	-0.788303	0.333153
17	6	0	-0.707245	-3.463422	-0.849829
18	6	0	1.513848	-4.600821	-1.123793
19	6	0	3.150963	1.269306	0.319001
20	6	0	-1.086604	2.672133	-0.331083
21	6	0	-2.825006	-4.280406	-0.839953
22	6	0	4.929560	0.007864	0.940726
23	6	0	4.483646	1.289560	0.926343
24	6	0	2.860631	-2.932684	-0.387129
25	6	0	-1.513621	-4.600652	-1.124562
26	6	0	3.961802	-2.170997	0.061161
27	6	0	2.825182	-4.280593	-0.838909
28	6	0	3.874470	-0.788160	0.333324

29	1	0	-1.376596	-1.471100	-0.260417
30	1	0	-5.862949	-0.366446	1.339676
31	1	0	1.337093	4.620530	-1.483004
32	1	0	-4.987510	2.163203	1.315597
33	1	0	-1.337735	4.620564	-1.482471
34	1	0	1.139847	-5.556220	-1.464386
35	1	0	-3.688326	-4.922419	-0.936384
36	1	0	5.862973	-0.365894	1.339605
37	1	0	4.987445	2.163746	1.314633
38	1	0	-1.139592	-5.555946	-1.465417
39	1	0	3.688480	-4.922697	-0.934920
40	7	0	-0.000045	1.923153	0.021349
41	1	0	1.376916	-1.470965	-0.260575
42	6	0	-3.298692	3.704806	-0.006520
43	6	0	-2.955335	4.818037	0.782182
44	6	0	-4.455690	3.800161	-0.801254
45	6	0	-3.737001	5.973531	0.783256
46	1	0	-2.066699	4.762062	1.403516
47	6	0	-5.235311	4.957225	-0.808731
48	1	0	-4.732516	2.955114	-1.424392
49	6	0	-4.881124	6.049703	-0.014077
50	1	0	-3.452372	6.815504	1.410544
51	1	0	-6.119241	5.006817	-1.441034
52	1	0	-5.489505	6.951382	-0.017294
53	6	0	-5.262825	-2.872653	0.234180
54	6	0	-5.369570	-4.030028	1.028631
55	6	0	-6.432427	-2.400969	-0.391257
56	6	0	-6.589262	-4.686556	1.190223
57	1	0	-4.482884	-4.402373	1.533102
58	6	0	-7.653743	-3.054234	-0.227244
59	1	0	-6.369040	-1.516732	-1.018009
60	6	0	-7.739455	-4.202011	0.563346
61	1	0	-6.642832	-5.574061	1.816995
62	1	0	-8.540022	-2.668896	-0.726533
63	1	0	-8.691228	-4.712542	0.690316
64	6	0	5.262877	-2.872539	0.235105
65	6	0	5.369534	-4.029668	1.029921
66	6	0	6.432500	-2.401115	-0.390474
67	6	0	6.589191	-4.686200	1.191756
68	1	0	4.482804	-4.401812	1.534464
69	6	0	7.653788	-3.054380	-0.226214
70	1	0	6.369161	-1.517084	-1.017519
71	6	0	7.739422	-4.201899	0.564754
72	1	0	6.642715	-5.573509	1.818808
73	1	0	8.540100	-2.669253	-0.725607
74	1	0	8.691165	-4.712439	0.691912
75	6	0	3.298607	3.704803	-0.007816
76	6	0	4.455344	3.799881	-0.802973
77	6	0	2.955616	4.818261	0.780725
78	6	0	5.235046	4.956885	-0.811024
79	1	0	4.731888	2.954643	-1.425977
80	6	0	3.737359	5.973700	0.781218
81	1	0	2.067206	4.762527	1.402406
82	6	0	4.881207	6.049598	-0.016536
83	1	0	6.118763	5.006237	-1.443643
84	1	0	3.453002	6.815856	1.408387
85	1	0	5.489636	6.951242	-0.020207

N_0SAPPh8$^{\ominus}$ (Energy = −2122.15024969)

Stoichiometry C48H32N5(1-)
Framework group C1[X(C48H32N5)]
Deg. of freedom 249



Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.700290	-2.580665	-0.233819
2	7	0	1.202100	-2.658512	-0.378244
3	7	0	2.737197	-0.024904	0.024250
4	7	0	-2.670854	0.112288	0.044609
5	6	0	-2.239653	2.560599	-0.401507
6	6	0	3.276827	1.119866	0.514578
7	6	0	-0.852851	2.800077	-0.408433
8	6	0	3.639772	-2.342659	-0.214518
9	6	0	-0.975002	-3.697855	-0.539990
10	6	0	4.854874	-0.434810	0.893483
11	6	0	2.707594	2.417635	0.388611
12	6	0	-0.301847	4.098965	-0.695223
13	6	0	4.590563	0.882038	1.099866
14	6	0	1.033296	4.084984	-0.423118
15	6	0	2.491929	-3.074238	-0.578705
16	6	0	3.691195	-0.986878	0.208280
17	6	0	0.432731	-3.700011	-0.728107
18	6	0	-1.866545	-4.797589	-0.498086
19	6	0	-3.031745	1.418812	-0.073562
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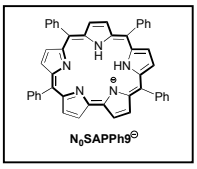
21	6	0	2.509262	-4.427960	-1.128749
22	6	0	-4.955221	0.349154	0.454675
23	6	0	-4.464252	1.581193	0.178746
24	6	0	-3.012832	-2.908607	0.027131
25	6	0	1.207424	-4.824700	-1.213700
26	6	0	-4.012315	-1.966671	0.353474
27	6	0	-3.111909	-4.320591	-0.122753
28	6	0	-3.837182	-0.570209	0.336297
29	1	0	5.730029	-0.987478	1.207347
30	1	0	-0.876088	4.939410	-1.050634
31	1	0	5.209441	1.609034	1.607957
32	1	0	1.726202	4.905238	-0.533252
33	1	0	-1.585701	-5.826715	-0.677146
34	1	0	3.386634	-4.986168	-1.426403
35	1	0	-5.978646	0.081170	0.677258
36	1	0	-5.012045	2.511978	0.161598
37	1	0	0.819429	-5.766258	-1.584468
38	1	0	-4.011018	-4.898157	0.035867
39	7	0	0.234713	2.009239	-0.044565
40	1	0	-1.358154	-1.622547	-0.198258
41	1	0	0.211497	1.011704	0.132442
42	6	0	3.628109	3.572287	0.650299
43	6	0	4.810654	3.740551	-0.091496
44	6	0	3.342774	4.516328	1.652073
45	6	0	5.670926	4.810717	0.155301
46	1	0	5.045761	3.020929	-0.869859
47	6	0	4.203106	5.585742	1.903927
48	1	0	2.437135	4.397230	2.239912
49	6	0	5.371857	5.738745	1.155406
50	1	0	6.575577	4.921782	-0.438428
51	1	0	3.961878	6.297265	2.690575
52	1	0	6.043229	6.572021	1.349780
53	6	0	4.944585	-3.076447	-0.247311
54	6	0	6.015390	-2.607772	-1.028993
55	6	0	5.142801	-4.250389	0.500641
56	6	0	7.232310	-3.288799	-1.068534
57	1	0	5.878182	-1.702968	-1.613468

58	6	0	6.361251	-4.929684	0.468076
59	1	0	4.329793	-4.620023	1.118110
60	6	0	7.411732	-4.453464	-0.319073
61	1	0	8.041574	-2.909386	-1.688631
62	1	0	6.490988	-5.830773	1.063555
63	1	0	8.361193	-4.983402	-0.346793
64	6	0	-5.364954	-2.513952	0.682190
65	6	0	-6.124375	-3.210043	-0.273279
66	6	0	-5.912241	-2.349390	1.965806
67	6	0	-7.382530	-3.724672	0.042545
68	1	0	-5.720864	-3.335837	-1.273899
69	6	0	-7.171472	-2.860118	2.282989
70	1	0	-5.334930	-1.815880	2.715499
71	6	0	-7.912290	-3.552269	1.322898
72	1	0	-7.953228	-4.254755	-0.716763
73	1	0	-7.571844	-2.720995	3.284711
74	1	0	-8.893154	-3.951948	1.569473
75	6	0	-3.060787	3.776408	-0.766973
76	6	0	-3.280460	4.818418	0.147536
77	6	0	-3.646012	3.879960	-2.037658
78	6	0	-4.059441	5.925369	-0.194387
79	1	0	-2.834361	4.750607	1.136170
80	6	0	-4.421860	4.987381	-2.386438
81	1	0	-3.487449	3.077627	-2.753010
82	6	0	-4.632810	6.014697	-1.464861
83	1	0	-4.220291	6.717916	0.533228
84	1	0	-4.862780	5.046260	-3.379064
85	1	0	-5.239300	6.876690	-1.733241

N_0SAPPh9$^{\ominus}$ (Energy = −2122.14095269)

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Stoichiometry    C48H32N5(1-)
Framework group  C1[X(C48H32N5)]
Deg. of freedom   249
Full point group                 C1
Largest Abelian subgroup         C1      NOp   1
Largest concise Abelian subgroup C1      NOp   1
                      Standard orientation:
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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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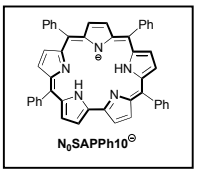
3	7	0	-2.762235	0.186642	0.070989
4	7	0	2.778820	-0.113917	0.038790
5	6	0	2.892315	2.319167	0.393593
6	6	0	-2.954793	1.548030	-0.075737
7	6	0	1.598733	2.713615	0.014629
8	6	0	-4.182828	-1.847717	0.351141
9	6	0	0.213188	-3.601257	-0.644625
10	6	0	-4.958337	0.564375	0.423658
11	6	0	-2.063700	2.611200	-0.398428
12	6	0	1.255742	4.036274	-0.395944
13	6	0	-4.352786	1.768798	0.160983
14	6	0	-0.079481	4.078646	-0.669507
15	6	0	-3.175160	-2.778288	0.049229
16	6	0	-3.970786	-0.451234	0.338716
17	6	0	-1.199327	-3.524885	-0.453749
18	6	0	0.903406	-4.789114	-1.134283
19	6	0	3.399990	0.998457	0.510948
20	6	0	-0.662134	2.790993	-0.393905
21	6	0	-3.310456	-4.219995	-0.060501

22	6	0	4.882427	-0.650714	0.865081
23	6	0	4.707900	0.682560	1.067547
24	6	0	2.318813	-3.136995	-0.533440
25	6	0	-2.074724	-4.683855	-0.409032
26	6	0	3.520729	-2.487265	-0.201070
27	6	0	2.229848	-4.494801	-1.076292
28	6	0	3.671079	-1.132103	0.210159
29	1	0	-6.004966	0.392851	0.628611
30	1	0	1.963143	4.845456	-0.495778
31	1	0	-4.830348	2.735528	0.146861
32	1	0	-0.632657	4.936656	-1.014474
33	1	0	0.441002	-5.700691	-1.494182
34	1	0	-4.211160	-4.795183	0.108499
35	1	0	5.727824	-1.256222	1.162691
36	1	0	5.383040	1.372127	1.555936
37	1	0	-1.776668	-5.712769	-0.568734
38	1	0	3.058766	-5.116609	-1.386897
39	7	0	0.411589	1.974509	-0.031305
40	1	0	0.414447	0.968213	0.103554
41	1	0	-1.944778	-0.402645	-0.123277
42	6	0	-2.820540	3.870792	-0.765345
43	6	0	-3.343416	4.031827	-2.056319
44	6	0	-3.037580	4.894356	0.169714
45	6	0	-4.055102	5.180963	-2.406950
46	1	0	-3.186299	3.242940	-2.786858
47	6	0	-3.753156	6.042880	-0.174154
48	1	0	-2.637019	4.780787	1.173529
49	6	0	-4.263861	6.190867	-1.465708
50	1	0	-4.447530	5.286099	-3.415858
51	1	0	-3.912516	6.822287	0.567702
52	1	0	-4.820207	7.085493	-1.735638
53	6	0	-5.563151	-2.330130	0.648669
54	6	0	-6.170042	-2.060604	1.887673
55	6	0	-6.295792	-3.069221	-0.295998
56	6	0	-7.458645	-2.512996	2.172728
57	1	0	-5.613506	-1.498010	2.631869
58	6	0	-7.583345	-3.525382	-0.011327
59	1	0	-5.845809	-3.275584	-1.262466
60	6	0	-8.171846	-3.249061	1.224334
61	1	0	-7.903092	-2.295553	3.141386
62	1	0	-8.130782	-4.092230	-0.761111
63	1	0	-9.175779	-3.603503	1.445902
64	6	0	4.773903	-3.304158	-0.259870
65	6	0	4.910464	-4.488035	0.486194
66	6	0	5.856816	-2.907213	-1.064388
67	6	0	6.080823	-5.245920	0.429376
68	1	0	4.088035	-4.803220	1.121059
69	6	0	7.025436	-3.666425	-1.127809
70	1	0	5.767280	-1.995704	-1.647765
71	6	0	7.143763	-4.839981	-0.379981
72	1	0	6.163376	-6.153505	1.023421
73	1	0	7.844690	-3.341239	-1.765403
74	1	0	8.055710	-5.431013	-0.426346
75	6	0	3.857744	3.435810	0.650981
76	6	0	5.046203	3.551916	-0.091431
77	6	0	3.611746	4.394848	1.649095
78	6	0	5.950376	4.586098	0.151751
79	1	0	5.251058	2.820698	-0.867477
80	6	0	4.515523	5.428823	1.896375
81	1	0	2.702495	4.315116	2.238004
82	6	0	5.689877	5.529894	1.147754
83	1	0	6.859050	4.656942	-0.441961
84	1	0	4.304068	6.152840	2.680174
85	1	0	6.395274	6.335281	1.339096

N_0SAPPh10$^{\ominus}$ (Energy = −2122.15368106)



Stoichiometry C48H32N5(1-)
Framework group C1[X(C48H32N5)]
Deg. of freedom 249
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.604958	-2.601500	-0.001404
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4	7	0	2.774913	0.033145	-0.002707
5	6	0	2.383974	2.531831	0.001346
6	6	0	-3.274805	1.292770	-0.000624
7	6	0	0.992919	2.812262	0.000366
8	6	0	-3.846485	-2.303754	0.000949
9	6	0	0.795793	-3.707248	-0.002384
10	6	0	-5.070260	-0.113400	-0.000760
11	6	0	-2.574686	2.514785	-0.001560
12	6	0	0.570560	4.221685	-0.001626
13	6	0	-4.709221	1.205613	-0.001256
14	6	0	-0.775979	4.226161	-0.002533
15	6	0	-2.691623	-3.106003	-0.000073
16	6	0	-3.881712	-0.902910	0.000887
17	6	0	-0.619339	-3.716760	-0.001616
18	6	0	1.647671	-4.846346	-0.004382
19	6	0	3.163660	1.338914	0.000620
20	6	0	-1.189267	2.821169	-0.001214
21	6	0	-2.700970	-4.557094	0.000700
22	6	0	5.105530	0.160920	0.003930
23	6	0	4.632179	1.428669	0.005157
24	6	0	2.933318	-2.981233	-0.002448
25	6	0	-1.393099	-4.941921	-0.000786
26	6	0	4.025923	-2.101505	-0.002029
27	6	0	2.953885	-4.405210	-0.005046
28	6	0	3.935729	-0.698914	-0.001332
29	1	0	-6.071555	-0.518920	-0.001747
30	1	0	1.216905	5.085625	-0.002580
31	1	0	-5.371829	2.056701	-0.002534
32	1	0	-1.426663	5.088031	-0.004084
33	1	0	1.305664	-5.871737	-0.005888
34	1	0	-3.579555	-5.188467	0.002245
35	1	0	6.137137	-0.164922	0.007342
36	1	0	5.217811	2.335377	0.009529
37	1	0	-1.000690	-5.951139	-0.000700
38	1	0	3.852231	-5.005983	-0.007329
39	7	0	-0.107608	1.987316	0.000062
40	1	0	-1.842124	-0.310872	0.001152
41	1	0	1.327939	-1.619016	-0.000191
42	6	0	3.245764	3.780848	0.003870
43	6	0	3.665313	4.370080	-1.197513
44	6	0	3.653639	4.373170	1.207723
45	6	0	4.462418	5.516665	-1.198010
46	1	0	3.357262	3.919499	-2.137285
47	6	0	4.450749	5.519740	1.213023
48	1	0	3.336485	3.924990	2.145610
49	6	0	4.858656	6.097191	0.008718
50	1	0	4.774144	5.956958	-2.142854
51	1	0	4.753375	5.962374	2.159726
52	1	0	5.479534	6.990344	0.010575

53	6	0	-3.494669	3.715051	-0.003182
54	6	0	-3.937329	4.285707	1.199179
55	6	0	-3.935746	4.283645	-1.207079
56	6	0	-4.790028	5.391542	1.200454
57	1	0	-3.602273	3.853685	2.138433
58	6	0	-4.788441	5.389493	-1.211358
59	1	0	-3.599465	3.850031	-2.145160
60	6	0	-5.219275	5.947996	-0.006215
61	1	0	-5.118725	5.818937	2.145318
62	1	0	-5.115887	5.815261	-2.157388
63	1	0	-5.882974	6.809736	-0.007376
64	6	0	5.387097	-2.734398	-0.001503
65	6	0	6.052672	-3.011506	-1.205103
66	6	0	6.023302	-3.071489	1.202643
67	6	0	7.317367	-3.603131	-1.206276
68	1	0	5.568401	-2.754786	-2.143380
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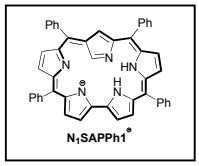
70	1	0	5.516279	-2.861321	2.140510
71	6	0	7.939624	-3.930820	-0.000123
72	1	0	7.816856	-3.807573	-2.150689
73	1	0	7.764507	-3.914365	2.150297
74	1	0	8.925232	-4.390828	0.000427
75	6	0	-5.175878	-3.004136	0.001681
76	6	0	-5.818348	-3.327532	1.206112
77	6	0	-5.803451	-3.357819	-1.202050
78	6	0	-7.051681	-3.982225	1.208746
79	1	0	-5.339613	-3.060028	2.144261
80	6	0	-7.036716	-4.012658	-1.203495
81	1	0	-5.313191	-3.113757	-2.140637
82	6	0	-7.665554	-4.326588	0.002915
83	1	0	-7.532798	-4.223620	2.153976
84	1	0	-7.506231	-4.277579	-2.148253
85	1	0	-8.626362	-4.836354	0.003401

Cartesian coordinates for the optimized structures of N-confused *meso*-tetraphenyl-sapphyrins (monoanion)

N_1SAPPh1$^{\ominus}$ (Energy = −2122.15711058)

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 Stoichiometry    C48H32N5(1-)
 Framework group  C1[X(C48H32N5)]
 Deg. of freedom   249
 Full point group                 C1
 Largest Abelian subgroup         C1      NOp   1
 Largest concise Abelian subgroup C1      NOp   1
                       Standard orientation:
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 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
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    2          7             0        2.979212    0.026532    0.120720
    3          7             0       -3.040562    0.254096   -0.200631
    4          6             0       -1.017260    2.312489   -0.420905
    5          6             0        0.146988    3.069236   -0.206789
    6          6             0        0.637364    0.970635   -0.931846
    7          6             0        1.247340    2.213091   -0.470101
    8          6             0        2.636938    2.398143   -0.272221
    9          6             0        3.484848    1.262637   -0.141022
   10          6             0        4.920213    1.188240   -0.371555
   11          6             0        5.246849   -0.134680   -0.280392
   12          6             0        4.005400   -0.846036    0.022217
   13          6             0        3.872067   -2.263926    0.131131
   14          6             0        2.670134   -3.004294    0.142700
   15          6             0        2.623519   -4.454806    0.330150
   16          6             0        1.316372   -4.818745    0.239331
   17          6             0        0.579409   -3.583469    0.019546
   18          6             0       -0.845470   -3.562605   -0.102609
   19          6             0       -1.698783   -4.668767   -0.287478
   20          6             0       -3.005836   -4.207293   -0.341531
   21          6             0       -3.001063   -2.798476   -0.166183
   22          6             0       -4.152000   -1.951491   -0.104005
   23          6             0       -4.149134   -0.548092   -0.062446
   24          6             0       -5.237615    0.349181    0.226245
   25          6             0       -4.754438    1.637090    0.241164
   26          6             0       -3.346159    1.595162   -0.026611
   27          6             0       -2.377961    2.613523   -0.109868
   28          1             0        0.193405    4.065683    0.209939
   29          1             0        1.160636    0.088164   -1.268400
   30          1             0        5.572309    2.011514   -0.635663
   31          1             0        6.220322   -0.580295   -0.439693
   32          1             0        3.468221   -5.099952    0.528639
   33          1             0        0.895924   -5.811144    0.348761
   34          1             0       -1.367013   -5.691476   -0.401850
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   36          1             0       -6.251553    0.037213    0.432326
   37          1             0       -5.322946    2.536432    0.431138
   38          7             0       -1.657823   -2.445670   -0.048754
   39          7             0        1.389300   -2.514967   -0.030181
   40          1             0       -2.129182    0.052347   -0.635348
   41          6             0       -2.760462    4.014651    0.195114
   42          6             0       -2.375689    5.063889   -0.661680
   43          6             0       -3.501306    4.350207    1.344316
   44          6             0       -2.729398    6.384299   -0.391082
   45          1             0       -1.797292    4.825609   -1.549059
   46          6             0       -3.859499    5.671166    1.613480
   47          1             0       -3.775684    3.563614    2.040686
   48          6             0       -3.477953    6.696628    0.746607
   49          1             0       -2.423006    7.172918   -1.074822
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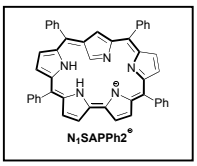
50	1	0	-4.427023	5.900442	2.512816
51	1	0	-3.753343	7.727116	0.958215
52	6	0	-5.483809	-2.622412	-0.046933
53	6	0	-6.481118	-2.330790	-0.995226
54	6	0	-5.795130	-3.552296	0.962810
55	6	0	-7.736829	-2.936521	-0.934874
56	1	0	-6.256008	-1.624956	-1.789480
57	6	0	-7.047059	-4.163218	1.021417
58	1	0	-5.042019	-3.785616	1.709623
59	6	0	-8.026538	-3.857870	0.073053
60	1	0	-8.486922	-2.694316	-1.684529
61	1	0	-7.261660	-4.873248	1.817088
62	1	0	-9.003467	-4.333310	0.119290
63	6	0	5.155216	-3.032786	0.193041
64	6	0	5.489046	-3.985666	-0.785329
65	6	0	6.079454	-2.802675	1.227197
66	6	0	6.694308	-4.686427	-0.728391
67	1	0	4.792628	-4.165206	-1.598944
68	6	0	7.283423	-3.504889	1.288648
69	1	0	5.837825	-2.067592	1.989285
70	6	0	7.597070	-4.451125	0.310531
71	1	0	6.930758	-5.413958	-1.501819
72	1	0	7.976935	-3.313682	2.104634
73	1	0	8.536467	-4.997395	0.356134
74	6	0	3.206376	3.762012	-0.182286
75	6	0	2.740240	4.799998	-1.013576
76	6	0	4.231523	4.068673	0.734400
77	6	0	3.280744	6.081511	-0.939072
78	1	0	1.953241	4.581249	-1.728379
79	6	0	4.771431	5.351933	0.809564
80	1	0	4.587280	3.289033	1.400258
81	6	0	4.300874	6.365865	-0.027169
82	1	0	2.907603	6.861341	-1.599313
83	1	0	5.556924	5.562403	1.532092
84	1	0	4.720612	7.367374	0.032958
85	1	0	-1.282513	-1.527417	0.148737

N_1SAPPh2$^{\ominus}$ (Energy = −2122.13095762)

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Stoichiometry    C48H32N5(1-)
Framework group  C1[X(C48H32N5)]
Deg. of freedom   249
Full point group                 C1
Largest Abelian subgroup         C1      NOp   1
Largest concise Abelian subgroup C1      NOp   1
                      Standard orientation:
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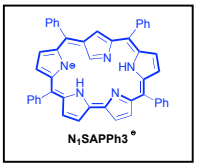
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.706678	1.325044	-1.632120
2	7	0	2.937405	0.040818	-0.252386
3	7	0	-2.889290	0.200647	-0.187938
4	6	0	-1.057013	2.385003	-0.781040
5	6	0	0.108426	3.076136	-0.341468
6	6	0	0.602356	1.300508	-1.636496
7	6	0	1.203461	2.339697	-0.803373
8	6	0	2.588663	2.482717	-0.434279
9	6	0	3.397820	1.361431	-0.249240
10	6	0	4.807974	1.260129	0.001267
11	6	0	5.142757	-0.059725	0.140817
12	6	0	3.961384	-0.868204	-0.028611
13	6	0	3.865766	-2.259473	0.056533

14	6	0	2.681581	-3.065417	-0.017237
15	6	0	2.642305	-4.462673	-0.238205
16	6	0	1.312437	-4.872637	-0.281680
17	6	0	0.501574	-3.743237	-0.090789
18	6	0	-0.925363	-3.655447	-0.064313
19	6	0	-1.806082	-4.803598	-0.203200
20	6	0	-3.068642	-4.298787	-0.147908
21	6	0	-2.934715	-2.849754	0.010742
22	6	0	-4.033631	-1.970708	0.012195
23	6	0	-4.010015	-0.543269	-0.058466
24	6	0	-5.192791	0.314961	0.030378
25	6	0	-4.736795	1.597846	-0.041101
26	6	0	-3.290409	1.500014	-0.189879
27	6	0	-2.371550	2.579005	-0.301766
28	1	0	0.137826	3.889582	0.371573
29	1	0	1.142916	0.633418	-2.306403
30	1	0	5.478718	2.105444	0.054572
31	1	0	6.122738	-0.457706	0.359445
32	1	0	3.515676	-5.081152	-0.383885
33	1	0	0.947706	-5.875948	-0.453886
34	1	0	-1.509070	-5.837368	-0.334404
35	1	0	-3.996277	-4.846016	-0.244699
36	1	0	-6.218986	-0.008285	0.144965
37	1	0	-5.323609	2.507917	-0.036317
38	7	0	-1.597894	-2.507864	0.067923
39	7	0	1.351336	-2.663488	0.056801
40	1	0	0.984130	-1.760034	0.323085
41	1	0	1.990809	-0.191932	-0.511595
42	6	0	-2.763058	3.928878	0.172890
43	6	0	-2.388805	5.078584	-0.549958
44	6	0	-3.509762	4.110272	1.353293
45	6	0	-2.753156	6.352240	-0.118160
46	1	0	-1.815495	4.954290	-1.463079
47	6	0	-3.873213	5.384898	1.785903
48	1	0	-3.786959	3.237922	1.936070
49	6	0	-3.498974	6.512677	1.052177
50	1	0	-2.457911	7.222549	-0.700002
51	1	0	-4.442736	5.497724	2.705761
52	1	0	-3.782469	7.506707	1.390574
53	6	0	3.119146	3.837304	-0.150899
54	6	0	2.790803	4.914812	-0.998824
55	6	0	3.932913	4.115182	0.965455
56	6	0	3.275885	6.197707	-0.759620
57	1	0	2.148835	4.725591	-1.853615
58	6	0	4.420581	5.400000	1.204027
59	1	0	4.158380	3.316048	1.664762
60	6	0	4.099548	6.449412	0.341559
61	1	0	3.011702	7.006151	-1.437841
62	1	0	5.040275	5.583755	2.079140
63	1	0	4.475607	7.452125	0.530241
64	6	0	-5.392718	-2.603138	0.059674
65	6	0	-6.297262	-2.461363	-1.006077
66	6	0	-5.799436	-3.354764	1.174385
67	6	0	-7.560449	-3.052103	-0.960647
68	1	0	-5.995321	-1.885751	-1.876168
69	6	0	-7.064167	-3.943074	1.224157
70	1	0	-5.111013	-3.469651	2.006600
71	6	0	-7.950659	-3.795026	0.155848
72	1	0	-8.240139	-2.934221	-1.801714
73	1	0	-7.357471	-4.516089	2.101083
74	1	0	-8.936043	-4.254004	0.192475
75	6	0	5.147862	-3.013375	0.214618
76	6	0	6.171517	-2.924128	-0.744961
77	6	0	5.366209	-3.842036	1.329985
78	6	0	7.370850	-3.621179	-0.589615

79	1	0	6.013777	-2.303772	-1.622611
80	6	0	6.561368	-4.543251	1.485350
81	1	0	4.584343	-3.926955	2.079109
82	6	0	7.572107	-4.434465	0.526706
83	1	0	8.144855	-3.535960	-1.349118
84	1	0	6.706628	-5.171366	2.361403
85	1	0	8.504655	-4.980606	0.647628

N_1SAPPh3$^{\ominus}$ (Energy = −2122.17724443)

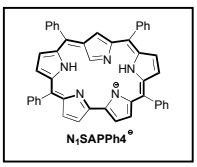


Stoichiometry C48H32N5(1-)
Framework group C1[X(C48H32N5)]
Deg. of freedom 249
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.708121	1.105046	-1.260611
2	7	0	2.965418	0.040913	-0.115864
3	7	0	-3.029232	0.141088	-0.233248
4	6	0	-1.088344	2.313675	-0.626405
5	6	0	0.054754	3.074996	-0.297614
6	6	0	0.594823	1.093614	-1.252419
7	6	0	1.171606	2.275798	-0.612550
8	6	0	2.543092	2.452979	-0.295429
9	6	0	3.405813	1.333891	-0.177103
10	6	0	4.861253	1.366565	-0.137420
11	6	0	5.278622	0.071286	-0.064543
12	6	0	4.072238	-0.746516	-0.059564
13	6	0	4.020544	-2.158031	0.035437
14	6	0	2.829211	-2.918512	0.044637
15	6	0	2.718507	-4.340180	0.011316
16	6	0	1.383028	-4.667914	-0.025542
17	6	0	0.615624	-3.467137	-0.017840
18	6	0	-0.807844	-3.430061	-0.049151
19	6	0	-1.576761	-4.663616	-0.107372
20	6	0	-2.886872	-4.298381	-0.106852
21	6	0	-2.907058	-2.845793	-0.043585
22	6	0	-4.094396	-2.072412	-0.039836
23	6	0	-4.132105	-0.661785	-0.099811
24	6	0	-5.254722	0.220048	0.019294
25	6	0	-4.790740	1.515695	-0.044681
26	6	0	-3.369212	1.477162	-0.205750
27	6	0	-2.442806	2.544713	-0.289614
28	1	0	0.065066	4.009855	0.245526
29	1	0	1.160653	0.301208	-1.724168
30	1	0	5.478306	2.253577	-0.196678
31	1	0	6.297544	-0.289151	-0.016073
32	1	0	3.556151	-5.021721	-0.005806
33	1	0	0.968045	-5.664495	-0.061169
34	1	0	-1.181931	-5.670072	-0.152591
35	1	0	-3.749977	-4.947050	-0.166047
36	1	0	-6.278562	-0.097675	0.154012
37	1	0	-5.381066	2.419774	0.000554
38	7	0	-1.624248	-2.348625	-0.019762
39	7	0	1.527336	-2.431990	0.027076
40	1	0	1.339928	-1.431808	0.025734
41	1	0	-2.087846	-0.215275	-0.402026
42	6	0	-2.881632	3.918284	0.058361

43	6	0	-2.497224	5.012441	-0.741410
44	6	0	-3.672787	4.185928	1.192367
45	6	0	-2.895874	6.310530	-0.429955
46	1	0	-1.883382	4.826052	-1.617153
47	6	0	-4.074194	5.484905	1.502854
48	1	0	-3.954105	3.363345	1.842483
49	6	0	-3.690442	6.555440	0.692995
50	1	0	-2.588819	7.134546	-1.070246
51	1	0	-4.678693	5.661696	2.389843
52	1	0	-4.001004	7.568714	0.936790
53	6	0	-5.408249	-2.774610	0.049247
54	6	0	-6.389564	-2.609827	-0.945007
55	6	0	-5.712036	-3.616742	1.134332
56	6	0	-7.622296	-3.257545	-0.858628
57	1	0	-6.169710	-1.972937	-1.797047
58	6	0	-6.942194	-4.268744	1.220491
59	1	0	-4.970439	-3.748786	1.916715
60	6	0	-7.905279	-4.091814	0.224665
61	1	0	-8.360141	-3.116239	-1.645392
62	1	0	-7.151564	-4.910810	2.073292
63	1	0	-8.865140	-4.598594	0.292085
64	6	0	5.305970	-2.914534	0.108054
65	6	0	6.247039	-2.848701	-0.934906
66	6	0	5.619313	-3.712465	1.222810
67	6	0	7.453001	-3.546917	-0.864621
68	1	0	6.017731	-2.246203	-1.809042
69	6	0	6.822200	-4.415677	1.293174
70	1	0	4.908560	-3.768337	2.042458
71	6	0	7.746810	-4.335362	0.249667
72	1	0	8.161364	-3.480806	-1.687533
73	1	0	7.040786	-5.021347	2.169943
74	1	0	8.685636	-4.881549	0.304163
75	6	0	3.051751	3.816347	-0.011190
76	6	0	2.673713	4.906799	-0.820218
77	6	0	3.911021	4.079086	1.074264
78	6	0	3.146270	6.192486	-0.568616
79	1	0	2.006274	4.726631	-1.657366
80	6	0	4.384013	5.366570	1.326733
81	1	0	4.189266	3.261497	1.731653
82	6	0	4.007533	6.431284	0.506098
83	1	0	2.843938	7.012270	-1.216727
84	1	0	5.040416	5.539398	2.176937
85	1	0	4.373938	7.435789	0.704765

N_1SAPPh4$^{\ominus}$ (Energy = −2122.17216974)



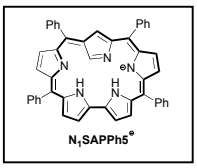
Stoichiometry C48H32N5(1-)
Framework group C1[X(C48H32N5)]
Deg. of freedom 249
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.584586	-2.322715	-0.036540
2	7	0	-1.572174	-2.333037	0.011626
3	7	0	-3.018095	0.068097	-0.147195
4	7	0	3.040380	0.112539	-0.219585
5	6	0	2.497819	2.526972	-0.260249
6	6	0	-3.384187	1.402054	-0.220888

7	6	0	-4.047799	-2.153342	0.037778
8	6	0	0.729325	-3.372254	-0.068700
9	6	0	-5.262996	0.110891	-0.097859
10	6	0	-2.493202	2.489656	-0.332277
11	6	0	-4.817017	1.409360	-0.190478
12	6	0	-2.832084	-2.884199	0.048128
13	6	0	-4.121950	-0.751992	-0.072694
14	6	0	-0.703597	-3.378787	-0.031576
15	6	0	1.470437	-4.632759	-0.134448
16	6	0	3.405410	1.441705	-0.184439
17	6	0	-2.757257	-4.332948	0.026119
18	6	0	5.268136	0.147975	0.020320
19	6	0	4.827351	1.453352	-0.029844
20	6	0	2.851539	-2.859526	-0.062209
21	6	0	-1.433552	-4.640509	-0.026388
22	6	0	4.057327	-2.122245	-0.053159
23	6	0	2.789112	-4.313030	-0.133078
24	6	0	4.128353	-0.709433	-0.099166
25	1	0	-6.290175	-0.221807	-0.055996
26	1	0	-5.423852	2.300203	-0.267835
27	1	0	1.049794	-5.627332	-0.186812
28	1	0	-3.594817	-5.017108	0.022910
29	1	0	6.286708	-0.190200	0.144854
30	1	0	5.434207	2.346419	0.016747
31	1	0	-1.005390	-5.632539	-0.059837
32	1	0	3.631751	-4.987746	-0.197417
33	6	0	-0.534906	1.123908	-1.292457
34	6	0	1.145953	2.319756	-0.621694
35	6	0	-1.114220	2.289281	-0.624488
36	1	0	-1.080698	0.337852	-1.802972
37	1	0	-0.012241	3.988245	0.301163
38	7	0	0.768361	1.137042	-1.296228
39	6	0	0.001565	3.071785	-0.272477
40	6	0	2.950249	3.885488	0.123430
41	6	0	2.571459	5.004407	-0.644589
42	6	0	3.750208	4.115193	1.259799
43	6	0	2.983350	6.289851	-0.300407
44	1	0	1.952151	4.847099	-1.522133
45	6	0	4.164655	5.401729	1.602861
46	1	0	4.027499	3.272883	1.885774
47	6	0	3.786018	6.497165	0.824408
48	1	0	2.680658	7.133554	-0.916658
49	1	0	4.775498	5.549194	2.490825
50	1	0	4.107004	7.500662	1.093737
51	6	0	5.354104	-2.856533	0.024197
52	6	0	6.337431	-2.701478	-0.969615
53	6	0	5.638864	-3.720492	1.097049
54	6	0	7.553815	-3.380646	-0.894987
55	1	0	6.131805	-2.047952	-1.812569
56	6	0	6.852821	-4.403672	1.171428
57	1	0	4.895304	-3.845351	1.878678
58	6	0	7.818042	-4.236645	0.176076
59	1	0	8.293423	-3.246790	-1.681392
60	1	0	7.047642	-5.062841	2.014543
61	1	0	8.765204	-4.767867	0.234303
62	6	0	-5.337906	-2.896932	0.142757
63	6	0	-6.301656	-2.834121	-0.879195
64	6	0	-5.631853	-3.679831	1.273246
65	6	0	-7.511889	-3.520922	-0.774065
66	1	0	-6.085922	-2.247501	-1.767701
67	6	0	-6.838708	-4.371512	1.378211
68	1	0	-4.900674	-3.735227	2.074447
69	6	0	-7.786715	-4.293933	0.355550
70	1	0	-8.237538	-3.459153	-1.582137
71	1	0	-7.041606	-4.967372	2.265362

72	1	0	-8.728460	-4.831604	0.437469
73	6	0	-2.990634	3.861008	-0.067257
74	6	0	-2.580549	4.938137	-0.879016
75	6	0	-3.867866	4.147463	0.997612
76	6	0	-3.040466	6.232286	-0.649983
77	1	0	-1.896625	4.740708	-1.698632
78	6	0	-4.329085	5.443581	1.226598
79	1	0	-4.169714	3.342441	1.660318
80	6	0	-3.921466	6.494501	0.403307
81	1	0	-2.712878	7.040902	-1.299759
82	1	0	-4.999734	5.633862	2.061795
83	1	0	-4.278171	7.505801	0.583747
84	1	0	2.093255	-0.240988	-0.368671
85	1	0	-2.085511	-0.342499	-0.057830

N_1SAPPh5$^{\ominus}$ (Energy = −2122.16498082)

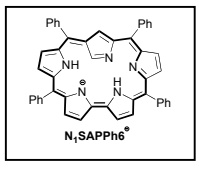


Stoichiometry C48H32N5(1-)
Framework group C1[X(C48H32N5)]
Deg. of freedom 249
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.672495	-2.323327	0.018883
2	7	0	-1.588786	-2.365325	0.027891
3	7	0	-3.005099	0.052195	-0.111107
4	7	0	3.010382	0.088795	-0.177575
5	6	0	2.435981	2.462236	-0.357366
6	6	0	-3.424636	1.353949	-0.132253
7	6	0	-4.080714	-2.133178	-0.010512
8	6	0	0.766963	-3.366082	0.050060
9	6	0	-5.316079	0.116389	-0.052312
10	6	0	-2.539511	2.454159	-0.230374
11	6	0	-4.878526	1.407159	-0.084460
12	6	0	-2.880856	-2.881445	0.009514
13	6	0	-4.122968	-0.719628	-0.074470
14	6	0	-0.653985	-3.386208	0.021001
15	6	0	1.540415	-4.562619	0.138854
16	6	0	3.369901	1.395971	-0.278077
17	6	0	-2.741541	-4.298183	-0.022867
18	6	0	5.319279	0.249329	-0.199549
19	6	0	4.822835	1.516713	-0.285540
20	6	0	2.976489	-2.809619	0.073689
21	6	0	-1.400082	-4.600020	-0.010758
22	6	0	4.157767	-2.038138	0.012246
23	6	0	2.872676	-4.228278	0.149164
24	6	0	4.160307	-0.631119	-0.134243
25	1	0	-1.456914	-1.352480	0.026891
26	1	0	-6.340280	-0.229969	-0.011714
27	1	0	-5.481549	2.305309	-0.113668
28	1	0	1.131929	-5.560669	0.197798
29	1	0	-3.563130	-4.997393	-0.070899
30	1	0	6.358524	-0.051672	-0.181889
31	1	0	5.383212	2.437931	-0.380189
32	1	0	-0.969279	-5.589858	-0.042953
33	1	0	3.711648	-4.906771	0.196064
34	6	0	-0.648167	1.092459	-1.316563
35	6	0	1.078036	2.231794	-0.671891

36	6	0	-1.181535	2.247729	-0.587716
37	1	0	-1.251037	0.355154	-1.832810
38	1	0	-0.008597	3.901184	0.330036
39	7	0	0.653134	1.073024	-1.371108
40	6	0	-0.039052	3.001187	-0.268812
41	6	0	2.873796	3.842716	-0.035496
42	6	0	2.449133	4.935149	-0.817523
43	6	0	3.719782	4.113420	1.058060
44	6	0	2.858558	6.234636	-0.526616
45	1	0	1.797884	4.745600	-1.665011
46	6	0	4.130271	5.414008	1.349190
47	1	0	4.038409	3.289979	1.689370
48	6	0	3.703815	6.482563	0.558246
49	1	0	2.520739	7.057348	-1.153059
50	1	0	4.777276	5.593602	2.205146
51	1	0	4.022088	7.497202	0.786522
52	6	0	5.460807	-2.758401	0.096836
53	6	0	6.395058	-2.688291	-0.952212
54	6	0	5.803388	-3.519273	1.228994
55	6	0	7.621042	-3.349234	-0.871956
56	1	0	6.143756	-2.113155	-1.838555
57	6	0	7.026451	-4.185675	1.308702
58	1	0	5.100843	-3.573114	2.055816
59	6	0	7.942971	-4.103291	0.258367
60	1	0	8.323548	-3.281020	-1.699671
61	1	0	7.267415	-4.763038	2.198625
62	1	0	8.897670	-4.620355	0.320356
63	6	0	-5.363524	-2.892043	0.025864
64	6	0	-6.310445	-2.764997	-1.007098
65	6	0	-5.674755	-3.754314	1.093292
66	6	0	-7.516711	-3.464899	-0.972651
67	1	0	-6.084246	-2.113688	-1.846294
68	6	0	-6.877449	-4.460224	1.126572
69	1	0	-4.963114	-3.857231	1.907565
70	6	0	-7.806740	-4.318366	0.093793
71	1	0	-8.228255	-3.349514	-1.787378
72	1	0	-7.093059	-5.115577	1.967694
73	1	0	-8.745701	-4.866373	0.119854
74	6	0	-3.008802	3.819943	0.102821
75	6	0	-2.606625	4.927592	-0.670565
76	6	0	-3.855224	4.067295	1.202111
77	6	0	-3.043078	6.215683	-0.370982
78	1	0	-1.949047	4.759056	-1.517748
79	6	0	-4.292584	5.357147	1.502054
80	1	0	-4.150797	3.234998	1.832984
81	6	0	-3.891993	6.439546	0.716701
82	1	0	-2.722087	7.049375	-0.991775
83	1	0	-4.939445	5.517543	2.361980
84	1	0	-4.230038	7.445928	0.952713
85	1	0	1.525917	-1.317344	-0.124277

N_1SAPPh6$^{\ominus}$ (Energy = −2122.16819736)



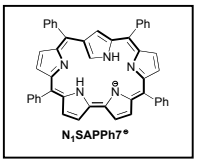
Stoichiometry C48H32N5(1-)
Framework group C1[X(C48H32N5)]
Deg. of freedom 249
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	7	0	1.608079	-2.355266	0.006854
2	7	0	-1.577989	-2.333880	0.025686
3	7	0	-3.032164	0.080653	-0.164650
4	7	0	2.994130	0.085222	-0.163422
5	6	0	2.477552	2.472255	-0.313385
6	6	0	-3.400586	1.415474	-0.205092
7	6	0	-4.059700	-2.143425	-0.002762
8	6	0	0.705702	-3.395490	0.035251
9	6	0	-5.276616	0.119898	-0.102537
10	6	0	-2.503871	2.497103	-0.297900
11	6	0	-4.833547	1.420166	-0.166385
12	6	0	-2.842435	-2.877664	0.024623
13	6	0	-4.133544	-0.743677	-0.098868
14	6	0	-0.720050	-3.390615	0.020596
15	6	0	1.482601	-4.593657	0.096983
16	6	0	3.387822	1.383958	-0.241697
17	6	0	-2.773483	-4.324122	0.006164
18	6	0	5.307537	0.190510	-0.180958
19	6	0	4.842728	1.471215	-0.242708
20	6	0	2.914069	-2.835869	0.042403
21	6	0	-1.449771	-4.644515	0.007193
22	6	0	4.098142	-2.071735	-0.011092
23	6	0	2.813712	-4.257965	0.097802
24	6	0	4.126721	-0.662032	-0.132402
25	1	0	-6.303012	-0.215560	-0.063225
26	1	0	-5.441634	2.311989	-0.220258
27	1	0	1.074773	-5.592489	0.138749
28	1	0	-3.614163	-5.003306	-0.027935
29	1	0	6.338965	-0.136501	-0.168717
30	1	0	5.424881	2.380537	-0.320681
31	1	0	-1.025092	-5.638931	-0.017109
32	1	0	3.655457	-4.934253	0.123546
33	6	0	-0.586469	1.152613	-1.383548
34	6	0	1.126108	2.268244	-0.669867
35	6	0	-1.134025	2.281348	-0.624244
36	1	0	-1.166150	0.428722	-1.948561
37	1	0	0.017483	3.895308	0.381184
38	7	0	0.716047	1.141273	-1.420550
39	6	0	0.000609	3.020081	-0.254014
40	6	0	2.928518	3.833907	0.060198
41	6	0	2.515253	4.959328	-0.680599
42	6	0	3.777393	4.054948	1.162985
43	6	0	2.937290	6.242699	-0.341052
44	1	0	1.863251	4.808184	-1.535150
45	6	0	4.200921	5.339494	1.502117
46	1	0	4.087170	3.205501	1.763342
47	6	0	3.785004	6.441265	0.752055
48	1	0	2.607951	7.091655	-0.936192
49	1	0	4.849783	5.480446	2.363853
50	1	0	4.113496	7.443359	1.018074
51	6	0	5.395320	-2.808112	0.056173
52	6	0	6.310492	-2.756562	-1.009853
53	6	0	5.747441	-3.563698	1.188192
54	6	0	7.529435	-3.432458	-0.946390
55	1	0	6.050585	-2.183754	-1.895250
56	6	0	6.964040	-4.243798	1.251906
57	1	0	5.057376	-3.604245	2.026170
58	6	0	7.862128	-4.180895	0.184525
59	1	0	8.217952	-3.379538	-1.786833
60	1	0	7.213764	-4.817558	2.141682
61	1	0	8.811443	-4.709150	0.233702
62	6	0	-5.350903	-2.887668	0.078466
63	6	0	-6.303057	-2.808740	-0.953453
64	6	0	-5.660423	-3.685628	1.194494

65	6	0	-7.516031	-3.493912	-0.871974
66	1	0	-6.075930	-2.209972	-1.830968
67	6	0	-6.869760	-4.375986	1.275706
68	1	0	-4.939619	-3.753410	2.004125
69	6	0	-7.805733	-4.282197	0.243239
70	1	0	-8.232126	-3.418763	-1.687410
71	1	0	-7.084541	-4.983041	2.152439
72	1	0	-8.749520	-4.818765	0.306701
73	6	0	-2.979856	3.865515	0.012448
74	6	0	-2.549321	4.964072	-0.759369
75	6	0	-3.857329	4.128698	1.083491
76	6	0	-2.989317	6.256482	-0.486215
77	1	0	-1.865079	4.784604	-1.582740
78	6	0	-4.299152	5.423079	1.355933
79	1	0	-4.173552	3.306330	1.717581
80	6	0	-3.871045	6.495733	0.571949
81	1	0	-2.645364	7.082157	-1.105354
82	1	0	-4.970143	5.594625	2.194947
83	1	0	-4.212048	7.505733	0.786796
84	1	0	1.429674	-1.354760	-0.103976
85	1	0	-2.095830	-0.317152	-0.081131

N_1SAPPh7$^{\ominus}$ (Energy = −2122.16001744)

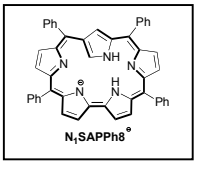


Stoichiometry C48H32N5(1-)
Framework group C1[X(C48H32N5)]
Deg. of freedom 249
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.471055	-2.390500	-0.081209
2	7	0	-1.647882	-2.410957	0.052722
3	7	0	-2.966786	0.112506	-0.047987
4	7	0	3.053579	0.088720	-0.184302
5	6	0	2.625297	2.471064	-0.087257
6	6	0	-3.343610	1.430511	-0.144333
7	6	0	-4.123411	-2.036455	0.114722
8	6	0	0.650270	-3.461561	-0.143467
9	6	0	-5.273773	0.254141	0.000345
10	6	0	-2.442371	2.500051	-0.307585
11	6	0	-4.800645	1.524462	-0.110505
12	6	0	-2.962811	-2.849879	0.082562
13	6	0	-4.104727	-0.622754	0.020828
14	6	0	-0.770992	-3.473798	-0.068278
15	6	0	1.401664	-4.704005	-0.289382
16	6	0	3.508545	1.367181	-0.022914
17	6	0	-2.903538	-4.271822	-0.016862
18	6	0	5.314105	0.023266	0.171224
19	6	0	4.947156	1.339769	0.193274
20	6	0	2.753848	-2.892243	-0.152848
21	6	0	-1.579499	-4.643360	-0.110828
22	6	0	3.971167	-2.169397	-0.100446
23	6	0	2.710794	-4.348732	-0.299736
24	6	0	4.096350	-0.749814	-0.064923
25	1	0	-1.424789	-1.422849	0.128293
26	1	0	-6.308053	-0.056561	0.063214
27	1	0	-5.381125	2.433183	-0.198816
28	1	0	0.993225	-5.702292	-0.381442

29	1	0	-3.765562	-4.921889	-0.046156
30	1	0	6.307041	-0.378543	0.324295
31	1	0	5.594121	2.196481	0.329385
32	1	0	-1.200705	-5.650434	-0.210412
33	1	0	3.563966	-5.002632	-0.415366
34	6	0	-0.512231	1.014786	-0.983466
35	6	0	1.245881	2.274090	-0.405172
36	6	0	-1.040831	2.252502	-0.523782
37	1	0	1.482304	0.239550	-0.873321
38	1	0	-1.046211	0.156926	-1.354110
39	1	0	0.072796	4.050061	0.202593
40	7	0	0.810326	1.041296	-0.908315
41	6	0	0.092380	3.051430	-0.208609
42	6	0	3.088969	3.840903	0.227621
43	6	0	2.712668	4.934286	-0.577644
44	6	0	3.908701	4.103561	1.342931
45	6	0	3.148622	6.226049	-0.291100
46	1	0	2.079502	4.754202	-1.441005
47	6	0	4.346083	5.396277	1.628133
48	1	0	4.180668	3.282284	1.998140
49	6	0	3.971103	6.465807	0.812605
50	1	0	2.847819	7.049075	-0.935545
51	1	0	4.972382	5.569603	2.500463
52	1	0	4.309120	7.474486	1.037850
53	6	0	5.247645	-2.945843	-0.053824
54	6	0	6.237402	-2.768931	-1.037742
55	6	0	5.513665	-3.860458	0.981574
56	6	0	7.438084	-3.478223	-0.992898
57	1	0	6.049534	-2.070796	-1.848489
58	6	0	6.712500	-4.572304	1.027923
59	1	0	4.767287	-4.001542	1.757810
60	6	0	7.682032	-4.385457	0.040192
61	1	0	8.182262	-3.325735	-1.771685
62	1	0	6.892457	-5.269615	1.843330
63	1	0	8.617315	-4.939368	0.076052
64	6	0	-5.436461	-2.737932	0.206091
65	6	0	-6.411650	-2.601838	-0.799167
66	6	0	-5.743524	-3.564230	1.302967
67	6	0	-7.642444	-3.252472	-0.706973
68	1	0	-6.188710	-1.983278	-1.663712
69	6	0	-6.970158	-4.222126	1.393718
70	1	0	-5.007054	-3.678035	2.093458
71	6	0	-7.928813	-4.067770	0.389751
72	1	0	-8.375782	-3.129974	-1.501176
73	1	0	-7.180887	-4.850078	2.256724
74	1	0	-8.886619	-4.577921	0.460705
75	6	0	-2.900725	3.901625	-0.182054
76	6	0	-2.443075	4.888676	-1.079734
77	6	0	-3.785394	4.312173	0.835975
78	6	0	-2.868917	6.210729	-0.982193
79	1	0	-1.752768	4.598177	-1.866081
80	6	0	-4.212862	5.636084	0.933010
81	1	0	-4.117900	3.581321	1.566237
82	6	0	-3.760731	6.594142	0.023837
83	1	0	-2.506227	6.945898	-1.697409
84	1	0	-4.891658	5.922433	1.733524
85	1	0	-4.090206	7.627460	0.102912

N_1SAPPh8$^{\ominus}$ (Energy = −2122.15698081)



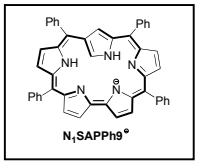
Stoichiometry C48H32N5(1-)
Framework group C1[X(C48H32N5)]
Deg. of freedom 249

Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.777569	-2.379727	0.022892
2	7	0	-1.318792	-2.483908	0.029660
3	7	0	-3.023460	-0.004415	0.139663
4	7	0	2.954744	0.232083	-0.087758
5	6	0	2.305675	2.609176	0.029310
6	6	0	-3.570429	1.215657	-0.150889
7	6	0	-3.817630	-2.326900	0.160788
8	6	0	0.952275	-3.486820	0.025384
9	6	0	-5.269362	-0.256396	-0.320575
10	6	0	-2.762633	2.362388	-0.301392
11	6	0	-4.998459	1.076389	-0.413660
12	6	0	-2.582870	-3.010892	0.212478
13	6	0	-4.005179	-0.915802	0.022200
14	6	0	-0.469276	-3.522330	0.139361
15	6	0	1.800881	-4.610246	-0.133609
16	6	0	3.261028	1.566931	0.053487
17	6	0	-2.488009	-4.450547	0.468124
18	6	0	5.241480	0.469499	0.088173
19	6	0	4.703859	1.719131	0.163424
20	6	0	3.108099	-2.747540	-0.109375
21	6	0	-1.170582	-4.771561	0.409255
22	6	0	4.225772	-1.868067	-0.116189
23	6	0	3.107316	-4.165612	-0.232237
24	6	0	4.130019	-0.459078	-0.068634
25	1	0	-6.219828	-0.743652	-0.496046
26	1	0	-5.676870	1.867241	-0.708068
27	1	0	1.458406	-5.632858	-0.210985
28	1	0	-3.312772	-5.113145	0.690960
29	1	0	6.287753	0.202747	0.152965
30	1	0	5.237555	2.654973	0.260843
31	1	0	-0.718220	-5.741299	0.576015
32	1	0	3.988207	-4.768947	-0.394937
33	6	0	-0.747996	0.976480	-0.882678
34	6	0	0.934974	2.348033	-0.279530
35	6	0	-1.343398	2.190398	-0.434968
36	1	0	1.295510	0.380697	-0.905738
37	1	0	-1.215391	0.064535	-1.215562
38	1	0	-0.343528	4.044357	0.325565
39	7	0	0.570822	1.100113	-0.802000
40	6	0	-0.260409	3.053057	-0.095097
41	6	0	2.692612	4.000075	0.359139
42	6	0	2.253905	5.081992	-0.430668
43	6	0	3.493264	4.297937	1.480003
44	6	0	2.611850	6.393344	-0.125622
45	1	0	1.633095	4.877590	-1.297772
46	6	0	3.855656	5.609924	1.782556
47	1	0	3.813481	3.485383	2.124666
48	6	0	3.418879	6.667061	0.981852
49	1	0	2.263500	7.205717	-0.759797
50	1	0	4.470766	5.807304	2.657884
51	1	0	3.696804	7.690792	1.221055
52	6	0	5.580292	-2.488154	-0.161888
53	6	0	6.492149	-2.159811	-1.182703
54	6	0	5.999718	-3.414680	0.811474
55	6	0	7.766670	-2.725467	-1.225642
56	1	0	6.183605	-1.457096	-1.951217
57	6	0	7.270769	-3.986794	0.766476

58	1	0	5.317011	-3.673967	1.615428
59	6	0	8.163281	-3.644353	-0.252102
60	1	0	8.448220	-2.454285	-2.029045
61	1	0	7.568747	-4.695049	1.536618
62	1	0	9.155292	-4.088678	-0.286493
63	6	0	-5.067590	-3.146929	0.214387
64	6	0	-5.331964	-4.147308	-0.738364
65	6	0	-6.033611	-2.922694	1.211904
66	6	0	-6.507134	-4.897827	-0.691714
67	1	0	-4.604449	-4.324385	-1.524917
68	6	0	-7.208742	-3.672929	1.262057
69	1	0	-5.846725	-2.154242	1.956440
70	6	0	-7.451677	-4.665687	0.310265
71	1	0	-6.688003	-5.661563	-1.445027
72	1	0	-7.934550	-3.483860	2.050027
73	1	0	-8.368098	-5.250227	0.347722
74	6	0	-3.351888	3.715073	-0.307043
75	6	0	-2.835855	4.729950	-1.139785
76	6	0	-4.447390	4.043845	0.518144
77	6	0	-3.399210	6.002856	-1.160814
78	1	0	-1.991211	4.499551	-1.781644
79	6	0	-5.010720	5.318585	0.495982
80	1	0	-4.837390	3.289444	1.193656
81	6	0	-4.492536	6.306244	-0.344185
82	1	0	-2.985535	6.762102	-1.820889
83	1	0	-5.851050	5.544614	1.148742
84	1	0	-4.929062	7.302134	-0.357380
85	1	0	1.503298	-1.422579	0.208569

N_1SAPPh9$^{\ominus}$ (Energy = −2122.15448281)

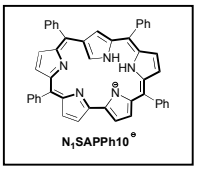


Stoichiometry C48H32N5(1-)
Framework group C1[X(C48H32N5)]
Deg. of freedom 249
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.449353	-2.329635	-0.136676
2	7	0	-1.692548	-2.270502	-0.001450
3	7	0	-3.050806	0.150080	-0.015245
4	7	0	3.091295	0.060704	-0.150869
5	6	0	2.674737	2.433364	-0.018892
6	6	0	-3.342117	1.498521	-0.150791
7	6	0	-4.165311	-2.017044	0.125198
8	6	0	0.580614	-3.360679	-0.207771
9	6	0	-5.291974	0.301697	-0.029591
10	6	0	-2.400932	2.522819	-0.312889
11	6	0	-4.783438	1.569195	-0.158004
12	6	0	-2.961417	-2.788056	0.077415
13	6	0	-4.192098	-0.620260	0.039301
14	6	0	-0.849804	-3.341106	-0.116037
15	6	0	1.295789	-4.634715	-0.368949
16	6	0	3.557125	1.331555	0.033719
17	6	0	-2.927110	-4.233099	0.012053
18	6	0	5.347147	-0.038755	0.201439
19	6	0	4.996609	1.282225	0.249866
20	6	0	2.712501	-2.880950	-0.204959
21	6	0	-1.612658	-4.575754	-0.114373

22	6	0	3.953781	-2.208595	-0.126009
23	6	0	2.615173	-4.335687	-0.372430
24	6	0	4.118132	-0.791122	-0.051259
25	1	0	-6.335389	0.021127	-0.005825
26	1	0	-5.347812	2.481673	-0.286223
27	1	0	0.854413	-5.615943	-0.479186
28	1	0	-3.782178	-4.895132	0.031451
29	1	0	6.335384	-0.455926	0.344609
30	1	0	5.655150	2.127444	0.402348
31	1	0	-1.214257	-5.577929	-0.192711
32	1	0	3.442803	-5.020780	-0.494437
33	6	0	-0.467294	0.983529	-0.927706
34	6	0	1.292523	2.235021	-0.342091
35	6	0	-0.995553	2.226656	-0.482818
36	1	0	1.514392	0.193439	-0.795477
37	1	0	-0.958976	0.102131	-1.309066
38	1	0	0.119942	4.018082	0.252755
39	7	0	0.855598	1.006919	-0.840695
40	6	0	0.139940	3.016598	-0.151391
41	6	0	3.137811	3.800690	0.306570
42	6	0	2.759773	4.901208	-0.487803
43	6	0	3.962336	4.051565	1.420890
44	6	0	3.198670	6.189731	-0.191183
45	1	0	2.123870	4.729556	-1.350811
46	6	0	4.402222	5.341114	1.716296
47	1	0	4.235621	3.223678	2.067178
48	6	0	4.025280	6.418252	0.911768
49	1	0	2.896752	7.018989	-0.826983
50	1	0	5.032146	5.505878	2.587622
51	1	0	4.365240	7.424454	1.144947
52	6	0	5.206010	-3.022803	-0.091237
53	6	0	6.211234	-2.842339	-1.058873
54	6	0	5.435842	-3.975721	0.917895
55	6	0	7.391169	-3.586054	-1.024703
56	1	0	6.051525	-2.114747	-1.849580
57	6	0	6.613760	-4.722333	0.953058
58	1	0	4.678105	-4.119048	1.682519
59	6	0	7.598539	-4.532040	-0.018687
60	1	0	8.147603	-3.430182	-1.790915
61	1	0	6.765415	-5.449806	1.747585
62	1	0	8.517546	-5.113014	0.008708
63	6	0	-5.471761	-2.727438	0.246727
64	6	0	-6.461730	-2.615689	-0.745604
65	6	0	-5.755695	-3.529571	1.366642
66	6	0	-7.688782	-3.268832	-0.619756
67	1	0	-6.253464	-2.018577	-1.628904
68	6	0	-6.978559	-4.188601	1.491418
69	1	0	-5.003174	-3.626080	2.143888
70	6	0	-7.953811	-4.059325	0.499726
71	1	0	-8.434934	-3.167750	-1.404933
72	1	0	-7.172748	-4.799682	2.370156
73	1	0	-8.908184	-4.571488	0.597475
74	6	0	-2.831718	3.936370	-0.247833
75	6	0	-2.313632	4.885056	-1.154606
76	6	0	-3.752019	4.399018	0.715032
77	6	0	-2.714154	6.217803	-1.117177
78	1	0	-1.594960	4.556330	-1.899294
79	6	0	-4.155753	5.733402	0.750125
80	1	0	-4.132114	3.701490	1.454971
81	6	0	-3.642640	6.652616	-0.166595
82	1	0	-2.303001	6.921461	-1.837851
83	1	0	-4.863246	6.058608	1.509957
84	1	0	-3.952865	7.694309	-0.135524
85	1	0	-2.149397	-0.314164	0.105384

N_1SAPPh10$^{\ominus}$ (Energy = −2122.14480364)

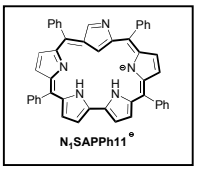


Stoichiometry C48H32N5(1-)
Framework group C1[X(C48H32N5)]
Deg. of freedom 249
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.793049	-2.211354	-0.031299
2	7	0	1.352953	-2.387993	0.000173
3	7	0	3.108136	-0.008731	-0.233513
4	7	0	-3.071437	0.231419	-0.220394
5	6	0	-2.288745	2.581491	-0.072762
6	6	0	3.633718	1.220316	0.054653
7	6	0	3.857117	-2.327122	-0.111875
8	6	0	-0.981863	-3.302440	-0.164607
9	6	0	5.314810	-0.245789	0.383319
10	6	0	2.796011	2.346594	0.164136
11	6	0	5.044319	1.091155	0.406321
12	6	0	2.596985	-2.957477	-0.193239
13	6	0	4.071120	-0.914963	-0.012983
14	6	0	0.452991	-3.364446	-0.223244
15	6	0	-1.778134	-4.507335	-0.262573
16	6	0	-3.290348	1.596219	-0.124981
17	6	0	2.450256	-4.370785	-0.553562
18	6	0	-5.273244	0.485495	0.136014
19	6	0	-4.706834	1.737154	0.076838
20	6	0	-3.084451	-2.693053	-0.038567
21	6	0	1.120949	-4.624123	-0.575540
22	6	0	-4.264421	-1.887964	0.005738
23	6	0	-3.087988	-4.129714	-0.176474
24	6	0	-4.238902	-0.488073	-0.046028
25	1	0	6.249271	-0.728759	0.639929
26	1	0	5.704633	1.891591	0.716102
27	1	0	-1.404321	-5.516885	-0.364680
28	1	0	3.253256	-5.050220	-0.804478
29	1	0	-6.310024	0.252703	0.334116
30	1	0	-5.207109	2.682752	0.230554
31	1	0	0.642201	-5.556309	-0.843551
32	1	0	-3.961604	-4.764608	-0.233714
33	6	0	0.816494	0.906007	0.724426
34	6	0	-0.912506	2.249567	0.149736
35	6	0	1.378289	2.127183	0.274724
36	1	0	-1.119746	0.233330	0.926894
37	1	0	1.289619	-0.005721	1.050540
38	1	0	0.326367	3.953372	-0.484831
39	7	0	-0.512253	0.995931	0.653031
40	6	0	0.271134	2.961190	-0.061608
41	1	0	-2.220684	-0.282218	-0.454062
42	6	0	-5.594645	-2.545140	0.124531
43	6	0	-6.631335	-2.265551	-0.784806
44	6	0	-5.865885	-3.455557	1.163513
45	6	0	-7.885567	-2.863929	-0.659191
46	1	0	-6.437211	-1.580198	-1.604759
47	6	0	-7.116845	-4.058459	1.287046
48	1	0	-5.081501	-3.678323	1.880477
49	6	0	-8.135665	-3.764954	0.377301
50	1	0	-8.665977	-2.632451	-1.380878
51	1	0	-7.299143	-4.754171	2.103187
52	1	0	-9.111833	-4.234274	0.474617

53	6	0	-2.665365	4.003589	-0.225313
54	6	0	-2.107264	5.005167	0.596280
55	6	0	-3.600196	4.412894	-1.198617
56	6	0	-2.472875	6.341669	0.458407
57	1	0	-1.387492	4.717216	1.355929
58	6	0	-3.971029	5.750122	-1.331519
59	1	0	-4.021276	3.666877	-1.865696
60	6	0	-3.410059	6.725548	-0.504941
61	1	0	-2.028987	7.088112	1.113559
62	1	0	-4.691018	6.032340	-2.096721
63	1	0	-3.693254	7.769748	-0.613143
64	6	0	3.350093	3.712778	0.184265
65	6	0	2.778781	4.724046	0.984545
66	6	0	4.474065	4.056174	-0.595798
67	6	0	3.314591	6.008608	1.016080
68	1	0	1.914545	4.481729	1.594977
69	6	0	5.010068	5.342208	-0.562458
70	1	0	4.908342	3.302971	-1.245318
71	6	0	4.435369	6.327077	0.243677
72	1	0	2.857884	6.765180	1.650309
73	1	0	5.873642	5.579211	-1.180024
74	1	0	4.850119	7.332064	0.264833
75	6	0	5.077319	-3.185475	-0.112362
76	6	0	5.234132	-4.239637	0.807082
77	6	0	6.126273	-2.952219	-1.021662
78	6	0	6.383146	-5.030427	0.812107
79	1	0	4.443246	-4.425343	1.527590
80	6	0	7.275792	-3.741988	-1.018735
81	1	0	6.022685	-2.147057	-1.743143
82	6	0	7.410804	-4.786633	-0.101499
83	1	0	6.478745	-5.835033	1.538048
84	1	0	8.066067	-3.544123	-1.739731
85	1	0	8.307348	-5.402370	-0.097674

N_1SAPPh11$^{\ominus}$ (Energy = −2122.15893888)



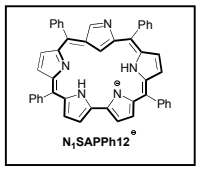
Stoichiometry C48H32N5(1-)
Framework group C1[X(C48H32N5)]
Deg. of freedom 249
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.633971	-2.445178	-0.406046
2	7	0	-1.511137	-2.501582	-0.237909
3	7	0	-2.834589	-0.028150	-0.007529
4	7	0	2.861202	0.048188	0.047311
5	6	0	2.468292	2.497602	0.283328
6	6	0	-3.279802	1.260898	0.063844
7	6	0	1.087506	2.636324	-0.042710
8	6	0	-3.923000	-2.226828	0.246659
9	6	0	0.765773	-3.475719	-0.701483
10	6	0	-5.053804	0.000815	0.682769
11	6	0	-2.561142	2.448932	-0.250717
12	6	0	0.574164	3.893057	-0.604218
13	6	0	-4.668302	1.292451	0.503567
14	6	0	-2.795729	-3.001674	-0.082895
15	6	0	-3.910007	-0.813404	0.317637
16	6	0	-0.640437	-3.514069	-0.578531

17	6	0	1.571774	-4.598271	-1.037634
18	6	0	3.230706	1.317308	0.414226
19	6	0	-1.163590	2.625230	-0.332949
20	6	0	-2.721971	-4.397585	-0.354165
21	6	0	5.080473	0.053020	0.738259
22	6	0	4.614343	1.318989	0.884569
23	6	0	2.946318	-2.879795	-0.489198
24	6	0	-1.415950	-4.705098	-0.662494
25	6	0	4.066831	-2.095252	-0.150990
26	6	0	2.895775	-4.238216	-0.914706
27	6	0	3.978568	-0.722677	0.189117
28	1	0	-6.010443	-0.361539	1.033292
29	1	0	1.185967	4.739578	-0.901535
30	1	0	-5.250629	2.184144	0.687444
31	1	0	1.189829	-5.565727	-1.331761
32	1	0	-3.561501	-5.076323	-0.322671
33	1	0	6.059133	-0.326864	0.998558
34	1	0	5.143869	2.168585	1.291700
35	1	0	-1.019021	-5.684187	-0.890664
36	1	0	3.759783	-4.858898	-1.100935
37	1	0	1.449942	-1.461171	-0.198665
38	7	0	-0.708841	3.893148	-0.794208
39	6	0	-0.058945	1.825556	0.070266
40	1	0	-0.114388	0.832605	0.491208
41	1	0	-1.371913	-1.488315	-0.219398
42	6	0	-3.409027	3.659775	-0.504406
43	6	0	-3.249495	4.844284	0.234701
44	6	0	-4.413260	3.629363	-1.486061
45	6	0	-4.067765	5.949056	0.008390
46	1	0	-2.474075	4.888679	0.991531
47	6	0	-5.226289	4.738975	-1.724398
48	1	0	-4.545621	2.724887	-2.072344
49	6	0	-5.060003	5.903685	-0.974731
50	1	0	-3.927890	6.851534	0.599584
51	1	0	-5.989752	4.690855	-2.497990
52	1	0	-5.694601	6.768772	-1.154763
53	6	0	3.203783	3.789583	0.481331
54	6	0	4.332755	4.126326	-0.287216
55	6	0	2.761425	4.722056	1.437094
56	6	0	4.996405	5.339591	-0.102583
57	1	0	4.678422	3.427534	-1.043045
58	6	0	3.426844	5.932984	1.628421
59	1	0	1.889005	4.480588	2.037211
60	6	0	4.548522	6.248264	0.858780
61	1	0	5.861312	5.578620	-0.717567
62	1	0	3.067381	6.631699	2.380548
63	1	0	5.065561	7.194150	1.003120
64	6	0	-5.199589	-2.958947	0.490052
65	6	0	-5.291951	-3.938361	1.495582
66	6	0	-6.348447	-2.700522	-0.279437
67	6	0	-6.481659	-4.630279	1.723662
68	1	0	-4.418637	-4.144159	2.107900
69	6	0	-7.539981	-3.388742	-0.050471
70	1	0	-6.293874	-1.955123	-1.067085
71	6	0	-7.613094	-4.358378	0.951821
72	1	0	-6.526459	-5.377407	2.512967
73	1	0	-8.412071	-3.171386	-0.663110
74	1	0	-8.541683	-4.895578	1.129867
75	6	0	5.399715	-2.759474	-0.145828
76	6	0	6.467316	-2.246732	-0.906699
77	6	0	5.641646	-3.916575	0.618534
78	6	0	7.719376	-2.861267	-0.902705
79	1	0	6.299155	-1.360039	-1.510545
80	6	0	6.891584	-4.535434	0.619791
81	1	0	4.837660	-4.319424	1.227597

82	6	0	7.938740	-4.010989	-0.141031
83	1	0	8.524156	-2.444261	-1.504135
84	1	0	7.050533	-5.424219	1.226592
85	1	0	8.914225	-4.491614	-0.139121

N_1SAPPh12$^{\ominus}$ (Energy = −2122.16485672)

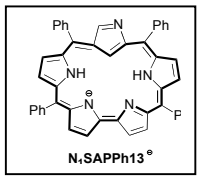


Stoichiometry C48H32N5(1-)
Framework group C1[X(C48H32N5)]
Deg. of freedom 249
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.586675	-2.490476	-0.373002
2	7	0	-1.483871	-2.475108	-0.321178
3	7	0	-2.890336	0.012558	0.029966
4	7	0	2.831680	0.038544	0.062914
5	6	0	2.499044	2.513202	-0.016744
6	6	0	-3.293914	1.325743	0.217726
7	6	0	1.098542	2.664891	-0.181190
8	6	0	-3.917394	-2.251147	0.034578
9	6	0	0.733356	-3.536835	-0.626419
10	6	0	-5.052674	-0.060407	0.653027
11	6	0	-2.567305	2.514832	0.007989
12	6	0	0.531440	3.934708	-0.648801
13	6	0	-4.663017	1.254597	0.633042
14	6	0	-2.758059	-2.984795	-0.306700
15	6	0	-3.944190	-0.859689	0.239665
16	6	0	-0.681777	-3.521446	-0.642678
17	6	0	1.544778	-4.703265	-0.737894
18	6	0	3.256886	1.333986	0.182650
19	6	0	-1.171728	2.675897	-0.184760
20	6	0	-2.755746	-4.387536	-0.679482
21	6	0	5.111544	0.083566	0.523414
22	6	0	4.683289	1.370878	0.494901
23	6	0	2.892569	-2.938566	-0.276425
24	6	0	-1.452790	-4.723001	-0.891577
25	6	0	3.999633	-2.137923	0.052725
26	6	0	2.853699	-4.346188	-0.508303
27	6	0	3.945397	-0.735774	0.235904
28	1	0	-6.019337	-0.450051	0.936242
29	1	0	1.105006	4.784533	-1.004187
30	1	0	-5.259565	2.112953	0.901894
31	1	0	1.169140	-5.699086	-0.925118
32	1	0	-3.626271	-5.021091	-0.780332
33	1	0	6.115387	-0.275179	0.704259
34	1	0	5.270948	2.259547	0.675209
35	1	0	-1.062331	-5.688245	-1.187386
36	1	0	3.714661	-4.997972	-0.484949
37	1	0	1.363326	-1.503470	-0.252188
38	7	0	-0.765662	3.955084	-0.657723
39	6	0	-0.041118	1.857974	0.061976
40	1	0	-0.032136	0.857836	0.474185
41	1	0	-1.979890	-0.334641	-0.262059
42	6	0	-5.206384	-2.988920	0.188566
43	6	0	-6.329499	-2.675865	-0.597781
44	6	0	-5.334266	-4.027494	1.128494
45	6	0	-7.531526	-3.368549	-0.448999

46	1	0	-6.247037	-1.885679	-1.338460
47	6	0	-6.534041	-4.723385	1.276998
48	1	0	-4.478805	-4.278875	1.748475
49	6	0	-7.640192	-4.396579	0.489630
50	1	0	-8.382688	-3.109096	-1.074644
51	1	0	-6.606474	-5.518641	2.015592
52	1	0	-8.576302	-4.937744	0.605727
53	6	0	-3.392469	3.767744	-0.008695
54	6	0	-4.444067	3.931922	-0.924229
55	6	0	-3.147428	4.806964	0.904156
56	6	0	-5.225499	5.088771	-0.927074
57	1	0	-4.639262	3.144929	-1.647022
58	6	0	-3.930935	5.959055	0.910455
59	1	0	-2.330864	4.700180	1.610959
60	6	0	-4.975282	6.106668	-0.006231
61	1	0	-6.028243	5.194439	-1.653731
62	1	0	-3.723645	6.746787	1.631496
63	1	0	-5.584216	7.008033	-0.004527
64	6	0	3.293361	3.789512	-0.059347
65	6	0	4.248969	4.021545	-1.063312
66	6	0	3.093069	4.795119	0.901340
67	6	0	4.977097	5.211184	-1.105250
68	1	0	4.411253	3.257282	-1.817807
69	6	0	3.824249	5.983222	0.866408
70	1	0	2.356627	4.632466	1.683099
71	6	0	4.769929	6.197268	-0.138264
72	1	0	5.704835	5.369308	-1.898162
73	1	0	3.653713	6.742931	1.625961
74	1	0	5.337652	7.124407	-0.169338
75	6	0	5.315339	-2.832116	0.201965
76	6	0	5.939589	-3.453464	-0.893029
77	6	0	5.964755	-2.888001	1.447143
78	6	0	7.163898	-4.107871	-0.749442
79	1	0	5.456527	-3.410660	-1.865194
80	6	0	7.191597	-3.536544	1.592197
81	1	0	5.492240	-2.418177	2.305089
82	6	0	7.796697	-4.151815	0.494329
83	1	0	7.627884	-4.577258	-1.614112
84	1	0	7.672123	-3.566920	2.567541
85	1	0	8.751790	-4.659508	0.606748

N_1SAPPh13$^{\ominus}$ (Energy = −2122.16396866)



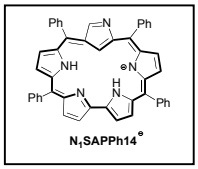
Stoichiometry C48H32N5(1-)
Framework group C1[X(C48H32N5)]
Deg. of freedom 249
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.582222	-2.382355	-0.389059
2	7	0	1.475172	-2.432109	-0.272225
3	7	0	2.882453	-0.010632	0.019463
4	7	0	-2.908384	0.073008	0.047924
5	6	0	-2.484657	2.547403	0.201501
6	6	0	3.293841	1.308415	0.099275
7	6	0	-1.093003	2.669589	-0.081703
8	6	0	3.885272	-2.272858	0.191799
9	6	0	-0.766677	-3.408047	-0.736117

10	6	0	5.037386	-0.046892	0.668585
11	6	0	2.566765	2.486915	-0.192315
12	6	0	-0.560575	3.918047	-0.633312
13	6	0	4.658407	1.266740	0.524761
14	6	0	2.725610	-2.987899	-0.166769
15	6	0	3.928441	-0.866668	0.310880
16	6	0	0.653448	-3.440161	-0.646497
17	6	0	-1.541516	-4.585052	-1.099415
18	6	0	-3.255716	1.380369	0.346066
19	6	0	1.167360	2.651704	-0.303944
20	6	0	2.695241	-4.398786	-0.519102
21	6	0	-5.073400	0.037512	0.669350
22	6	0	-4.627824	1.330204	0.767017
23	6	0	-2.856707	-2.878708	-0.462773
24	6	0	1.402593	-4.677027	-0.834799
25	6	0	-4.012356	-2.143651	-0.110656
26	6	0	-2.851067	-4.254881	-0.926922
27	6	0	-3.996384	-0.769819	0.190912
28	1	0	5.998171	-0.416704	0.995209
29	1	0	-1.160181	4.764962	-0.952347
30	1	0	5.259404	2.141603	0.721737
31	1	0	-1.147904	-5.533631	-1.439937
32	1	0	3.544450	-5.068113	-0.545715
33	1	0	-6.056036	-0.334731	0.919966
34	1	0	-5.189640	2.184330	1.113537
35	1	0	0.997640	-5.631690	-1.143221
36	1	0	-3.720445	-4.872238	-1.108959
37	7	0	0.729281	3.915813	-0.778918
38	6	0	0.049604	1.851562	0.069216
39	1	0	0.085256	0.864099	0.513555
40	1	0	1.976949	-0.392687	-0.257849
41	1	0	-2.003284	-0.305903	-0.231026
42	6	0	5.149215	-3.027932	0.432223
43	6	0	5.205529	-4.035928	1.411721
44	6	0	6.316335	-2.769030	-0.308892
45	6	0	6.379011	-4.753996	1.642238
46	1	0	4.314855	-4.245369	1.996657
47	6	0	7.491884	-3.483776	-0.077453
48	1	0	6.289306	-2.006057	-1.081361
49	6	0	7.529695	-4.480387	0.899913
50	1	0	6.395494	-5.524973	2.409343
51	1	0	8.378202	-3.267038	-0.669660
52	1	0	8.445474	-5.038527	1.080051
53	6	0	3.412110	3.711932	-0.376829
54	6	0	3.228239	4.855876	0.418036
55	6	0	4.430235	3.740791	-1.343664
56	6	0	4.035621	5.980089	0.257868
57	1	0	2.441119	4.853681	1.164413
58	6	0	5.234478	4.869033	-1.513632
59	1	0	4.580249	2.869187	-1.974091
60	6	0	5.043056	5.993732	-0.710412
61	1	0	3.875945	6.851011	0.889821
62	1	0	6.008891	4.868045	-2.277652
63	1	0	5.669847	6.873528	-0.838277
64	6	0	-3.233309	3.836815	0.357976
65	6	0	-2.829525	4.783587	1.316609
66	6	0	-4.337337	4.156469	-0.452836
67	6	0	-3.505518	5.994623	1.465919
68	1	0	-1.977745	4.554408	1.950194
69	6	0	-5.013519	5.368049	-0.307665
70	1	0	-4.653174	3.446315	-1.211474
71	6	0	-4.602024	6.293037	0.654610
72	1	0	-3.174970	6.705950	2.219401
73	1	0	-5.857904	5.593900	-0.955170
74	1	0	-5.127923	7.238195	0.767624

75	6	0	-5.324340	-2.849351	-0.043833
76	6	0	-5.497535	-3.975741	0.781212
77	6	0	-6.427901	-2.418537	-0.802488
78	6	0	-6.721122	-4.642081	0.845772
79	1	0	-4.658657	-4.318827	1.379214
80	6	0	-7.653647	-3.081648	-0.736664
81	1	0	-6.310186	-1.560327	-1.457649
82	6	0	-7.806945	-4.197781	0.088102
83	1	0	-6.828169	-5.507274	1.496288
84	1	0	-8.488273	-2.729966	-1.339167
85	1	0	-8.761482	-4.716363	0.139034

N_1SAPPh14$^{\ominus}$ (Energy = −2122.16529917)

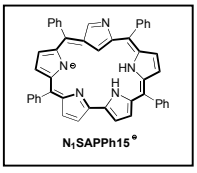


Stoichiometry C48H32N5(1-)
Framework group C1[X(C48H32N5)]
Deg. of freedom 249
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.567512	-2.419354	-0.422269
2	7	0	-1.493572	-2.525221	-0.269281
3	7	0	-2.792705	-0.017386	0.034635
4	7	0	2.899453	0.088650	0.049981
5	6	0	2.477847	2.546009	0.349855
6	6	0	-3.267222	1.260149	-0.023213
7	6	0	1.092735	2.674137	0.020866
8	6	0	-3.880845	-2.219291	0.303868
9	6	0	0.777164	-3.485650	-0.708836
10	6	0	-5.069156	0.001862	0.509276
11	6	0	-2.541624	2.445184	-0.341467
12	6	0	0.584150	3.931907	-0.537780
13	6	0	-4.692238	1.287739	0.279385
14	6	0	-2.767447	-3.010809	-0.023434
15	6	0	-3.877109	-0.804411	0.325266
16	6	0	-0.628647	-3.552654	-0.544903
17	6	0	1.561632	-4.640946	-1.083879
18	6	0	3.249309	1.377242	0.425436
19	6	0	-1.146960	2.640192	-0.349907
20	6	0	-2.689011	-4.429139	-0.157781
21	6	0	5.071569	0.018816	0.643143
22	6	0	4.626097	1.299225	0.832145
23	6	0	2.853377	-2.876870	-0.549649
24	6	0	-1.395796	-4.753404	-0.500363
25	6	0	4.007677	-2.121013	-0.221343
26	6	0	2.867937	-4.256301	-0.994307
27	6	0	3.988460	-0.763232	0.130619
28	1	0	-6.057539	-0.364409	0.750438
29	1	0	1.196032	4.791324	-0.795688
30	1	0	-5.310749	2.172337	0.329075
31	1	0	1.177976	-5.606632	-1.388224
32	1	0	-3.513199	-5.109631	-0.001457
33	1	0	6.056906	-0.367828	0.858880
34	1	0	5.190891	2.129017	1.229108
35	1	0	-0.993156	-5.744877	-0.652026
36	1	0	3.746786	-4.847249	-1.213377
37	7	0	-0.691059	3.917599	-0.774985
38	6	0	-0.044793	1.847794	0.089111

39	1	0	-0.117748	0.849997	0.500020
40	1	0	-1.306456	-1.523175	-0.254935
41	1	0	1.988430	-0.256984	-0.240195
42	6	0	5.333233	-2.807174	-0.209769
43	6	0	5.562812	-3.931073	0.604613
44	6	0	6.396038	-2.351558	-1.010437
45	6	0	6.801561	-4.571996	0.617990
46	1	0	4.756245	-4.292749	1.235317
47	6	0	7.637021	-2.989369	-0.996489
48	1	0	6.234523	-1.492437	-1.655146
49	6	0	7.846286	-4.103953	-0.182181
50	1	0	6.953098	-5.435490	1.261906
51	1	0	8.439546	-2.618570	-1.630301
52	1	0	8.812531	-4.602871	-0.171456
53	6	0	3.201767	3.830180	0.616151
54	6	0	2.736748	4.711849	1.608967
55	6	0	4.335595	4.216542	-0.121713
56	6	0	3.385027	5.920013	1.864771
57	1	0	1.858592	4.433139	2.183979
58	6	0	4.984839	5.425245	0.130867
59	1	0	4.696432	3.562755	-0.910325
60	6	0	4.514438	6.282585	1.127942
61	1	0	3.006661	6.579186	2.642793
62	1	0	5.853970	5.702896	-0.461488
63	1	0	5.018968	7.225813	1.323974
64	6	0	-3.387199	3.636166	-0.690998
65	6	0	-3.337279	4.825065	0.054820
66	6	0	-4.278377	3.576801	-1.774308
67	6	0	-4.153275	5.908812	-0.264028
68	1	0	-2.647860	4.890937	0.889675
69	6	0	-5.088173	4.665086	-2.104590
70	1	0	-4.326556	2.666411	-2.364743
71	6	0	-5.032430	5.835770	-1.347746
72	1	0	-4.099473	6.816414	0.333454
73	1	0	-5.763123	4.595288	-2.954997
74	1	0	-5.665363	6.683952	-1.599680
75	6	0	-5.158042	-2.933808	0.607854
76	6	0	-5.738984	-2.849773	1.884777
77	6	0	-5.815545	-3.705297	-0.365193
78	6	0	-6.931348	-3.511961	2.178354
79	1	0	-5.241001	-2.259306	2.648485
80	6	0	-7.006371	-4.371781	-0.072586
81	1	0	-5.387516	-3.768867	-1.361579
82	6	0	-7.570225	-4.278112	1.201163
83	1	0	-7.359093	-3.433222	3.175280
84	1	0	-7.498453	-4.958509	-0.845075
85	1	0	-8.499037	-4.795451	1.429709

N_1SAPPh15$^{\ominus}$ (Energy = −2122.14111156)



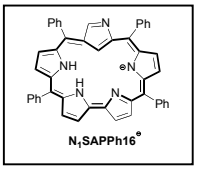
Stoichiometry C48H32N5(1-)
Framework group C1[X(C48H32N5)]
Deg. of freedom 249
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.317569	-2.676478	-0.236588
2	7	0	-1.529664	-2.648277	-0.373360

3	7	0	-2.790479	0.136348	-0.005965
4	7	0	2.769346	-0.003701	-0.039568
5	6	0	2.611794	2.459251	-0.153779
6	6	0	-3.139421	1.459209	0.299291
7	6	0	1.236625	2.648604	-0.404771
8	6	0	-3.948005	-2.095305	-0.016369
9	6	0	0.642899	-3.699522	-0.776413
10	6	0	-4.842332	0.075841	0.928781
11	6	0	-2.414760	2.620234	0.019520
12	6	0	0.689895	3.878423	-0.975503
13	6	0	-4.422903	1.377901	0.931156
14	6	0	-2.882350	-2.925040	-0.480221
15	6	0	-3.850550	-0.731387	0.279867
16	6	0	-0.777063	-3.688848	-0.874604
17	6	0	1.508864	-4.797265	-1.159231
18	6	0	3.256603	1.241866	0.206765
19	6	0	-1.026789	2.714907	-0.331298
20	6	0	-2.970777	-4.177929	-1.131222
21	6	0	4.843185	-0.146337	0.995832
22	6	0	4.554768	1.177551	0.865383
23	6	0	2.635688	-3.065267	-0.231471
24	6	0	-1.678425	-4.643081	-1.372595
25	6	0	3.724596	-2.281423	0.190176
26	6	0	2.763843	-4.408061	-0.795852
27	6	0	3.728621	-0.867471	0.390695
28	1	0	-5.751807	-0.314575	1.361448
29	1	0	1.270453	4.674594	-1.431285
30	1	0	-4.934084	2.222797	1.368371
31	1	0	1.207986	-5.726369	-1.628998
32	1	0	-3.898215	-4.657850	-1.409096
33	1	0	5.709571	-0.586906	1.470821
34	1	0	5.136731	2.018958	1.217696
35	1	0	-1.398552	-5.566612	-1.861405
36	1	0	3.688435	-4.949913	-0.942780
37	7	0	-0.610632	3.930069	-0.941694
38	6	0	0.078172	1.889656	-0.062875
39	1	0	0.091768	0.925839	0.427683
40	1	0	-2.064876	-0.073582	-0.679436
41	1	0	-1.094899	-1.914649	0.171399
42	6	0	-5.278042	-2.749623	0.140849
43	6	0	-6.434519	-2.220298	-0.462334
44	6	0	-5.418342	-3.932763	0.891532
45	6	0	-7.676924	-2.836264	-0.310739
46	1	0	-6.346652	-1.320279	-1.063592
47	6	0	-6.658285	-4.552061	1.040168
48	1	0	-4.539388	-4.358986	1.365676
49	6	0	-7.796595	-4.006193	0.441548
50	1	0	-8.551896	-2.405867	-0.792801
51	1	0	-6.737038	-5.460393	1.633377
52	1	0	-8.764093	-4.488746	0.557881
53	6	0	-3.169624	3.905619	0.128797
54	6	0	-4.398140	4.090721	-0.528246
55	6	0	-2.675537	4.970505	0.904037
56	6	0	-5.112238	5.284029	-0.407142
57	1	0	-4.784673	3.291354	-1.153476
58	6	0	-3.388432	6.159890	1.031424
59	1	0	-1.723378	4.851387	1.409960
60	6	0	-4.612755	6.324032	0.377081
61	1	0	-6.056437	5.401757	-0.934580
62	1	0	-2.986487	6.964226	1.643632
63	1	0	-5.166653	7.255187	0.473361
64	6	0	5.019518	-2.999346	0.400630
65	6	0	5.098135	-4.095505	1.278101
66	6	0	6.191549	-2.613540	-0.274689
67	6	0	6.299635	-4.776575	1.476733

68	1	0	4.203303	-4.401675	1.811503
69	6	0	7.391882	-3.297215	-0.082768
70	1	0	6.147102	-1.774452	-0.962039
71	6	0	7.452668	-4.381382	0.795940
72	1	0	6.334727	-5.615748	2.167973
73	1	0	8.281610	-2.984450	-0.624798
74	1	0	8.389526	-4.912451	0.948336
75	6	0	3.492819	3.665303	-0.228231
76	6	0	4.664133	3.653273	-1.008196
77	6	0	3.187708	4.841586	0.480264
78	6	0	5.489850	4.774216	-1.085283
79	1	0	4.912291	2.754556	-1.564209
80	6	0	4.017165	5.961107	0.410720
81	1	0	2.296573	4.863374	1.099762
82	6	0	5.171191	5.933737	-0.374523
83	1	0	6.383149	4.742823	-1.705088
84	1	0	3.762197	6.855181	0.975151
85	1	0	5.816749	6.807174	-0.431852

N_1SAPPh16$^{\ominus}$ (Energy = −2122.14245935)

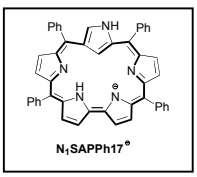


Stoichiometry C48H32N5(1-)
Framework group C1[X(C48H32N5)]
Deg. of freedom 249
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.651484	-2.578594	-0.441479
2	7	0	1.181680	-2.691590	-0.193082
3	7	0	2.736608	-0.074339	-0.055987
4	7	0	-2.803148	0.228660	0.002880
5	6	0	-2.303571	2.671649	0.230166
6	6	0	3.278956	1.155623	0.108165
7	6	0	-0.925290	2.727341	-0.194626
8	6	0	3.583076	-2.370604	0.335994
9	6	0	-0.914540	-3.634805	-0.927872
10	6	0	4.783687	-0.241748	1.028917
11	6	0	2.691864	2.384764	-0.340736
12	6	0	-0.381674	3.914242	-0.858113
13	6	0	4.562231	1.081763	0.789636
14	6	0	2.481748	-3.129882	-0.105934
15	6	0	3.649244	-0.953348	0.456121
16	6	0	0.499809	-3.700119	-0.751070
17	6	0	-1.822060	-4.537482	-1.502123
18	6	0	-3.088634	1.537718	0.413531
19	6	0	1.319283	2.624541	-0.505635
20	6	0	2.588023	-4.488333	-0.628573
21	6	0	-4.877437	0.201161	0.893809
22	6	0	-4.388001	1.469465	1.024162
23	6	0	-3.006257	-2.795255	-0.632134
24	6	0	1.340549	-4.836588	-1.060332
25	6	0	-4.058941	-1.940081	-0.178256
26	6	0	-3.107989	-4.022613	-1.323744
27	6	0	-3.912474	-0.604412	0.199480
28	1	0	5.621375	-0.683455	1.551756
29	1	0	-0.970499	4.760644	-1.201437
30	1	0	5.179333	1.921095	1.082300
31	1	0	-1.551793	-5.458603	-2.000670

32	1	0	3.497111	-5.069135	-0.708769
33	1	0	-5.814768	-0.175724	1.276577
34	1	0	-4.861447	2.297343	1.531035
35	1	0	1.030334	-5.765018	-1.525445
36	1	0	-4.036224	-4.457329	-1.666246
37	7	0	0.904619	3.862163	-1.053337
38	6	0	0.183429	1.887207	-0.035390
39	1	0	0.238597	0.919281	0.444347
40	1	0	-2.076349	0.037814	-0.675066
41	1	0	-1.218515	-1.871651	0.138734
42	6	0	4.826984	-3.139876	0.652482
43	6	0	4.800929	-4.178232	1.600070
44	6	0	6.047710	-2.865096	0.010915
45	6	0	5.950948	-4.908481	1.901838
46	1	0	3.865628	-4.400297	2.104944
47	6	0	7.196497	-3.599531	0.305070
48	1	0	6.082796	-2.072809	-0.730335
49	6	0	7.154525	-4.623221	1.254418
50	1	0	5.906034	-5.700605	2.645976
51	1	0	8.126349	-3.373627	-0.212160
52	1	0	8.051280	-5.193319	1.486428
53	6	0	3.647272	3.500248	-0.609258
54	6	0	3.459579	4.793000	-0.087959
55	6	0	4.793573	3.266662	-1.390228
56	6	0	4.382669	5.807240	-0.334621
57	1	0	2.581774	4.992494	0.514701
58	6	0	5.710972	4.285103	-1.649978
59	1	0	4.950957	2.276370	-1.805727
60	6	0	5.511740	5.560380	-1.119636
61	1	0	4.218346	6.796458	0.087074
62	1	0	6.582413	4.079738	-2.267846
63	1	0	6.228343	6.355070	-1.315848
64	6	0	-2.951216	3.987120	0.516226
65	6	0	-2.323183	4.920939	1.362849
66	6	0	-4.182684	4.353571	-0.058716
67	6	0	-2.907215	6.157091	1.634767
68	1	0	-1.370818	4.658432	1.813452
69	6	0	-4.768344	5.590578	0.211768
70	1	0	-4.671289	3.661092	-0.737864
71	6	0	-4.134667	6.498981	1.061955
72	1	0	-2.402582	6.854984	2.299012
73	1	0	-5.716598	5.849729	-0.254104
74	1	0	-4.588676	7.464776	1.270940
75	6	0	-5.421356	-2.539612	-0.102743
76	6	0	-5.644179	-3.753645	0.574867
77	6	0	-6.528743	-1.920452	-0.712013
78	6	0	-6.916951	-4.317149	0.647898
79	1	0	-4.803975	-4.248116	1.052741
80	6	0	-7.804015	-2.480942	-0.636056
81	1	0	-6.375981	-0.994472	-1.258447
82	6	0	-8.005925	-3.683119	0.044140
83	1	0	-7.060165	-5.251440	1.186112
84	1	0	-8.639817	-1.981561	-1.121072
85	1	0	-8.998824	-4.122802	0.100952

N_1SAPPh17$^{\ominus}$ (Energy = −2122.12942358)



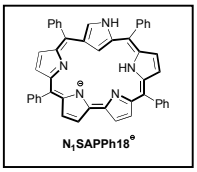
Stoichiometry C48H32N5(1-)
Framework group C1[X(C48H32N5)]
Deg. of freedom 249
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.691931	-2.566288	-0.095392
2	7	0	1.301003	-2.625470	0.123101
3	7	0	2.856991	-0.023780	0.052358
4	7	0	-2.794872	0.087244	-0.029063
5	6	0	-2.348470	2.502844	0.460814
6	6	0	3.413105	1.160199	-0.353695
7	6	0	-0.923694	2.669657	0.254941
8	6	0	3.752507	-2.333945	0.288487
9	6	0	-0.896485	-3.685630	-0.010491
10	6	0	5.104419	-0.322430	-0.454086
11	6	0	2.734274	2.380064	-0.444242
12	6	0	-0.396962	3.980616	0.211016
13	6	0	4.826873	0.980443	-0.697591
14	6	0	2.567282	-3.088335	0.365622
15	6	0	3.849962	-0.935210	0.007186
16	6	0	0.501121	-3.702162	0.196599
17	6	0	-1.746455	-4.806277	-0.202289
18	6	0	-3.158149	1.376033	0.307032
19	6	0	1.334776	2.590080	-0.194568
20	6	0	2.534262	-4.530228	0.652128
21	6	0	-5.110181	0.233776	0.175982
22	6	0	-4.616715	1.456723	0.467587
23	6	0	-3.006873	-2.918547	-0.309625
24	6	0	1.240482	-4.917483	0.521511
25	6	0	-4.087509	-2.011292	-0.339934
26	6	0	-3.029446	-4.343775	-0.413534
27	6	0	-3.956410	-0.616664	-0.117322
28	1	0	6.043666	-0.834928	-0.612947
29	1	0	-0.896398	4.928244	0.338087
30	1	0	5.494436	1.732884	-1.095130
31	1	0	-1.413249	-5.835201	-0.216111
32	1	0	3.379123	-5.147346	0.925378
33	1	0	-6.143366	-0.084667	0.199848
34	1	0	-5.176547	2.332000	0.764457
35	1	0	0.824396	-5.907264	0.666693
36	1	0	-3.910638	-4.933759	-0.617577
37	1	0	-1.404893	-1.594275	0.006804
38	7	0	0.910973	3.922668	-0.061497
39	6	0	0.190094	1.800946	0.001412
40	1	0	0.187495	0.722194	-0.031140
41	1	0	1.529543	4.715374	-0.136790
42	6	0	-5.453383	-2.572764	-0.548324
43	6	0	-6.252524	-2.136825	-1.621777
44	6	0	-5.997103	-3.543921	0.313218
45	6	0	-7.534953	-2.646679	-1.825611
46	1	0	-5.849350	-1.391561	-2.301548
47	6	0	-7.276545	-4.060591	0.107827
48	1	0	-5.406893	-3.881568	1.160142
49	6	0	-8.053990	-3.614801	-0.963425
50	1	0	-8.127265	-2.291664	-2.666334
51	1	0	-7.671852	-4.805779	0.795001
52	1	0	-9.052430	-4.015466	-1.122899
53	6	0	-3.059733	3.772489	0.853374
54	6	0	-3.832129	4.498674	-0.067818
55	6	0	-2.943822	4.281074	2.157782
56	6	0	-4.474151	5.682668	0.301703
57	1	0	-3.927373	4.119769	-1.081729
58	6	0	-3.584562	5.463544	2.532102
59	1	0	-2.347273	3.731971	2.881379
60	6	0	-4.353230	6.170385	1.604481

61	1	0	-5.067841	6.225484	-0.430698
62	1	0	-3.486392	5.830978	3.551315
63	1	0	-4.853110	7.091789	1.894312
64	6	0	3.535019	3.590888	-0.808104
65	6	0	3.225874	4.352803	-1.952849
66	6	0	4.615850	4.018137	-0.013385
67	6	0	3.967878	5.485508	-2.290652
68	1	0	2.404582	4.033285	-2.588711
69	6	0	5.361180	5.147572	-0.352787
70	1	0	4.862125	3.450489	0.878843
71	6	0	5.040634	5.888713	-1.492442
72	1	0	3.713321	6.047121	-3.186691
73	1	0	6.190344	5.454214	0.280869
74	1	0	5.619991	6.770421	-1.755575
75	6	0	5.050061	-3.060323	0.455920
76	6	0	5.423772	-4.118803	-0.391659
77	6	0	5.952450	-2.686711	1.468625
78	6	0	6.640895	-4.781633	-0.228542
79	1	0	4.748965	-4.410497	-1.190968
80	6	0	7.169954	-3.347187	1.634355
81	1	0	5.681972	-1.870829	2.132877
82	6	0	7.520683	-4.400276	0.786743
83	1	0	6.905786	-5.593258	-0.902919
84	1	0	7.844568	-3.040846	2.431049
85	1	0	8.469840	-4.915982	0.914017

N_1SAPPh18$^{\ominus}$ (Energy = −2122.12557907)



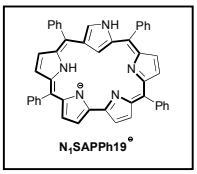
Stoichiometry C48H32N5(1-)
Framework group C1[X(C48H32N5)]
Deg. of freedom 249
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.197520	-2.613071	-0.164451
2	7	0	1.806507	-2.418711	-0.140304
3	7	0	2.880755	0.160811	-0.039772
4	7	0	-2.884035	-0.117685	-0.040245
5	6	0	-2.879980	2.326305	0.130731
6	6	0	3.116259	1.524619	0.004427
7	6	0	-1.485676	2.570162	-0.181083
8	6	0	4.192852	-1.942315	0.144651
9	6	0	-0.345877	-3.593953	-0.490252
10	6	0	5.072807	0.421241	0.448962
11	6	0	2.254644	2.604743	-0.205324
12	6	0	-1.086850	3.796885	-0.734752
13	6	0	4.519618	1.662410	0.333279
14	6	0	3.103695	-2.832038	-0.086921
15	6	0	4.054888	-0.554063	0.188882
16	6	0	1.074512	-3.528606	-0.419911
17	6	0	-1.056770	-4.816623	-0.896911
18	6	0	-3.473949	1.077585	0.299988
19	6	0	0.811681	2.625783	-0.319828
20	6	0	3.210196	-4.250878	-0.353165
21	6	0	-5.020180	-0.484547	0.787974
22	6	0	-4.817197	0.853647	0.843183
23	6	0	-2.454717	-3.140142	-0.312093
24	6	0	1.931422	-4.684257	-0.575680

25	6	0	-3.659221	-2.473603	-0.053556
26	6	0	-2.374695	-4.535064	-0.784783
27	6	0	-3.797907	-1.066734	0.212043
28	1	0	6.095075	0.185720	0.707238
29	1	0	-1.685842	4.625271	-1.081515
30	1	0	5.016602	2.607896	0.489462
31	1	0	-0.605910	-5.740031	-1.238647
32	1	0	4.122814	-4.831068	-0.391396
33	1	0	-5.886801	-1.033649	1.131720
34	1	0	-5.480122	1.606918	1.247523
35	1	0	1.612749	-5.694481	-0.800123
36	1	0	-3.211198	-5.175515	-1.029795
37	7	0	0.252354	3.813110	-0.825469
38	6	0	-0.277013	1.821312	0.039048
39	1	0	-0.239920	0.819186	0.443046
40	1	0	2.010733	-0.351501	-0.202852
41	1	0	0.804774	4.575651	-1.185340
42	6	0	5.554088	-2.520060	0.336621
43	6	0	5.795414	-3.457456	1.357873
44	6	0	6.633083	-2.164604	-0.492402
45	6	0	7.062312	-4.008346	1.547815
46	1	0	4.973517	-3.744481	2.006878
47	6	0	7.902670	-2.711988	-0.301723
48	1	0	6.462095	-1.460213	-1.301361
49	6	0	8.124571	-3.636780	0.720159
50	1	0	7.221514	-4.726129	2.349574
51	1	0	8.717848	-2.421985	-0.961254
52	1	0	9.112955	-4.065745	0.868267
53	6	0	2.919601	3.947113	-0.286666
54	6	0	2.622510	4.969959	0.636629
55	6	0	3.845874	4.242681	-1.305362
56	6	0	3.228925	6.223453	0.551155
57	1	0	1.914019	4.763093	1.434165
58	6	0	4.457769	5.494166	-1.390215
59	1	0	4.080201	3.471969	-2.034089
60	6	0	4.151955	6.492491	-0.462760
61	1	0	2.987037	6.989056	1.285069
62	1	0	5.168305	5.692145	-2.189687
63	1	0	4.625357	7.469074	-0.529784
64	6	0	-3.739378	3.534154	0.290545
65	6	0	-3.367489	4.589596	1.147088
66	6	0	-4.949204	3.665868	-0.418318
67	6	0	-4.173176	5.717645	1.296883
68	1	0	-2.444553	4.503802	1.712563
69	6	0	-5.753511	4.796319	-0.273002
70	1	0	-5.243699	2.872090	-1.097550
71	6	0	-5.370915	5.828467	0.586226
72	1	0	-3.867826	6.509948	1.976890
73	1	0	-6.678343	4.873837	-0.840333
74	1	0	-5.997674	6.709874	0.700080
75	6	0	-4.916945	-3.278780	-0.055363
76	6	0	-5.059027	-4.416563	0.760815
77	6	0	-6.008248	-2.922245	-0.870185
78	6	0	-6.234148	-5.168768	0.757036
79	1	0	-4.235020	-4.699178	1.409073
80	6	0	-7.184099	-3.672008	-0.875363
81	1	0	-5.918438	-2.049964	-1.510970
82	6	0	-7.303850	-4.801093	-0.061598
83	1	0	-6.316347	-6.040574	1.402655
84	1	0	-8.007452	-3.376679	-1.522320
85	1	0	-8.220834	-5.386046	-0.064268

N_1SAPPh19$^{\ominus}$ (Energy = −2122.12942358)

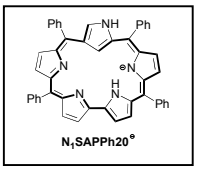


Stoichiometry C48H32N5(1-)
Framework group C1[X(C48H32N5)]
Deg. of freedom 249
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.763103	-2.445231	-0.099926
2	7	0	-1.254739	-2.597548	-0.152276
3	7	0	-2.897865	-0.078642	-0.049573
4	7	0	2.857927	0.124903	0.033717
5	6	0	2.294226	2.575502	-0.285627
6	6	0	-3.472894	1.114002	0.300479
7	6	0	0.846791	2.683094	-0.309021
8	6	0	-3.716853	-2.420812	-0.117290
9	6	0	1.008463	-3.564163	-0.261561
10	6	0	-5.079672	-0.418993	0.668018
11	6	0	-2.839611	2.357084	0.217180
12	6	0	0.262460	3.921256	-0.655114
13	6	0	-4.845838	0.910981	0.774478
14	6	0	-2.511072	-3.113060	-0.318184
15	6	0	-3.843761	-1.017403	0.139767
16	6	0	-0.406523	-3.612538	-0.379562
17	6	0	1.837003	-4.752584	-0.228958
18	6	0	3.132188	1.483162	-0.078588
19	6	0	-1.441768	2.566323	-0.059222
20	6	0	-2.437976	-4.532656	-0.710026
21	6	0	5.099328	0.353661	0.246705
22	6	0	4.569553	1.596464	0.078116
23	6	0	3.045882	-2.879319	0.046281
24	6	0	-1.122015	-4.845945	-0.737283
25	6	0	4.146977	-1.994900	0.224414
26	6	0	3.116442	-4.326336	-0.007509
27	6	0	4.030552	-0.603618	0.203170
28	1	0	-5.976534	-0.953697	0.951029
29	1	0	0.728643	4.828816	-1.004715
30	1	0	-5.509930	1.668819	1.168279
31	1	0	1.492222	-5.775453	-0.313785
32	1	0	-3.275010	-5.173006	-0.953427
33	1	0	6.141495	0.101180	0.378047
34	1	0	5.108050	2.531814	0.071547
35	1	0	-0.673873	-5.795901	-1.001325
36	1	0	4.005004	-4.931826	0.111634
37	7	0	-1.065096	3.845136	-0.488360
38	6	0	-0.253877	1.823583	0.029498
39	1	0	-0.224744	0.782098	0.319336
40	1	0	1.978069	-0.380396	-0.095086
41	1	0	-1.723176	4.585789	-0.675531
42	6	0	5.512746	-2.571968	0.403095
43	6	0	6.246145	-2.351594	1.582078
44	6	0	6.107729	-3.356093	-0.601132
45	6	0	7.524386	-2.886629	1.749209
46	1	0	5.796391	-1.760106	2.374696
47	6	0	7.382663	-3.897213	-0.434179
48	1	0	5.557602	-3.532685	-1.520765
49	6	0	8.099089	-3.663658	0.741830
50	1	0	8.068200	-2.702873	2.673343
51	1	0	7.820715	-4.497026	-1.229022
52	1	0	9.093749	-4.083885	0.871975

53	6	0	3.018172	3.882367	-0.477208
54	6	0	3.026216	4.863739	0.528980
55	6	0	3.696449	4.165214	-1.674070
56	6	0	3.690976	6.077809	0.349592
57	1	0	2.507092	4.659700	1.461666
58	6	0	4.362183	5.379134	-1.858829
59	1	0	3.697350	3.417048	-2.462031
60	6	0	4.362232	6.341110	-0.847054
61	1	0	3.689635	6.817127	1.147635
62	1	0	4.878815	5.573693	-2.796121
63	1	0	4.880616	7.286626	-0.988711
64	6	0	-3.669670	3.581047	0.419233
65	6	0	-3.305716	4.567019	1.360083
66	6	0	-4.840057	3.801780	-0.333848
67	6	0	-4.079792	5.712295	1.545160
68	1	0	-2.415197	4.412404	1.962840
69	6	0	-5.615976	4.945726	-0.146876
70	1	0	-5.128454	3.062719	-1.074786
71	6	0	-5.240333	5.908518	0.792626
72	1	0	-3.780522	6.448649	2.287709
73	1	0	-6.512616	5.089528	-0.745545
74	1	0	-5.843762	6.801578	0.936169
75	6	0	-4.986794	-3.208041	-0.153576
76	6	0	-5.193227	-4.311055	0.695468
77	6	0	-6.027079	-2.862689	-1.036445
78	6	0	-6.381887	-5.040899	0.658848
79	1	0	-4.409034	-4.584763	1.395044
80	6	0	-7.216619	-3.590064	-1.074880
81	1	0	-5.886137	-2.016666	-1.702854
82	6	0	-7.400712	-4.684798	-0.227223
83	1	0	-6.514843	-5.885924	1.331086
84	1	0	-7.999937	-3.304081	-1.773708
85	1	0	-8.327963	-5.252655	-0.255957

N_1SAPPh20$^{\ominus}$ (Energy = −2122.13056960)



Stoichiometry C48H32N5(1-)
Framework group C1[X(C48H32N5)]
Deg. of freedom 249
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

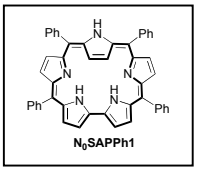
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.251176	-2.635718	0.104230
2	7	0	-1.741958	-2.542626	-0.120783
3	7	0	-2.795576	0.113121	-0.034011
4	7	0	2.854491	-0.049184	0.042609
5	6	0	2.782968	2.355889	-0.460815
6	6	0	-3.130283	1.399873	0.313019
7	6	0	1.388914	2.616641	-0.180583
8	6	0	-4.130079	-1.954768	-0.361296
9	6	0	0.439700	-3.699734	0.178901
10	6	0	-5.108265	0.304830	0.170243
11	6	0	-2.289921	2.507032	0.487716
12	6	0	0.954572	3.942901	0.007219
13	6	0	-4.586656	1.513703	0.474369
14	6	0	-3.059140	-2.880387	-0.338836
15	6	0	-3.974893	-0.569048	-0.130034
16	6	0	-0.959047	-3.670655	-0.038506

17	6	0	1.160457	-4.922500	0.523538
18	6	0	3.432604	1.125391	-0.382743
19	6	0	-0.866550	2.619025	0.286398
20	6	0	-3.098003	-4.301918	-0.449727
21	6	0	5.086778	-0.398629	-0.491658
22	6	0	4.836012	0.907459	-0.744965
23	6	0	2.512559	-3.112330	0.366207
24	6	0	-1.818018	-4.779976	-0.237706
25	6	0	3.704019	-2.376351	0.293772
26	6	0	2.456805	-4.551452	0.666404
27	6	0	3.824853	-0.977247	-0.006642
28	1	0	-6.148622	0.010410	0.191660
29	1	0	1.514945	4.864696	-0.021152
30	1	0	-5.127625	2.396968	0.782906
31	1	0	0.728905	-5.904895	0.673468
32	1	0	-3.984828	-4.882053	-0.657786
33	1	0	6.011085	-0.935473	-0.658425
34	1	0	5.514761	1.641059	-1.157997
35	1	0	-1.496223	-5.812527	-0.255848
36	1	0	3.289983	-5.176475	0.956778
37	7	0	-0.352886	3.932738	0.288854
38	6	0	0.229165	1.789354	0.009003
39	1	0	0.220217	0.711665	-0.046728
40	1	0	-1.447697	-1.573029	-0.010632
41	1	0	-0.920166	4.749716	0.453400
42	6	0	4.992189	-3.112781	0.486282
43	6	0	5.888691	-2.727509	1.499928
44	6	0	5.363811	-4.190292	-0.337744
45	6	0	7.097076	-3.397331	1.691257
46	1	0	5.620724	-1.895374	2.144770
47	6	0	6.572514	-4.862012	-0.149363
48	1	0	4.694814	-4.489855	-1.138984
49	6	0	7.445398	-4.470340	0.867734
50	1	0	7.766890	-3.082235	2.488537
51	1	0	6.836117	-5.688735	-0.805632
52	1	0	8.387940	-4.992881	1.014614
53	6	0	3.605491	3.542797	-0.854159
54	6	0	4.708246	3.955278	-0.084872
55	6	0	3.293677	4.290394	-2.005020
56	6	0	5.471167	5.064579	-0.452227
57	1	0	4.956960	3.396394	0.812373
58	6	0	4.056752	5.397923	-2.375740
59	1	0	2.449957	3.982705	-2.616168
60	6	0	5.149732	5.791681	-1.600176
61	1	0	6.315633	5.364507	0.164381
62	1	0	3.800424	5.950601	-3.276950
63	1	0	5.744146	6.655852	-1.887582
64	6	0	-2.964633	3.791898	0.892443
65	6	0	-2.796536	4.313687	2.188469
66	6	0	-3.753467	4.527369	-0.010345
67	6	0	-3.404369	5.510865	2.571826
68	1	0	-2.188575	3.759603	2.898826
69	6	0	-4.366322	5.722731	0.370942
70	1	0	-3.886244	4.142771	-1.017665
71	6	0	-4.194535	6.220134	1.664486
72	1	0	-3.266172	5.885410	3.583627
73	1	0	-4.975352	6.268500	-0.346302
74	1	0	-4.670197	7.151614	1.962086
75	6	0	-5.504223	-2.495102	-0.568563
76	6	0	-6.056153	-3.469028	0.284834
77	6	0	-6.303642	-2.035797	-1.631993
78	6	0	-7.344166	-3.964599	0.081938
79	1	0	-5.465294	-3.825390	1.123543
80	6	0	-7.594706	-2.524730	-1.833261
81	1	0	-5.893516	-1.289170	-2.306026

82	6	0	-8.122156	-3.495108	-0.978895
83	1	0	-7.745760	-4.712130	0.762916
84	1	0	-8.187085	-2.151680	-2.666114
85	1	0	-9.127184	-3.879745	-1.136509

Cartesian coordinates for the optimized structures of normal *meso*-tetraphenyl-sapphyrins (neutral)

N_0SAPPh1 (Energy = −2122.71865352)

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 Stoichiometry    C48H33N5
 Framework group  C1[X(C48H33N5)]
 Deg. of freedom   252
 Full point group                 C1
 Largest Abelian subgroup         C1      NOp   1
 Largest concise Abelian subgroup C1      NOp   1
                       Standard orientation:
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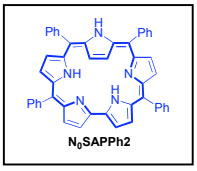
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          7             0        1.618614   -2.360313   -0.001990
    2          7             0       -1.618709   -2.360268   -0.001966
    3          7             0       -2.978152    0.065017   -0.254546
    4          7             0        2.978149    0.064943   -0.254608
    5          6             0        2.433494    2.437638   -0.422917
    6          6             0       -3.360916    1.367160   -0.280896
    7          6             0       -4.105778   -2.074886   -0.002414
    8          6             0        0.712651   -3.399062    0.012049
    9          6             0       -5.282912    0.201691   -0.060458
   10          6             0       -2.433405    2.437697   -0.422863
   11          6             0       -4.807891    1.475174   -0.146924
   12          6             0       -2.920179   -2.849843    0.020608
   13          6             0       -4.118575   -0.672860   -0.124750
   14          6             0       -0.712773   -3.399042    0.012021
   15          6             0        1.480106   -4.598907    0.040293
   16          6             0        3.360968    1.367072   -0.280952
   17          6             0       -2.815279   -4.267132    0.043097
   18          6             0        5.282914    0.201524   -0.060512
   19          6             0        4.807949    1.475027   -0.146990
   20          6             0        2.920070   -2.849920    0.020650
   21          6             0       -1.480263   -4.598868    0.040167
   22          6             0        4.105691   -2.074997   -0.002387
   23          6             0        2.815131   -4.267206    0.043221
   24          6             0        4.118537   -0.672976   -0.124770
   25          1             0       -1.469540   -1.350952   -0.054079
   26          1             0       -6.311664   -0.112910    0.048529
   27          1             0       -5.378611    2.394163   -0.157399
   28          1             0        1.070157   -5.597521    0.052622
   29          1             0       -3.653486   -4.947475    0.047453
   30          1             0        6.311652   -0.113121    0.048474
   31          1             0        5.378709    2.393991   -0.157469
   32          1             0       -1.070341   -5.597495    0.052403
   33          1             0        3.653319   -4.947571    0.047647
   34          1             0        1.469477   -1.350994   -0.054182
   35          6             0       -0.685852    1.012873   -1.641907
   36          6             0        0.685884    1.012845   -1.641904
   37          6             0        1.137482    2.134139   -0.878965
   38          6             0       -1.137408    2.134168   -0.878942
   39          7             0        0.000049    2.845708   -0.538260
   40          1             0        1.346576    0.318922   -2.136571
   41          1             0       -1.346568    0.318975   -2.136576
   42          1             0        0.000066    3.596128    0.138948
   43          6             0        2.771935    3.812610    0.006533
   44          6             0        2.345020    4.927157   -0.744295
   45          6             0        3.516562    4.053836    1.178212
   46          6             0        2.656108    6.224946   -0.344571
   47          1             0        1.785767    4.764207   -1.661287
   48          6             0        3.830835    5.352871    1.573444
   49          1             0        3.831948    3.211647    1.786041
```

50	6	0	3.402467	6.444655	0.815582
51	1	0	2.323974	7.066824	-0.946542
52	1	0	4.402760	5.512707	2.483810
53	1	0	3.645901	7.456929	1.126661
54	6	0	-2.771796	3.812668	0.006613
55	6	0	-2.344849	4.927219	-0.744192
56	6	0	-3.516408	4.053896	1.178302
57	6	0	-2.655890	6.225010	-0.344437
58	1	0	-1.785608	4.764273	-1.661193
59	6	0	-3.830636	5.352933	1.573564
60	1	0	-3.831819	3.211706	1.786116
61	6	0	-3.402236	6.444720	0.815724
62	1	0	-2.323728	7.066889	-0.946392
63	1	0	-4.402553	5.512767	2.483935
64	1	0	-3.645633	7.456996	1.126826
65	6	0	-5.404867	-2.802169	0.106661
66	6	0	-6.356069	-2.725646	-0.924686
67	6	0	-5.713658	-3.569405	1.242578
68	6	0	-7.575856	-3.394909	-0.823472
69	1	0	-6.126604	-2.144965	-1.813488
70	6	0	-6.933708	-4.237936	1.344066
71	1	0	-4.994332	-3.626304	2.054642
72	6	0	-7.869249	-4.153612	0.311049
73	1	0	-8.295256	-3.327441	-1.635470
74	1	0	-7.155734	-4.819873	2.234857
75	1	0	-8.819607	-4.674775	0.389886
76	6	0	5.404765	-2.802310	0.106708
77	6	0	6.355949	-2.725858	-0.924660
78	6	0	5.713556	-3.569490	1.242660
79	6	0	7.575718	-3.395152	-0.823437
80	1	0	6.126485	-2.145208	-1.813483
81	6	0	6.933588	-4.238052	1.344157
82	1	0	4.994246	-3.626327	2.054743
83	6	0	7.869109	-4.153809	0.311115
84	1	0	8.295102	-3.327744	-1.635454
85	1	0	7.155617	-4.819948	2.234974
86	1	0	8.819453	-4.674997	0.389960

N_0SAPPh2 (Energy = −2122.72151660)



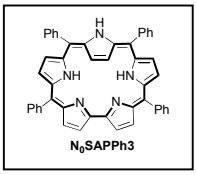
Stoichiometry C48H33N5
Framework group C1[X(C48H33N5)]
Deg. of freedom 252
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.583774	-2.330529	-0.024589
2	7	0	-1.577041	-2.378064	-0.026961
3	7	0	-2.967322	0.072076	-0.237252
4	7	0	3.009138	0.081106	-0.284017
5	6	0	2.418446	2.471690	-0.477456
6	6	0	-3.367057	1.369740	-0.235637
7	6	0	-4.067946	-2.086598	-0.016369
8	6	0	0.750855	-3.397444	-0.021627
9	6	0	-5.270523	0.177744	-0.012224
10	6	0	-2.450828	2.450169	-0.377598
11	6	0	-4.812392	1.459030	-0.080027
12	6	0	-2.881771	-2.857269	-0.017182

13	6	0	-4.096108	-0.680423	-0.108276
14	6	0	-0.678163	-3.418030	-0.032907
15	6	0	1.497369	-4.645840	0.014785
16	6	0	3.352571	1.414757	-0.338076
17	6	0	-2.784619	-4.278205	-0.030475
18	6	0	5.243399	0.171574	-0.092924
19	6	0	4.775364	1.462793	-0.216584
20	6	0	2.861504	-2.857329	0.022297
21	6	0	-1.452236	-4.616207	-0.037378
22	6	0	4.062533	-2.113358	0.010663
23	6	0	2.812303	-4.307184	0.043795
24	6	0	4.122019	-0.711956	-0.127293
25	1	0	-1.390599	-1.377205	-0.043786
26	1	0	-6.293823	-0.151488	0.104550
27	1	0	-5.394499	2.370867	-0.066548
28	1	0	1.084076	-5.644580	0.016378
29	1	0	-3.627645	-4.952412	-0.047626
30	1	0	6.272204	-0.140114	0.012842
31	1	0	5.362956	2.368911	-0.254329
32	1	0	-1.046231	-5.616129	-0.052120
33	1	0	3.664485	-4.971370	0.058839
34	6	0	-0.726741	1.054287	-1.654570
35	6	0	0.645954	1.056358	-1.682168
36	6	0	1.111917	2.165564	-0.911274
37	6	0	-1.163734	2.160766	-0.866891
38	7	0	-0.018431	2.866192	-0.532218
39	1	0	1.283839	0.369599	-2.219206
40	1	0	-1.393265	0.364253	-2.146078
41	1	0	-0.005622	3.603641	0.158879
42	1	0	2.078341	-0.335131	-0.221483
43	6	0	2.771273	3.849204	-0.066726
44	6	0	2.330037	4.955151	-0.821834
45	6	0	3.539208	4.103430	1.086796
46	6	0	2.649468	6.257054	-0.443021
47	1	0	1.750817	4.782045	-1.724402
48	6	0	3.862890	5.406605	1.460062
49	1	0	3.866016	3.269169	1.699667
50	6	0	3.419981	6.490013	0.698651
51	1	0	2.305004	7.091959	-1.047702
52	1	0	4.452835	5.576141	2.357047
53	1	0	3.670415	7.505557	0.992782
54	6	0	-2.787836	3.814900	0.082299
55	6	0	-2.372959	4.945254	-0.651678
56	6	0	-3.519779	4.030424	1.266944
57	6	0	-2.683482	6.233871	-0.223174
58	1	0	-1.824597	4.802093	-1.578485
59	6	0	-3.833157	5.320456	1.691077
60	1	0	-3.825518	3.175296	1.861362
61	6	0	-3.416825	6.428211	0.949764
62	1	0	-2.361309	7.088498	-0.812432
63	1	0	-4.395088	5.460731	2.610807
64	1	0	-3.659802	7.433379	1.283388
65	6	0	5.363439	-2.833499	0.157112
66	6	0	6.327056	-2.793283	-0.864248
67	6	0	5.657638	-3.557480	1.324319
68	6	0	7.545725	-3.457951	-0.723894
69	1	0	6.108033	-2.248093	-1.778063
70	6	0	6.876588	-4.220900	1.465206
71	1	0	4.924949	-3.588555	2.125537
72	6	0	7.825080	-4.173587	0.441688
73	1	0	8.274528	-3.421398	-1.529487
74	1	0	7.086789	-4.771594	2.378423
75	1	0	8.774335	-4.691211	0.551340
76	6	0	-5.363986	-2.821912	0.084526
77	6	0	-6.318146	-2.732646	-0.942880

78	6	0	-5.666114	-3.608040	1.209075
79	6	0	-7.534544	-3.409120	-0.849362
80	1	0	-6.093855	-2.136496	-1.822733
81	6	0	-6.883323	-4.282846	1.303355
82	1	0	-4.943652	-3.675579	2.017470
83	6	0	-7.821782	-4.186478	0.274073
84	1	0	-8.256278	-3.332189	-1.658447
85	1	0	-7.100392	-4.879870	2.185330
86	1	0	-8.769696	-4.712932	0.347135

N_0SAPPh3 (Energy = −2122.71617287)

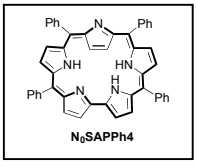


Stoichiometry C48H33N5
Framework group C1[X(C48H33N5)]
Deg. of freedom 252
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.578600	-2.297523	-0.044392
2	7	0	-1.578918	-2.297359	-0.044135
3	7	0	-3.018684	0.078807	-0.260776
4	7	0	3.018630	0.078440	-0.261450
5	6	0	2.437744	2.472089	-0.427512
6	6	0	-3.368936	1.411260	-0.294414
7	6	0	-4.055716	-2.125358	-0.005432
8	6	0	0.719127	-3.341658	-0.049638
9	6	0	-5.253465	0.156292	-0.069636
10	6	0	-2.437473	2.472350	-0.427009
11	6	0	-4.790842	1.452497	-0.171290
12	6	0	-2.846184	-2.849539	-0.005450
13	6	0	-4.127626	-0.719230	-0.118712
14	6	0	-0.719558	-3.341611	-0.049849
15	6	0	1.450647	-4.608326	-0.029862
16	6	0	3.369069	1.410851	-0.295141
17	6	0	-2.771220	-4.300252	-0.002000
18	6	0	5.253424	0.155655	-0.070261
19	6	0	4.790974	1.451926	-0.172057
20	6	0	2.845803	-2.849828	-0.005097
21	6	0	-1.451216	-4.608177	-0.030988
22	6	0	4.055391	-2.125813	-0.005403
23	6	0	2.770662	-4.300547	-0.000777
24	6	0	4.127466	-0.719696	-0.119220
25	1	0	-6.280715	-0.162219	0.030818
26	1	0	-5.382451	2.356546	-0.195221
27	1	0	1.022949	-5.599951	-0.041957
28	1	0	-3.610308	-4.981183	0.000538
29	1	0	6.280641	-0.162932	0.030259
30	1	0	5.382725	2.355877	-0.196137
31	1	0	-1.023684	-5.599864	-0.043911
32	1	0	3.609684	-4.981560	0.002408
33	6	0	-0.686690	1.076923	-1.679178
34	6	0	0.686604	1.076904	-1.679349
35	6	0	1.138919	2.173750	-0.886848
36	6	0	-1.138772	2.173837	-0.886631
37	7	0	0.000134	2.868412	-0.515300
38	1	0	1.330432	0.391323	-2.210003
39	1	0	-1.330647	0.391369	-2.209704
40	1	0	0.000225	3.595667	0.186499

41	1	0	2.087149	-0.344266	-0.201194
42	6	0	2.786258	3.841254	0.011904
43	6	0	2.348345	4.961735	-0.723681
44	6	0	3.549113	4.072518	1.173625
45	6	0	2.665798	6.255868	-0.317890
46	1	0	1.774472	4.806426	-1.632854
47	6	0	3.870369	5.368153	1.574032
48	1	0	3.873621	3.226166	1.770821
49	6	0	3.430558	6.466232	0.832040
50	1	0	2.324611	7.102535	-0.907869
51	1	0	4.456214	5.520196	2.476782
52	1	0	3.679362	7.475809	1.147310
53	6	0	-2.785722	3.841542	0.012490
54	6	0	-2.347741	4.962007	-0.723081
55	6	0	-3.548411	4.072867	1.174317
56	6	0	-2.664983	6.256162	-0.317199
57	1	0	-1.773980	4.806677	-1.632323
58	6	0	-3.869466	5.368522	1.574808
59	1	0	-3.872937	3.226538	1.771535
60	6	0	-3.429601	6.466580	0.832815
61	1	0	-2.323736	7.102808	-0.907174
62	1	0	-4.455194	5.520600	2.477629
63	1	0	-3.678241	7.476177	1.148155
64	1	0	-2.087260	-0.344017	-0.200468
65	6	0	-5.349114	-2.860545	0.126793
66	6	0	-6.316417	-2.803148	-0.890386
67	6	0	-5.633168	-3.616060	1.276382
68	6	0	-7.528369	-3.482441	-0.763436
69	1	0	-6.105240	-2.233564	-1.791070
70	6	0	-6.845649	-4.293938	1.403922
71	1	0	-4.897800	-3.660263	2.074431
72	6	0	-7.797619	-4.229648	0.384629
73	1	0	-8.259841	-3.432603	-1.565881
74	1	0	-7.047914	-4.869406	2.303526
75	1	0	-8.741740	-4.758623	0.483847
76	6	0	5.348714	-2.861064	0.127045
77	6	0	6.315844	-2.804404	-0.890342
78	6	0	5.632946	-3.615873	1.277064
79	6	0	7.527765	-3.483709	-0.763187
80	1	0	6.104554	-2.235380	-1.791357
81	6	0	6.845385	-4.293775	1.404805
82	1	0	4.897732	-3.659492	2.075291
83	6	0	7.797174	-4.230219	0.385294
84	1	0	8.259086	-3.434422	-1.565803
85	1	0	7.047755	-4.868690	2.304739
86	1	0	8.741276	-4.759197	0.484678

N_0SAPPh4 (Energy = −2122.70658126)



Stoichiometry C48H33N5
Framework group C1[X(C48H33N5)]
Deg. of freedom 252
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

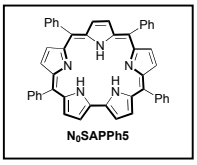
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.868457	-2.224967	0.029793
2	7	0	-1.220380	-2.531185	0.048516
3	7	0	-3.014673	-0.073199	-0.090212

4	7	0	2.979091	0.322476	-0.188666
5	6	0	2.099086	2.632796	-0.192877
6	6	0	-3.548930	1.184764	-0.353658
7	6	0	-3.763341	-2.425479	0.083169
8	6	0	1.158948	-3.361771	0.186951
9	6	0	-5.200865	-0.378089	-0.472225
10	6	0	-2.733461	2.327088	-0.435990
11	6	0	-4.943323	0.969408	-0.579611
12	6	0	-2.500489	-3.059285	0.247295
13	6	0	-3.983444	-1.057739	-0.132488
14	6	0	-0.254917	-3.493439	0.298328
15	6	0	2.026811	-4.528375	0.236756
16	6	0	3.162091	1.689046	-0.182967
17	6	0	-2.299553	-4.394112	0.688779
18	6	0	5.194849	0.666132	-0.201898
19	6	0	4.573093	1.898530	-0.187116
20	6	0	3.195557	-2.617340	-0.009933
21	6	0	-0.944184	-4.656899	0.709828
22	6	0	4.297199	-1.747853	-0.110604
23	6	0	3.295405	-4.064518	0.094023
24	6	0	4.181441	-0.338382	-0.187902
25	1	0	-6.142387	-0.874472	-0.657314
26	1	0	-5.638905	1.741732	-0.876156
27	1	0	1.709118	-5.558376	0.327852
28	1	0	-3.094179	-5.061481	0.986179
29	1	0	6.257258	0.472266	-0.218849
30	1	0	5.047088	2.868890	-0.218644
31	1	0	-0.470902	-5.573572	1.030473
32	1	0	4.208620	-4.640940	0.055774
33	6	0	-0.836593	1.002582	-1.534133
34	6	0	0.519195	1.088995	-1.485208
35	6	0	0.817371	2.234895	-0.632337
36	6	0	-1.343244	2.105943	-0.715418
37	7	0	-0.335380	2.860813	-0.239649
38	1	0	1.234369	0.488888	-2.030526
39	1	0	-1.435047	0.331656	-2.136959
40	1	0	2.109095	-0.200492	-0.077876
41	6	0	2.344722	4.002775	0.304636
42	6	0	1.741212	5.111326	-0.319760
43	6	0	3.186825	4.239812	1.407905
44	6	0	1.985575	6.404645	0.131393
45	1	0	1.084619	4.945051	-1.165908
46	6	0	3.426513	5.535814	1.861363
47	1	0	3.632375	3.397058	1.926913
48	6	0	2.830393	6.624134	1.222813
49	1	0	1.515823	7.246301	-0.370763
50	1	0	4.072117	5.693504	2.721413
51	1	0	3.016834	7.635065	1.575635
52	6	0	-3.285934	3.673631	-0.222300
53	6	0	-2.729266	4.790595	-0.877719
54	6	0	-4.387965	3.889587	0.629600
55	6	0	-3.266796	6.061745	-0.704351
56	1	0	-1.873719	4.645939	-1.527392
57	6	0	-4.926569	5.163366	0.798516
58	1	0	-4.802999	3.053968	1.184532
59	6	0	-4.371070	6.255726	0.130376
60	1	0	-2.824605	6.906769	-1.225723
61	1	0	-5.772470	5.304587	1.466382
62	1	0	-4.787638	7.250346	0.265477
63	1	0	-2.127807	-0.174930	0.379985
64	6	0	-4.974291	-3.298586	0.159701
65	6	0	-5.153327	-4.362936	-0.740664
66	6	0	-5.969506	-3.067128	1.124056
67	6	0	-6.290409	-5.167669	-0.679350
68	1	0	-4.397121	-4.548944	-1.497875

69	6	0	-7.107103	-3.872585	1.185864
70	1	0	-5.839403	-2.255995	1.834730
71	6	0	-7.271690	-4.925575	0.284469
72	1	0	-6.412831	-5.980970	-1.389837
73	1	0	-7.861711	-3.680285	1.944038
74	1	0	-8.157499	-5.553178	0.332553
75	6	0	5.681085	-2.311312	-0.104650
76	6	0	6.528921	-2.136653	-1.210930
77	6	0	6.170974	-3.014804	1.007943
78	6	0	7.824552	-2.653961	-1.206918
79	1	0	6.160126	-1.602938	-2.082382
80	6	0	7.466867	-3.531383	1.012126
81	1	0	5.530376	-3.144909	1.875325
82	6	0	8.298185	-3.353060	-0.095175
83	1	0	8.461997	-2.514853	-2.076190
84	1	0	7.828651	-4.068746	1.884869
85	1	0	9.307645	-3.755417	-0.091606
86	1	0	-1.000277	-1.675503	-0.444846

N_0SAPPh5 (Energy = −2122.70456168)

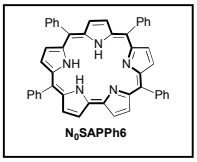


Stoichiometry C48H33N5
Framework group C1[X(C48H33N5)]
Deg. of freedom 252
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.559031	-2.471178	-0.562554
2	7	0	1.493406	-2.540951	-0.273436
3	7	0	2.700717	-0.015825	0.008828
4	7	0	-2.700385	0.024342	0.124502
5	6	0	-2.358914	2.455389	0.582290
6	6	0	3.196162	1.238764	-0.176727
7	6	0	-1.073191	2.743594	0.084053
8	6	0	3.821404	-2.192219	0.442139
9	6	0	-0.724514	-3.516376	-0.861315
10	6	0	4.991438	0.023732	0.454604
11	6	0	2.503166	2.419823	-0.562219
12	6	0	-0.717974	4.030607	-0.440742
13	6	0	4.630512	1.277422	0.090907
14	6	0	0.585304	4.001244	-0.837622
15	6	0	2.737578	-3.020795	0.088413
16	6	0	3.790937	-0.788475	0.360899
17	6	0	0.664335	-3.581940	-0.604770
18	6	0	-1.540345	-4.579457	-1.329365
19	6	0	-3.053869	1.220125	0.676646
20	6	0	1.134062	2.715030	-0.513152
21	6	0	2.676049	-4.437327	-0.011352
22	6	0	-4.892239	-0.070626	0.916738
23	6	0	-4.404743	1.153267	1.232502
24	6	0	-2.876452	-2.844356	-0.745217
25	6	0	1.416423	-4.776880	-0.462550
26	6	0	-3.967751	-2.059978	-0.320510
27	6	0	-2.855958	-4.165702	-1.271415
28	6	0	-3.827672	-0.760882	0.208108
29	1	0	1.350330	-1.531682	-0.346668
30	1	0	5.976415	-0.332943	0.719181
31	1	0	-1.410298	4.851902	-0.542433

32	1	0	5.259176	2.153382	0.029263
33	1	0	1.140131	4.799353	-1.304934
34	1	0	-1.170576	-5.535304	-1.673013
35	1	0	3.482671	-5.110384	0.237817
36	1	0	-5.860136	-0.484547	1.161625
37	1	0	-4.902760	1.938468	1.781669
38	1	0	1.025102	-5.772909	-0.614569
39	1	0	-3.730445	-4.730584	-1.557771
40	7	0	0.070944	1.961776	-0.023391
41	1	0	0.169843	1.021204	0.331537
42	1	0	-1.345544	-1.538162	-0.210093
43	6	0	-3.143932	3.685316	0.951319
44	6	0	-2.732440	4.493549	2.023138
45	6	0	-4.288270	4.065857	0.230969
46	6	0	-3.448794	5.638600	2.374020
47	1	0	-1.847531	4.212457	2.587350
48	6	0	-4.999613	5.216006	0.573631
49	1	0	-4.613107	3.455331	-0.606504
50	6	0	-4.584196	6.004454	1.648924
51	1	0	-3.118819	6.244516	3.213894
52	1	0	-5.877759	5.497582	-0.001749
53	1	0	-5.140458	6.898412	1.918304
54	6	0	3.383850	3.547845	-1.033223
55	6	0	4.019866	3.464073	-2.281067
56	6	0	3.608684	4.685521	-0.242849
57	6	0	4.849033	4.492318	-2.731415
58	1	0	3.857209	2.585318	-2.898863
59	6	0	4.442890	5.711935	-0.688701
60	1	0	3.129569	4.757944	0.729714
61	6	0	5.063700	5.619346	-1.936012
62	1	0	5.327855	4.411743	-3.703850
63	1	0	4.609673	6.582494	-0.059544
64	1	0	5.712037	6.419015	-2.284313
65	6	0	5.087813	-2.866715	0.861843
66	6	0	5.807505	-3.684474	-0.024455
67	6	0	5.583392	-2.694364	2.164499
68	6	0	6.985197	-4.313386	0.380896
69	1	0	5.445802	-3.812444	-1.040775
70	6	0	6.760565	-3.323616	2.569960
71	1	0	5.033769	-2.066629	2.860171
72	6	0	7.465006	-4.136482	1.679929
73	1	0	7.531755	-4.936452	-0.322306
74	1	0	7.125087	-3.180897	3.583898
75	1	0	8.382224	-4.626490	1.995448
76	6	0	-5.328597	-2.665177	-0.400985
77	6	0	-5.628044	-3.881518	0.237224
78	6	0	-6.349837	-2.023502	-1.123055
79	6	0	-6.904523	-4.437430	0.154342
80	1	0	-4.857068	-4.380094	0.817315
81	6	0	-7.625146	-2.581299	-1.208554
82	1	0	-6.130505	-1.087229	-1.627516
83	6	0	-7.907272	-3.790717	-0.570661
84	1	0	-7.117504	-5.373507	0.664061
85	1	0	-8.397844	-2.071848	-1.778371
86	1	0	-8.901364	-4.224906	-0.635986

N_0SAPPh6 (Energy = −2122.68474194)



Stoichiometry C48H33N5
Framework group C1[X(C48H33N5)]
Deg. of freedom 252
Full point group C1
Largest Abelian subgroup C1 NOp 1

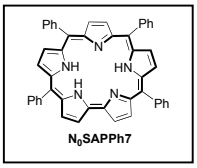
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.726458	-2.540919	-0.541000
2	7	0	1.040286	-2.707503	-0.298944
3	7	0	2.642433	-0.101817	0.020378
4	7	0	-2.683457	0.232601	0.007012
5	6	0	-2.114954	2.684602	0.202089
6	6	0	3.290543	1.087094	0.147249
7	6	0	-0.786483	2.832786	-0.283044
8	6	0	3.418067	-2.449349	0.336102
9	6	0	-1.040432	-3.603812	-1.070493
10	6	0	4.718338	-0.401119	1.033093
11	6	0	2.812285	2.338306	-0.319559
12	6	0	-0.324109	4.030855	-0.912005
13	6	0	4.589190	0.926693	0.789997
14	6	0	1.030094	3.940430	-1.094966
15	6	0	2.321553	-3.168567	-0.179301
16	6	0	3.518343	-1.039357	0.492213
17	6	0	0.362206	-3.700403	-0.899925
18	6	0	-1.995520	-4.473739	-1.640730
19	6	0	-2.874083	1.533574	0.474255
20	6	0	1.474710	2.693426	-0.564285
21	6	0	2.430427	-4.520208	-0.733344
22	6	0	-4.665392	0.266158	1.093331
23	6	0	-4.100601	1.510275	1.209423
24	6	0	-3.090741	-2.724655	-0.675703
25	6	0	1.197995	-4.841378	-1.213647
26	6	0	-4.074645	-1.856524	-0.147915
27	6	0	-3.252372	-3.937563	-1.398557
28	6	0	-3.818052	-0.549525	0.290305
29	1	0	5.538326	-0.902950	1.526040
30	1	0	-0.968077	4.849199	-1.196267
31	1	0	5.274664	1.721500	1.049185
32	1	0	1.675911	4.673082	-1.554319
33	1	0	-1.766849	-5.386995	-2.172492
34	1	0	3.334242	-5.110360	-0.789471
35	1	0	-5.578924	-0.080066	1.554338
36	1	0	-4.482809	2.346354	1.775321
37	1	0	0.890175	-5.752539	-1.711254
38	1	0	-4.204443	-4.338493	-1.714942
39	7	0	0.325642	2.012252	-0.160927
40	1	0	0.381582	1.100177	0.278473
41	1	0	-1.254026	-1.887888	0.071784
42	6	0	-2.832832	3.981989	0.444904
43	6	0	-2.328792	4.919417	1.362683
44	6	0	-4.022762	4.291644	-0.235295
45	6	0	-2.994448	6.122081	1.597649
46	1	0	-1.411648	4.692981	1.898811
47	6	0	-4.686095	5.497544	-0.006905
48	1	0	-4.421192	3.581749	-0.954563
49	6	0	-4.175206	6.416106	0.912170
50	1	0	-2.592263	6.828458	2.319141
51	1	0	-5.599817	5.721353	-0.551328
52	1	0	-4.692619	7.354663	1.092121
53	6	0	3.838575	3.405074	-0.536680
54	6	0	4.911980	3.177555	-1.415423
55	6	0	3.778859	4.637407	0.136667
56	6	0	5.884336	4.154842	-1.624758
57	1	0	4.970332	2.229470	-1.941424
58	6	0	4.756669	5.611511	-0.065299
59	1	0	2.967661	4.820927	0.835048

60	6	0	5.810665	5.375072	-0.949899
61	1	0	6.700229	3.962653	-2.316586
62	1	0	4.697750	6.553372	0.473986
63	1	0	6.571065	6.134960	-1.109599
64	6	0	4.628222	-3.266862	0.671265
65	6	0	5.854383	-3.075571	0.012218
66	6	0	4.547096	-4.273986	1.647486
67	6	0	6.963127	-3.863134	0.321899
68	1	0	5.928308	-2.311257	-0.755571
69	6	0	5.658844	-5.054435	1.965877
70	1	0	3.604711	-4.433274	2.163405
71	6	0	6.870560	-4.852856	1.302809
72	1	0	7.899624	-3.705490	-0.206980
73	1	0	5.577012	-5.821035	2.732150
74	1	0	7.735888	-5.463670	1.546590
75	6	0	-5.468480	-2.371626	-0.041934
76	6	0	-5.735664	-3.605073	0.579367
77	6	0	-6.551533	-1.643276	-0.566082
78	6	0	-7.039166	-4.089915	0.675545
79	1	0	-4.912943	-4.174622	1.000822
80	6	0	-7.854858	-2.129294	-0.470514
81	1	0	-6.361259	-0.698022	-1.065545
82	6	0	-8.104102	-3.354422	0.150958
83	1	0	-7.223607	-5.040898	1.168258
84	1	0	-8.675557	-1.553588	-0.890328
85	1	0	-9.119786	-3.733480	0.225278
86	1	0	-2.085273	0.034670	-0.785470

N_0SAPPh7 (Energy = −2122.70262837)

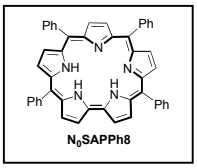


Stoichiometry C48H33N5
Framework group C1[X(C48H33N5)]
Deg. of freedom 252
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.388813	-2.573130	-0.542055
2	7	0	1.476124	-2.529738	-0.248917
3	7	0	2.681490	0.025855	0.032928
4	7	0	-2.735069	0.072931	0.071501
5	6	0	-2.458856	2.527179	0.413449
6	6	0	3.051072	1.350619	-0.017316
7	6	0	-1.160757	2.753718	-0.146359
8	6	0	3.797288	-2.164708	0.455045
9	6	0	-0.570481	-3.569227	-1.024104
10	6	0	4.784047	0.144577	0.831536
11	6	0	2.338198	2.479505	-0.512819
12	6	0	-0.862561	4.020896	-0.812473
13	6	0	4.383058	1.415220	0.494415
14	6	0	0.444957	3.972518	-1.148744
15	6	0	2.751884	-2.979926	-0.003240
16	6	0	3.732952	-0.751497	0.488176
17	6	0	0.823767	-3.583214	-0.774376
18	6	0	-1.399941	-4.520778	-1.652340
19	6	0	-3.104224	1.302685	0.600897
20	6	0	0.956093	2.703220	-0.626602
21	6	0	2.885857	-4.374229	-0.397050
22	6	0	-4.770148	-0.195927	1.006563

23	6	0	-4.369976	1.089769	1.243159
24	6	0	-2.718847	-2.893627	-0.762338
25	6	0	1.678872	-4.744263	-0.909615
26	6	0	-3.827940	-2.161821	-0.270833
27	6	0	-2.715022	-4.106268	-1.498729
28	6	0	-3.765154	-0.854931	0.227154
29	1	0	5.728840	-0.149476	1.263077
30	1	0	-1.576234	4.805586	-1.021107
31	1	0	4.945642	2.328442	0.613923
32	1	0	1.017621	4.716163	-1.682781
33	1	0	-1.050673	-5.401661	-2.173044
34	1	0	3.785638	-4.969106	-0.325114
35	1	0	-5.668026	-0.677693	1.364533
36	1	0	-4.890450	1.837633	1.821945
37	1	0	1.390830	-5.709491	-1.306293
38	1	0	-3.601193	-4.593186	-1.878566
39	7	0	-0.072684	1.944209	-0.098494
40	1	0	-1.046119	-1.891495	0.122774
41	6	0	-3.226330	3.752529	0.800047
42	6	0	-2.671757	4.675144	1.704833
43	6	0	-4.497918	4.029377	0.267760
44	6	0	-3.368562	5.824904	2.074754
45	1	0	-1.690600	4.474892	2.125122
46	6	0	-5.193590	5.182078	0.633002
47	1	0	-4.932841	3.340516	-0.450685
48	6	0	-4.632664	6.082854	1.540389
49	1	0	-2.924246	6.519058	2.783393
50	1	0	-6.171399	5.380257	0.201469
51	1	0	-5.174713	6.980506	1.825934
52	6	0	3.242649	3.625153	-0.878543
53	6	0	4.141545	3.502281	-1.950298
54	6	0	3.230361	4.826534	-0.151995
55	6	0	4.988713	4.554593	-2.297975
56	1	0	4.165078	2.576014	-2.517568
57	6	0	4.086679	5.875260	-0.490295
58	1	0	2.547362	4.930362	0.685995
59	6	0	4.965728	5.744204	-1.567022
60	1	0	5.667673	4.444280	-3.139541
61	1	0	4.067144	6.794540	0.089343
62	1	0	5.629570	6.562409	-1.833493
63	6	0	5.078673	-2.818946	0.855599
64	6	0	6.286601	-2.546062	0.191438
65	6	0	5.090597	-3.752827	1.905314
66	6	0	7.468884	-3.182424	0.569207
67	1	0	6.289791	-1.843566	-0.636706
68	6	0	6.273944	-4.385843	2.285826
69	1	0	4.163754	-3.970843	2.427836
70	6	0	7.467416	-4.102619	1.619389
71	1	0	8.390961	-2.963903	0.036858
72	1	0	6.262872	-5.099082	3.105848
73	1	0	8.389232	-4.596852	1.914353
74	6	0	-5.153233	-2.846270	-0.268085
75	6	0	-5.315677	-4.106044	0.335848
76	6	0	-6.273653	-2.250611	-0.873892
77	6	0	-6.555129	-4.744266	0.337572
78	1	0	-4.463265	-4.575824	0.817351
79	6	0	-7.513240	-2.889566	-0.872731
80	1	0	-6.161522	-1.285807	-1.359696
81	6	0	-7.659043	-4.138764	-0.266822
82	1	0	-6.660117	-5.713158	0.818702
83	1	0	-8.363974	-2.413743	-1.353482
84	1	0	-8.624701	-4.637148	-0.266173
85	1	0	-1.956455	-0.012765	-0.568959
86	1	0	1.796400	-0.387692	-0.250657

N_0SAPPh8 (Energy = −2122.69118107)



Stoichiometry C48H33N5
Framework group C1[X(C48H33N5)]
Deg. of freedom 252
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.327013	-2.542977	-0.521158
2	7	0	1.640786	-2.487866	-0.218027
3	7	0	2.653714	0.025773	-0.037058
4	7	0	-2.759949	0.036687	0.133879
5	6	0	-2.552177	2.471312	0.568873
6	6	0	2.951889	1.338481	-0.056654
7	6	0	-1.274432	2.710440	-0.049177
8	6	0	3.930457	-1.999319	0.529559
9	6	0	-0.463584	-3.507930	-1.006772
10	6	0	4.759285	0.369566	0.902010
11	6	0	2.188599	2.429559	-0.613801
12	6	0	-1.028047	3.952098	-0.783081
13	6	0	4.270422	1.579285	0.525273
14	6	0	0.251237	3.883849	-1.211098
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24	6	0	-2.639297	-2.880941	-0.830069
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27	6	0	-2.571751	-4.047120	-1.622172
28	6	0	-3.770994	-0.920627	0.221167
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31	1	0	4.730279	2.548377	0.657882
32	1	0	0.779603	4.599887	-1.822598
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34	1	0	3.873546	-4.898400	-0.047008
35	1	0	-5.697732	-0.842276	1.336078
36	1	0	-4.985313	1.659529	1.938573
37	1	0	1.472578	-5.676109	-0.988185
38	1	0	-3.424794	-4.529322	-2.076378
39	7	0	-0.192633	1.907958	-0.031759
40	1	0	-1.080416	-1.911027	0.230028
41	6	0	-3.299119	3.682051	1.021526
42	6	0	-2.679626	4.603115	1.886068
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50	1	0	-6.289674	5.299327	0.667797
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56	1	0	3.973482	2.288167	-2.633755
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76	6	0	-6.218404	-2.328266	-0.982906
77	6	0	-6.441198	-4.897578	0.071572
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81	6	0	-7.554653	-4.289450	-0.512781
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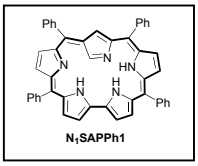
Cartesian coordinates for the optimized structures of N-confused *meso*-tetraphenyl-sapphyrins (neutral)

N_1SAPPh1 (Energy = −2122.71279475)

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 Stoichiometry    C48H33N5
 Framework group  C1[X(C48H33N5)]
 Deg. of freedom   252
 Full point group                 C1
 Largest Abelian subgroup         C1      NOp   1
 Largest concise Abelian subgroup C1      NOp   1
                       Standard orientation:
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 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
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    9          6             0        3.363281    1.344897   -0.257701
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   14          6             0        2.910925   -2.894486    0.110241
   15          6             0        2.813363   -4.318560    0.100462
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   21          6             0       -2.908445   -2.847463   -0.168546
   22          6             0       -4.101881   -2.086522   -0.084292
   23          6             0       -4.156949   -0.680006   -0.039859
   24          6             0       -5.255573    0.172515    0.313777
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   26          6             0       -3.432760    1.481248   -0.063402
   27          6             0       -2.501117    2.528734   -0.188117
   28          1             0        0.020972    4.004995    0.148485
   29          1             0        1.058579    0.214975   -1.695653
   30          1             0        5.403743    2.325134   -0.312617
   31          1             0        6.297429   -0.185626   -0.028593
   32          1             0        3.656936   -4.991497    0.134763
   33          1             0        1.077803   -5.657983   -0.005129
   34          1             0       -1.090099   -5.604317   -0.542777
   35          1             0       -3.657095   -4.890975   -0.599450
   36          1             0       -6.241234   -0.177291    0.584277
   37          1             0       -5.399190    2.358295    0.526511
   38          7             0       -1.592655   -2.398612   -0.033647
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   40          1             0       -1.342225   -1.469217    0.273212
   41          1             0        1.455233   -1.405725   -0.009556
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   44          6             0       -2.612324    4.982614   -0.688295
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   46          6             0       -2.977367    6.286580   -0.358954
   47          1             0       -2.113556    4.778249   -1.630774
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63	1	0	4.853817	5.671764	1.994597
64	1	0	4.203544	7.479061	0.412597
65	6	0	-5.394573	-2.827746	-0.015177
66	6	0	-6.421873	-2.563976	-0.938046
67	6	0	-5.628778	-3.793716	0.979687
68	6	0	-7.639367	-3.241161	-0.868988
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71	1	0	-4.852293	-3.999311	1.710840
72	6	0	-7.855454	-4.199300	0.123107
73	1	0	-8.416745	-3.024956	-1.597212
74	1	0	-7.005872	-5.210421	1.829061
75	1	0	-8.803324	-4.728074	0.176384
76	6	0	5.383593	-2.837475	0.203838
77	6	0	6.316255	-2.807750	-0.846402
78	6	0	5.706916	-3.562205	1.362926
79	6	0	7.533633	-3.480442	-0.739761
80	1	0	6.075170	-2.260543	-1.753203
81	6	0	6.924596	-4.234886	1.469669
82	1	0	5.000298	-3.583498	2.187915
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84	1	0	8.239194	-3.449613	-1.565974
85	1	0	7.158111	-4.784122	2.378098
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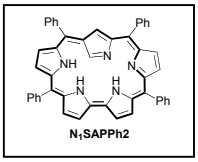
N_1SAPPh2 (Energy = −2122.69832692)



Stoichiometry C48H33N5
Framework group C1[X(C48H33N5)]
Deg. of freedom 252
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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9	6	0	3.607910	1.191953	-0.370011
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11	6	0	5.234995	-0.392732	-0.564181
12	6	0	4.034662	-1.053446	-0.131045

13	6	0	3.816213	-2.408666	0.135958
14	6	0	2.543500	-3.013491	0.364418
15	6	0	2.319053	-4.296926	0.914539
16	6	0	0.956764	-4.538067	0.941366
17	6	0	0.289617	-3.412054	0.416915
18	6	0	-1.122951	-3.319726	0.261544
19	6	0	-1.987731	-4.447657	0.366086
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21	6	0	-3.255038	-2.609801	-0.018939
22	6	0	-4.355059	-1.729680	-0.135006
23	6	0	-4.215626	-0.326215	-0.134629
24	6	0	-5.261258	0.670363	-0.312871
25	6	0	-4.641687	1.881506	-0.232105
26	6	0	-3.222239	1.605430	-0.048912
27	6	0	-2.178712	2.579493	-0.008364
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29	1	0	1.239391	0.334047	-1.843311
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31	1	0	6.158216	-0.903187	-0.797314
32	1	0	3.099028	-4.947434	1.280605
33	1	0	0.467404	-5.413678	1.342590
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35	1	0	-4.178769	-4.618048	0.221776
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37	1	0	-5.086082	2.861397	-0.344242
38	7	0	-1.917344	-2.229540	0.013095
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41	1	0	1.107120	-1.677010	-0.485008
42	1	0	2.235511	-0.143166	0.503012
43	6	0	5.012622	-3.298077	0.205198
44	6	0	6.082175	-3.004290	1.068970
45	6	0	5.107406	-4.447047	-0.600417
46	6	0	7.208600	-3.825672	1.121575
47	1	0	6.018153	-2.130694	1.711213
48	6	0	6.231990	-5.269036	-0.546603
49	1	0	4.294285	-4.685357	-1.279842
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63	1	0	6.042683	5.367668	1.071310
64	1	0	5.071918	7.234694	-0.258529
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67	6	0	-3.347091	4.190579	1.523649
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80	1	0	-5.260554	-3.485545	-2.003312
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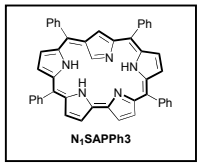
N_1SAPPh3 (Energy = −2122.71064662)



Stoichiometry C48H33N5
Framework group C1[X(C48H33N5)]
Deg. of freedom 252
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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25	6	0	-4.630771	1.850481	0.023216
26	6	0	-3.217124	1.678833	-0.079453
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30	1	0	5.660026	1.691350	-0.908560
31	1	0	6.128569	-0.923533	-0.653947
32	1	0	3.091003	-5.094892	0.979393
33	1	0	0.470797	-5.634899	0.923268
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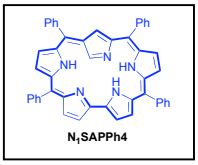
39	7	0	1.220102	-2.555095	0.070349
40	1	0	1.002875	-1.675757	-0.378434

41	1	0	2.171016	-0.145610	0.520292
42	1	0	-2.092680	-0.116650	-0.334185
43	6	0	4.972896	-3.304154	0.212792
44	6	0	5.959667	-3.087087	1.188841
45	6	0	5.163949	-4.350734	-0.705763
46	6	0	7.100361	-3.888825	1.245083
47	1	0	5.821086	-2.288701	1.912397
48	6	0	6.303667	-5.152150	-0.650162
49	1	0	4.414388	-4.525817	-1.472120
50	6	0	7.276327	-4.924414	0.325973
51	1	0	7.848424	-3.707209	2.012408
52	1	0	6.435120	-5.951533	-1.374761
53	1	0	8.164195	-5.549500	0.369574
54	6	0	-5.662130	-2.350653	-0.203153
55	6	0	-6.512267	-2.107081	-1.294728
56	6	0	-6.149436	-3.124030	0.863317
57	6	0	-7.805611	-2.629057	-1.323401
58	1	0	-6.146737	-1.514804	-2.128848
59	6	0	-7.443633	-3.644315	0.835478
60	1	0	-5.508116	-3.305435	1.720832
61	6	0	-8.275819	-3.399835	-0.258407
62	1	0	-8.444479	-2.436716	-2.181433
63	1	0	-7.803395	-4.236364	1.673016
64	1	0	-9.283791	-3.805481	-0.280172
65	6	0	-2.523234	4.033293	0.400171
66	6	0	-2.090784	5.149915	-0.338749
67	6	0	-3.265816	4.258583	1.573626
68	6	0	-2.397673	6.444176	0.076402
69	1	0	-1.526319	4.990180	-1.252158
70	6	0	-3.567718	5.554278	1.990427
71	1	0	-3.587353	3.409321	2.168696
72	6	0	-3.137225	6.651991	1.242771
73	1	0	-2.063361	7.292223	-0.515457
74	1	0	-4.134249	5.706044	2.905443
75	1	0	-3.374729	7.661596	1.567198
76	6	0	3.455104	3.678221	-0.324434
77	6	0	2.968459	4.752056	-1.096804
78	6	0	4.565669	3.915851	0.509500
79	6	0	3.578275	6.002462	-1.049917
80	1	0	2.114385	4.588331	-1.746344
81	6	0	5.175498	5.168354	0.553946
82	1	0	4.931798	3.115833	1.145607
83	6	0	4.686791	6.217534	-0.226370
84	1	0	3.190901	6.811939	-1.663249
85	1	0	6.026295	5.328124	1.211305
86	1	0	5.159766	7.195134	-0.188576

N_1SAPPh4 (Energy = −2122.71742510)



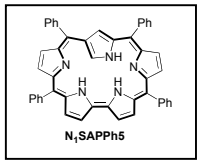
Stoichiometry C48H33N5
Framework group C1[X(C48H33N5)]
Deg. of freedom 252
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.807962	1.064710	-1.179717
2	7	0	2.993207	0.065065	-0.059962
3	7	0	-3.078875	0.152849	-0.254120

4	6	0	-1.177873	2.292887	-0.575552
5	6	0	-0.028647	3.056602	-0.304905
6	6	0	0.497470	1.048202	-1.214751
7	6	0	1.082223	2.252150	-0.637948
8	6	0	2.462397	2.469699	-0.386176
9	6	0	3.357879	1.389332	-0.242540
10	6	0	4.787834	1.394269	-0.296754
11	6	0	5.235215	0.099872	-0.167004
12	6	0	4.095404	-0.749642	-0.011057
13	6	0	4.039450	-2.155186	0.122767
14	6	0	2.843091	-2.901433	0.131065
15	6	0	2.796103	-4.352971	0.232359
16	6	0	1.489624	-4.702650	0.129032
17	6	0	0.742223	-3.459601	0.001429
18	6	0	-0.673394	-3.480491	-0.105732
19	6	0	-1.466069	-4.641978	-0.305262
20	6	0	-2.789889	-4.268012	-0.346822
21	6	0	-2.873981	-2.857468	-0.156902
22	6	0	-4.069182	-2.098226	-0.082454
23	6	0	-4.140323	-0.692508	-0.048338
24	6	0	-5.253213	0.147059	0.293855
25	6	0	-4.831186	1.457304	0.277717
26	6	0	-3.443580	1.477236	-0.071791
27	6	0	-2.524741	2.537429	-0.188525
28	1	0	0.000061	4.015447	0.192197
29	1	0	1.027986	0.232070	-1.692238
30	1	0	5.387682	2.276023	-0.469132
31	1	0	6.258621	-0.243699	-0.200885
32	1	0	3.646055	-5.006720	0.364746
33	1	0	1.072096	-5.699335	0.171869
34	1	0	-1.076071	-5.640357	-0.438057
35	1	0	-3.640970	-4.910084	-0.516102
36	1	0	-6.236521	-0.214635	0.557009
37	1	0	-5.426655	2.330928	0.499859
38	7	0	-1.555166	-2.417244	-0.043300
39	7	0	1.567433	-2.384389	0.015224
40	1	0	2.062249	-0.333249	0.049530
41	1	0	-2.214748	-0.020881	-0.780294
42	6	0	5.350185	-2.868000	0.220314
43	6	0	6.206655	-2.643067	1.310668
44	6	0	5.766240	-3.761450	-0.780713
45	6	0	7.436816	-3.295193	1.401333
46	1	0	5.895139	-1.959730	2.095761
47	6	0	6.996208	-4.413651	-0.690548
48	1	0	5.121004	-3.933679	-1.637369
49	6	0	7.835794	-4.183385	0.400936
50	1	0	8.081086	-3.112420	2.257462
51	1	0	7.301096	-5.097797	-1.478226
52	1	0	8.793886	-4.691519	0.470730
53	6	0	-5.360003	-2.844662	-0.004741
54	6	0	-6.376468	-2.615485	-0.948057
55	6	0	-5.601597	-3.777674	1.018902
56	6	0	-7.591733	-3.296154	-0.871843
57	1	0	-6.201565	-1.905864	-1.751684
58	6	0	-6.815739	-4.459289	1.094352
59	1	0	-4.832282	-3.956263	1.764550
60	6	0	-7.815832	-4.221516	0.149077
61	1	0	-8.361034	-3.107878	-1.616209
62	1	0	-6.983494	-5.171241	1.898344
63	1	0	-8.762018	-4.752691	0.208312
64	6	0	-2.933070	3.914664	0.185383
65	6	0	-2.643243	4.993784	-0.669640
66	6	0	-3.599556	4.185681	1.394063
67	6	0	-3.020621	6.292885	-0.335534
68	1	0	-2.129788	4.799869	-1.606460

69	6	0	-3.975429	5.486382	1.728077
70	1	0	-3.798049	3.371672	2.084695
71	6	0	-3.690515	6.544939	0.863805
72	1	0	-2.795250	7.109991	-1.015920
73	1	0	-4.481997	5.673730	2.671317
74	1	0	-3.983241	7.558422	1.124771
75	6	0	2.967158	3.852077	-0.208656
76	6	0	2.550302	4.876189	-1.080770
77	6	0	3.857444	4.186048	0.829327
78	6	0	3.020281	6.178353	-0.931135
79	1	0	1.864400	4.634231	-1.886574
80	6	0	4.322616	5.491519	0.981124
81	1	0	4.163438	3.418032	1.532875
82	6	0	3.909305	6.492312	0.100275
83	1	0	2.695364	6.950153	-1.623964
84	1	0	5.001723	5.728492	1.795952
85	1	0	4.272324	7.509706	0.218759
86	1	0	-1.263179	-1.480723	0.197222

N_1SAPPh5 (Energy = −2122.71135401)

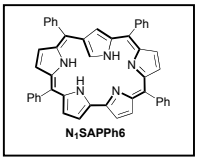


Stoichiometry C48H33N5
Framework group C1[X(C48H33N5)]
Deg. of freedom 252
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.670234	-2.355143	0.026213
2	7	0	-1.558254	-2.403732	0.122585
3	7	0	-2.977742	0.013336	-0.164790
4	7	0	2.991547	0.127809	-0.155694
5	6	0	2.464628	2.521247	-0.067711
6	6	0	-3.424927	1.314946	-0.285431
7	6	0	-4.040499	-2.172906	0.102579
8	6	0	0.775306	-3.411929	0.042907
9	6	0	-5.292784	0.052300	-0.139815
10	6	0	-2.574454	2.416414	-0.423903
11	6	0	-4.882570	1.340875	-0.267473
12	6	0	-2.851960	-2.913429	0.169082
13	6	0	-4.081004	-0.760563	-0.076818
14	6	0	-0.630947	-3.430556	0.121530
15	6	0	1.566309	-4.598221	-0.083827
16	6	0	3.370164	1.450110	-0.015375
17	6	0	-2.718311	-4.338210	0.222066
18	6	0	5.284015	0.255250	0.091728
19	6	0	4.812336	1.531442	0.142748
20	6	0	2.977807	-2.818348	-0.082366
21	6	0	-1.386488	-4.646555	0.190798
22	6	0	4.141858	-2.031220	-0.102707
23	6	0	2.885987	-4.243595	-0.168059
24	6	0	4.125704	-0.609501	-0.085366
25	1	0	-1.428915	-1.393731	0.068346
26	1	0	-6.308303	-0.314634	-0.086684
27	1	0	-5.500272	2.221168	-0.379187
28	1	0	1.169568	-5.601114	-0.137519
29	1	0	-3.546567	-5.029731	0.257539
30	1	0	6.310432	-0.071485	0.183655
31	1	0	5.387090	2.441391	0.245794

32	1	0	-0.957834	-5.637304	0.216057
33	1	0	3.729899	-4.904391	-0.296754
34	1	0	1.501692	-1.361208	0.158256
35	6	0	-0.596689	1.080985	-1.269012
36	6	0	1.106752	2.308067	-0.462613
37	6	0	-1.165148	2.215922	-0.644443
38	1	0	1.426378	0.432861	-1.352696
39	1	0	-1.090998	0.276008	-1.789102
40	1	0	-0.142018	3.925867	0.365787
41	7	0	0.732974	1.156503	-1.162646
42	6	0	-0.073391	3.001752	-0.188472
43	6	0	2.868307	3.889189	0.330233
44	6	0	2.492141	5.003608	-0.444059
45	6	0	3.622100	4.116952	1.497176
46	6	0	2.871647	6.292242	-0.075950
47	1	0	1.912174	4.847156	-1.348466
48	6	0	3.999059	5.407523	1.865214
49	1	0	3.889379	3.273645	2.126097
50	6	0	3.628234	6.500481	1.079748
51	1	0	2.579776	7.136148	-0.695595
52	1	0	4.574224	5.559828	2.774757
53	1	0	3.920925	7.506419	1.368360
54	6	0	-3.075294	3.799660	-0.264819
55	6	0	-2.642548	4.817511	-1.137722
56	6	0	-3.972717	4.147279	0.763312
57	6	0	-3.110738	6.122036	-1.005868
58	1	0	-1.946666	4.568819	-1.933361
59	6	0	-4.435657	5.455420	0.897902
60	1	0	-4.283367	3.386975	1.472741
61	6	0	-4.011075	6.447315	0.012346
62	1	0	-2.774584	6.887295	-1.700711
63	1	0	-5.121135	5.701891	1.704562
64	1	0	-4.371567	7.466963	0.118686
65	6	0	5.459123	-2.731622	-0.124112
66	6	0	6.372799	-2.505686	-1.168382
67	6	0	5.828881	-3.622837	0.898325
68	6	0	7.609946	-3.149394	-1.191193
69	1	0	6.099726	-1.826002	-1.970615
70	6	0	7.064891	-4.269061	0.874716
71	1	0	5.143616	-3.794497	1.723655
72	6	0	7.960584	-4.035126	-0.170311
73	1	0	8.298057	-2.963178	-2.011782
74	1	0	7.331636	-4.949295	1.679542
75	1	0	8.924169	-4.537301	-0.188198
76	6	0	-5.327588	-2.924253	0.204986
77	6	0	-6.237572	-2.946204	-0.865578
78	6	0	-5.662294	-3.625283	1.375714
79	6	0	-7.441883	-3.643381	-0.767789
80	1	0	-5.988833	-2.418471	-1.782047
81	6	0	-6.865264	-4.325486	1.473147
82	1	0	-4.975284	-3.606640	2.217272
83	6	0	-7.760156	-4.336450	0.401842
84	1	0	-8.129185	-3.650700	-1.609893
85	1	0	-7.106138	-4.856347	2.390609
86	1	0	-8.698099	-4.880076	0.477672

N_1SAPPh6 (Energy = −2122.69176454)



Stoichiometry C48H33N5
Framework group C1[X(C48H33N5)]
Deg. of freedom 252
Full point group C1
Largest Abelian subgroup C1 NOp 1

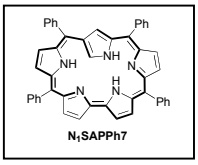
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.632148	-2.363562	-0.116728
2	7	0	-1.405192	-2.543589	0.061864
3	7	0	-2.994504	0.040773	0.009672
4	7	0	3.013124	0.234296	-0.191110
5	6	0	2.437299	2.566779	0.109173
6	6	0	-3.458775	1.331505	-0.304814
7	6	0	-3.921311	-2.251469	0.228455
8	6	0	0.919213	-3.490784	-0.029938
9	6	0	-5.213202	-0.131746	-0.357938
10	6	0	-2.625901	2.432441	-0.448760
11	6	0	-4.870693	1.179840	-0.537939
12	6	0	-2.695968	-2.991429	0.324264
13	6	0	-4.039064	-0.881529	0.012457
14	6	0	-0.494120	-3.579199	0.171773
15	6	0	1.752800	-4.687524	-0.143877
16	6	0	3.384860	1.528490	0.090502
17	6	0	-2.564792	-4.358655	0.664224
18	6	0	5.271133	0.299438	0.201423
19	6	0	4.817286	1.579130	0.335048
20	6	0	2.956077	-2.771333	-0.247050
21	6	0	-1.227401	-4.717451	0.553536
22	6	0	4.096192	-1.960853	-0.238505
23	6	0	3.018790	-4.237597	-0.305616
24	6	0	4.107158	-0.526647	-0.116524
25	1	0	-1.150237	-1.645884	-0.320892
26	1	0	-6.185249	-0.574177	-0.521767
27	1	0	-5.516350	1.974016	-0.885114
28	1	0	1.408406	-5.713520	-0.135358
29	1	0	-3.382992	-4.993957	0.967878
30	1	0	6.285099	-0.053189	0.329786
31	1	0	5.398564	2.462976	0.559239
32	1	0	-0.799820	-5.687422	0.764208
33	1	0	3.912397	-4.827268	-0.450011
34	6	0	-0.583909	1.064493	-1.077320
35	6	0	1.082602	2.321141	-0.284691
36	6	0	-1.186968	2.220340	-0.522295
37	1	0	1.450615	0.376024	-0.954069
38	1	0	-1.045105	0.246241	-1.610421
39	1	0	-0.202056	3.975266	0.442441
40	7	0	0.738540	1.138485	-0.932286
41	6	0	-0.115546	3.020705	-0.055605
42	6	0	2.800890	3.926370	0.571036
43	6	0	2.416029	5.061380	-0.166838
44	6	0	3.530845	4.118538	1.758447
45	6	0	2.764088	6.341410	0.259170
46	1	0	1.859065	4.928966	-1.089269
47	6	0	3.872356	5.400579	2.185980
48	1	0	3.806562	3.254848	2.355073
49	6	0	3.493507	6.516458	1.437274
50	1	0	2.468243	7.203907	-0.332148
51	1	0	4.428485	5.527784	3.110959
52	1	0	3.761021	7.515337	1.771212
53	6	0	-3.177386	3.800500	-0.512013
54	6	0	-2.608930	4.762070	-1.371977
55	6	0	-4.273065	4.194311	0.281565
56	6	0	-3.130412	6.050147	-1.453037
57	1	0	-1.761108	4.481841	-1.989644
58	6	0	-4.794843	5.484171	0.197758
59	1	0	-4.696151	3.487292	0.988538

60	6	0	-4.228882	6.418410	-0.671253
61	1	0	-2.681061	6.769226	-2.133195
62	1	0	-5.636653	5.763962	0.825968
63	1	0	-4.632449	7.425427	-0.732512
64	6	0	5.442164	-2.614427	-0.293693
65	6	0	6.309936	-2.352452	-1.367109
66	6	0	5.884491	-3.472096	0.726792
67	6	0	7.571963	-2.943389	-1.427752
68	1	0	5.982705	-1.688049	-2.162015
69	6	0	7.149294	-4.058912	0.669564
70	1	0	5.232329	-3.667010	1.573155
71	6	0	7.996305	-3.799082	-0.409092
72	1	0	8.223546	-2.735870	-2.272646
73	1	0	7.474115	-4.715924	1.472283
74	1	0	8.980825	-4.257130	-0.454225
75	6	0	-5.192712	-3.030963	0.337689
76	6	0	-5.487104	-4.069865	-0.562476
77	6	0	-6.135823	-2.727876	1.333808
78	6	0	-6.684335	-4.778422	-0.470352
79	1	0	-4.772379	-4.311444	-1.343769
80	6	0	-7.335280	-3.435341	1.425393
81	1	0	-5.916661	-1.936260	2.044770
82	6	0	-7.613640	-4.463672	0.524004
83	1	0	-6.895185	-5.573013	-1.181400
84	1	0	-8.048480	-3.186677	2.207006
85	1	0	-8.546467	-5.016565	0.595473
86	1	0	-2.183662	-0.070190	0.603349

N_1SAPPh7 (Energy = −2122.71461042)

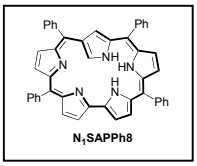


Stoichiometry C48H33N5
Framework group C1[X(C48H33N5)]
Deg. of freedom 252
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.643791	-2.360495	-0.035823
2	7	0	-1.511570	-2.363057	0.065639
3	7	0	-3.019694	0.023354	-0.161223
4	7	0	2.987691	0.145587	-0.137576
5	6	0	2.464004	2.533298	0.000120
6	6	0	-3.425401	1.345299	-0.314091
7	6	0	-3.997817	-2.204536	0.136165
8	6	0	0.758945	-3.418392	-0.066188
9	6	0	-5.270411	0.011168	-0.132962
10	6	0	-2.573128	2.433764	-0.472151
11	6	0	-4.867395	1.306429	-0.302754
12	6	0	-2.764657	-2.914088	0.154117
13	6	0	-4.097271	-0.819399	-0.042800
14	6	0	-0.650353	-3.423927	0.027592
15	6	0	1.559175	-4.595886	-0.240560
16	6	0	3.368142	1.461191	0.050342
17	6	0	-2.690214	-4.366353	0.185116
18	6	0	5.271764	0.252765	0.173297
19	6	0	4.805931	1.530236	0.249877
20	6	0	2.956521	-2.805269	-0.154143
21	6	0	-1.374467	-4.684071	0.095658
22	6	0	4.120250	-2.021581	-0.128865

23	6	0	2.875397	-4.229470	-0.303159
24	6	0	4.113166	-0.598584	-0.061144
25	1	0	-6.285345	-0.355285	-0.085633
26	1	0	-5.499514	2.170583	-0.445767
27	1	0	1.167385	-5.597170	-0.337822
28	1	0	-3.531124	-5.042330	0.242354
29	1	0	6.293491	-0.082849	0.283570
30	1	0	5.382828	2.433056	0.395013
31	1	0	-0.942733	-5.675129	0.090974
32	1	0	3.725921	-4.876409	-0.456874
33	6	0	-0.563564	1.106826	-1.294441
34	6	0	1.115177	2.324489	-0.433070
35	6	0	-1.153044	2.222647	-0.655762
36	1	0	1.461427	0.461737	-1.329328
37	1	0	-1.023634	0.300587	-1.847101
38	1	0	-0.161237	3.914965	0.411797
39	7	0	0.765027	1.190735	-1.164788
40	6	0	-0.075254	3.002391	-0.159020
41	6	0	2.854288	3.891836	0.438642
42	6	0	2.487348	5.022882	-0.315954
43	6	0	3.586281	4.094029	1.624126
44	6	0	2.856100	6.303528	0.088810
45	1	0	1.924215	4.885760	-1.233990
46	6	0	3.951818	5.376746	2.028941
47	1	0	3.844459	3.237038	2.238085
48	6	0	3.591313	6.486569	1.262457
49	1	0	2.572488	7.160938	-0.515878
50	1	0	4.509845	5.509671	2.952050
51	1	0	3.875405	7.486309	1.579720
52	6	0	-3.084845	3.817731	-0.370178
53	6	0	-2.624465	4.809200	-1.259711
54	6	0	-4.019788	4.196521	0.612707
55	6	0	-3.100944	6.115125	-1.187476
56	1	0	-1.898268	4.538579	-2.020342
57	6	0	-4.494929	5.505384	0.684559
58	1	0	-4.350377	3.462020	1.340466
59	6	0	-4.041697	6.469973	-0.216625
60	1	0	-2.740617	6.858573	-1.893824
61	1	0	-5.210544	5.774520	1.457130
62	1	0	-4.410038	7.490596	-0.158141
63	6	0	5.437242	-2.722814	-0.156455
64	6	0	6.368238	-2.455515	-1.175328
65	6	0	5.788763	-3.654397	0.835852
66	6	0	7.604878	-3.099820	-1.203448
67	1	0	6.109102	-1.743833	-1.954045
68	6	0	7.024956	-4.300088	0.807340
69	1	0	5.088875	-3.858553	1.641155
70	6	0	7.937798	-4.025740	-0.212666
71	1	0	8.306589	-2.882378	-2.004567
72	1	0	7.277863	-5.012296	1.588559
73	1	0	8.901271	-4.527961	-0.234554
74	6	0	-5.273328	-2.970124	0.292450
75	6	0	-6.209404	-3.039672	-0.752268
76	6	0	-5.568889	-3.632914	1.495241
77	6	0	-7.404938	-3.743183	-0.598290
78	1	0	-5.987768	-2.546416	-1.694785
79	6	0	-6.761616	-4.340027	1.648788
80	1	0	-4.856783	-3.583478	2.314309
81	6	0	-7.685279	-4.396171	0.603094
82	1	0	-8.113386	-3.787489	-1.421557
83	1	0	-6.971923	-4.842583	2.589424
84	1	0	-8.615050	-4.945856	0.723240
85	1	0	-2.078501	-0.342434	-0.026215
86	1	0	1.432600	-1.383383	0.134278

N_1SAPPh8 (Energy = −2122.67727262)

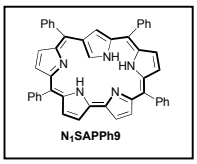


Stoichiometry C48H33N5
Framework group C1[X(C48H33N5)]
Deg. of freedom 252
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.390723	-2.616405	0.012643
2	7	0	-1.572758	-2.480543	-0.045119
3	7	0	-2.932457	0.176806	-0.112056
4	7	0	2.951183	0.046572	-0.223564
5	6	0	2.586445	2.483752	-0.437163
6	6	0	-3.343269	1.487708	0.029951
7	6	0	-4.025159	-2.024321	-0.000204
8	6	0	0.545116	-3.680243	-0.260077
9	6	0	-5.199743	0.249600	0.323819
10	6	0	-2.454657	2.551220	-0.125191
11	6	0	-4.773826	1.539867	0.313225
12	6	0	-2.909605	-2.855099	-0.104186
13	6	0	-4.017038	-0.580151	0.055157
14	6	0	-0.881311	-3.601593	-0.249171
15	6	0	1.359279	-4.787012	-0.538357
16	6	0	3.394948	1.373084	-0.244321
17	6	0	-3.008971	-4.300176	-0.358521
18	6	0	5.162806	-0.015389	0.170554
19	6	0	4.816521	1.290914	-0.013541
20	6	0	2.719607	-3.027177	-0.046376
21	6	0	-1.741890	-4.764977	-0.459987
22	6	0	3.903816	-2.228560	0.116037
23	6	0	2.688330	-4.391948	-0.404349
24	6	0	3.986919	-0.844478	0.035177
25	1	0	-6.202791	-0.107862	0.511214
26	1	0	-5.370668	2.432299	0.442448
27	1	0	1.002271	-5.764047	-0.832378
28	1	0	-3.926086	-4.858861	-0.477677
29	1	0	6.150777	-0.399349	0.376503
30	1	0	5.478907	2.143976	-0.004301
31	1	0	-1.419292	-5.779696	-0.655188
32	1	0	3.565776	-4.994650	-0.586022
33	6	0	-0.695876	1.232840	-1.388106
34	6	0	1.174780	2.333636	-0.723829
35	6	0	-1.108605	2.311108	-0.593485
36	1	0	1.199493	0.691801	-2.097745
37	1	0	-1.286816	0.477737	-1.879543
38	1	0	0.132548	3.866642	0.441782
39	7	0	0.655609	1.247381	-1.451279
40	6	0	0.079546	3.016818	-0.223040
41	6	0	3.102029	3.857259	-0.230373
42	6	0	2.756311	4.886090	-1.128133
43	6	0	3.919994	4.188797	0.866610
44	6	0	3.232454	6.182885	-0.953054
45	1	0	2.115287	4.654213	-1.973567
46	6	0	4.398479	5.487035	1.039497
47	1	0	4.156305	3.425765	1.601890
48	6	0	4.060860	6.489950	0.129507
49	1	0	2.959354	6.956203	-1.666476
50	1	0	5.023401	5.718003	1.898391
51	1	0	4.430415	7.502476	0.267160
52	6	0	-2.834193	3.933033	0.244472

53	6	0	-2.474339	5.015019	-0.582164
54	6	0	-3.542515	4.208686	1.429503
55	6	0	-2.834602	6.318713	-0.251086
56	1	0	-1.923496	4.820202	-1.497324
57	6	0	-3.894625	5.515447	1.763514
58	1	0	-3.790288	3.391678	2.099310
59	6	0	-3.547225	6.574677	0.923132
60	1	0	-2.559358	7.137240	-0.910940
61	1	0	-4.432989	5.706821	2.687980
62	1	0	-3.822244	7.592980	1.184566
63	6	0	5.174783	-2.993033	0.315579
64	6	0	6.227040	-2.915886	-0.611844
65	6	0	5.336897	-3.823421	1.437617
66	6	0	7.409542	-3.630971	-0.415454
67	1	0	6.107404	-2.298005	-1.497402
68	6	0	6.517092	-4.539254	1.634090
69	1	0	4.529439	-3.898114	2.160415
70	6	0	7.559395	-4.443831	0.709011
71	1	0	8.209735	-3.559472	-1.147642
72	1	0	6.624548	-5.169343	2.513188
73	1	0	8.479051	-5.002337	0.861682
74	6	0	-5.373077	-2.674882	0.041704
75	6	0	-6.325023	-2.427617	-0.961768
76	6	0	-5.721541	-3.540468	1.091570
77	6	0	-7.580001	-3.034635	-0.922201
78	1	0	-6.069505	-1.762686	-1.782045
79	6	0	-6.979688	-4.142692	1.135424
80	1	0	-4.999255	-3.730648	1.880201
81	6	0	-7.912648	-3.893645	0.127730
82	1	0	-8.298068	-2.838135	-1.714244
83	1	0	-7.230766	-4.804797	1.960112
84	1	0	-8.892002	-4.363715	0.160211
85	1	0	1.029554	-1.795457	0.479241
86	1	0	1.981876	-0.207626	-0.309562

N_1SAPPh9 (Energy = −2122.70923914)



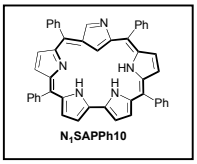
Stoichiometry C48H33N5
Framework group C1[X(C48H33N5)]
Deg. of freedom 252
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.592543	-2.323681	0.014738
2	7	0	-1.575974	-2.390210	0.039585
3	7	0	-2.988122	0.061540	-0.125194
4	7	0	3.017576	0.093022	-0.171308
5	6	0	2.499672	2.513483	-0.242198
6	6	0	-3.424321	1.371656	-0.135785
7	6	0	-4.059939	-2.129060	0.012317
8	6	0	0.747849	-3.400485	0.022345
9	6	0	-5.299852	0.119716	-0.026993
10	6	0	-2.559130	2.463364	-0.245293
11	6	0	-4.879682	1.411474	-0.064226
12	6	0	-2.878810	-2.878850	0.033445
13	6	0	-4.094636	-0.705018	-0.063296
14	6	0	-0.664873	-3.423737	0.029807
15	6	0	1.498253	-4.645515	0.016372

16	6	0	3.383875	1.437868	-0.171995
17	6	0	-2.765917	-4.309202	0.011261
18	6	0	5.270913	0.154967	-0.115737
19	6	0	4.822870	1.447770	-0.152391
20	6	0	2.857665	-2.853210	0.011991
21	6	0	-1.439631	-4.634053	0.011536
22	6	0	4.074647	-2.113146	-0.018585
23	6	0	2.812027	-4.304180	0.008528
24	6	0	4.130856	-0.720213	-0.108848
25	1	0	-6.317122	-0.241964	0.029973
26	1	0	-5.490240	2.303556	-0.087955
27	1	0	1.088382	-5.645580	0.011952
28	1	0	-3.604957	-4.987876	-0.020859
29	1	0	6.298461	-0.177922	-0.102807
30	1	0	5.423858	2.344227	-0.201855
31	1	0	-1.024840	-5.630112	-0.012335
32	1	0	3.666225	-4.965454	-0.012769
33	6	0	-0.676230	1.159492	-1.315675
34	6	0	1.111105	2.304236	-0.542629
35	6	0	-1.171863	2.246583	-0.570662
36	1	0	1.277959	0.554716	-1.767504
37	1	0	-1.216006	0.404456	-1.863848
38	1	0	-0.042932	3.852747	0.502748
39	7	0	0.666175	1.201184	-1.287848
40	6	0	-0.032707	2.978976	-0.131817
41	6	0	2.958106	3.890195	0.048079
42	6	0	2.521244	4.973686	-0.739278
43	6	0	3.827724	4.162893	1.121810
44	6	0	2.953102	6.271041	-0.476234
45	1	0	1.847729	4.785244	-1.569737
46	6	0	4.260145	5.462145	1.382629
47	1	0	4.142201	3.349182	1.767920
48	6	0	3.827589	6.522340	0.584267
49	1	0	2.610190	7.088848	-1.104745
50	1	0	4.925519	5.647502	2.221847
51	1	0	4.161768	7.535530	0.790385
52	6	0	-3.017570	3.841516	0.032304
53	6	0	-2.597087	4.911756	-0.782010
54	6	0	-3.864598	4.130511	1.119846
55	6	0	-3.028217	6.212292	-0.535255
56	1	0	-1.940597	4.708710	-1.622796
57	6	0	-4.290053	5.434358	1.369260
58	1	0	-4.164523	3.326332	1.784025
59	6	0	-3.878089	6.480022	0.541424
60	1	0	-2.702301	7.019751	-1.185751
61	1	0	-4.936138	5.634567	2.219992
62	1	0	-4.209159	7.496330	0.737345
63	6	0	5.373417	-2.849980	0.058471
64	6	0	6.284059	-2.822553	-1.010501
65	6	0	5.719498	-3.579690	1.208017
66	6	0	7.502172	-3.499350	-0.932397
67	1	0	6.024588	-2.275025	-1.912567
68	6	0	6.935119	-4.259359	1.285883
69	1	0	5.028362	-3.604051	2.045855
70	6	0	7.831907	-4.220633	0.216159
71	1	0	8.190000	-3.468939	-1.773605
72	1	0	7.184380	-4.814824	2.186376
73	1	0	8.779422	-4.749403	0.277012
74	6	0	-5.355000	-2.872177	0.064716
75	6	0	-6.267102	-2.803903	-1.002073
76	6	0	-5.697136	-3.650172	1.183371
77	6	0	-7.479547	-3.491847	-0.952319
78	1	0	-6.013554	-2.213847	-1.878370
79	6	0	-6.909045	-4.339825	1.233068
80	1	0	-5.008820	-3.700691	2.022417

81	6	0	-7.804983	-4.262979	0.165352
82	1	0	-8.168055	-3.429952	-1.791160
83	1	0	-7.155632	-4.931797	2.110712
84	1	0	-8.749596	-4.798915	0.203916
85	1	0	2.103300	-0.318591	0.023140
86	1	0	-1.400011	-1.388949	0.066880

N_1SAPPh10 (Energy = −2122.69108579)

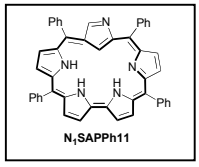


Stoichiometry C48H33N5
Framework group C1[X(C48H33N5)]
Deg. of freedom 252
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.640144	-2.475978	-0.277277
2	7	0	-1.402986	-2.502617	-0.499534
3	7	0	-2.833522	0.039564	0.114002
4	7	0	2.749355	0.042527	0.018626
5	6	0	2.368798	2.458079	-0.508856
6	6	0	-3.229582	1.264530	0.659832
7	6	0	0.970993	2.588514	-0.507895
8	6	0	-3.868489	-2.200794	-0.274356
9	6	0	0.853799	-3.531211	-0.658695
10	6	0	-4.865142	-0.274573	1.045772
11	6	0	-2.568283	2.481211	0.489701
12	6	0	0.295357	3.788163	-1.025566
13	6	0	-4.486258	1.017807	1.299194
14	6	0	-2.719363	-2.880362	-0.756492
15	6	0	-3.853582	-0.902517	0.251185
16	6	0	-0.534451	-3.493507	-0.931388
17	6	0	1.649823	-4.704319	-0.570805
18	6	0	3.152096	1.336502	-0.093499
19	6	0	-1.242581	2.626782	-0.032715
20	6	0	-2.647375	-4.092866	-1.481905
21	6	0	4.999862	0.227064	0.586229
22	6	0	4.559251	1.469811	0.259636
23	6	0	2.908112	-2.924241	0.056093
24	6	0	-1.314740	-4.470689	-1.576826
25	6	0	3.960189	-2.070063	0.435128
26	6	0	2.896344	-4.338068	-0.104904
27	6	0	3.869001	-0.661446	0.399100
28	1	0	-5.752073	-0.776931	1.403489
29	1	0	0.763330	4.567029	-1.616873
30	1	0	-5.014331	1.744760	1.898268
31	1	0	1.290501	-5.705903	-0.762212
32	1	0	-3.500825	-4.610316	-1.894441
33	1	0	5.994548	-0.065828	0.890609
34	1	0	5.120128	2.392928	0.276842
35	1	0	-0.918591	-5.338341	-2.086406
36	1	0	3.726466	-4.992155	0.116769
37	1	0	1.478041	-1.465060	-0.341773
38	7	0	-0.968550	3.832420	-0.736243
39	6	0	-0.091309	1.829966	0.070045
40	1	0	0.022198	0.912254	0.631325
41	1	0	-2.148280	0.008354	-0.631505
42	6	0	-3.308196	3.729013	0.824259
43	6	0	-4.618538	3.958149	0.369986

44	6	0	-2.697113	4.719225	1.614195
45	6	0	-5.299803	5.127749	0.706512
46	1	0	-5.093140	3.224970	-0.275093
47	6	0	-3.379271	5.883685	1.956275
48	1	0	-1.682647	4.560742	1.965956
49	6	0	-4.685016	6.092730	1.505255
50	1	0	-6.308343	5.288829	0.334344
51	1	0	-2.890565	6.631414	2.575503
52	1	0	-5.215365	7.004225	1.768286
53	6	0	-5.167398	-2.931517	-0.299197
54	6	0	-5.292523	-4.213369	0.266836
55	6	0	-6.305719	-2.354039	-0.889839
56	6	0	-6.510619	-4.890845	0.244240
57	1	0	-4.427904	-4.670340	0.738951
58	6	0	-7.524591	-3.031264	-0.911018
59	1	0	-6.223853	-1.372057	-1.346443
60	6	0	-7.632174	-4.302691	-0.344687
61	1	0	-6.585803	-5.876648	0.695771
62	1	0	-8.389005	-2.567615	-1.379064
63	1	0	-8.581465	-4.831218	-0.362325
64	6	0	5.251379	-2.703032	0.838937
65	6	0	5.743529	-2.537285	2.144012
66	6	0	5.999292	-3.474386	-0.065472
67	6	0	6.944125	-3.130342	2.534304
68	1	0	5.172624	-1.945366	2.853683
69	6	0	7.201049	-4.066063	0.325108
70	1	0	5.641304	-3.594108	-1.084037
71	6	0	7.676652	-3.897836	1.626651
72	1	0	7.305369	-2.994727	3.550338
73	1	0	7.769233	-4.653092	-0.391751
74	1	0	8.612510	-4.358910	1.930674
75	6	0	3.162787	3.653297	-0.947409
76	6	0	4.041587	3.559254	-2.040015
77	6	0	3.056927	4.885375	-0.281051
78	6	0	4.778410	4.665342	-2.462147
79	1	0	4.133741	2.612661	-2.564580
80	6	0	3.803461	5.988977	-0.695171
81	1	0	2.392918	4.969226	0.574258
82	6	0	4.663639	5.883851	-1.789479
83	1	0	5.442524	4.575017	-3.317799
84	1	0	3.712436	6.931012	-0.160823
85	1	0	5.241554	6.744664	-2.115238
86	1	0	-1.164409	-1.847396	0.233698

N_1SAPPh11 (Energy = −2122.69377701)



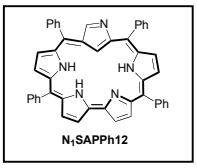
Stoichiometry C48H33N5
Framework group C1[X(C48H33N5)]
Deg. of freedom 252
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.481371	-2.449811	-0.530474
2	7	0	1.529257	-2.477688	-0.210576
3	7	0	2.725481	0.005790	-0.032991
4	7	0	-2.833302	0.102766	0.143572
5	6	0	-2.482407	2.503560	0.645806
6	6	0	3.132606	1.291041	-0.078978

7	6	0	-1.159584	2.627079	0.080725
8	6	0	3.852485	-2.109184	0.537387
9	6	0	-0.623395	-3.427389	-1.006482
10	6	0	4.872301	0.191389	0.850644
11	6	0	2.399185	2.423391	-0.598708
12	6	0	-0.774736	3.799768	-0.716345
13	6	0	4.474056	1.434342	0.465247
14	6	0	2.790963	-2.945476	0.121581
15	6	0	3.794347	-0.705514	0.487110
16	6	0	0.758350	-3.507176	-0.681981
17	6	0	-1.400516	-4.330111	-1.747506
18	6	0	-3.194789	1.316422	0.740544
19	6	0	1.015593	2.591275	-0.559505
20	6	0	2.791571	-4.339623	-0.138366
21	6	0	-4.900815	-0.173756	1.015638
22	6	0	-4.476401	1.081749	1.348523
23	6	0	-2.794608	-2.764088	-0.866110
24	6	0	1.548684	-4.681065	-0.645369
25	6	0	-3.941438	-2.071989	-0.372266
26	6	0	-2.730565	-3.920075	-1.670550
27	6	0	-3.895404	-0.804695	0.206919
28	1	0	5.800711	-0.089057	1.327416
29	1	0	-1.450088	4.598976	-1.008349
30	1	0	5.010973	2.366389	0.570601
31	1	0	-1.009262	-5.170269	-2.304741
32	1	0	3.629182	-4.999857	0.031959
33	1	0	-5.813255	-0.658804	1.331116
34	1	0	-4.986469	1.792497	1.981943
35	1	0	1.197619	-5.668751	-0.910333
36	1	0	-3.581617	-4.382911	-2.148092
37	1	0	-1.250801	-1.841638	0.244431
38	7	0	0.459659	3.769940	-1.116256
39	6	0	-0.007592	1.844816	0.124882
40	1	0	0.154942	0.935042	0.686879
41	1	0	1.394689	-1.464724	-0.299423
42	1	0	-2.142521	0.084750	-0.597449
43	6	0	3.248577	3.510544	-1.166953
44	6	0	4.248395	3.184762	-2.101490
45	6	0	3.105712	4.857016	-0.788612
46	6	0	5.064340	4.171003	-2.653934
47	1	0	4.368474	2.150256	-2.408865
48	6	0	3.933660	5.839505	-1.327240
49	1	0	2.345104	5.125489	-0.065728
50	6	0	4.912132	5.502734	-2.265365
51	1	0	5.819185	3.897533	-3.386639
52	1	0	3.812309	6.873330	-1.014326
53	1	0	5.551881	6.272869	-2.688706
54	6	0	-3.131881	3.768069	1.087751
55	6	0	-2.413521	4.679497	1.885360
56	6	0	-4.442935	4.113388	0.708599
57	6	0	-2.990913	5.875804	2.306485
58	1	0	-1.399988	4.430896	2.185693
59	6	0	-5.019820	5.310904	1.129541
60	1	0	-4.999363	3.447663	0.055827
61	6	0	-4.298020	6.195732	1.933140
62	1	0	-2.419375	6.558492	2.929807
63	1	0	-6.030372	5.559835	0.815938
64	1	0	-4.747252	7.130235	2.258407
65	6	0	-5.256954	-2.766046	-0.455125
66	6	0	-5.420053	-4.077651	0.027635
67	6	0	-6.373708	-2.125525	-1.021593
68	6	0	-6.654328	-4.720524	-0.048471
69	1	0	-4.572042	-4.585969	0.476670
70	6	0	-7.609213	-2.768299	-1.095937
71	1	0	-6.261153	-1.121196	-1.419286

72	6	0	-7.754775	-4.068635	-0.610022
73	1	0	-6.759023	-5.730487	0.339357
74	1	0	-8.456125	-2.255100	-1.543902
75	1	0	-8.716425	-4.571132	-0.669777
76	6	0	5.102828	-2.785298	0.989189
77	6	0	6.328775	-2.558140	0.341433
78	6	0	5.073631	-3.681608	2.071259
79	6	0	7.489540	-3.204273	0.766096
80	1	0	6.361909	-1.881829	-0.507199
81	6	0	6.236134	-4.322233	2.499233
82	1	0	4.133828	-3.860489	2.585671
83	6	0	7.448010	-4.086626	1.847275
84	1	0	8.426780	-3.021081	0.247321
85	1	0	6.194973	-5.003026	3.345404
86	1	0	8.353481	-4.587653	2.178913

N_1SAPPh12 (Energy = −2122.69300356)



N_1SAPPh12

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Stoichiometry    C48H33N5
Framework group  C1[X(C48H33N5)]
Deg. of freedom   252
Full point group                 C1
Largest Abelian subgroup         C1      NOp   1
Largest concise Abelian subgroup C1      NOp   1
                      Standard orientation:
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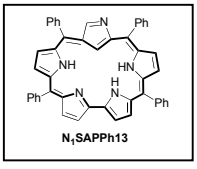
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.459762	-2.458091	-0.528037
2	7	0	1.566777	-2.476494	-0.236750
3	7	0	2.706342	0.023661	0.001553
4	7	0	-2.824115	0.088047	0.152898
5	6	0	-2.482022	2.482827	0.689789
6	6	0	3.133730	1.295097	-0.160428
7	6	0	-1.164427	2.619274	0.117670
8	6	0	3.863499	-2.083451	0.559728
9	6	0	-0.599990	-3.453469	-0.963129
10	6	0	4.934448	0.202599	0.656309
11	6	0	2.377179	2.416384	-0.664405
12	6	0	-0.795864	3.801910	-0.672428
13	6	0	4.525627	1.431885	0.241997
14	6	0	2.809810	-2.937325	0.165927
15	6	0	3.802047	-0.681272	0.467585
16	6	0	0.778522	-3.526533	-0.621510
17	6	0	-1.372111	-4.380207	-1.678886
18	6	0	-3.191009	1.291926	0.766708
19	6	0	0.995642	2.588606	-0.570561
20	6	0	2.777696	-4.351235	0.047210
21	6	0	-4.895667	-0.204810	1.010111
22	6	0	-4.474505	1.045987	1.365025
23	6	0	-2.771164	-2.783920	-0.861246
24	6	0	1.541539	-4.709414	-0.463178
25	6	0	-3.922193	-2.088365	-0.384901
26	6	0	-2.701547	-3.964539	-1.629533
27	6	0	-3.884113	-0.822809	0.199829
28	1	0	5.911887	-0.084812	1.016773
29	1	0	-1.476403	4.605400	-0.939481
30	1	0	5.095744	2.349576	0.227435
31	1	0	-0.976700	-5.238951	-2.204005
32	1	0	3.583166	-5.014679	0.325310
33	1	0	-5.808978	-0.695948	1.313375
34	1	0	-4.988999	1.746034	2.006694

35	1	0	1.169273	-5.709181	-0.638725
36	1	0	-3.548956	-4.441587	-2.099389
37	1	0	-1.235134	-1.830599	0.233320
38	7	0	0.428218	3.773774	-1.102105
39	6	0	-0.010693	1.837325	0.131386
40	1	0	0.164507	0.920053	0.676884
41	1	0	1.428235	-1.466026	-0.346628
42	1	0	-2.131687	0.084488	-0.586926
43	6	0	3.195595	3.497604	-1.291260
44	6	0	4.113645	3.167575	-2.303968
45	6	0	3.099481	4.841686	-0.892519
46	6	0	4.897290	4.148790	-2.910170
47	1	0	4.197266	2.134060	-2.626811
48	6	0	3.895846	5.819012	-1.485707
49	1	0	2.399462	5.112890	-0.111426
50	6	0	4.793923	5.478570	-2.499772
51	1	0	5.589186	3.872541	-3.701640
52	1	0	3.812137	6.851477	-1.156351
53	1	0	5.408950	6.244360	-2.965511
54	6	0	-3.134415	3.738801	1.151540
55	6	0	-2.416660	4.639254	1.961932
56	6	0	-4.446240	4.087611	0.778497
57	6	0	-2.995517	5.828258	2.401417
58	1	0	-1.402249	4.387895	2.256988
59	6	0	-5.024474	5.277946	1.217561
60	1	0	-5.002111	3.430986	0.116120
61	6	0	-4.303369	6.151694	2.033833
62	1	0	-2.424414	6.502554	3.034184
63	1	0	-6.035557	5.530144	0.908331
64	1	0	-4.753755	7.080590	2.373252
65	6	0	-5.238290	-2.781067	-0.478977
66	6	0	-5.414361	-4.084754	0.019925
67	6	0	-6.343302	-2.143481	-1.070855
68	6	0	-6.650135	-4.723634	-0.066729
69	1	0	-4.575879	-4.589852	0.490017
70	6	0	-7.580163	-2.782329	-1.156212
71	1	0	-6.220468	-1.144403	-1.478705
72	6	0	-7.738665	-4.075286	-0.654925
73	1	0	-6.765383	-5.727485	0.333752
74	1	0	-8.417917	-2.271765	-1.623945
75	1	0	-8.701367	-4.574720	-0.722863
76	6	0	5.123152	-2.723458	1.043546
77	6	0	5.891954	-3.544858	0.203117
78	6	0	5.563400	-2.511540	2.360164
79	6	0	7.065482	-4.139465	0.667644
80	1	0	5.574051	-3.700648	-0.823724
81	6	0	6.735226	-3.108942	2.824504
82	1	0	4.975139	-1.880464	3.020083
83	6	0	7.489904	-3.925486	1.980167
84	1	0	7.651882	-4.765086	-0.000174
85	1	0	7.056776	-2.937480	3.848382
86	1	0	8.403654	-4.389474	2.341561

N_1SAPPh13 (Energy = −2122.70046900)



N_1SAPPh13

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Stoichiometry    C48H33N5
Framework group  C1[X(C48H33N5)]
Deg. of freedom   252
Full point group                 C1
Largest Abelian subgroup         C1      NOp   1
Largest concise Abelian subgroup C1      NOp   1
                      Standard orientation:
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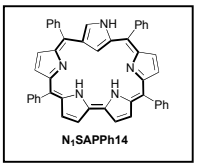
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.561210	-2.445727	-0.339211
2	7	0	1.373447	-2.542978	-0.495461
3	7	0	2.821470	0.030253	0.063073
4	7	0	-2.820444	0.080427	0.036984
5	6	0	-2.414762	2.549905	-0.250785
6	6	0	3.234940	1.292190	0.490086
7	6	0	-1.016890	2.642852	-0.419804
8	6	0	3.821822	-2.254883	-0.101658
9	6	0	-0.872991	-3.482377	-0.863989
10	6	0	4.817852	-0.236607	1.074864
11	6	0	2.591610	2.506676	0.214680
12	6	0	-0.388310	3.821300	-1.030007
13	6	0	4.474155	1.088700	1.170439
14	6	0	2.698955	-2.937959	-0.627002
15	6	0	3.810502	-0.917303	0.324422
16	6	0	0.532120	-3.503232	-1.019761
17	6	0	-1.723203	-4.631267	-1.108712
18	6	0	-3.172509	1.414209	0.125350
19	6	0	1.239211	2.644535	-0.215176
20	6	0	2.674120	-4.157971	-1.354179
21	6	0	-4.919619	0.144592	0.845957
22	6	0	-4.500171	1.439139	0.652216
23	6	0	-2.850636	-2.905000	-0.195344
24	6	0	1.353966	-4.500335	-1.591307
25	6	0	-3.928303	-2.131277	0.267882
26	6	0	-2.959792	-4.278610	-0.664608
27	6	0	-3.877678	-0.725327	0.412421
28	1	0	5.682541	-0.719041	1.506247
29	1	0	-0.913837	4.600411	-1.571584
30	1	0	5.012397	1.864789	1.694029
31	1	0	-1.412637	-5.579965	-1.527101
32	1	0	3.555082	-4.693131	-1.676834
33	1	0	-5.866293	-0.182089	1.249392
34	1	0	-5.046552	2.341514	0.881580
35	1	0	0.994049	-5.365078	-2.131201
36	1	0	-3.863674	-4.871021	-0.680097
37	7	0	0.903897	3.836530	-0.908477
38	6	0	0.087194	1.865065	0.027311
39	1	0	0.037573	0.967324	0.631612
40	1	0	-1.963241	-0.326664	-0.330351
41	1	0	2.134127	-0.072907	-0.673101
42	1	0	1.036992	-1.853979	0.163650
43	6	0	3.395067	3.750347	0.378008
44	6	0	2.880166	4.843287	1.098012
45	6	0	4.683559	3.866941	-0.172307
46	6	0	3.632581	6.001090	1.275889
47	1	0	1.885735	4.771612	1.525758
48	6	0	5.434430	5.029788	-0.001658
49	1	0	5.085893	3.046794	-0.759231
50	6	0	4.913651	6.099827	0.727037
51	1	0	3.218157	6.829973	1.843851
52	1	0	6.423577	5.101771	-0.446560
53	1	0	5.498247	7.006127	0.861803
54	6	0	5.102719	-3.011233	-0.004681
55	6	0	6.290157	-2.502641	-0.560939
56	6	0	5.155148	-4.257973	0.644802
57	6	0	7.487050	-3.212047	-0.466630
58	1	0	6.264864	-1.550490	-1.082562
59	6	0	6.351657	-4.967217	0.738317
60	1	0	4.250198	-4.661615	1.089120
61	6	0	7.522901	-4.447000	0.183561
62	1	0	8.390843	-2.802683	-0.910254

63	1	0	6.370333	-5.924474	1.252666
64	1	0	8.455418	-5.000096	0.256436
65	6	0	-3.211707	3.803456	-0.438278
66	6	0	-2.905711	4.967924	0.287404
67	6	0	-4.283809	3.847818	-1.347113
68	6	0	-3.646568	6.136399	0.110983
69	1	0	-2.089311	4.945530	1.002957
70	6	0	-5.018184	5.018610	-1.530846
71	1	0	-4.526548	2.959307	-1.922493
72	6	0	-4.703492	6.166748	-0.800489
73	1	0	-3.398244	7.022954	0.688406
74	1	0	-5.834031	5.035251	-2.248712
75	1	0	-5.277815	7.078487	-0.941368
76	6	0	-5.219130	-2.816284	0.573038
77	6	0	-5.267029	-3.833022	1.542102
78	6	0	-6.406792	-2.480389	-0.099174
79	6	0	-6.463680	-4.487351	1.834305
80	1	0	-4.357614	-4.098804	2.073069
81	6	0	-7.602792	-3.136793	0.190932
82	1	0	-6.383105	-1.711012	-0.865382
83	6	0	-7.636216	-4.141246	1.160257
84	1	0	-6.479871	-5.265639	2.592780
85	1	0	-8.508164	-2.867576	-0.346822
86	1	0	-8.568551	-4.651423	1.386987

N_1SAPPh14 (Energy = −2122.69404851)

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Stoichiometry    C48H33N5
Framework group  C1[X(C48H33N5)]
Deg. of freedom   252
Full point group                 C1
Largest Abelian subgroup         C1      NOp   1
Largest concise Abelian subgroup C1      NOp   1
                      Standard orientation:
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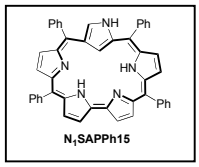
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.557249	-2.500656	-0.306734
2	7	0	-1.592270	-2.495551	-0.225163
3	7	0	-2.864465	-0.004055	0.028582
4	7	0	2.865146	-0.016791	0.054817
5	6	0	2.583648	2.450193	0.145863
6	6	0	-3.291228	1.300507	0.133542
7	6	0	1.173883	2.600749	-0.138483
8	6	0	-4.016721	-2.181038	0.134552
9	6	0	0.674613	-3.527684	-0.562340
10	6	0	-5.125499	0.057632	0.578581
11	6	0	-2.544521	2.458860	-0.093291
12	6	0	0.709129	3.788915	-0.743997
13	6	0	-4.709597	1.342127	0.495108
14	6	0	-2.890944	-2.966558	-0.143272
15	6	0	-3.967183	-0.767188	0.248955
16	6	0	-0.725962	-3.530860	-0.507856
17	6	0	1.467524	-4.695105	-0.805524
18	6	0	3.300285	1.267871	0.319849
19	6	0	-1.120792	2.562660	-0.244030
20	6	0	-2.834832	-4.371971	-0.408066
21	6	0	5.108899	-0.041510	0.671623
22	6	0	4.702485	1.246680	0.741324
23	6	0	2.860623	-2.969784	-0.330984
24	6	0	-1.527344	-4.709561	-0.634508
25	6	0	3.995479	-2.208083	-0.040096

26	6	0	2.786916	-4.360149	-0.668417
27	6	0	3.953556	-0.807652	0.214612
28	1	0	-6.107941	-0.306116	0.843831
29	1	0	1.272013	4.617543	-1.145876
30	1	0	-5.285779	2.235114	0.690381
31	1	0	1.070658	-5.670176	-1.047535
32	1	0	-3.692640	-5.027263	-0.425042
33	1	0	6.079392	-0.446752	0.920753
34	1	0	5.276797	2.101411	1.067766
35	1	0	-1.143888	-5.696391	-0.849223
36	1	0	3.642292	-5.008088	-0.786981
37	1	0	1.387709	-1.504986	-0.159616
38	7	0	-0.623812	3.753005	-0.802519
39	6	0	0.006583	1.821951	0.134540
40	1	0	-0.020795	0.868587	0.638431
41	1	0	-1.425597	-1.489047	-0.167932
42	1	0	-1.215632	4.470111	-1.196111
43	6	0	3.344197	3.736441	0.236580
44	6	0	4.436565	4.000345	-0.608928
45	6	0	2.964069	4.730338	1.157529
46	6	0	5.127577	5.210036	-0.531788
47	1	0	4.731293	3.251087	-1.337462
48	6	0	3.661772	5.934607	1.243111
49	1	0	2.126394	4.540413	1.822449
50	6	0	4.745206	6.180264	0.396566
51	1	0	5.963159	5.395651	-1.201709
52	1	0	3.360955	6.680729	1.974132
53	1	0	5.285958	7.120885	0.459061
54	6	0	-3.301066	3.749705	-0.198614
55	6	0	-3.045215	4.815779	0.684587
56	6	0	-4.274698	3.935464	-1.196433
57	6	0	-3.748187	6.016225	0.583180
58	1	0	-2.302395	4.687014	1.467208
59	6	0	-4.974098	5.138537	-1.301356
60	1	0	-4.475095	3.126242	-1.892296
61	6	0	-4.714931	6.182431	-0.411392
62	1	0	-3.545130	6.819907	1.286203
63	1	0	-5.719997	5.260362	-2.082428
64	1	0	-5.260965	7.118475	-0.492047
65	6	0	-5.326349	-2.883099	0.284555
66	6	0	-5.521544	-3.832743	1.302037
67	6	0	-6.395483	-2.617973	-0.588291
68	6	0	-6.742255	-4.493468	1.442983
69	1	0	-4.709697	-4.040232	1.993603
70	6	0	-7.617163	-3.276248	-0.446740
71	1	0	-6.257662	-1.895643	-1.387849
72	6	0	-7.795464	-4.217263	0.569292
73	1	0	-6.872201	-5.219079	2.241908
74	1	0	-8.428646	-3.058173	-1.136389
75	1	0	-8.747112	-4.730440	0.679405
76	6	0	5.312052	-2.910681	-0.002107
77	6	0	6.352225	-2.536039	-0.870302
78	6	0	5.548091	-3.962455	0.899896
79	6	0	7.583150	-3.191083	-0.839308
80	1	0	6.183511	-1.730124	-1.578752
81	6	0	6.778775	-4.619014	0.930769
82	1	0	4.761233	-4.252983	1.590325
83	6	0	7.801200	-4.236064	0.060878
84	1	0	8.371096	-2.888205	-1.524157
85	1	0	6.940853	-5.425287	1.641614
86	1	0	8.760364	-4.746484	0.085128

N_1SAPPh15 (Energy = −2122.69808205)

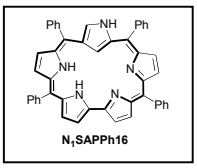


Stoichiometry C48H33N5
Framework group C1[X(C48H33N5)]
Deg. of freedom 252
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.489807	-2.534957	-0.334392
2	7	0	1.575047	-2.454092	-0.261069
3	7	0	2.888794	0.043856	0.065535
4	7	0	-2.841994	-0.031719	0.061364
5	6	0	-2.608550	2.435976	0.175283
6	6	0	3.278240	1.374500	0.074780
7	6	0	-1.206967	2.609503	-0.130484
8	6	0	3.989787	-2.174215	0.156656
9	6	0	-0.613530	-3.560107	-0.587596
10	6	0	5.113791	0.076517	0.471674
11	6	0	2.517227	2.514573	-0.156491
12	6	0	-0.769216	3.798601	-0.747547
13	6	0	4.694613	1.367894	0.362805
14	6	0	2.840654	-2.951112	-0.146597
15	6	0	3.982579	-0.783678	0.257520
16	6	0	0.789718	-3.536583	-0.525618
17	6	0	-1.411041	-4.727188	-0.837092
18	6	0	-3.299990	1.239191	0.354184
19	6	0	1.085967	2.600318	-0.270777
20	6	0	2.860703	-4.389999	-0.352304
21	6	0	-5.071359	-0.112349	0.722750
22	6	0	-4.691644	1.183838	0.803672
23	6	0	-2.795922	-2.994883	-0.354950
24	6	0	1.577391	-4.753226	-0.612600
25	6	0	-3.930464	-2.245669	-0.046814
26	6	0	-2.727596	-4.387707	-0.701830
27	6	0	-3.908382	-0.845423	0.231016
28	1	0	6.115314	-0.273177	0.673760
29	1	0	-1.348384	4.619102	-1.142591
30	1	0	5.292998	2.258655	0.480045
31	1	0	-1.014604	-5.700283	-1.086925
32	1	0	3.732209	-5.026750	-0.300138
33	1	0	-6.027458	-0.542407	0.985499
34	1	0	-5.276815	2.021274	1.154900
35	1	0	1.203893	-5.749690	-0.806001
36	1	0	-3.587018	-5.029239	-0.826544
37	1	0	-1.276908	-1.556246	-0.158328
38	7	0	0.564986	3.776094	-0.832751
39	6	0	-0.023256	1.846682	0.132529
40	1	0	0.009236	0.899359	0.650427
41	1	0	1.984972	-0.358136	-0.178167
42	1	0	1.141745	4.498567	-1.238677
43	6	0	3.267689	3.805948	-0.294106
44	6	0	3.042810	4.871350	0.598072
45	6	0	4.198402	3.996325	-1.331091
46	6	0	3.732727	6.076398	0.465523
47	1	0	2.332138	4.739649	1.409554
48	6	0	4.888942	5.201917	-1.463860
49	1	0	4.373595	3.188698	-2.036015
50	6	0	4.659289	6.245989	-0.565967
51	1	0	3.552099	6.880688	1.173943
52	1	0	5.602414	5.326418	-2.274230

53	1	0	5.196531	7.184812	-0.669533
54	6	0	5.302030	-2.869882	0.350078
55	6	0	5.967717	-3.471746	-0.729755
56	6	0	5.898640	-2.931580	1.619200
57	6	0	7.190894	-4.117484	-0.545546
58	1	0	5.520451	-3.425596	-1.718904
59	6	0	7.124310	-3.573465	1.804058
60	1	0	5.388975	-2.478034	2.464995
61	6	0	7.774057	-4.169692	0.722102
62	1	0	7.691359	-4.575240	-1.395069
63	1	0	7.567636	-3.612624	2.795803
64	1	0	8.727286	-4.671734	0.865248
65	6	0	-5.242300	-2.959042	-0.006754
66	6	0	-6.287419	-2.587694	-0.870060
67	6	0	-5.467677	-4.014265	0.893459
68	6	0	-7.513540	-3.251502	-0.837458
69	1	0	-6.126735	-1.777675	-1.575706
70	6	0	-6.694342	-4.678424	0.927004
71	1	0	-4.676056	-4.301954	1.579522
72	6	0	-7.721685	-4.300014	0.061089
73	1	0	-8.305695	-2.952210	-1.518972
74	1	0	-6.848847	-5.487615	1.636149
75	1	0	-8.677432	-4.816713	0.087120
76	6	0	-3.389717	3.707530	0.283181
77	6	0	-3.003306	4.711350	1.190727
78	6	0	-4.509869	3.947476	-0.532793
79	6	0	-3.721824	5.901974	1.292566
80	1	0	-2.144509	4.539470	1.833100
81	6	0	-5.221134	5.144132	-0.440181
82	1	0	-4.809792	3.190705	-1.251271
83	6	0	-4.832305	6.124181	0.475125
84	1	0	-3.415815	6.655862	2.013357
85	1	0	-6.077732	5.311937	-1.087823
86	1	0	-5.389098	7.054473	0.549983

N_1SAPPh16 (Energy = −2122.67550363)

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Stoichiometry    C48H33N5
Framework group  C1[X(C48H33N5)]
Deg. of freedom   252
Full point group                 C1
Largest Abelian subgroup         C1      NOp   1
Largest concise Abelian subgroup C1      NOp   1
                      Standard orientation:
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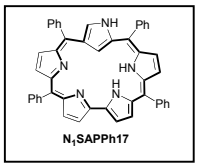
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.584475	-2.634178	-0.321640
2	7	0	1.280545	-2.686554	-0.191215
3	7	0	2.780892	-0.051959	-0.007278
4	7	0	-2.809496	0.137319	-0.005321
5	6	0	-2.417557	2.609785	0.006683
6	6	0	3.312478	1.199753	0.215950
7	6	0	-1.004693	2.678536	-0.346078
8	6	0	3.702411	-2.347190	0.188728
9	6	0	-0.832287	-3.688521	-0.792632
10	6	0	4.888954	-0.221368	0.955258
11	6	0	2.687749	2.400632	-0.118184
12	6	0	-0.487075	3.789963	-1.040054
13	6	0	4.636819	1.103330	0.829165
14	6	0	2.595871	-3.106188	-0.185597
15	6	0	3.727159	-0.918062	0.386939

16	6	0	0.586133	-3.710307	-0.687191
17	6	0	-1.729319	-4.648736	-1.286688
18	6	0	-3.156861	1.470926	0.260737
19	6	0	1.286832	2.555723	-0.394587
20	6	0	2.688140	-4.480070	-0.704469
21	6	0	-4.906206	0.127286	0.856110
22	6	0	-4.471232	1.415863	0.856327
23	6	0	-2.932616	-2.910135	-0.447130
24	6	0	1.429026	-4.848558	-1.042308
25	6	0	-4.005147	-2.066853	-0.012137
26	6	0	-3.021813	-4.173046	-1.074210
27	6	0	-3.899082	-0.708824	0.254651
28	1	0	5.758067	-0.688431	1.396795
29	1	0	-1.011695	4.610371	-1.506597
30	1	0	5.248584	1.930819	1.161030
31	1	0	-1.448445	-5.581354	-1.756081
32	1	0	3.599470	-5.045964	-0.835571
33	1	0	-5.832877	-0.247077	1.265517
34	1	0	-4.981537	2.273461	1.269064
35	1	0	1.100309	-5.783460	-1.478485
36	1	0	-3.947889	-4.653960	-1.353005
37	1	0	-1.162553	-1.896734	0.227717
38	7	0	0.852801	3.710089	-1.054106
39	6	0	0.125535	1.884286	0.012940
40	1	0	0.133392	0.966773	0.583058
41	1	0	1.477887	4.378292	-1.480788
42	1	0	-2.105320	-0.089515	-0.696124
43	6	0	3.522322	3.637600	-0.168455
44	6	0	3.156889	4.796962	0.543548
45	6	0	4.698593	3.675188	-0.940169
46	6	0	3.945672	5.945501	0.494872
47	1	0	2.262310	4.780820	1.159525
48	6	0	5.482499	4.827481	-0.993853
49	1	0	4.984773	2.793901	-1.505462
50	6	0	5.110348	5.965736	-0.276187
51	1	0	3.654467	6.822968	1.066226
52	1	0	6.383575	4.836496	-1.601310
53	1	0	5.722787	6.862421	-0.317177
54	6	0	5.002200	-3.068976	0.352038
55	6	0	6.131450	-2.720279	-0.409362
56	6	0	5.122052	-4.123550	1.273143
57	6	0	7.335573	-3.407075	-0.259816
58	1	0	6.053786	-1.912963	-1.131731
59	6	0	6.329240	-4.805727	1.429401
60	1	0	4.260679	-4.396453	1.875699
61	6	0	7.439948	-4.451284	0.662206
62	1	0	8.193011	-3.128580	-0.867186
63	1	0	6.401288	-5.613067	2.153675
64	1	0	8.380008	-4.983543	0.781592
65	6	0	-5.341669	-2.715266	0.138902
66	6	0	-6.471264	-2.223453	-0.537871
67	6	0	-5.500793	-3.847773	0.957489
68	6	0	-7.718052	-2.832335	-0.391162
69	1	0	-6.361847	-1.364352	-1.193434
70	6	0	-6.745875	-4.457295	1.103447
71	1	0	-4.638902	-4.241915	1.487774
72	6	0	-7.860675	-3.951129	0.430864
73	1	0	-8.576282	-2.437023	-0.928515
74	1	0	-6.846797	-5.326117	1.748764
75	1	0	-8.830992	-4.427272	0.544129
76	6	0	-3.121255	3.921393	0.132292
77	6	0	-2.606179	4.940702	0.956426
78	6	0	-4.306093	4.186419	-0.578624
79	6	0	-3.257074	6.167167	1.075615
80	1	0	-1.697074	4.753310	1.520564

81	6	0	-4.956723	5.415339	-0.462248
82	1	0	-4.707027	3.421705	-1.237554
83	6	0	-4.436132	6.410652	0.366249
84	1	0	-2.847424	6.932514	1.729980
85	1	0	-5.866918	5.597398	-1.027942
86	1	0	-4.941993	7.368171	0.456945

N_1SAPPh17 (Energy = −2122.67611625)



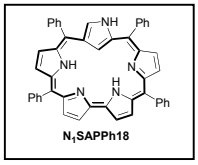
Stoichiometry C48H33N5
Framework group C1[X(C48H33N5)]
Deg. of freedom 252
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.211633	-2.707922	-0.186962
2	7	0	1.652578	-2.611554	-0.308361
3	7	0	2.820605	0.176983	-0.010680
4	7	0	-2.772444	-0.090823	-0.005438
5	6	0	-2.745890	2.363963	-0.124337
6	6	0	3.131903	1.515469	0.252840
7	6	0	-1.347098	2.570519	-0.423159
8	6	0	4.063421	-1.999110	-0.003074
9	6	0	-0.501442	-3.719710	-0.680816
10	6	0	4.916826	0.222023	0.848267
11	6	0	2.354735	2.631503	0.001329
12	6	0	-0.892713	3.715128	-1.099937
13	6	0	4.448091	1.499388	0.845635
14	6	0	3.005877	-2.864408	-0.434937
15	6	0	3.930344	-0.642742	0.253859
16	6	0	0.919313	-3.676440	-0.782813
17	6	0	-1.324680	-4.870178	-1.041013
18	6	0	-3.333813	1.151140	0.224230
19	6	0	0.943616	2.632564	-0.339119
20	6	0	3.116667	-4.123026	-1.063755
21	6	0	-4.868204	-0.312939	0.971292
22	6	0	-4.648923	1.017995	0.849344
23	6	0	-2.522955	-3.148130	-0.187020
24	6	0	1.831134	-4.620070	-1.278342
25	6	0	-3.641007	-2.408703	0.184222
26	6	0	-2.591012	-4.521838	-0.708627
27	6	0	-3.695150	-0.978079	0.390533
28	1	0	5.854850	-0.125862	1.255247
29	1	0	-1.453472	4.482084	-1.612335
30	1	0	4.937142	2.371791	1.253144
31	1	0	-0.979434	-5.799106	-1.477168
32	1	0	4.050618	-4.587668	-1.344054
33	1	0	-5.721005	-0.803081	1.419682
34	1	0	-5.277492	1.828770	1.190472
35	1	0	1.566246	-5.556048	-1.750278
36	1	0	-3.492648	-5.101621	-0.845550
37	7	0	0.449966	3.734231	-1.052158
38	6	0	-0.170296	1.872951	0.012623
39	1	0	-0.174091	0.964910	0.597440
40	1	0	2.109304	-0.070768	-0.686865
41	1	0	1.041945	4.452219	-1.443730
42	1	0	1.217351	-1.883723	0.243449
43	6	0	3.003093	3.971962	0.121595

44	6	0	2.432045	4.979545	0.924804
45	6	0	4.185183	4.279946	-0.578018
46	6	0	3.027801	6.234419	1.036095
47	1	0	1.523400	4.760224	1.478628
48	6	0	4.783063	5.535586	-0.464228
49	1	0	4.627962	3.525530	-1.221902
50	6	0	4.207683	6.518180	0.343074
51	1	0	2.575121	6.990017	1.673033
52	1	0	5.694522	5.748689	-1.016773
53	1	0	4.671421	7.497066	0.429443
54	6	0	-3.615740	3.574302	-0.157502
55	6	0	-3.267468	4.744970	0.542853
56	6	0	-4.810926	3.575947	-0.900456
57	6	0	-4.089742	5.870154	0.511176
58	1	0	-2.358417	4.755117	1.136504
59	6	0	-5.625826	4.706684	-0.942777
60	1	0	-5.084447	2.686151	-1.458607
61	6	0	-5.270289	5.856620	-0.235177
62	1	0	-3.811060	6.756869	1.074635
63	1	0	-6.538306	4.689935	-1.532926
64	1	0	-5.908150	6.736005	-0.265027
65	6	0	5.411265	-2.621497	0.152034
66	6	0	6.533468	-2.107746	-0.520761
67	6	0	5.588830	-3.751461	0.970409
68	6	0	7.791119	-2.692807	-0.369877
69	1	0	6.409714	-1.251335	-1.177248
70	6	0	6.844895	-4.336665	1.120838
71	1	0	4.732653	-4.162574	1.496944
72	6	0	7.952197	-3.808813	0.452466
73	1	0	8.643423	-2.281266	-0.904441
74	1	0	6.960166	-5.203706	1.766097
75	1	0	8.931010	-4.266396	0.568916
76	6	0	-4.930275	-3.151483	0.336976
77	6	0	-5.038419	-4.213230	1.251132
78	6	0	-6.061068	-2.814013	-0.427184
79	6	0	-6.236183	-4.914020	1.397635
80	1	0	-4.175875	-4.476849	1.856085
81	6	0	-7.255118	-3.520075	-0.288112
82	1	0	-5.992534	-1.999995	-1.142854
83	6	0	-7.348181	-4.571513	0.627015
84	1	0	-6.299734	-5.726568	2.116846
85	1	0	-8.113810	-3.250500	-0.897683
86	1	0	-8.280808	-5.118320	0.738669

N_1SAPPh18 (Energy = −2122.69815924)

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Stoichiometry    C48H33N5
Framework group  C1[X(C48H33N5)]
Deg. of freedom   252
Full point group                 C1
Largest Abelian subgroup         C1      NOp   1
Largest concise Abelian subgroup C1      NOp   1
                      Standard orientation:
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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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4	7	0	-2.905743	0.033507	0.038418
5	6	0	-2.561782	2.515599	0.157745
6	6	0	3.297484	1.282865	0.098188

7	6	0	-1.146541	2.654177	-0.114462
8	6	0	3.942117	-2.212415	0.168974
9	6	0	-0.733017	-3.517150	-0.634385
10	6	0	5.120360	0.006698	0.483417
11	6	0	2.570013	2.452166	-0.138514
12	6	0	-0.671002	3.847740	-0.699638
13	6	0	4.735095	1.298788	0.374127
14	6	0	2.822902	-2.989626	-0.137822
15	6	0	3.919239	-0.794781	0.268578
16	6	0	0.669523	-3.554084	-0.553153
17	6	0	-1.513917	-4.710889	-0.913981
18	6	0	-3.294428	1.344213	0.290003
19	6	0	1.147515	2.586306	-0.251149
20	6	0	2.761881	-4.411422	-0.323767
21	6	0	-5.094427	-0.027677	0.596334
22	6	0	-4.685875	1.268920	0.675028
23	6	0	-2.807432	-2.943048	-0.399303
24	6	0	1.464482	-4.746995	-0.597267
25	6	0	-3.974320	-2.201860	-0.083343
26	6	0	-2.815011	-4.350899	-0.770069
27	6	0	-3.978446	-0.826818	0.169730
28	1	0	6.112671	-0.376609	0.673531
29	1	0	-1.226915	4.694666	-1.071948
30	1	0	5.349458	2.180750	0.483350
31	1	0	-1.126652	-5.683203	-1.187032
32	1	0	3.609680	-5.075512	-0.246402
33	1	0	-6.073216	-0.421577	0.825990
34	1	0	-5.274210	2.118027	0.987710
35	1	0	1.074896	-5.739179	-0.771550
36	1	0	-3.692889	-4.966419	-0.905277
37	7	0	0.660707	3.794228	-0.774042
38	6	0	0.012438	1.853074	0.130381
39	1	0	0.048800	0.889094	0.616589
40	1	0	1.258229	4.513302	-1.155474
41	1	0	1.324330	-1.524087	-0.222966
42	1	0	-1.992362	-0.320938	-0.235307
43	6	0	-5.281759	-2.922338	0.002153
44	6	0	-6.342796	-2.603721	-0.861603
45	6	0	-5.481170	-3.938376	0.952173
46	6	0	-7.563017	-3.275595	-0.777731
47	1	0	-6.199765	-1.830057	-1.610918
48	6	0	-6.700062	-4.611351	1.036380
49	1	0	-4.672648	-4.191086	1.632133
50	6	0	-7.746196	-4.282061	0.172037
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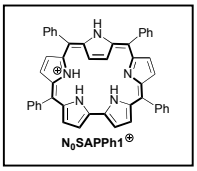
52	1	0	-6.834174	-5.390280	1.782647
53	1	0	-8.695877	-4.806450	0.237637
54	6	0	5.243623	-2.924880	0.365740
55	6	0	5.849798	-2.968257	1.631731
56	6	0	5.889086	-3.564344	-0.704678
57	6	0	7.063411	-3.629912	1.821628
58	1	0	5.357805	-2.482936	2.470189
59	6	0	7.101570	-4.229168	-0.515096
60	1	0	5.437434	-3.528448	-1.692287
61	6	0	7.693209	-4.263813	0.748716
62	1	0	7.513994	-3.654703	2.810521
63	1	0	7.586787	-4.714708	-1.357995
64	1	0	8.637983	-4.780242	0.896417
65	6	0	-3.316636	3.801849	0.287781
66	6	0	-4.392164	4.110719	-0.563823
67	6	0	-2.943670	4.753713	1.254758
68	6	0	-5.075975	5.321512	-0.446920
69	1	0	-4.680225	3.396325	-1.329580
70	6	0	-3.630311	5.961161	1.376170
71	1	0	-2.117628	4.529588	1.923696

72	6	0	-4.699339	6.250425	0.524932
73	1	0	-5.899353	5.541453	-1.121556
74	1	0	-3.333309	6.675135	2.140098
75	1	0	-5.232738	7.192745	0.617007
76	6	0	3.354443	3.722136	-0.299808
77	6	0	3.184738	4.797436	0.592233
78	6	0	4.266745	3.875606	-1.358622
79	6	0	3.912750	5.977738	0.439223
80	1	0	2.490201	4.692263	1.421360
81	6	0	4.991286	5.058177	-1.514459
82	1	0	4.401195	3.057326	-2.059802
83	6	0	4.818259	6.112392	-0.615556
84	1	0	3.777307	6.789686	1.148959
85	1	0	5.689716	5.155703	-2.341406
86	1	0	5.384250	7.032168	-0.735887

Cartesian coordinates for the optimized structures of normal *meso*-tetraphenyl-sapphyrins (monocation)

N_0SAPPh1$^{\oplus}$ (Energy = −2123.14412552)

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 Stoichiometry    C48H34N5(1+)
 Framework group  C1[X(C48H34N5)]
 Deg. of freedom   255
 Full point group                 C1
 Largest Abelian subgroup         C1      NOp   1
 Largest concise Abelian subgroup C1      NOp   1
                         Standard orientation:
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 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
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    8          6             0        0.904627   -3.451098   -0.111162
    9          6             0       -5.196406   -0.020805    0.271875
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   11          6             0       -4.826687    1.287984    0.089462
   12          6             0       -2.736337   -2.979613   -0.074351
   13          6             0       -4.061391   -0.860942    0.008572
   14          6             0       -0.512463   -3.504918   -0.174167
   15          6             0        1.736425   -4.610307   -0.127606
   16          6             0        3.238544    1.475872   -0.207004
   17          6             0       -2.606349   -4.343828   -0.424231
   18          6             0        5.211723    0.418913    0.061232
   19          6             0        4.667947    1.663574   -0.004639
   20          6             0        3.065285   -2.777439   -0.003510
   21          6             0       -1.261764   -4.659471   -0.489756
   22          6             0        4.190733   -1.929422    0.010852
   23          6             0        3.045821   -4.202318   -0.060211
   24          6             0        4.103586   -0.517461   -0.079223
   25          1             0       -1.208433   -1.671066    0.603152
   26          1             0       -6.165082   -0.384324    0.581440
   27          1             0       -5.453499    2.160690    0.199777
   28          1             0        1.377183   -5.628352   -0.163725
   29          1             0       -3.436093   -4.995971   -0.652413
   30          1             0        6.250232    0.157830    0.205588
   31          1             0        5.181903    2.613774    0.036954
   32          1             0       -0.841013   -5.610161   -0.783367
   33          1             0        3.924280   -4.829547   -0.061433
   34          1             0        1.537012   -1.363308   -0.097635
   35          6             0       -0.762469    1.095780   -1.815473
   36          6             0        0.617102    1.105352   -1.735124
   37          6             0        1.001727    2.172281   -0.879661
   38          6             0       -1.266437    2.148175   -0.995942
   39          7             0       -0.166082    2.829029   -0.533151
   40          1             0        1.313159    0.464027   -2.253169
   41          1             0       -1.366203    0.468626   -2.458688
   42          1             0       -0.213175    3.564243    0.160572
   43          1             0       -2.132053   -0.291248   -0.663613
   44          6             0        2.531910    3.874476    0.129487
   45          6             0        2.105159    4.987056   -0.625228
   46          6             0        3.201179    4.108066    1.347510
   47          6             0        2.354032    6.284046   -0.183906
   48          1             0        1.609715    4.827155   -1.578600
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50	1	0	3.510097	3.263808	1.955677
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54	1	0	3.215885	7.510862	1.367406
55	6	0	-2.964094	3.791714	-0.142695
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57	6	0	-3.613598	4.074037	1.074860
58	6	0	-2.988715	6.173630	-0.654402
59	1	0	-2.159979	4.667047	-1.946808
60	6	0	-3.954127	5.382326	1.413522
61	1	0	-3.827313	3.265696	1.767609
62	6	0	-3.645588	6.435835	0.550390
63	1	0	-2.750916	6.987265	-1.333678
64	1	0	-4.450452	5.580358	2.359252
65	1	0	-3.911895	7.454616	0.816237
66	6	0	5.534318	-2.564724	0.115767
67	6	0	6.500083	-2.357915	-0.884284
68	6	0	5.863372	-3.376059	1.215280
69	6	0	7.757802	-2.951871	-0.788760
70	1	0	6.253739	-1.744441	-1.746095
71	6	0	7.125198	-3.961816	1.312240
72	1	0	5.133734	-3.527009	2.005856
73	6	0	8.074479	-3.753672	0.309832
74	1	0	8.489233	-2.791077	-1.575598
75	1	0	7.367993	-4.576251	2.174524
76	1	0	9.056034	-4.212628	0.384762
77	6	0	-5.201001	-3.053518	0.244530
78	6	0	-6.297298	-2.876752	-0.618422
79	6	0	-5.304337	-4.001176	1.278514
80	6	0	-7.463799	-3.620957	-0.447009
81	1	0	-6.222681	-2.169120	-1.439064
82	6	0	-6.472646	-4.741652	1.449640
83	1	0	-4.470014	-4.141544	1.959661
84	6	0	-7.555663	-4.553601	0.588023
85	1	0	-8.297437	-3.478776	-1.128727
86	1	0	-6.539400	-5.461564	2.260300
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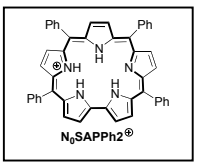
N_0SAPPh2$^{\oplus}$ (Energy = −2123.13443276)



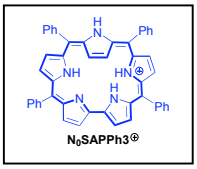
Stoichiometry C48H34N5(1+)
Framework group C1[X(C48H34N5)]
Deg. of freedom 255
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.477651	-2.448717	-0.674506
2	7	0	1.464395	-2.527024	-0.361701
3	7	0	2.605552	-0.017469	0.032271
4	7	0	-2.699884	0.111989	0.097312
5	6	0	-2.328408	2.523372	0.639057
6	6	0	3.115888	1.230794	-0.150660
7	6	0	-1.086343	2.764694	-0.004186
8	6	0	3.707495	-2.179308	0.576020
9	6	0	-0.670379	-3.447752	-1.177674
10	6	0	4.840757	0.056202	0.703055
11	6	0	2.457107	2.380066	-0.684388

12	6	0	-0.789252	3.952249	-0.738157
13	6	0	4.511352	1.295167	0.262720
14	6	0	0.499839	3.873956	-1.190818
15	6	0	2.677588	-3.010207	0.088315
16	6	0	3.663202	-0.770693	0.506913
17	6	0	0.701230	-3.557820	-0.842760
18	6	0	-1.493317	-4.319189	-1.919079
19	6	0	-2.978562	1.287432	0.793677
20	6	0	1.086427	2.666735	-0.692093
21	6	0	2.654037	-4.420470	-0.100396
22	6	0	-4.645832	-0.206684	1.205940
23	6	0	-4.165169	1.033721	1.547296
24	6	0	-2.810010	-2.724987	-0.970006
25	6	0	1.456260	-4.750122	-0.705824
26	6	0	-3.900745	-2.029129	-0.394995
27	6	0	-2.802077	-3.871028	-1.801989
28	6	0	-3.762842	-0.791979	0.253921
29	1	0	1.334111	-1.515494	-0.450117
30	1	0	5.795370	-0.283937	1.076434
31	1	0	-1.507350	4.735001	-0.933037
32	1	0	5.134353	2.176863	0.236825
33	1	0	1.013854	4.587174	-1.816351
34	1	0	-1.142269	-5.162230	-2.497885
35	1	0	3.440894	-5.097627	0.196103
36	1	0	-5.514847	-0.703827	1.611961
37	1	0	-4.585497	1.718947	2.268213
38	1	0	1.099153	-5.739813	-0.954450
39	1	0	-3.678238	-4.296926	-2.268568
40	7	0	0.052817	1.971561	-0.058209
41	1	0	0.237377	1.174908	0.538438
42	1	0	-1.212025	-1.890087	0.126405
43	1	0	-2.139997	0.124436	-0.747012
44	6	0	-3.059054	3.743957	1.094256
45	6	0	-4.381277	4.003463	0.689316
46	6	0	-2.420789	4.674339	1.934797
47	6	0	-5.044680	5.151906	1.118131
48	1	0	-4.880837	3.310988	0.018338
49	6	0	-3.087649	5.818770	2.368042
50	1	0	-1.402525	4.485403	2.262242
51	6	0	-4.401490	6.060874	1.961169
52	1	0	-6.061444	5.341629	0.786240
53	1	0	-2.582848	6.519348	3.026981
54	1	0	-4.920190	6.954358	2.296304
55	6	0	3.359714	3.439680	-1.238230
56	6	0	4.196997	3.138202	-2.325983
57	6	0	3.415638	4.728421	-0.680860
58	6	0	5.050692	4.105393	-2.854402
59	1	0	4.165675	2.144299	-2.762847
60	6	0	4.280845	5.690596	-1.201849
61	1	0	2.794606	4.967277	0.177700
62	6	0	5.096314	5.383235	-2.292690
63	1	0	5.681732	3.860184	-3.703856
64	1	0	4.321505	6.678211	-0.751296
65	1	0	5.767218	6.134074	-2.700017
66	6	0	4.932449	-2.840577	1.114196
67	6	0	5.741534	-3.649449	0.299319
68	6	0	5.292824	-2.658807	2.459590
69	6	0	6.881151	-4.262873	0.819673
70	1	0	5.488998	-3.776684	-0.749524
71	6	0	6.428719	-3.279417	2.978649
72	1	0	4.671316	-2.039081	3.099744
73	6	0	7.225536	-4.082715	2.160554
74	1	0	7.503486	-4.876268	0.174312
75	1	0	6.689548	-3.136273	4.023378
76	1	0	8.111882	-4.562939	2.564868

77	6	0	-5.245287	-2.659654	-0.430392
78	6	0	-5.427339	-4.003002	-0.050809
79	6	0	-6.369358	-1.919522	-0.842482
80	6	0	-6.693232	-4.583991	-0.081447
81	1	0	-4.575943	-4.581585	0.294128
82	6	0	-7.633260	-2.505308	-0.877198
83	1	0	-6.241953	-0.888871	-1.159707
84	6	0	-7.799190	-3.838427	-0.496215
85	1	0	-6.817866	-5.617819	0.227490
86	1	0	-8.487444	-1.922646	-1.209785
87	1	0	-8.784747	-4.294075	-0.521971

N_0SAPPh3$^{\oplus}$ (Energy = −2123.1482290)

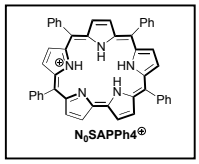


Stoichiometry C48H34N5(1+)
Framework group C1[X(C48H34N5)]
Deg. of freedom 255
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.677037	-2.333689	-0.070804
2	7	0	-1.399459	-2.496982	-0.031943
3	7	0	-3.019586	0.007314	-0.330831
4	7	0	2.961029	0.169799	-0.252423
5	6	0	2.272730	2.541935	-0.388759
6	6	0	-3.437411	1.327708	-0.284073
7	6	0	-3.923214	-2.260721	0.055057
8	6	0	0.922633	-3.445094	-0.213689
9	6	0	-5.172687	-0.033635	0.291391
10	6	0	-2.588630	2.424885	-0.509669
11	6	0	-4.812749	1.280132	0.116590
12	6	0	-2.709781	-2.983097	-0.105901
13	6	0	-4.037861	-0.863121	0.004370
14	6	0	-0.496264	-3.521106	-0.264985
15	6	0	1.741916	-4.647607	-0.293285
16	6	0	3.237799	1.524126	-0.235106
17	6	0	-2.598002	-4.354090	-0.456185
18	6	0	5.175644	0.375722	0.072907
19	6	0	4.648163	1.642119	-0.029564
20	6	0	2.984498	-2.785002	-0.043543
21	6	0	-1.259902	-4.676975	-0.556714
22	6	0	4.134425	-1.975644	0.024886
23	6	0	3.027217	-4.235917	-0.172802
24	6	0	4.103546	-0.561907	-0.054453
25	1	0	-1.121852	-1.662751	0.467396
26	1	0	-6.134609	-0.405502	0.611649
27	1	0	-5.442512	2.148185	0.245001
28	1	0	1.384246	-5.661259	-0.409344
29	1	0	-3.439172	-5.000730	-0.656448
30	1	0	6.211256	0.110760	0.224548
31	1	0	5.187619	2.577759	-0.004710
32	1	0	-0.851231	-5.633981	-0.845594
33	1	0	3.921850	-4.840447	-0.197902
34	6	0	-0.774735	1.140880	-1.839369
35	6	0	0.605606	1.154803	-1.775435
36	6	0	0.997808	2.212085	-0.909854
37	6	0	-1.273456	2.177717	-0.999236
38	7	0	-0.167922	2.856799	-0.538824

39	1	0	1.286933	0.524867	-2.329529
40	1	0	-1.381197	0.517676	-2.483523
41	1	0	-0.210119	3.579079	0.168614
42	1	0	-2.117772	-0.276881	-0.679873
43	1	0	2.052599	-0.295195	-0.246922
44	6	0	5.471106	-2.620556	0.177608
45	6	0	6.472539	-2.439303	-0.791434
46	6	0	5.753217	-3.418719	1.298937
47	6	0	7.720678	-3.043541	-0.643764
48	1	0	6.262180	-1.840434	-1.673221
49	6	0	7.004335	-4.016699	1.447460
50	1	0	4.991644	-3.555552	2.061319
51	6	0	7.990696	-3.831713	0.476757
52	1	0	8.479960	-2.903228	-1.407881
53	1	0	7.209195	-4.624129	2.324443
54	1	0	8.963961	-4.299889	0.592161
55	6	0	2.550800	3.918805	0.072797
56	6	0	2.129047	5.022935	-0.696536
57	6	0	3.228288	4.164794	1.283499
58	6	0	2.391153	6.324080	-0.276075
59	1	0	1.624760	4.852515	-1.643405
60	6	0	3.486117	5.468643	1.701258
61	1	0	3.530782	3.328373	1.905819
62	6	0	3.071044	6.551701	0.923369
63	1	0	2.074678	7.162015	-0.890457
64	1	0	4.003977	5.639137	2.640650
65	1	0	3.274584	7.567234	1.250117
66	6	0	-2.964217	3.793388	-0.087104
67	6	0	-2.667473	4.889595	-0.922106
68	6	0	-3.596187	4.044515	1.146426
69	6	0	-3.008946	6.185982	-0.544693
70	1	0	-2.193111	4.713145	-1.883561
71	6	0	-3.937810	5.343046	1.519774
72	1	0	-3.795868	3.219407	1.823328
73	6	0	-3.648145	6.417303	0.675883
74	1	0	-2.786563	7.016002	-1.209197
75	1	0	-4.420579	5.517114	2.477150
76	1	0	-3.915824	7.428339	0.968568
77	6	0	-5.167833	-3.057291	0.248102
78	6	0	-6.274388	-2.882999	-0.602100
79	6	0	-5.258075	-4.001078	1.286714
80	6	0	-7.438094	-3.627617	-0.414703
81	1	0	-6.209997	-2.177594	-1.425513
82	6	0	-6.424180	-4.741110	1.474417
83	1	0	-4.415247	-4.138721	1.957767
84	6	0	-7.517136	-4.556638	0.624747
85	1	0	-8.279775	-3.488431	-1.087078
86	1	0	-6.481001	-5.458245	2.288257
87	1	0	-8.424447	-5.135665	0.770275

N_0SAPPh4$^{\oplus}$ (Energy = −2123.14006537)

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Stoichiometry    C48H34N5(1+)
Framework group  C1[X(C48H34N5)]
Deg. of freedom   255
Full point group                 C1
Largest Abelian subgroup         C1      NOp   1
Largest concise Abelian subgroup C1      NOp   1
                      Standard orientation:
```
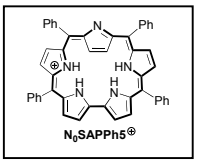

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	7	0	1.377569	-2.507518	0.641836
2	7	0	-1.478811	-2.447451	0.469366
3	7	0	-2.715401	0.045329	-0.046780
4	7	0	2.718543	0.054970	-0.061111
5	6	0	2.494601	2.541267	-0.262715
6	6	0	-3.081725	1.367613	-0.191616
7	6	0	1.204337	2.778930	0.254351
8	6	0	-3.792306	-2.180233	-0.312437
9	6	0	0.581542	-3.436563	1.265633
10	6	0	-4.711097	0.062787	-1.094263
11	6	0	-2.429312	2.537341	0.288756
12	6	0	0.824473	3.933180	1.002860
13	6	0	-4.336116	1.366892	-0.872543
14	6	0	-0.530962	3.908995	1.188867
15	6	0	-2.757125	-2.920231	0.286324
16	6	0	-3.720434	-0.782932	-0.521074
17	6	0	-0.824629	-3.445663	1.098180
18	6	0	1.439940	-4.364950	1.901854
19	6	0	3.072562	1.292849	-0.587171
20	6	0	-1.066340	2.754431	0.535118
21	6	0	-2.897141	-4.254954	0.848756
22	6	0	4.598249	-0.245927	-1.275620
23	6	0	4.223605	1.072652	-1.396117
24	6	0	2.714460	-2.864683	0.760494
25	6	0	-1.687069	-4.573348	1.385174
26	6	0	3.786409	-2.201265	0.126086
27	6	0	2.742812	-4.018850	1.591202
28	6	0	3.696549	-0.894185	-0.387499
29	1	0	-5.596643	-0.284844	-1.604520
30	1	0	1.524125	4.664424	1.379704
31	1	0	-4.863121	2.259171	-1.175226
32	1	0	-1.124495	4.618564	1.745186
33	1	0	1.115722	-5.186854	2.524539
34	1	0	-3.802772	-4.844230	0.858188
35	1	0	5.414066	-0.741135	-1.781529
36	1	0	4.689825	1.829863	-2.009002
37	1	0	-1.402203	-5.487778	1.888623
38	1	0	3.645704	-4.504739	1.931261
39	7	0	0.040114	2.023863	0.076547
40	1	0	-0.041839	1.341343	-0.666516
41	1	0	0.999483	-1.897308	-0.070791
42	1	0	-1.923818	-0.350626	0.455405
43	1	0	2.155164	-0.025097	0.776666
44	6	0	-3.335034	3.707639	0.516325
45	6	0	-4.428820	3.596102	1.393061
46	6	0	-3.123734	4.930547	-0.144484
47	6	0	-5.275740	4.680673	1.614345
48	1	0	-4.601280	2.658890	1.914089
49	6	0	-3.980162	6.010355	0.067481
50	1	0	-2.295596	5.025168	-0.840778
51	6	0	-5.055132	5.889679	0.950446
52	1	0	-6.107120	4.582347	2.306408
53	1	0	-3.810549	6.944044	-0.461080
54	1	0	-5.719299	6.732536	1.118413
55	6	0	3.360737	3.743160	-0.452166
56	6	0	2.898555	4.849683	-1.188103
57	6	0	4.654469	3.797970	0.098463
58	6	0	3.705391	5.971178	-1.371564
59	1	0	1.908530	4.817715	-1.633442
60	6	0	5.457374	4.923110	-0.079528
61	1	0	5.021035	2.960627	0.684872
62	6	0	4.986319	6.011914	-0.816731
63	1	0	3.336300	6.810882	-1.953432
64	1	0	6.448689	4.952662	0.363565
65	1	0	5.613856	6.887145	-0.957662

66	6	0	-5.046814	-2.885089	-0.695906
67	6	0	-6.297588	-2.486772	-0.191903
68	6	0	-4.991522	-3.985137	-1.570072
69	6	0	-7.458403	-3.168291	-0.554777
70	1	0	-6.353581	-1.657302	0.506819
71	6	0	-6.155191	-4.657986	-1.939564
72	1	0	-4.032450	-4.296776	-1.973151
73	6	0	-7.391293	-4.252095	-1.432747
74	1	0	-8.415200	-2.856252	-0.145906
75	1	0	-6.096032	-5.497987	-2.625727
76	1	0	-8.297162	-4.779317	-1.717729
77	6	0	5.078110	-2.924538	-0.003497
78	6	0	5.115203	-4.235370	-0.514886
79	6	0	6.288132	-2.319361	0.384297
80	6	0	6.325092	-4.914871	-0.640408
81	1	0	4.192855	-4.709020	-0.836937
82	6	0	7.495572	-3.004550	0.264452
83	1	0	6.274106	-1.318344	0.804738
84	6	0	7.518194	-4.302647	-0.250117
85	1	0	6.336792	-5.920872	-1.049736
86	1	0	8.418555	-2.527306	0.580881
87	1	0	8.460281	-4.834658	-0.345316

N_0SAPPh5$^{\oplus}$ (Energy = −2123.11956034)



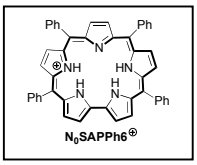
Stoichiometry C48H34N5(1+)
Framework group C1[X(C48H34N5)]
Deg. of freedom 255
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.562629	-2.485536	0.089404
2	7	0	-1.562668	-2.485449	0.089372
3	7	0	-2.975246	0.106299	-0.263002
4	7	0	2.975290	0.106297	-0.263274
5	6	0	2.387441	2.497716	-0.428845
6	6	0	-3.314388	1.454073	-0.229364
7	6	0	-4.054114	-2.105449	0.071130
8	6	0	0.703859	-3.564476	-0.103089
9	6	0	-5.151629	0.201676	0.263020
10	6	0	-2.387362	2.497718	-0.428623
11	6	0	-4.699586	1.493161	0.112537
12	6	0	-2.896967	-2.906680	-0.018281
13	6	0	-4.062017	-0.692299	0.020246
14	6	0	-0.703913	-3.564466	-0.103128
15	6	0	1.525857	-4.687588	-0.385245
16	6	0	3.314479	1.454073	-0.229619
17	6	0	-2.843079	-4.295228	-0.327585
18	6	0	5.151646	0.201626	0.262864
19	6	0	4.699632	1.493130	0.112407
20	6	0	2.896911	-2.906696	-0.018199
21	6	0	-1.525888	-4.687469	-0.385650
22	6	0	4.054076	-2.105477	0.071037
23	6	0	2.843028	-4.295354	-0.327137
24	6	0	4.062045	-0.692327	0.020032
25	1	0	-1.305590	-1.660379	0.613727
26	1	0	-6.148862	-0.110023	0.535312
27	1	0	-5.278885	2.398623	0.215680

28	1	0	1.161318	-5.672116	-0.640579
29	1	0	-3.709791	-4.903984	-0.537152
30	1	0	6.148846	-0.110094	0.535256
31	1	0	5.278929	2.398577	0.215692
32	1	0	-1.161354	-5.671925	-0.641275
33	1	0	3.709771	-4.904164	-0.536415
34	1	0	1.305362	-1.659857	0.612678
35	6	0	-0.683706	1.115379	-1.816003
36	6	0	0.683672	1.115438	-1.816146
37	6	0	1.083001	2.206810	-0.933932
38	6	0	-1.082945	2.206776	-0.933805
39	7	0	0.000034	2.885351	-0.483355
40	1	0	1.334057	0.526482	-2.453193
41	1	0	-1.334183	0.526327	-2.452860
42	1	0	-2.091433	-0.221502	-0.625630
43	1	0	2.091651	-0.221416	-0.626409
44	6	0	2.715781	3.871684	-0.006627
45	6	0	2.327620	4.959686	-0.812873
46	6	0	3.408740	4.137114	1.190666
47	6	0	2.649393	6.262998	-0.449175
48	1	0	1.788923	4.770129	-1.735175
49	6	0	3.719267	5.444279	1.557539
50	1	0	3.667129	3.317645	1.853985
51	6	0	3.347846	6.510370	0.735668
52	1	0	2.356517	7.088848	-1.091019
53	1	0	4.241469	5.631572	2.491404
54	1	0	3.593979	7.529233	1.020733
55	6	0	-2.715696	3.871693	-0.006484
56	6	0	-2.327537	4.959673	-0.812772
57	6	0	-3.408689	4.137191	1.190778
58	6	0	-2.649334	6.262991	-0.449143
59	1	0	-1.788817	4.770085	-1.735054
60	6	0	-3.719248	5.444368	1.557583
61	1	0	-3.667083	3.317756	1.854142
62	6	0	-3.347818	6.510427	0.735674
63	1	0	-2.356418	7.088804	-1.091018
64	1	0	-4.241497	5.631687	2.491417
65	1	0	-3.593983	7.529298	1.020673
66	6	0	-5.364436	-2.806273	0.188649
67	6	0	-6.398676	-2.560683	-0.731871
68	6	0	-5.589567	-3.731054	1.223684
69	6	0	-7.621959	-3.219421	-0.617829
70	1	0	-6.232791	-1.865789	-1.550081
71	6	0	-6.814962	-4.385950	1.337571
72	1	0	-4.805091	-3.920104	1.950915
73	6	0	-7.834305	-4.132293	0.417563
74	1	0	-8.406790	-3.025144	-1.343200
75	1	0	-6.975592	-5.089257	2.149637
76	1	0	-8.788450	-4.643496	0.506324
77	6	0	5.364388	-2.806314	0.188654
78	6	0	6.398605	-2.560912	-0.731940
79	6	0	5.589520	-3.730916	1.223849
80	6	0	7.621879	-3.219652	-0.617808
81	1	0	6.232713	-1.866166	-1.550273
82	6	0	6.814906	-4.385816	1.337823
83	1	0	4.805060	-3.919814	1.951135
84	6	0	7.834230	-4.132342	0.417743
85	1	0	8.406698	-3.025525	-1.343231
86	1	0	6.975547	-5.088979	2.150010
87	1	0	8.788368	-4.643548	0.506572

N_0SAPPh6$^{\oplus}$ (Energy = −2123.11941782)



Stoichiometry C48H34N5(1+)
Framework group C1[X(C48H34N5)]
Deg. of freedom 255
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.422686	-2.585501	0.267930
2	7	0	-1.422860	-2.585416	-0.267965
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4	7	0	2.595829	0.092520	-0.119749
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6	6	0	-2.936056	1.164163	0.935806
7	6	0	0.913893	2.629607	-0.588298
8	6	0	-3.774600	-1.984795	-0.712638
9	6	0	0.656026	-3.731843	0.264167
10	6	0	-4.769194	-0.155485	0.688647
11	6	0	-2.164227	2.314359	1.178154
12	6	0	0.547080	4.028811	-0.396809
13	6	0	-4.287010	0.947652	1.346338
14	6	0	-0.546998	4.028823	0.396637
15	6	0	-2.666165	-2.848601	-0.829620
16	6	0	-3.712130	-0.723294	-0.081702
17	6	0	-0.656278	-3.731817	-0.264125
18	6	0	1.392176	-4.736727	0.924779
19	6	0	2.936112	1.164044	-0.935816
20	6	0	-0.913759	2.629617	0.588242
21	6	0	-2.606926	-4.186491	-1.306879
22	6	0	4.769141	-0.155746	-0.688711
23	6	0	4.287028	0.947445	-1.346382
24	6	0	2.665977	-2.848725	0.829599
25	6	0	-1.392484	-4.736685	-0.924690
26	6	0	3.774453	-1.984983	0.712601
27	6	0	2.606656	-4.186594	1.306922
28	6	0	3.712053	-0.723474	0.081650
29	1	0	-1.274980	-1.831097	0.391502
30	1	0	-5.748463	-0.599764	0.789443
31	1	0	1.098195	4.879996	-0.767648
32	1	0	-4.818063	1.564386	2.054676
33	1	0	-1.098142	4.880017	0.767411
34	1	0	1.025505	-5.728886	1.149204
35	1	0	-3.386913	-4.672411	-1.873777
36	1	0	5.748375	-0.600097	-0.789534
37	1	0	4.818120	1.564154	-2.054713
38	1	0	-1.025874	-5.728880	-1.149055
39	1	0	3.386615	-4.672537	1.873839
40	7	0	0.000065	1.788747	0.000011
41	1	0	1.274808	-1.831178	-0.391529
42	1	0	1.769184	0.142528	0.468794
43	1	0	-1.769215	0.142584	-0.468832
44	6	0	2.784190	3.370946	-2.041563
45	6	0	3.964916	4.036559	-1.673033
46	6	0	2.156743	3.727337	-3.246403
47	6	0	4.507810	5.025427	-2.493682
48	1	0	4.445046	3.792258	-0.729610
49	6	0	2.705563	4.709869	-4.070315
50	1	0	1.240200	3.222689	-3.538828
51	6	0	3.882395	5.361060	-3.696322
52	1	0	5.415808	5.538357	-2.189400

53	1	0	2.212722	4.966963	-5.003608
54	1	0	4.307439	6.129551	-4.335490
55	6	0	-2.783955	3.371045	2.041590
56	6	0	-2.156426	3.727372	3.246409
57	6	0	-3.964636	4.036767	1.673115
58	6	0	-2.705127	4.709941	4.070352
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63	1	0	-2.212228	4.966983	5.003630
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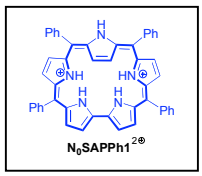
66	6	0	-5.119894	-2.471153	-1.120394
67	6	0	-5.631379	-3.702596	-0.671277
68	6	0	-5.918062	-1.678037	-1.964980
69	6	0	-6.897232	-4.130878	-1.066965
70	1	0	-5.046508	-4.308872	0.013666
71	6	0	-7.180551	-2.112499	-2.364446
72	1	0	-5.532985	-0.727733	-2.323001
73	6	0	-7.673016	-3.340407	-1.917914
74	1	0	-7.282541	-5.078423	-0.701503
75	1	0	-7.777854	-1.493386	-3.027483
76	1	0	-8.658114	-3.677637	-2.226890
77	6	0	5.119722	-2.471394	1.120370
78	6	0	5.631142	-3.702885	0.671310
79	6	0	5.917940	-1.678273	1.964907
80	6	0	6.896975	-4.131213	1.067014
81	1	0	5.046240	-4.309160	-0.013607
82	6	0	7.180406	-2.112783	2.364390
83	1	0	5.532918	-0.727927	2.322873
84	6	0	7.672804	-3.340740	1.917921
85	1	0	7.282233	-5.078794	0.701594
86	1	0	7.777746	-1.493664	3.027389
87	1	0	8.657885	-3.678008	2.226907

Cartesian coordinates for the optimized structures of normal *meso*-tetraphenyl-sapphyrins (dication)

N_0SAPPh1$^{2⊕}$ (Energy = −2123.46581760)

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 Stoichiometry    C48H35N5(2+)
 Framework group  C1[X(C48H35N5)]
 Deg. of freedom   258
 Full point group                 C1
 Largest Abelian subgroup         C1      NOp   1
 Largest concise Abelian subgroup C1      NOp   1
                       Standard orientation:
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 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
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    2          7             0       -1.565556   -2.488841    0.078697
    3          7             0       -2.997301    0.090724   -0.290314
    4          7             0        2.997273    0.090599   -0.290636
    5          6             0        2.427335    2.490672   -0.456510
    6          6             0       -3.334344    1.436287   -0.233204
    7          6             0       -4.064321   -2.120272    0.080198
    8          6             0        0.706957   -3.553742   -0.176239
    9          6             0       -5.148943    0.187361    0.343951
   10          6             0       -2.427441    2.490789   -0.456223
   11          6             0       -4.704562    1.477309    0.175877
   12          6             0       -2.897732   -2.912285   -0.053126
   13          6             0       -4.072617   -0.707409    0.043415
   14          6             0       -0.706937   -3.553720   -0.176274
   15          6             0        1.521658   -4.659456   -0.529922
   16          6             0        3.334238    1.436197   -0.233506
   17          6             0       -2.842318   -4.275755   -0.446522
   18          6             0        5.148798    0.187375    0.344058
   19          6             0        4.704414    1.477281    0.175756
   20          6             0        2.897755   -2.912350   -0.053114
   21          6             0       -1.521649   -4.659330   -0.530227
   22          6             0        4.064357   -2.120320    0.080171
   23          6             0        2.842329   -4.275902   -0.446243
   24          6             0        4.072606   -0.707467    0.043259
   25          1             0       -1.316669   -1.707866    0.671649
   26          1             0       -6.130399   -0.123973    0.669176
   27          1             0       -5.276806    2.382990    0.312620
   28          1             0        1.156085   -5.624759   -0.848902
   29          1             0       -3.706627   -4.872631   -0.697170
   30          1             0        6.130181   -0.123911    0.669549
   31          1             0        5.276570    2.383003    0.312599
   32          1             0       -1.156093   -5.624554   -0.849467
   33          1             0        3.706641   -4.872860   -0.696681
   34          6             0       -0.692843    1.171732   -1.869193
   35          6             0        0.692489    1.171781   -1.869378
   36          6             0        1.136091    2.198132   -0.988604
   37          6             0       -1.136264    2.198171   -0.988433
   38          7             0       -0.000045    2.843785   -0.553963
   39          1             0        1.334974    0.581418   -2.510234
   40          1             0       -1.335484    0.581304   -2.509830
   41          1             0        0.000026    3.572291    0.150243
   42          1             0       -2.130788   -0.252923   -0.676547
   43          1             0        2.130995   -0.253154   -0.677297
   44          1             0        1.316662   -1.707384    0.670786
   45          6             0       -5.359978   -2.829745    0.221335
   46          6             0       -6.445679   -2.525813   -0.623142
   47          6             0       -5.522154   -3.824808    1.205202
   48          6             0       -7.657158   -3.198807   -0.484640
   49          1             0       -6.326461   -1.785810   -1.409193
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50	6	0	-6.739311	-4.487136	1.346218
51	1	0	-4.701299	-4.054337	1.878423
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53	1	0	-8.481028	-2.966526	-1.152593
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56	6	0	5.360022	-2.829728	0.221440
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58	6	0	5.522234	-3.824684	1.205416
59	6	0	7.657270	-3.198702	-0.484390
60	1	0	6.326525	-1.785876	-1.409131
61	6	0	6.739421	-4.486927	1.346539
62	1	0	4.701375	-4.054181	1.878645
63	6	0	7.808444	-4.177066	0.502101
64	1	0	8.481161	-2.966416	-1.152315
65	1	0	6.856093	-5.239983	2.119953
66	1	0	8.755336	-4.697125	0.610796
67	6	0	2.733062	3.866613	-0.018610
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69	6	0	3.348223	4.132649	1.222688
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71	1	0	1.942860	4.765846	-1.822731
72	6	0	3.633652	5.440913	1.604340
73	1	0	3.572026	3.314074	1.899891
74	6	0	3.312264	6.505890	0.758414
75	1	0	2.451345	7.083223	-1.134002
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77	1	0	3.542081	7.524459	1.056067
78	6	0	-2.733108	3.866692	-0.018262
79	6	0	-2.396238	4.954247	-0.853168
80	6	0	-3.348299	4.132698	1.223037
81	6	0	-2.691944	6.258818	-0.469323
82	1	0	-1.942722	4.766023	-1.822257
83	6	0	-3.633640	5.440952	1.604778
84	1	0	-3.572189	3.314091	1.900171
85	6	0	-3.312110	6.505973	0.758960
86	1	0	-2.451017	7.083376	-1.133363
87	1	0	-4.099535	5.631240	2.566872
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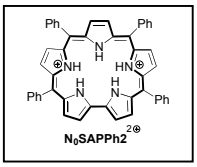
$N_0SAPPh2^{2\oplus}$ (Energy = −2123.44806048)



Stoichiometry C48H35N5(2+)
Framework group C1[X(C48H35N5)]
Deg. of freedom 258
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

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10	6	0	4.840233	-0.223166	-0.733387

11	6	0	2.399444	2.465396	-0.754850
12	6	0	-0.644023	4.158956	0.223501
13	6	0	4.388947	0.997016	-1.185443
14	6	0	0.645078	4.159056	-0.220261
15	6	0	2.725351	-2.940831	0.737750
16	6	0	3.825399	-0.814727	0.055629
17	6	0	0.665090	-3.743114	0.250187
18	6	0	-1.382228	-4.773333	-0.889881
19	6	0	-3.098230	1.239368	0.641122
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21	6	0	2.631939	-4.271299	1.224010
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24	6	0	-2.725306	-2.941138	-0.736917
25	6	0	1.382133	-4.772778	0.892483
26	6	0	-3.868253	-2.124606	-0.589861
27	6	0	-2.631877	-4.271960	-1.222182
28	6	0	-3.825553	-0.814584	-0.056490
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30	1	0	-1.261446	5.020466	0.423285
31	1	0	4.901288	1.664531	-1.860926
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34	1	0	3.409010	-4.782503	1.772865
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40	1	0	-0.000185	0.999297	-0.001446
41	1	0	-1.346472	-1.879034	0.454271
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45	6	0	-3.190492	3.591304	1.355559
46	6	0	-4.327294	4.100813	0.705729
47	6	0	-2.795719	4.150876	2.582446
48	6	0	-5.049915	5.151214	1.270553
49	1	0	-4.633343	3.685311	-0.250414
50	6	0	-3.529516	5.191454	3.151232
51	1	0	-1.922397	3.759332	3.096824
52	6	0	-4.655002	5.695281	2.495269
53	1	0	-5.918770	5.546553	0.753003
54	1	0	-3.222917	5.607553	4.106179
55	1	0	-5.221903	6.509676	2.936077
56	6	0	3.190467	3.591492	-1.355429
57	6	0	4.328757	4.099469	-0.706957
58	6	0	2.794001	4.152823	-2.580993
59	6	0	5.051141	5.150017	-1.271785
60	1	0	4.636107	3.682694	0.248210
61	6	0	3.527563	5.193526	-3.149826
62	1	0	1.919550	3.762475	-3.094356
63	6	0	4.654531	5.695782	-2.495201
64	1	0	5.921133	5.544169	-0.755241
65	1	0	3.219640	5.610946	-4.103768
66	1	0	5.221261	6.510287	-2.936027
67	6	0	-5.205658	-2.691259	-0.873804
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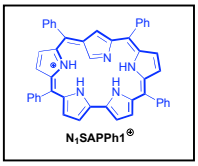
73	1	0	-4.919873	-4.514500	0.258465
74	6	0	-7.756048	-3.723022	-1.441162
75	1	0	-8.074768	-1.897931	-2.546737

76	1	0	-7.156581	-5.423436	-0.256090
77	1	0	-8.741122	-4.123040	-1.661404
78	6	0	5.205800	-2.691159	0.873044
79	6	0	6.125947	-1.950536	1.643471
80	6	0	5.594869	-3.953615	0.379592
81	6	0	7.385270	-2.468883	1.931575
82	1	0	5.835042	-0.983949	2.043705
83	6	0	6.861566	-4.459458	0.657939
84	1	0	4.919019	-4.515093	-0.257861
85	6	0	7.756407	-3.722947	1.439413
86	1	0	8.076136	-1.897175	2.543573
87	1	0	7.155906	-5.424046	0.255849
88	1	0	8.741564	-4.122971	1.659276

Cartesian coordinates for the optimized structures of N-confused *meso*-tetraphenyl-sapphyrins (monocation)

N_1SAPPh1$^{\oplus}$ (Energy = −2123.14019416)

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 Stoichiometry    C48H34N5(1+)
 Framework group  C1[X(C48H34N5)]
 Deg. of freedom   255
 Full point group                 C1
 Largest Abelian subgroup         C1      NOp   1
 Largest concise Abelian subgroup C1      NOp   1
                         Standard orientation:
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 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
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   13          6             0        3.820430   -2.390629    0.202368
   14          6             0        2.578229   -3.048338    0.350125
   15          6             0        2.381787   -4.403850    0.739942
   16          6             0        1.042151   -4.706997    0.638457
   17          6             0        0.350578   -3.544038    0.218717
   18          6             0       -1.042000   -3.458018    0.006975
   19          6             0       -1.902661   -4.560076   -0.250052
   20          6             0       -3.180486   -4.080688   -0.416112
   21          6             0       -3.169622   -2.664882   -0.232054
   22          6             0       -4.283878   -1.802879   -0.206452
   23          6             0       -4.200262   -0.394286   -0.084367
   24          6             0       -5.222866    0.526831    0.303754
   25          6             0       -4.659261    1.781950    0.402561
   26          6             0       -3.275202    1.673454    0.074738
   27          6             0       -2.250699    2.649806    0.044904
   28          1             0        0.364697    3.971330    0.363573
   29          1             0        1.105900    0.253233   -1.746860
   30          1             0        5.555491    1.729259   -1.130507
   31          1             0        6.106203   -0.863232   -0.771920
   32          1             0        3.170010   -5.059421    1.077609
   33          1             0        0.569210   -5.644004    0.897008
   34          1             0       -1.574513   -5.584086   -0.359182
   35          1             0       -4.059499   -4.653331   -0.670518
   36          1             0       -6.245176    0.254343    0.520936
   37          1             0       -5.159843    2.696057    0.685718
   38          7             0       -1.828282   -2.320879   -0.027449
   39          7             0        1.298760   -2.532341    0.099445
   40          1             0       -1.538690   -1.432164    0.357428
   41          1             0        1.143612   -1.714948   -0.476637
   42          1             0       -2.199005    0.113789   -0.742724
   43          1             0        2.199612   -0.124631    0.557856
   44          6             0        5.060130   -3.215198    0.322274
   45          6             0        6.040411   -2.888622    1.274946
   46          6             0        5.281982   -4.316184   -0.523019
   47          6             0        7.205898   -3.646443    1.383737
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56	6	0	2.831644	4.732225	-1.259342
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60	6	0	5.061665	5.212776	0.350535
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62	6	0	4.542375	6.235615	-0.445913
63	1	0	3.022379	6.780478	-1.876840
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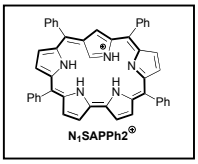
65	1	0	5.001761	7.219782	-0.437006
66	6	0	-2.544408	4.024939	0.517328
67	6	0	-2.199988	5.132811	-0.278551
68	6	0	-3.162535	4.254073	1.760133
69	6	0	-2.479724	6.428703	0.150163
70	1	0	-1.735492	4.968313	-1.246071
71	6	0	-3.431822	5.552216	2.190210
72	1	0	-3.404798	3.411521	2.401028
73	6	0	-3.095471	6.642623	1.385314
74	1	0	-2.222117	7.272441	-0.483641
75	1	0	-3.898747	5.712198	3.157850
76	1	0	-3.310400	7.653454	1.719618
77	6	0	-5.646147	-2.404564	-0.252129
78	6	0	-6.567688	-1.989592	-1.230026
79	6	0	-6.046091	-3.377074	0.681507
80	6	0	-7.847393	-2.540228	-1.278702
81	1	0	-6.268807	-1.247446	-1.964659
82	6	0	-7.328184	-3.922533	0.633257
83	1	0	-5.355273	-3.687005	1.460256
84	6	0	-8.231216	-3.507777	-0.347832
85	1	0	-8.542963	-2.217058	-2.047848
86	1	0	-7.624522	-4.665386	1.368307
87	1	0	-9.229345	-3.934413	-0.385139

N_1SAPPh2$^{\oplus}$ (Energy = −2123.13858153)



Stoichiometry C48H34N5(1+)
Framework group C1[X(C48H34N5)]
Deg. of freedom 255
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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10	6	0	4.928017	0.905052	-0.794202
11	6	0	5.185490	-0.423154	-0.581205

12	6	0	3.981400	-1.064781	-0.128283
13	6	0	3.795582	-2.407470	0.222278
14	6	0	2.536032	-3.033286	0.425001
15	6	0	2.314692	-4.349973	0.908404
16	6	0	0.964545	-4.626083	0.837249
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18	6	0	-1.095524	-3.387924	0.124601
19	6	0	-1.957027	-4.520422	-0.030315
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21	6	0	-3.212057	-2.633672	-0.210653
22	6	0	-4.296834	-1.751042	-0.267761
23	6	0	-4.155167	-0.332349	-0.150378
24	6	0	-5.236999	0.606369	0.092691
25	6	0	-4.655680	1.824103	0.282832
26	6	0	-3.226677	1.628112	0.130613
27	6	0	-2.229034	2.619934	0.186355
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32	1	0	3.091029	-5.000529	1.281415
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35	1	0	-4.106966	-4.661246	-0.457849
36	1	0	-6.289093	0.363777	0.135305
37	1	0	-5.148028	2.767872	0.469859
38	7	0	-1.879349	-2.270066	-0.017063
39	7	0	1.272226	-2.504859	0.146589
40	1	0	-1.652136	-1.292315	0.156593
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42	1	0	2.208449	-0.121690	0.488278
43	1	0	-1.402567	0.637768	-1.408404
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45	6	0	6.005808	-2.914687	1.315323
46	6	0	5.212702	-4.392696	-0.424485
47	6	0	7.154931	-3.693455	1.452222
48	1	0	5.861784	-2.044943	1.950282
49	6	0	6.362621	-5.169312	-0.287637
50	1	0	4.464927	-4.659167	-1.166171
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63	1	0	2.977610	6.702985	-2.123732
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66	6	0	-2.509955	3.950661	0.760365
67	6	0	-2.048339	5.120979	0.125324
68	6	0	-3.236814	4.078889	1.960517
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70	1	0	-1.502475	5.040512	-0.809519
71	6	0	-3.497278	5.335535	2.501681
72	1	0	-3.568399	3.185595	2.480175
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75	1	0	-4.048144	5.415616	3.434304
76	1	0	-3.251030	7.466341	2.275852

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78	6	0	-6.492011	-1.929425	-1.466999
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80	6	0	-7.776589	-2.453587	-1.600762
81	1	0	-6.113521	-1.228115	-2.205219
82	6	0	-7.460945	-3.749283	0.412959
83	1	0	-5.560284	-3.516481	1.396265
84	6	0	-8.264935	-3.364579	-0.661468
85	1	0	-8.395368	-2.152371	-2.441203
86	1	0	-7.839064	-4.446564	1.155145
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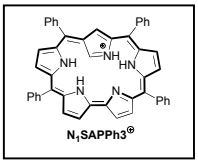
N_1SAPPh3$^{\oplus}$ (Energy = −2123.13693333)



Stoichiometry C48H34N5(1+)
Framework group C1[X(C48H34N5)]
Deg. of freedom 255
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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8	6	0	2.770906	2.369807	-0.465943
9	6	0	3.549837	1.219710	-0.416425
10	6	0	4.931871	0.996107	-0.725674
11	6	0	5.199268	-0.341577	-0.595168
12	6	0	4.006008	-1.014688	-0.161992
13	6	0	3.834866	-2.370846	0.145713
14	6	0	2.587259	-3.001538	0.391727
15	6	0	2.402650	-4.303898	0.935631
16	6	0	1.053972	-4.577511	0.973592
17	6	0	0.350155	-3.452514	0.469801
18	6	0	-1.052756	-3.351724	0.320412
19	6	0	-1.903825	-4.528153	0.469860
20	6	0	-3.169175	-4.111816	0.233344
21	6	0	-3.090081	-2.677354	-0.025475
22	6	0	-4.226202	-1.859297	-0.182122
23	6	0	-4.163828	-0.446896	-0.189779
24	6	0	-5.226355	0.510028	-0.272743
25	6	0	-4.684862	1.763605	-0.129188
26	6	0	-3.263498	1.631572	-0.001499
27	6	0	-2.289740	2.638384	0.054062
28	1	0	0.391255	3.751522	0.749257
29	1	0	1.150484	0.524609	-2.056182
30	1	0	5.605613	1.759995	-1.086974
31	1	0	6.130685	-0.842035	-0.816232
32	1	0	3.206079	-4.937803	1.278798
33	1	0	0.591924	-5.473518	1.361013
34	1	0	-1.573598	-5.531175	0.701362
35	1	0	-4.076778	-4.696585	0.261171
36	1	0	-6.264974	0.262285	-0.433680
37	1	0	-5.206107	2.708840	-0.176521
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45	6	0	6.093502	-2.892566	1.133658
46	6	0	5.214532	-4.349727	-0.582774
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48	1	0	5.981817	-2.030724	1.785602
49	6	0	6.366309	-5.131754	-0.507322
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51	6	0	7.383988	-4.798111	0.389010
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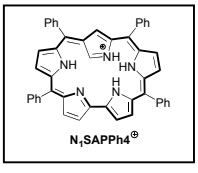
63	1	0	2.929930	6.847494	-1.700895
64	1	0	5.976437	5.423011	0.981768
65	1	0	4.969877	7.271949	-0.342817
66	6	0	-2.649426	3.997465	0.496807
67	6	0	-2.108525	5.132848	-0.140585
68	6	0	-3.541835	4.192254	1.570736
69	6	0	-2.461234	6.413995	0.272278
70	1	0	-1.432525	5.002314	-0.979736
71	6	0	-3.887830	5.476421	1.983579
72	1	0	-3.936142	3.330024	2.099235
73	6	0	-3.351380	6.590995	1.335295
74	1	0	-2.047693	7.277461	-0.240687
75	1	0	-4.567744	5.607147	2.820376
76	1	0	-3.621785	7.592007	1.658421
77	6	0	-5.573863	-2.491588	-0.299150
78	6	0	-5.866309	-3.337070	-1.382370
79	6	0	-6.572568	-2.255366	0.660091
80	6	0	-7.124442	-3.926624	-1.504255
81	1	0	-5.105768	-3.520314	-2.136336
82	6	0	-7.829312	-2.848251	0.538067
83	1	0	-6.354132	-1.621660	1.515245
84	6	0	-8.109326	-3.683656	-0.545002
85	1	0	-7.335934	-4.572396	-2.351839
86	1	0	-8.587135	-2.662827	1.294050
87	1	0	-9.088591	-4.143878	-0.639853

N_1SAPPh4$^{\oplus}$ (Energy = −2123.13265940)



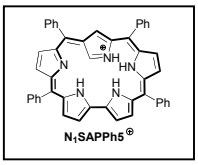
Stoichiometry C48H34N5(1+)
Framework group C1[X(C48H34N5)]
Deg. of freedom 255
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	7	0	-0.824673	1.304584	-1.533690
2	7	0	2.982741	0.205201	-0.144412
3	7	0	-3.012468	-0.013398	-0.185014
4	6	0	-1.322610	2.304957	-0.680408
5	6	0	-0.219329	2.941810	-0.140085
6	6	0	0.531030	1.312768	-1.524654
7	6	0	0.959541	2.303276	-0.628448
8	6	0	2.325535	2.589975	-0.242475
9	6	0	3.265190	1.569744	-0.130949
10	6	0	4.696020	1.672736	-0.022308
11	6	0	5.218618	0.409527	0.036499
12	6	0	4.130704	-0.525899	-0.027353
13	6	0	4.183027	-1.940280	0.028196
14	6	0	3.041201	-2.756318	-0.020502
15	6	0	3.101504	-4.211576	-0.153893
16	6	0	1.823928	-4.637675	-0.263162
17	6	0	0.986664	-3.441720	-0.169301
18	6	0	-0.422063	-3.538733	-0.217824
19	6	0	-1.169888	-4.698879	-0.531977
20	6	0	-2.512305	-4.392836	-0.448190
21	6	0	-2.644066	-3.027873	-0.080431
22	6	0	-3.871336	-2.326124	0.073180
23	6	0	-4.014438	-0.934852	0.047500
24	6	0	-5.215703	-0.159946	0.231610
25	6	0	-4.913533	1.165079	0.091240
26	6	0	-3.503574	1.294956	-0.168939
27	6	0	-2.722678	2.430997	-0.336230
28	1	0	-0.255913	3.721032	0.606998
29	1	0	1.102930	0.677408	-2.185883
30	1	0	5.242712	2.604040	-0.036139
31	1	0	6.259758	0.134223	0.111936
32	1	0	4.005060	-4.802299	-0.187292
33	1	0	1.475848	-5.654646	-0.378877
34	1	0	-0.747151	-5.646542	-0.832014
35	1	0	-3.343514	-5.045664	-0.668013
36	1	0	-6.183942	-0.586873	0.445913
37	1	0	-5.599916	1.996787	0.150126
38	7	0	-1.345171	-2.521256	0.015352
39	7	0	1.730736	-2.320489	-0.027176
40	1	0	2.075919	-0.259739	-0.096670
41	1	0	-1.381177	0.846403	-2.244752
42	1	0	-2.062731	-0.250773	-0.420994
43	1	0	-1.091640	-1.726596	0.587536
44	6	0	5.532874	-2.573492	0.129871
45	6	0	6.478436	-2.426565	-0.898433
46	6	0	5.879894	-3.327454	1.262824
47	6	0	7.736986	-3.019357	-0.796013
48	1	0	6.217874	-1.860630	-1.788864
49	6	0	7.139688	-3.917987	1.364503
50	1	0	5.161105	-3.438668	2.069885
51	6	0	8.071213	-3.765461	0.335945
52	1	0	8.453586	-2.903847	-1.604286
53	1	0	7.394179	-4.493290	2.250142
54	1	0	9.051728	-4.225939	0.415322
55	6	0	2.689182	3.981208	0.087752
56	6	0	2.221483	5.043927	-0.712386
57	6	0	3.490312	4.286422	1.206540
58	6	0	2.570314	6.358809	-0.421411
59	1	0	1.603936	4.826827	-1.578540
60	6	0	3.827807	5.605676	1.500767
61	1	0	3.816504	3.486736	1.864039
62	6	0	3.374955	6.644776	0.685641
63	1	0	2.217543	7.163318	-1.060172
64	1	0	4.435666	5.822856	2.374241
65	1	0	3.639965	7.672683	0.915288

66	6	0	-3.241811	3.783041	-0.041965
67	6	0	-2.918336	4.861638	-0.888856
68	6	0	-4.044852	4.037920	1.086875
69	6	0	-3.405820	6.139965	-0.632823
70	1	0	-2.297728	4.685172	-1.762441
71	6	0	-4.527947	5.319607	1.342462
72	1	0	-4.259683	3.233211	1.783148
73	6	0	-4.215140	6.373857	0.482048
74	1	0	-3.158351	6.955139	-1.306791
75	1	0	-5.137791	5.497642	2.223539
76	1	0	-4.591977	7.372412	0.683043
77	6	0	-5.107033	-3.156982	0.205198
78	6	0	-6.145136	-3.063967	-0.737095
79	6	0	-5.247447	-4.057066	1.275046
80	6	0	-7.295184	-3.842734	-0.607577
81	1	0	-6.040475	-2.389986	-1.582848
82	6	0	-6.398152	-4.833925	1.404031
83	1	0	-4.454634	-4.136050	2.013616
84	6	0	-7.425321	-4.728337	0.463798
85	1	0	-8.085250	-3.763498	-1.348933
86	1	0	-6.494238	-5.518356	2.242081
87	1	0	-8.320794	-5.334780	0.564194

N_1SAPPh5$^{\oplus}$ (Energy = −2123.12980006)



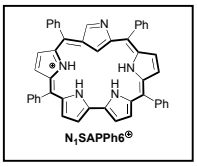
Stoichiometry C48H34N5(1+)
Framework group C1[X(C48H34N5)]
Deg. of freedom 255
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.800576	1.249024	-1.516882
2	7	0	2.947290	0.185771	-0.146311
3	7	0	-3.021890	-0.023752	-0.186363
4	6	0	-1.318073	2.282489	-0.710723
5	6	0	-0.226033	2.939227	-0.171849
6	6	0	0.554021	1.258808	-1.476198
7	6	0	0.962487	2.278774	-0.605280
8	6	0	2.315844	2.556497	-0.186451
9	6	0	3.262191	1.532175	-0.093751
10	6	0	4.701650	1.706287	0.036606
11	6	0	5.241407	0.460164	0.051099
12	6	0	4.123654	-0.468577	-0.054241
13	6	0	4.236318	-1.897028	-0.000559
14	6	0	3.135093	-2.752339	0.019225
15	6	0	3.131482	-4.184423	-0.054869
16	6	0	1.833169	-4.608623	-0.086398
17	6	0	0.978896	-3.456405	-0.031839
18	6	0	-0.428650	-3.532221	-0.075514
19	6	0	-1.163166	-4.696925	-0.389779
20	6	0	-2.510292	-4.396102	-0.350925
21	6	0	-2.660720	-3.029422	-0.013893
22	6	0	-3.891937	-2.327282	0.100172
23	6	0	-4.031652	-0.936611	0.043201
24	6	0	-5.234505	-0.154903	0.184604
25	6	0	-4.925177	1.165761	0.019717
26	6	0	-3.510199	1.286581	-0.214316
27	6	0	-2.722526	2.415850	-0.393503

28	1	0	-0.279745	3.743371	0.547256
29	1	0	1.150748	0.597832	-2.085911
30	1	0	5.223981	2.651870	0.062527
31	1	0	6.284511	0.192150	0.136189
32	1	0	4.019368	-4.797124	-0.094053
33	1	0	1.486270	-5.630570	-0.129483
34	1	0	-0.729449	-5.645268	-0.672762
35	1	0	-3.329288	-5.058854	-0.586275
36	1	0	-6.208253	-0.574520	0.388226
37	1	0	-5.610368	2.000215	0.045209
38	7	0	-1.364278	-2.504138	0.109450
39	7	0	1.797110	-2.359036	0.047592
40	1	0	-1.339804	0.777854	-2.232870
41	1	0	-2.070961	-0.270979	-0.408326
42	1	0	-1.172320	-1.739970	0.746291
43	1	0	1.577698	-1.362174	0.011661
44	6	0	5.595129	-2.508013	0.030930
45	6	0	6.506162	-2.279916	-1.014995
46	6	0	5.992053	-3.320665	1.106713
47	6	0	7.775084	-2.856351	-0.988048
48	1	0	6.208963	-1.662626	-1.858008
49	6	0	7.265110	-3.889888	1.134739
50	1	0	5.306104	-3.485483	1.932863
51	6	0	8.158644	-3.661558	0.086935
52	1	0	8.463477	-2.679312	-1.809480
53	1	0	7.560049	-4.506561	1.978972
54	1	0	9.149289	-4.106352	0.108332
55	6	0	-5.129760	-3.157302	0.216214
56	6	0	-6.144630	-3.080601	-0.752545
57	6	0	-5.296412	-4.040532	1.296303
58	6	0	-7.297389	-3.857864	-0.638725
59	1	0	-6.019968	-2.419674	-1.605870
60	6	0	-6.449272	-4.816721	1.409234
61	1	0	-4.522272	-4.106809	2.055752
62	6	0	-7.453347	-4.726772	0.442766
63	1	0	-8.069382	-3.790477	-1.400056
64	1	0	-6.565562	-5.487849	2.255481
65	1	0	-8.350839	-5.332144	0.530920
66	6	0	2.657560	3.942711	0.188249
67	6	0	2.207582	5.024345	-0.596258
68	6	0	3.421376	4.221381	1.339440
69	6	0	2.537295	6.333243	-0.258245
70	1	0	1.621578	4.827588	-1.488843
71	6	0	3.736087	5.534223	1.683001
72	1	0	3.738690	3.403704	1.978542
73	6	0	3.301552	6.592946	0.882999
74	1	0	2.200516	7.152996	-0.886242
75	1	0	4.314750	5.730914	2.580861
76	1	0	3.551169	7.615762	1.150001
77	6	0	-3.246251	3.775052	-0.141686
78	6	0	-2.909491	4.832025	-1.010095
79	6	0	-4.066236	4.057370	0.968191
80	6	0	-3.401046	6.116184	-0.793455
81	1	0	-2.275099	4.633713	-1.868897
82	6	0	-4.552802	5.344889	1.184687
83	1	0	-4.291768	3.269965	1.680717
84	6	0	-4.226996	6.377384	0.302959
85	1	0	-3.143180	6.914477	-1.483535
86	1	0	-5.175602	5.544774	2.051921
87	1	0	-4.606598	7.380580	0.473430

N_1SAPPh6$^{\oplus}$ (Energy = −2123.11217758)

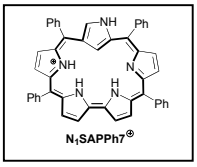


Stoichiometry C48H34N5(1+)
Framework group C1[X(C48H34N5)]
Deg. of freedom 255
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.540632	-2.546506	-0.215963
2	7	0	1.435891	-2.583998	0.222562
3	7	0	2.797262	0.056504	0.008353
4	7	0	-2.821518	0.119064	-0.009789
5	6	0	-2.401801	2.478775	0.733008
6	6	0	3.192548	1.235633	-0.628583
7	6	0	-1.052534	2.652669	0.324852
8	6	0	3.864355	-2.163608	0.544212
9	6	0	-0.737783	-3.675336	-0.207001
10	6	0	4.939447	-0.224292	-0.655405
11	6	0	2.455576	2.433718	-0.756090
12	6	0	-0.516456	4.006407	0.099591
13	6	0	4.519561	1.012127	-1.090647
14	6	0	2.706333	-2.951915	0.671049
15	6	0	3.871644	-0.839534	0.048405
16	6	0	0.603714	-3.689751	0.228696
17	6	0	-1.492284	-4.734434	-0.757894
18	6	0	-3.183790	1.317605	0.612944
19	6	0	1.107672	2.651947	-0.384703
20	6	0	2.598931	-4.305858	1.095529
21	6	0	-4.985597	-0.075400	0.618237
22	6	0	-4.528977	1.144598	1.054302
23	6	0	-2.818650	-2.885830	-0.661702
24	6	0	1.330605	-4.763194	0.791998
25	6	0	-3.956976	-2.063236	-0.544384
26	6	0	-2.748164	-4.246076	-1.069811
27	6	0	-3.926379	-0.737816	-0.062728
28	1	0	5.883631	-0.704048	-0.867094
29	1	0	-1.075191	4.926195	0.226419
30	1	0	5.073395	1.704072	-1.705958
31	1	0	-1.109097	-5.725152	-0.960412
32	1	0	3.388975	-4.859623	1.580284
33	1	0	-5.950822	-0.518689	0.814077
34	1	0	-5.068933	1.858999	1.656683
35	1	0	0.920444	-5.740392	1.006691
36	1	0	-3.552641	-4.784659	-1.547791
37	1	0	-1.394103	-1.774355	0.423249
38	7	0	0.703084	4.008923	-0.330213
39	6	0	0.027024	1.803087	-0.010003
40	1	0	0.036906	0.720514	0.026146
41	1	0	1.306589	-1.813252	-0.421900
42	1	0	-2.086808	0.096059	-0.707086
43	1	0	2.076030	0.062822	0.719301
44	6	0	3.213055	3.598573	-1.310523
45	6	0	4.371706	4.074620	-0.676602
46	6	0	2.781205	4.226266	-2.490052
47	6	0	5.080962	5.151546	-1.208896
48	1	0	4.703214	3.614232	0.249851
49	6	0	3.499982	5.289558	-3.029641
50	1	0	1.881594	3.872511	-2.983512
51	6	0	4.650805	5.757212	-2.389992
52	1	0	5.966776	5.517932	-0.697785

53	1	0	3.158690	5.758242	-3.948269
54	1	0	5.205568	6.592402	-2.807955
55	6	0	5.189415	-2.784608	0.819646
56	6	0	6.088558	-2.152283	1.697458
57	6	0	5.580916	-3.988255	0.205738
58	6	0	7.334256	-2.716264	1.966380
59	1	0	5.797414	-1.225319	2.182848
60	6	0	6.830811	-4.545646	0.470538
61	1	0	4.913369	-4.470966	-0.501756
62	6	0	7.708791	-3.914224	1.354194
63	1	0	8.011160	-2.221299	2.656652
64	1	0	7.122773	-5.468926	-0.021525
65	1	0	8.681336	-4.351167	1.561082
66	6	0	-5.297997	-2.651990	-0.817424
67	6	0	-6.173222	-2.012075	-1.713286
68	6	0	-5.726930	-3.832477	-0.184301
69	6	0	-7.433258	-2.545266	-1.979363
70	1	0	-5.852584	-1.103490	-2.214755
71	6	0	-6.990184	-4.359934	-0.447378
72	1	0	-5.077008	-4.321272	0.535372
73	6	0	-7.845045	-3.720631	-1.347891
74	1	0	-8.091700	-2.044501	-2.683229
75	1	0	-7.310450	-5.265987	0.058948
76	1	0	-8.828035	-4.134259	-1.553388
77	6	0	-3.086641	3.671084	1.325736
78	6	0	-4.229875	4.234253	0.733569
79	6	0	-2.572300	4.259688	2.493778
80	6	0	-4.842508	5.353357	1.297056
81	1	0	-4.623923	3.806239	-0.183882
82	6	0	-3.192569	5.371819	3.061467
83	1	0	-1.689824	3.832932	2.961911
84	6	0	-4.328341	5.922120	2.464192
85	1	0	-5.717538	5.785017	0.819596
86	1	0	-2.787643	5.808677	3.969762
87	1	0	-4.807861	6.792222	2.903116

N_1SAPPh7$^{\oplus}$ (Energy = −2123.13051234)



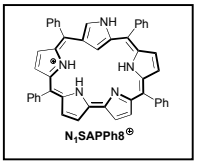
Stoichiometry C48H34N5(1+)
Framework group C1[X(C48H34N5)]
Deg. of freedom 255
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.444598	-2.497462	-0.462837
2	7	0	1.597411	-2.502680	-0.198802
3	7	0	2.762772	0.013161	0.043224
4	7	0	-2.854286	0.045330	0.108494
5	6	0	-2.568577	2.473463	0.542513
6	6	0	3.205237	1.302714	-0.144976
7	6	0	-1.218489	2.613996	0.023279
8	6	0	3.936658	-2.125657	0.462401
9	6	0	-0.579232	-3.518151	-0.832409
10	6	0	5.051553	0.148114	0.447330
11	6	0	2.442749	2.420643	-0.518415
12	6	0	-0.863916	3.753618	-0.735213
13	6	0	4.640624	1.392376	0.103612
14	6	0	2.864422	-2.957966	0.137281

15	6	0	3.872835	-0.701790	0.369691
16	6	0	0.800230	-3.556661	-0.552630
17	6	0	-1.357524	-4.513484	-1.462937
18	6	0	-3.251121	1.274370	0.654805
19	6	0	1.021432	2.541418	-0.472679
20	6	0	2.829761	-4.385303	0.017534
21	6	0	-4.922281	-0.241933	0.983530
22	6	0	-4.531879	1.036850	1.263237
23	6	0	-2.755642	-2.873604	-0.739967
24	6	0	1.587506	-4.744405	-0.439367
25	6	0	-3.912658	-2.178787	-0.305498
26	6	0	-2.681526	-4.114511	-1.423568
27	6	0	-3.893886	-0.879315	0.213039
28	1	0	6.050657	-0.175760	0.699248
29	1	0	-1.490533	4.562633	-1.081284
30	1	0	5.234997	2.292761	0.053311
31	1	0	-0.961078	-5.403818	-1.931148
32	1	0	3.651870	-5.042370	0.258547
33	1	0	-5.823235	-0.737548	1.314170
34	1	0	-5.060466	1.760079	1.866493
35	1	0	1.216986	-5.745068	-0.611854
36	1	0	-3.530785	-4.634343	-1.841140
37	1	0	-1.224489	-1.838832	0.273890
38	7	0	0.434798	3.689099	-1.029084
39	6	0	-0.028756	1.844771	0.152797
40	1	0	0.105610	0.944770	0.734760
41	1	0	1.441085	-1.494717	-0.286415
42	1	0	-2.174839	0.008220	-0.642108
43	1	0	0.953948	4.373575	-1.563254
44	6	0	-3.261384	3.732472	0.921489
45	6	0	-4.558033	4.031776	0.459849
46	6	0	-2.611502	4.675759	1.742719
47	6	0	-5.186867	5.222218	0.820619
48	1	0	-5.059761	3.338035	-0.207941
49	6	0	-3.245714	5.860964	2.108663
50	1	0	-1.616011	4.456959	2.117765
51	6	0	-4.535476	6.138418	1.649367
52	1	0	-6.182575	5.439552	0.444645
53	1	0	-2.735261	6.566401	2.758201
54	1	0	-5.027570	7.064717	1.931265
55	6	0	3.198484	3.626675	-0.986842
56	6	0	4.021058	3.544933	-2.124547
57	6	0	3.104180	4.857933	-0.310695
58	6	0	4.724153	4.662032	-2.574768
59	1	0	4.098460	2.601758	-2.656991
60	6	0	3.818591	5.970184	-0.756461
61	1	0	2.493565	4.931185	0.585319
62	6	0	4.626734	5.876078	-1.891612
63	1	0	5.349055	4.582947	-3.459651
64	1	0	3.749965	6.907417	-0.211615
65	1	0	5.179777	6.743504	-2.239884
66	6	0	-5.221210	-2.891360	-0.366259
67	6	0	-5.390986	-4.149539	0.238621
68	6	0	-6.317602	-2.312137	-1.028905
69	6	0	-6.619375	-4.806039	0.182202
70	1	0	-4.559718	-4.603111	0.770539
71	6	0	-7.545134	-2.970967	-1.085988
72	1	0	-6.197504	-1.348651	-1.516044
73	6	0	-7.699726	-4.219565	-0.480827
74	1	0	-6.735043	-5.772912	0.663723
75	1	0	-8.378535	-2.511906	-1.610196
76	1	0	-8.655957	-4.732780	-0.525287
77	6	0	5.229020	-2.762997	0.849079
78	6	0	5.765677	-2.542035	2.128709
79	6	0	5.931148	-3.587791	-0.045249

80	6	0	6.966277	-3.141562	2.506973
81	1	0	5.229796	-1.909274	2.830664
82	6	0	7.135578	-4.181212	0.333739
83	1	0	5.541595	-3.744144	-1.047260
84	6	0	7.654292	-3.962809	1.611063
85	1	0	7.362724	-2.968978	3.503515
86	1	0	7.671260	-4.808923	-0.372764
87	1	0	8.591114	-4.426708	1.905818

N_1SAPPh8$^{\oplus}$ (Energy = −2123.13611503)

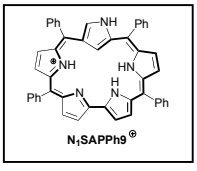


Stoichiometry C48H34N5(1+)
Framework group C1[X(C48H34N5)]
Deg. of freedom 255
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.404173	-2.529166	-0.470652
2	7	0	1.543121	-2.450606	-0.280996
3	7	0	2.829087	0.049608	0.051357
4	7	0	-2.848415	0.031717	0.070063
5	6	0	-2.612929	2.498484	0.285502
6	6	0	3.208614	1.383111	0.077021
7	6	0	-1.237407	2.631883	-0.149279
8	6	0	3.920459	-2.163749	0.308088
9	6	0	-0.554776	-3.501167	-0.963345
10	6	0	4.965984	0.112911	0.776011
11	6	0	2.466878	2.513705	-0.277432
12	6	0	-0.825658	3.753384	-0.904310
13	6	0	4.565974	1.400861	0.552212
14	6	0	2.822292	-2.925788	-0.130440
15	6	0	3.888103	-0.755833	0.408598
16	6	0	0.842019	-3.489735	-0.790700
17	6	0	-1.369169	-4.502576	-1.550068
18	6	0	-3.270474	1.294545	0.500116
19	6	0	1.044384	2.592581	-0.404583
20	6	0	2.915878	-4.315743	-0.572756
21	6	0	-4.883988	-0.228880	1.018325
22	6	0	-4.535585	1.087153	1.146194
23	6	0	-2.724495	-2.922889	-0.634346
24	6	0	1.681584	-4.658074	-1.016006
25	6	0	-3.862095	-2.241483	-0.141676
26	6	0	-2.688737	-4.151609	-1.353431
27	6	0	-3.853747	-0.907435	0.289512
28	1	0	5.918986	-0.220684	1.157592
29	1	0	-1.425872	4.536839	-1.343097
30	1	0	5.133406	2.301011	0.734798
31	1	0	-1.000390	-5.371712	-2.076290
32	1	0	3.813001	-4.917613	-0.570454
33	1	0	-5.761437	-0.714671	1.418737
34	1	0	-5.079077	1.855290	1.676311
35	1	0	1.360176	-5.608007	-1.421658
36	1	0	-3.564679	-4.682996	-1.694613
37	1	0	-1.087084	-1.850662	0.209022
38	7	0	0.500079	3.711917	-1.051565
39	6	0	-0.050798	1.886952	0.121382
40	1	0	0.024053	1.016998	0.759583
41	1	0	-2.162463	-0.070551	-0.667803

42	1	0	1.059338	4.390671	-1.551241
43	1	0	1.962917	-0.364594	-0.288869
44	6	0	5.201809	-2.863068	0.620070
45	6	0	5.241227	-3.833868	1.635264
46	6	0	6.380938	-2.585671	-0.092279
47	6	0	6.428462	-4.501458	1.935089
48	1	0	4.338148	-4.052381	2.198124
49	6	0	7.566202	-3.257472	0.205912
50	1	0	6.360609	-1.856451	-0.897316
51	6	0	7.593906	-4.215135	1.221736
52	1	0	6.442971	-5.243001	2.728815
53	1	0	8.466355	-3.038158	-0.361406
54	1	0	8.517857	-4.736782	1.454162
55	6	0	3.239065	3.771880	-0.513578
56	6	0	2.950860	4.947015	0.207843
57	6	0	4.270146	3.807516	-1.470678
58	6	0	3.678392	6.115147	-0.015637
59	1	0	2.174085	4.930746	0.967419
60	6	0	4.989874	4.979978	-1.698217
61	1	0	4.494068	2.912785	-2.043864
62	6	0	4.697686	6.135614	-0.970791
63	1	0	3.455577	7.006988	0.563068
64	1	0	5.776864	4.991127	-2.446703
65	1	0	5.261590	7.047124	-1.145973
66	6	0	-3.367096	3.760207	0.504354
67	6	0	-2.804201	4.805705	1.263979
68	6	0	-4.646609	3.954545	-0.052157
69	6	0	-3.502933	5.992797	1.473124
70	1	0	-1.827537	4.666321	1.718022
71	6	0	-5.339551	5.146349	0.151303
72	1	0	-5.082638	3.174823	-0.669247
73	6	0	-4.772153	6.167790	0.916677
74	1	0	-3.059985	6.779224	2.077613
75	1	0	-6.319719	5.281763	-0.296936
76	1	0	-5.314682	7.095082	1.076209
77	6	0	-5.148365	-2.993294	-0.083951
78	6	0	-5.227467	-4.226729	0.587069
79	6	0	-6.307599	-2.487573	-0.698333
80	6	0	-6.430171	-4.928979	0.645461
81	1	0	-4.344551	-4.624329	1.079060
82	6	0	-7.509077	-3.192737	-0.641036
83	1	0	-6.258011	-1.546677	-1.238891
84	6	0	-7.574233	-4.414513	0.031623
85	1	0	-6.475227	-5.875319	1.176882
86	1	0	-8.392477	-2.791295	-1.129430
87	1	0	-8.510587	-4.963140	0.076322

N_1SAPPh9$^{\oplus}$ (Energy = −2123.13612733)

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Stoichiometry    C48H34N5(1+)
Framework group  C1[X(C48H34N5)]
Deg. of freedom   255
Full point group                 C1
Largest Abelian subgroup         C1      NOp   1
Largest concise Abelian subgroup C1      NOp   1
                       Standard orientation:
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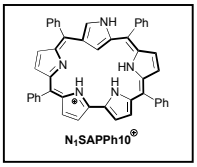
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.502802	-2.465146	-0.308776
2	7	0	-1.446946	-2.521872	-0.457784
3	7	0	-2.849199	0.050813	0.075129

4	7	0	2.830246	0.026464	0.038298
5	6	0	2.512926	2.502767	-0.259622
6	6	0	-3.252635	1.325493	0.477778
7	6	0	1.088727	2.620329	-0.420964
8	6	0	-3.899837	-2.205648	-0.105321
9	6	0	0.789764	-3.493904	-0.814046
10	6	0	-4.896873	-0.157523	1.013579
11	6	0	-2.570313	2.513443	0.253566
12	6	0	0.525703	3.737018	-1.081663
13	6	0	-4.527831	1.153936	1.117416
14	6	0	-2.771567	-2.903153	-0.609652
15	6	0	-3.873418	-0.869901	0.304379
16	6	0	-0.611907	-3.495840	-0.970532
17	6	0	1.616414	-4.670161	-1.055008
18	6	0	3.229510	1.356699	0.096148
19	6	0	-1.191322	2.595901	-0.160114
20	6	0	-2.756154	-4.125139	-1.334508
21	6	0	4.954617	0.043033	0.797010
22	6	0	4.576667	1.342230	0.596833
23	6	0	2.781997	-2.953985	-0.170313
24	6	0	-1.439560	-4.485636	-1.551734
25	6	0	3.885692	-2.210547	0.271264
26	6	0	2.857569	-4.342913	-0.622313
27	6	0	3.869909	-0.798949	0.394648
28	1	0	-5.786372	-0.619319	1.415890
29	1	0	1.012483	4.506026	-1.661985
30	1	0	-5.063038	1.943166	1.624606
31	1	0	1.281224	-5.614164	-1.463310
32	1	0	-3.640458	-4.647962	-1.667307
33	1	0	5.895377	-0.313621	1.187760
34	1	0	5.153545	2.228797	0.812603
35	1	0	-1.085456	-5.354322	-2.088646
36	1	0	3.749022	-4.953009	-0.632858
37	7	0	-0.797997	3.713099	-0.912072
38	6	0	-0.020759	1.884570	0.113917
39	1	0	0.041731	1.021362	0.762390
40	1	0	1.960511	-0.366060	-0.317037
41	1	0	-1.451665	4.393015	-1.277675
42	1	0	-2.160031	-0.074617	-0.656078
43	1	0	-1.115522	-1.849958	0.221604
44	6	0	-5.190120	-2.948182	-0.025871
45	6	0	-6.353094	-2.442138	-0.632713
46	6	0	-5.268323	-4.174995	0.657305
47	6	0	-7.558154	-3.139336	-0.554297
48	1	0	-6.303633	-1.507885	-1.184652
49	6	0	-6.474458	-4.869009	0.736958
50	1	0	-4.381725	-4.573928	1.141503
51	6	0	-7.622737	-4.353591	0.131632
52	1	0	-8.444628	-2.737740	-1.036969
53	1	0	-6.518851	-5.810030	1.277798
54	1	0	-8.561661	-4.896232	0.192604
55	6	0	-3.298716	3.799809	0.436014
56	6	0	-4.555417	4.018297	-0.160985
57	6	0	-2.732790	4.839849	1.200941
58	6	0	-5.228228	5.226826	0.014390
59	1	0	-4.993766	3.240013	-0.778537
60	6	0	-3.408655	6.045458	1.376638
61	1	0	-1.771450	4.683747	1.682547
62	6	0	-4.658762	6.242934	0.784477
63	1	0	-6.194076	5.378063	-0.459117
64	1	0	-2.964036	6.828367	1.984433
65	1	0	-5.184079	7.183727	0.920493
66	6	0	3.310302	3.748159	-0.448500
67	6	0	4.394708	3.776666	-1.345760
68	6	0	2.993248	4.924184	0.258776

69	6	0	5.132014	4.944342	-1.533962
70	1	0	4.639784	2.883057	-1.911763
71	6	0	3.742205	6.085967	0.080177
72	1	0	2.177447	4.911418	0.975610
73	6	0	4.810467	6.100796	-0.819565
74	1	0	5.955627	4.952187	-2.242023
75	1	0	3.496411	6.978022	0.649211
76	1	0	5.390027	7.008202	-0.962323
77	6	0	5.161510	-2.924666	0.571960
78	6	0	6.342667	-2.644599	-0.136183
79	6	0	5.193925	-3.911212	1.572136
80	6	0	7.522520	-3.330516	0.150431
81	1	0	6.328172	-1.901732	-0.928779
82	6	0	6.376116	-4.592622	1.860811
83	1	0	4.289551	-4.130889	2.132401
84	6	0	7.543211	-4.304357	1.151118
85	1	0	8.424118	-3.109302	-0.413815
86	1	0	6.385299	-5.346374	2.643016
87	1	0	8.463249	-4.836628	1.374788

N_1SAPPh10$^{\oplus}$ (Energy = −2123.13035388)

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Stoichiometry    C48H34N5(1+)
Framework group  C1[X(C48H34N5)]
Deg. of freedom   255
Full point group                 C1
Largest Abelian subgroup         C1      NOp   1
Largest concise Abelian subgroup C1      NOp   1
                      Standard orientation:
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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.563872	-2.512866	-0.220235
2	7	0	-1.483574	-2.506942	-0.407752
3	7	0	-2.873201	0.047054	0.106319
4	7	0	2.793482	-0.005670	0.014753
5	6	0	2.491971	2.444037	-0.331001
6	6	0	-3.268196	1.314326	0.547145
7	6	0	1.065382	2.570924	-0.446820
8	6	0	-3.947895	-2.184941	-0.173382
9	6	0	0.766535	-3.538544	-0.650621
10	6	0	-4.946597	-0.162414	0.992087
11	6	0	-2.571509	2.496119	0.360445
12	6	0	0.485908	3.687189	-1.094553
13	6	0	-4.556754	1.135075	1.161068
14	6	0	-2.802064	-2.883724	-0.642673
15	6	0	-3.918733	-0.864282	0.275385
16	6	0	-0.626500	-3.500870	-0.860514
17	6	0	1.581140	-4.709244	-0.732834
18	6	0	3.220201	1.304043	0.046569
19	6	0	-1.200757	2.569004	-0.093510
20	6	0	-2.751169	-4.100213	-1.364907
21	6	0	5.000981	0.104651	0.743943
22	6	0	4.601587	1.378555	0.510158
23	6	0	2.859558	-2.973877	-0.022152
24	6	0	-1.424847	-4.478666	-1.490635
25	6	0	3.942343	-2.169274	0.335413
26	6	0	2.848862	-4.370881	-0.334077
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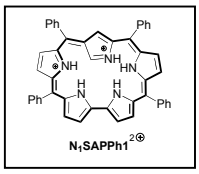
Cartesian coordinates for the optimized structures of N-confused *meso*-tetraphenyl-sapphyrins (dication)

N_1SAPPh1$^{2\oplus}$ (Energy = −2123.45257857)

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 Stoichiometry    C48H35N5(2+)
 Framework group  C1[X(C48H35N5)]
 Deg. of freedom   258
 Full point group                 C1
 Largest Abelian subgroup         C1      NOp   1
 Largest concise Abelian subgroup C1      NOp   1
                        Standard orientation:
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 Number     Number      Type              X           Y           Z
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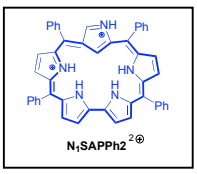
N_1SAPPh2$^{2\oplus}$ (Energy = −2123.45566447)



Stoichiometry C48H35N5(2+)
Framework group C1[X(C48H35N5)]
Deg. of freedom 258
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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83	6	0	-6.904631	-4.489224	-0.458138
84	1	0	-5.003497	-4.411888	0.542789
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87	1	0	-7.214053	-5.397513	0.050067
88	1	0	-8.736183	-4.300787	-1.580375

Calculation details. All the DFT calculations were performed with a Gaussian 03 program package[1] without symmetry assumption. Initial structures are arbitrarily generated. The geometries were fully optimized at the Becke's three-parameter hybrid functional[2] combined with the Lee-Yang-Parr correlation functional[3] abbreviated as the B3LYP level of density functional theory.

[1] Gaussian 03, Revision D.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; and Pople, J. A.; Gaussian, Inc., Wallingford CT, 2004.

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

[3] C. Lee, W. Yang, R. G. Parr, *Phys. Rev. B* **1988**, *37*, 785-789.