Supporting Information

for

N-Confused and N-Fused meso-Aryl Sapphyrins

Iti Gupta, a Alagar Srinivasan, Tatsuki Morimoto, Motoki Toganoh, and Hiroyuki Furuta*

Department of Chemistry and Biochemistry, Graduate School of Engineering
Kyushu University, Fukuoka 819-0395, Japan
Fax: (+81) 92-802-2865, E-mail: hfuruta@cstf.kyushu-u.ac.jp

aCurrent address: BITS-Pilani, Goa Campus, Near NH-17B,
Bye Pass Road Zuarinagar, Goa 403 726 (India)

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S1
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 pentapyrane* (3, 234 mg, 0.223 mmol) and NH₄Cl (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 °C (dec). ¹H NMR (300 MHz, CDCl₃, 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), 1.07 (s, 1H).

1H NMR (300 MHz, CD₂Cl₂, 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: C₄₈H₁₃N₅F₂₀, calcd 1039.1, obsd m/z 1039.5 (M+). HRMS (ESI+) m/z; found: 1040.07969, calcd for C₄₈H₁₄F₂₀N₅ (MH⁺): 1040.09298. UV-Vis λₓmax/nm (ε/mol¹ dm³ 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 °C (dec). ¹H NMR (300 MHz, CDCl₃, 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: C₄₈H₁₁N₂F₂₀, calcd 1037.1, obsd m/z 1037.6 (M⁺). HRMS (ESI−) m/z; found: 1036.06466, calcd for C₄₈H₁₀F₂₀N₅ ([M–H]⁻): 1036.06168. UV-Vis λₓmax/nm (ε/mol¹ dm³ 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).

S2
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’-Bipyrrrole (14 mg, 0.106 mmol) and bis-carbinol derivative of N-confused pentafluorophenyl tripyrrane** (4, 100 mg, 0.106 mmol) were dissolved in dry CH₂Cl₂ (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 CH₂Cl₂ (200 mL) was added, the solution was stirred at room temperature under N₂ atm. After 1 h, a solution of N-confused tripyrrane (3.0 g, 5.38 mmol) in 100 mL of CH₂Cl₂ was added dropwise at room temperature. After stirring for 12 h, water and aqueous NaOH solution were added. The aqueous layer was extracted with CH₂Cl₂ and the combined extracts were washed with brine, dried over anhydrous Na₂SO₄. After evaporation, the products were separated by silica gel column chromatography (eluted with 90% CH₂Cl₂/n-hexane). Bis(benzoyl/pentafluorophenyl) tripyrrane was obtained in
25% yield (1.29 g). Brown solid. \(^1\)H NMR (300 MHz, CDCl\(_3\), \(\delta\) in ppm) 5.89 (s, 2H, meso-H), 6.08 (m, 2H, \(\beta\)H), 6.14 (m, 2H, \(\beta\)H), 6.64 (m, 2H, \(\beta\)H and \(\epsilon\)CH), 8.27 (s, br, 1H, NH), 9.62 (s, br, 2H, NH). MALDI-TOF-MS: C\(_{48}\)H\(_{11}\)N\(_3\)F\(_{20}\)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\(_2\)SO\(_4\). 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 \(\mu\)L, 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\(_2\)SO\(_4\), 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\(_2\)Cl\(_2\)/hexane) affording N-confused pentaapyrrane (3) in 71% yield (0.54 g). Brown flaky solid. \(^1\)H NMR (300 MHz, CDCl\(_3\), \(\delta\) in ppm) 5.63 (s, 1H, meso-H), 5.73 (s, 1H, meso-H), 5.82 (m, 4H, \(\beta\)H + meso-H), 5.90-5.97 (m, 5H, \(\beta\)H), 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](image)


**[3+2] route for normal sapphyrin**

2,2’-Bipyrrrole (17 mg, 0.128 mmol) and bis-carbinol derivative of pentafluorophenyl tripyrrane (120 mg, 0.170 mmol) were dissolved in dry CH\(_2\)Cl\(_2\) (60 mL) under argon atmosphere. After few minutes TFA (0.128 mmol, 10 \(\mu\)L) 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 \(\mu\)m] column chromatography. Normal sapphyrin, mesotetakis(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\(_2\)Cl\(_2\), \(\delta\) in ppm): –1.39 (s, 2H, inner \(\beta\)-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\(_2\)Cl\(_2\), \(\delta\) in ppm at 203 K): –2.98 (br s, 2H, inner NH), –1.59 (s, 2H, inner \(\beta\)-CH), 11.78 (br s, 1H, outer NH). MALDI-TOF-MS: C\(_{48}\)H\(_{11}\)N\(_3\)F\(_{20}\), calcd 1039.1, obsd \(m/z\) 1039.2 (M\(^+\)). UV-Vis \(\lambda_{\text{max}}\) nm (toluene, \(\varepsilon\)/mol\(^{-1}\) 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\textsubscript{2}Cl\textsubscript{2} (3 mL), to this added dropwise NBS (N-bromosuccinimide, 0.68 mg solution in 2 mL dry CH\textsubscript{2}Cl\textsubscript{2}). Progress of the reaction was judged by TLC and also by the appearance of M\textsuperscript{+} 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\textsubscript{2} and 1-Br, respectively, were unsuccessful due to the unstable nature of 1-Br\textsubscript{2}. Thus the crude mixture of 1-Br\textsubscript{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)

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 Re₂(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 (25:75) 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 dichloromethylene/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. ¹H NMR (300 MHz, CD₂Cl₂, 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: C₅₁H₁₀N₅F₂₀ReO₃, calc 1307.0, obsd m/z 1305.8 (M⁺). UV-Vis: λₘₐₓ/nm (ε/mol⁻¹ dm³ 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. ¹H NMR (500 MHz, CD₂Cl₂, 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: C₅₁H₈N₅F₁₉ReO₃, calc 1287.0, obsd m/z 1286.2 (M⁺). HRMS (ESI−) m/z: calc for C₅₁H₂₀N₅O₁₈²⁵Re (M−): 1284.99316, found: 1285.00225. UV-Vis: λₘₐₓ/nm (ε/mol⁻¹ dm³ 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$_2$Cl$_2$ at –90 °C.

Figure S3. $^1$H NMR spectrum of N-confused sapphyrin (1) (0.5 eq. TFA) in CD$_2$Cl$_2$ at –90 °C.
Figure S4. $^1$H NMR spectrum of N-confused sapphyrin (1) (1 eq. TFA) in CD$_2$Cl$_2$ at –90 $^\circ$C.

Figure S5. $^1$H NMR spectrum of N-confused sapphyrin (1) (2 eq. TFA) in CD$_2$Cl$_2$ at –90 $^\circ$C.
Figure S6. $^1$H NMR spectrum of N-confused sapphyrin (1) (5 eq. TFA) in CD$_2$Cl$_2$ 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

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Mol. Formula: $C_{48}H_{12}BrN_5F_{20}$

Exact Mass: 1194.9

Mol. Formula: $C_{48}H_{12}BrN_5F_{20}$

Exact Mass: 1117.0
**Figure S11.** MALDI-TOF-MS spectrum of Re complex of N-fused sapphyrin (6).

![MALDI-TOF-MS spectrum of Re complex of N-fused sapphyrin (6).](image)

**Mol. Formula:** C$_{51}$H$_{10}$N$_{5}$F$_{20}$O$_{3}$Re  
**Exact Mass:** 1307.0

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

![MALDI-TOF-MS spectrum of Re complex of domino-fused sapphyrin (7).](image)

**Mol. Formula:** C$_{51}$H$_{8}$N$_{5}$F$_{19}$O$_{3}$Re  
**Exact Mass:** 1286.0
**Figure S13.** $^1$H NMR spectrum of Re complex of N-fused sapphyrin (6) in CD$_2$Cl$_2$.

![NMR spectrum of Re complex of N-fused sapphyrin (6) in CD$_2$Cl$_2$.](image1)

**Figure S14.** $^1$H NMR spectrum of Re complex of domino-fused sapphyrin (7) in CD$_2$Cl$_2$.

![NMR spectrum of Re complex of domino-fused sapphyrin (7) in CD$_2$Cl$_2$.](image2)
Figure S15. UV-Vis-NIR spectra of 2, 6, and 7 in CH₂Cl₂.
Figure S16. X-ray crystal structure and packing diagram of [1•Bu₄N⁺]

Solid state structure of [1•Bu₄N⁺] complex

Packing diagram of [1•Bu₄N⁺] complex. Meso-aryl groups are omitted for clarity.

Table S1. Selected bond distances (Å) and bond angles (deg) of 1⁻.

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

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:

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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 sapphryns (monoanion)

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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)

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 sapphryns (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 sapphryins (neutral)**

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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)

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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)

\[ \text{N}_1\text{SAP}^\oplus \]

\begin{align*}
\text{N}_1\text{SAP}^\oplus & : -1198.91151773 (+11.6) \\
\text{N}_1\text{SAP}1 & : -1198.90822543 (+13.7) \\
\text{N}_1\text{SAP}2 & : -1198.90754616 (+14.1) \\
\text{N}_1\text{SAP}3 & : -1198.90629443 (+14.9) \\
\text{N}_1\text{SAP}5 & : -1198.90193045 (+17.6) \\
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\text{N}_1\text{SAP}7 & : -1198.91760453 (+7.8) \\
\text{N}_1\text{SAP}8 & : -1198.91914304 (+6.8) \\
\text{N}_1\text{SAP}9 & : -1198.92247979 (+4.7) \\
\text{N}_1\text{SAP}10 & : -1198.9178048 (+8.0)
\end{align*}

Diprotonated N-confused sapphyrins (dication)

\[ \text{N}_2\text{SAP}^{2\oplus} \]

\begin{align*}
\text{N}_2\text{SAP}1^{2\oplus} & : -1199.19808533 (+13.1) \\
\text{N}_2\text{SAP}2^{2\oplus} & : -1199.22031598 (+0.86)
\end{align*}

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)

\[
\begin{align*}
\text{N}_0\text{SAPPh}^\ominus &: -2122.16998297 (+3.4) \\
\text{N}_0\text{SAPPh1}^\ominus &: -2122.14158179 (+22.0) \\
\text{N}_0\text{SAPPh2}^\ominus &: -2122.17536400 (0) \\
\text{N}_0\text{SAPPh3}^\ominus &: -2122.17270659 (+1.7) \\
\text{N}_0\text{SAPPh4}^\ominus &: -2122.1778131 (+17.3) \\
\text{N}_0\text{SAPPh5}^\ominus &: -2122.15524133 (+12.6) \\
\text{N}_0\text{SAPPh6}^\ominus &: -2122.14803314 (+17.2) \\
\text{N}_0\text{SAPPh7}^\ominus &: -2122.15024969 (+15.8) \\
\text{N}_0\text{SAPPh8}^\ominus &: -2122.14099269 (+21.6) \\
\text{N}_0\text{SAPPh9}^\ominus &: -2122.15368106 (+13.6) \\
\text{N}_0\text{SAPPh10}^\ominus &: -2122.14009297 (+22.0)
\end{align*}
\]

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)

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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-sapphryns (neutral)

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

N-confused meso-tetraphenyl-sapphrysins (neutral)

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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)

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Diprotonated normal *meso*-tetraphenyl-sapphyrins

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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 \textit{meso}-tetraphenyl-sapphyrins (monocation)

\begin{align*}
\text{N}_1\text{SAPPh}^{\text{+}} & \quad -2123.14019416 \quad (+5.0) \\
\text{N}_1\text{SAPPh}^1 & \quad -2123.12980006 \quad (+11.6) \\
\text{N}_1\text{SAPPh}^6 & \quad -2123.13051234 \quad (+11.1) \\
\text{N}_1\text{SAPPh}^9 & \quad -2123.13612733 \quad (+7.6) \\
\end{align*}

Diprotonated N-confused \textit{meso}-tetraphenyl-sapphyrins (dication)

\begin{align*}
\text{N}_1\text{SAPPh}^{\text{2+}} & \quad -2123.45257857 \quad (+8.3) \\
\text{N}_1\text{SAPPh}^1 & \quad -2123.45566447 \quad (+6.4) \\
\end{align*}

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)

\( \text{N}_{2}\text{SAP1}^\ominus \) (Energy = \(-1197.94601276\))

Stoichiometry \( \text{C}_{24}\text{H}_{16}\text{N}_{5}(\text{1}) \)
Framework group \( \text{C}_1[\text{X(C}_{24}\text{H}_{16}\text{N}_{5})] \)
Deg. of freedom 129
Full point group \( \text{C}_1 \)
Largest Abelian subgroup \( \text{C}_1 \) \( \text{NOp} \) 1
Largest concise Abelian subgroup \( \text{C}_1 \) \( \text{NOp} \) 1

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Stoichiometry \( \text{C24H16N5}(1-) \)
Framework group \( \text{Cl}[\text{C24H16N5}] \)
Deg. of freedom 129

Full point group \( \text{Cl} \)
Largest Abelian subgroup \( \text{Cl} \)

Largest concise Abelian subgroup \( \text{Cl} \)

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S33
\( \text{N}_{3}\text{SAP3}^\Theta \) (Energy = \(-1197.95264239\))

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Framework group  \( \text{Cl}[\text{X(C24H16N5)}] \)
Deg. of freedom  129
Full point group  \( \text{Cl} \)
Largest Abelian subgroup  \( \text{Cl} \)  NOp  1
Largest concise Abelian subgroup  \( \text{Cl} \)  NOp  1

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**N₆SAP₄**

(Energy = \(-1197.94983557\))

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Framework group: \(Cl[X(C_{24}H_{16}N_{5})]\)
Deg. of freedom: 129
Full point group: \(Cl\)
Largest Abelian subgroup: \(Cl\) NOp 1
Largest concise Abelian subgroup: \(Cl\) NOp 1

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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
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Deg. of freedom  129
Full point group  \(\text{C}_1\)
Largest Abelian subgroup  \(\text{C}_1\)  \(\text{NOp}\)  1
Largest concise Abelian subgroup  \(\text{C}_1\)  \(\text{NOp}\)  1

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Deg. of freedom  129
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Largest Abelian subgroup  C1  NOP  1
Largest concise Abelian subgroup  C1  NOP  1

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Deg. of freedom 129

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S39
NdSAP9\textsuperscript{2} (Energy = -1197.95296246)

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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

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C$_{24}$H$_{16}$N$_{5}$(1-)

Framework group  
Cl[X(C$_{24}$H$_{16}$N$_{5}$)]

Deg. of freedom  
129

Full point group  
Cl

Largest Abelian subgroup  
Cl  NOp  1

Largest concise Abelian subgroup  
Cl  NOp  1

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**N$_1$SAP1**\(^\ominus\) (Energy = \(-1197.93772367\))

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Framework group  \(\text{Cl}\left[\text{X(C24H16N5)}\right]\)
Deg. of freedom  129
Full point group  \(\text{Cl}\)
Largest Abelian subgroup  \(\text{Cl} \quad \text{NOp} \quad 1\)
Largest concise Abelian subgroup  \(\text{Cl} \quad \text{NOp}\)

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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  
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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

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Framework group  \( \text{Cl}[\text{X(C}_{24}\text{H}_{16}\text{N}_5)] \)
Deg. of freedom  129
Full point group  \( \text{Cl} \)
Largest Abelian subgroup  \( \text{Cl} \)
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S45
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Deg. of freedom 129
Full point group \( C1 \)
Largest Abelian subgroup \( C1 \) \( \text{NOP} \) 1
Largest concise Abelian subgroup \( C1 \) \( \text{NOP} \) 1

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Framework group  \(C1[X(C_{24}H_{16}N_5)]\)
Deg. of freedom  129

Full point group  \(C1\)
Largest Abelian subgroup  \(C1\)  \(\text{NOp} 1\)
Largest concise Abelian subgroup  \(C1\)  \(\text{NOp} 1\)

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Deg. of freedom  129
Full point group  \(\text{Cl}\)
Largest Abelian subgroup  \(\text{Cl}\) \(\text{NOP} \) 1
Largest concise Abelian subgroup  \(\text{Cl}\) \(\text{NOP} \) 1

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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

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Stoichiometry  C$_{24}$H$_{16}$N$_5$(1$-$)
Framework group  C$_1[X(C_{24}H_{16}N_5)]$
Deg. of freedom  129

Full point group  C$_1$
Largest Abelian subgroup  C$_1$                  NOp 1
Largest concise Abelian subgroup  C$_1$                  NOp 1

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**Stoichiometry**  \( C_{24}H_{16}N_{5}(1-) \)

**Framework group**  \( C_1[X(C_{24}H_{16}N_{5})] \)

**Deg. of freedom**  129

**Full point group**  \( C_1 \)

**Largest Abelian subgroup**  \( C_1 \) \( \text{NOp} \) 1

**Largest concise Abelian subgroup**  \( C_1 \) \( \text{NOp} \) 1

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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
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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

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C$_{24}$H$_{16}$N$_5$(1⁻)

Framework group  
C1[X(C$_{24}$H$_{16}$N$_5$)]

Deg. of freedom  
129

Full point group  
C1

Largest Abelian subgroup  
C1  NOp  1

Largest concise Abelian subgroup  
C1  NOp  1

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

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N$_{17}$SAP$^\ominus$ (Energy = $-197.94584085$)

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Framework group C$_1[X(C_{24}H_{16}N_5)]$
Deg. of freedom 129

Full point group C$_1$
Largest Abelian subgroup C$_1$  NOp 1
Largest concise Abelian subgroup C$_1$  NOp 1

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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

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Deg. of freedom  129
Full point group  \[\text{Cl}\]
Largest Abelian subgroup  \[\text{Cl}\] \[\text{NOP} 1\]
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Framework group: $\text{C1[X(C24H16N5)]}$

Deg. of freedom: 129

Full point group: $\text{C1}$

Largest Abelian subgroup: $\text{C1}$  NOp 1

Largest concise Abelian subgroup: $\text{C1}$  NOp 1

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S61
Cartesian coordinates for the optimized structures of normal sapphryns (neutral)

**N₆SAP1** (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

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Deg. of freedom  132
Full point group  C₁
Largest Abelian subgroup  C₁      NOp   1
Largest concise Abelian subgroup C₁      NOp   1

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Deg. of freedom  132
Full point group  C₁
Largest Abelian subgroup  C₁  NOp  1
Largest concise Abelian subgroup  C₁  NOp  1

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S64
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**N₅SAP5** (Energy = −1198.5179866)

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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

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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

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Stoichiometry  
C$_{24}$H$_{17}$N$_5$

Framework group  
C$_1[X(C_{24}H_{17}N_5)]$

Deg. of freedom  
132

Full point group  
C$_1$

Largest Abelian subgroup  
C$_1$  NOp  1

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

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

**N$_5$SAP1** (Energy = $-1198.49635445$)

Stoichiometry: C$_{24}$H$_{17}$N$_5$

Framework group: C$_1$[X(C$_{24}$H$_{17}$N$_5$)]

Deg. of freedom: 132

Full point group: C$_1$

Largest Abelian subgroup: C$_1$     NOp 1

Largest concise Abelian subgroup: C$_1$     NOp 1

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Framework group  \( \text{C}_1[\text{X(C}_{24}\text{H}_{17}\text{N}_5)] \)
Deg. of freedom  132
Full point group  \( \text{C}_1 \)
Largest Abelian subgroup  \( \text{C}_1 \)  \( \text{NOp} \)  1
Largest concise Abelian subgroup  \( \text{C}_1 \)  \( \text{NOp} \)  1

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Framework group  C$_1[X(C_{24}H_{17}N_5)]$
Deg. of freedom  132
Full point group  C$_1$
Largest Abelian subgroup  C$_1$  NOp  1
Largest concise Abelian subgroup C$_1$  NOp  1

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S72
**N1SAP4** (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

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S73
**S74**

**N$_1$SAP$_5$** (Energy = $-1198.49318193$)

Stoichiometry: C$_{24}$H$_{17}$N$_5$

Framework group: C$_1[X(C_{24}H_{17}N_5)]$

Deg. of freedom: 132

Full point group: C$_1$

Largest Abelian subgroup: C$_1$  NOp  1

Largest concise Abelian subgroup: C$_1$  NOp  1

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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

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Framework group  \( \text{C1}[\text{X(C24H17N5)}] \)
Deg. of freedom  132
Full point group  \( \text{C1} \)

Largest Abelian subgroup  \( \text{C1} \)  NOp  1
Largest concise Abelian subgroup  \( \text{C1} \)  NOp  1

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Deg. of freedom  132
Full point group  C1

Largest Abelian subgroup  C1  NOP  1
Largest concise Abelian subgroup  C1  NOP  1

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S77
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Deg. of freedom  132
Full point group  C$_{1}$

Largest Abelian subgroup  C$_{1}$  NOp  1
Largest concise Abelian subgroup  C$_{1}$  NOp  1

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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

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Deg. of freedom   132

Full point group  C1
Largest Abelian subgroup  C1  NOp  1
Largest concise Abelian subgroup  C1  NOp  1

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Deg. of freedom 132
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Largest Abelian subgroup C1
Largest concise Abelian subgroup C1
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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  

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Deg. of freedom  132  
Full point group  Cl  
Largest Abelian subgroup  Cl  
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Deg. of freedom  132  
Full point group  C1  
Largest Abelian subgroup  C1  
Largest concise Abelian subgroup  C1  
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**N$_8$SAP17** (Energy = $-1198.47530040$)

Stoichiometry: C$_{24}$H$_{17}$N$_5$

Framework group: C1[X(C$_{24}$H$_{17}$N$_5$)]

Deg. of freedom: 132

Full point group: C1

Largest Abelian subgroup: C1

Largest concise Abelian subgroup: C1

**Standard orientation:**

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**Diagram:**

![Diagram of N$_8$SAP17](image)

S86
**N$_1$ SAP18** (Energy = $-1198.50018236$)

Stoichiometry \( \text{C24H17N5} \)

Framework group \( \text{Cl}[\text{X(C24H17N5)}] \)

Deg. of freedom 132

Full point group \( \text{Cl} \)

Largest Abelian subgroup \( \text{Cl} \) \( \text{NOp} \) 1

Largest concise Abelian subgroup \( \text{Cl} \) \( \text{NOp} \) 1

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S87
### Cartesian coordinates for the optimized structures of normal sapphyrins (monocation)

**N$_8$SAP1**

(Energy = $-1198.91180770$)

Stoichiometry: $C_{24}H_{18}N_5(1+)$
Framework group: C1[$X(C_{24}H_{18}N_5)$]
Deg. of freedom: 135

Full point group: C1

Largest Abelian subgroup: C1

Largest concise Abelian subgroup: C1

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**N₄SAP2**<sup>+</sup> (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

Standard orientation:

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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

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Framework group  \( \text{C1[X(C24H18N5)]} \)
Deg. of freedom  135
Full point group  \( \text{C1} \)
Largest Abelian subgroup  \( \text{C1 NOp 1} \)
Largest concise Abelian subgroup  \( \text{C1 NOp} \)

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**Stoichiometry**  \(\text{C24H18N5(1+)}\)

**Framework group**  \(\text{C1}[\text{X(C24H18N5)}]\)

**Deg. of freedom**  135

**Full point group**  \(\text{C1}\)

**Largest Abelian subgroup**  \(\text{C1} \quad \text{NOP} \quad 1\)

**Largest concise Abelian subgroup**  \(\text{C1} \quad \text{NOP} \quad 1\)

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Largest Abelian subgroup  C1  NOp 1
Largest concise Abelian subgroup  C1  NOp

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Full point group  
Largest Abelian subgroup  
Largest concise Abelian subgroup  

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\( \text{N}_{1}\text{SAP}^+ \) (Energy = \(-1198.9115773\))

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S96
\[\text{N}_1\text{SAP}_2^+\] (Energy = -1198.90822543)

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Largest Abelian subgroup  \(\text{C}_1\quad \text{NOp} 1\)
Largest concise Abelian subgroup  \(\text{C}_1\quad \text{NOp} 1\)

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Stoichiometry \textit{C24H18N5}(1+)

Framework group \textit{C1}[\text{X(C24H18N5)}]

Deg. of freedom 135

Full point group \textit{C1}

Largest Abelian subgroup \textit{C1} \textit{NoP} 1

Largest concise Abelian subgroup \textit{C1} \textit{NoP} 1

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S98
**N$_2$SAP$_4^\oplus$ (Energy = -1198.90629443)**

Stoichiometry  C$_{24}$H$_{18}$N$_5$(1+)

Framework group  C$_1$[X(C$_{24}$H$_{18}$N$_5$)]

Deg. of freedom  135

Full point group  C$_1$

Largest Abelian subgroup  C$_1$  NOp  1

Largest concise Abelian subgroup  C$_1$  NOp  1

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Largest Abelian subgroup  C$_1$  NOP  1
Largest concise Abelian subgroup  C$_1$  NOP  1

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\[ \text{C24H18N5}(1+) \]

### Framework group

\[ \text{C1}[\text{X(C24H18N5)}] \]

### Deg. of freedom

135

### Full point group

C1

### Largest Abelian subgroup

C1  NOp  1

### Largest concise Abelian subgroup

C1  NOp  1

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**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

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Framework group \ C_1[X(C_{24}H_{18}N_{5})]\
Deg. of freedom 135\
Full point group \ C_1\
Largest Abelian subgroup \ C_1 \ NOp 1\
Largest concise Abelian subgroup \ C_1 \ NOp 1

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Framework group  C₁[XC₂₄H₁₈N₅]
Deg. of freedom  135
Full point group  C₁
Largest Abelian subgroup  C₁    NOP   1
Largest concise Abelian subgroup  C₁    NOP  1

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**Stoichiometry** C$_{24}$H$_{18}$N$_5$ (1+)

**Framework group** C1[X(C$_{24}$H$_{18}$N$_5$)]

**Deg. of freedom** 135

**Full point group** C1

**Largest Abelian subgroup** C1  NOp  1

**Largest concise Abelian subgroup** C1  NOp  1

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Framework group C\textsubscript{1}[X(C\textsubscript{24}H\textsubscript{19}N\textsubscript{5})]
Deg. of freedom 138
Full point group C\textsubscript{1}
Largest Abelian subgroup C\textsubscript{1} NOp 1
Largest concise Abelian subgroup C\textsubscript{1} NOp 1

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Stoichiometry  
\[ C_{24}H_{19}N_{5}(2+) \]

Framework group  
\[ C1[X(C_{24}H_{19}N_{5})] \]

Deg. of freedom  
138

Full point group  
\[ C1 \]

Largest Abelian subgroup  
\[ C1 \quad NOp \quad 1 \]

Largest concise Abelian subgroup  
\[ C1 \quad NOp \]

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\[ N_5SAPPh1 \] (Energy = \(-2122.16998297\))

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

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\]
Framework group \[
C1[X(\text{C}_{48}\text{H}_{32}\text{N}_5)]\
\]
Deg. of freedom \[
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Full point group \[
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Largest Abelian subgroup \[
C1 \quad \text{NOp} \quad 1\]
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Stoichiometry \( \text{C4H32N5}(1-) \)
Framework group \( \text{C1}[^\text{X(C4H32N5)}] \)
Deg. of freedom 249
Full point group \( \text{C1} \)
Largest Abelian subgroup \( \text{C1 \ NOp 1} \)
Largest concise Abelian subgroup \( \text{C1 \ NOp 1} \)

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S113
### N$_2$SAPPh$_5$ (Energy = $-2122.14778131$)

Stoichiometry: C$_{48}$H$_{32}$N$_5$(1-)

Framework group: C$_1[X(C48H32N5)]$

Deg. of freedom: 249

Full point group: C$_1$

Largest Abelian subgroup: C$_1$ NOp 1

Largest concise Abelian subgroup: C$_1$ NOp 1

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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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Stoichiometry    C48H32N5(1

N0SAPPh88 (Energy = -2122.15024969)

S18
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Largest concise Abelian subgroup: C1, NOP 1

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Deg. of freedom  249

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Largest Abelian subgroup  C₁  NOp  1
Largest concise Abelian subgroup  C₁  NOp  1

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S123
Cartesian coordinates for the optimized structures of N-confused meso-tetraphenylsapphyrins (monoanion)

\[ \text{N$_n$SAPPh}^{1\Theta} \] (Energy = -2122.15711058)

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

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\( \text{N}_8\text{SAPPh}_2 \) \((\text{Energy} = -2122.13095762)\)

Stoichiometry  \( \text{C}_{48}\text{H}_{32}\text{N}_5(1-) \)

Framework group  \( \text{C}_1[\text{X(C}_{48}\text{H}_{32}\text{N}_5)] \)

Deg. of freedom 249

Full point group  \( \text{C}_1 \)

Largest Abelian subgroup  \( \text{C}_1 \)  \(\text{NOp} \)  1

Largest concise Abelian subgroup  \(\text{C}_1 \)  \(\text{NOp} \)  1

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**Note:**

- The coordinates are given in Angstroms.
- The table lists the atomic positions for each atom in the molecule, with the X, Y, and Z coordinates provided.
- The energy value is given in Hartrees.
- The stoichiometry indicates the composition of the molecule, with \( \text{C}_{48}\text{H}_{32}\text{N}_5 \) as the main component.
- The framework group and deg. of freedom provide structural information about the molecule.
- The point group and Abelian subgroup information give insights into the symmetry of the molecule.
- The standard orientation shows the arrangement of the atoms in the molecule.
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| 18| 6 | 0 | -0.925363 | -3.655447 | -0.064313 |
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\[N_8\text{SAPPh}_3\] (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

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Stoichiometry \( \text{C}_{48}\text{H}_{32}\text{N}_5(1-) \)
Framework group \( \text{C}1[\text{X(C}_{48}\text{H}_{32}\text{N}_5)] \)
Deg. of freedom \( 249 \)

Full point group \( \text{C}1 \)
Largest Abelian subgroup \( \text{C}1 \) \( \text{NOp} \) \( 1 \)
Largest concise Abelian subgroup \( \text{C}1 \) \( \text{NOp} \) \( 1 \)

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Deg. of freedom 249

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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

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Deg. of freedom  249

Full point group  C$_1$

Largest Abelian subgroup  C$_1$  NOp  1
Largest concise Abelian subgroup  C$_1$  NOp  1

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N₈SAPh₈² (Energy = -2122.15698081)

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

S134
### Full point group
- **Cl**

### Largest Abelian subgroup
- **Cl**
- NOp 1

### Largest concise Abelian subgroup
- **Cl**
- NOp 1

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N_SAPPh9\textsuperscript{\textdegree} (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

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S136
**N₈SAPPh₁₀**\(^\ominus\) (Energy = -2122.14480364)

Stoichiometry \(\text{C}_{48}\text{H}_{32}\text{N}_5\)
Framework group \(\text{Cl}[\text{X(C}_{48}\text{H}_{32}\text{N}_5}]\)
Deg. of freedom \(249\)
Full point group \(\text{Cl}\)
Largest Abelian subgroup \(\text{Cl} \ NOp 1\)
Largest concise Abelian subgroup \(\text{Cl} \ NOp 1\)

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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
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S139
N,SAPPh12\(^\Theta\) (Energy = -2122.16485672)

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

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**N,SAPPh13**\(^\circ\) (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

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Deg. of freedom 249
Full point group C₁
Largest Abelian subgroup C₁ NOP 1
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N,SAPPh16 (Energy = -2122.14245935)

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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

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N,SAPPh16 (Energy = -2122.14245935)

Stoichiometry  C48H32N5(1-)
Framework group  C1[X(C48H32N5)]
Deg. of freedom  249
Full point group  C1
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  \item Full point group \(\text{C1}\)
  \item Largest Abelian subgroup \(\text{C1}\) \(\text{NOP}\) \(1\)
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Deg. of freedom 249

Full point group \( \text{C}1 \)

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Largest concise Abelian subgroup \( \text{C}1 \) NoP 1

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**N,SAPPh20** (Energy = -2122.13056960)

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

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**Sapphyrins (neutral)**

**N$_{SAPPh1}$ (Energy = -2122.71865352)**

Stoichiometry C$_{48}$H$_{33}$N$_{5}$

Framework group C$_1[X(C_{48}H_{33}N_{5})]]$

Deg. of freedom 252

Full point group C$_1$

Largest Abelian subgroup C$_1$ NOp 1

Largest concise Abelian subgroup C$_1$ NOp 1

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S156
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        | Framework group C1[X(C48H33N5)] | | | |
        | Full point group C1 | | | |
        | Largest concise Abelian subgroup C1 | NOp | 1 | |

**N₈SAPPh₂** (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

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N₅SAPPh₃ (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:
N$_8$SAPPh$_4$ (Energy = $-2122.70658126$)

Stoichiometry C$_{48}$H$_{33}$N$_5$5
Framework group C$_1[X(C48H33N5)]$
Deg. of freedom 252
Full point group C$_1$
Largest Abelian subgroup C$_1$ NOp 1
Largest concise Abelian subgroup C$_1$ NOp 1

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Stoichiometry C$_{48}$H$_{33}$N$_5$

Framework group C1[X(C$_{48}$H$_{33}$N$_5$)]

Deg. of freedom 252

Full point group C1

Largest Abelian subgroup C1

Largest concise Abelian subgroup C1

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Cartesian coordinates for the optimized structures of N-confused *meso*-tetraphenylsapphyrins (neutral)

N$_2$SAPPh1 (Energy = -2122.71279475)

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**Framework group** C1[X(C48H33N5)]  
**Deg. of freedom** 252  

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Framework group \( \text{Cl}[\text{X(C48H33N5)}] \)

Deg. of freedom 252

Full point group \( \text{Cl} \)

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Largest concise Abelian subgroup \( \text{Cl} \) \( \text{NOp} \) 1

Standard orientation:

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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

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Stoichiometry: C_{48}H_{33}N_{5}

Framework group: C_{1}[X(C_{48}H_{33}N_{5})]

Deg. of freedom: 252

Full point group: C_{1}

Largest Abelian subgroup: C_{1} NOp 1

Largest concise Abelian subgroup: C_{1} NOp 1

Standard orientation:

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Full point group: C$_1$
Largest Abelian subgroup: C$_1$, NOp 1
Largest concise Abelian subgroup: C$_1$, NOp 1

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Stoichiometry  \( \text{C}_{48}\text{H}_{33}\text{N}_5\)
Framework group  \( \text{C}_1[\text{X} (\text{C}_{48}\text{H}_{33}\text{N}_5)] \)
Deg. of freedom  252
Full point group  \( \text{C}_1 \)
Largest Abelian subgroup  \( \text{C}_1 \)

S176
Largest concise Abelian subgroup Cl

Standard orientation:

Center  Atomic  Atomic  Coordinates (Angstroms)
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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
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9       6        0       -5.213202  -0.131746  -0.357938
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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
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19      6        0        4.817286   1.579130   0.335048
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21      6        0       -1.227401  -4.717451   0.553536
22      6        0        4.096192  -1.960853  -0.238505
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27      6        0       -5.516350   1.974016  -0.885114
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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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Stoichiometry  C_{48}H_{33}N_{5}
Framework group  C_{1}[X(C_{48}H_{33}N_{5})]
Deg. of freedom  252
Full point group  C_{1}
Largest Abelian subgroup  C_{1}  NOp  1
Largest concise Abelian subgroup  C_{1}  NOp  1

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**N$_7$SAPPh9** (Energy = $-2122.70923914$)

**Stoichiometry**: C$_{48}$H$_{33}$N$_5$

**Framework group**: C$_1[X(C_{48}H_{33}N_5)]$

**Deg. of freedom**: 252

**Full point group**: C$_1$

**Largest Abelian subgroup**: C$_1$ NOp 1

**Largest concise Abelian subgroup**: C$_1$ NOp 1

**Standard orientation**: 

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N$_4$SAPPh10 (Energy = -2122.69108579)

Stoichiometry C$_{48}$H$_{33}$N$_5$

Framework group C$_1[X(C_{48}H_{33}N_5)]$

Deg. of freedom 252

Full point group C$_1$

Largest concise Abelian subgroup C$_1$ NOp 1

Largest Abelian subgroup C$_1$ NOp 1

Standard orientation:
N$_1$SAPPh11 (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

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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
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N$_6$SAPPh12 (Energy = -2122.69300356)

Stoichiometry  C$_{48}$H$_{33}$N$_5$

Framework group  C$_1$[X(C$_{48}$H$_{33}$N$_5$)]

Deg. of freedom  252

Full point group  C$_1$

Largest Abelian subgroup  C$_1$  NOp  1

Largest concise Abelian subgroup  C$_1$  NOp  1

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Stoichiometry C\textsubscript{48}H\textsubscript{33}N\textsubscript{5}
Framework group C\textsubscript{1}[X(C\textsubscript{48}H\textsubscript{33}N\textsubscript{5})]
Deg. of freedom 252
Full point group C\textsubscript{1}
Largest Abelian subgroup C\textsubscript{1} No p 1
Largest concise Abelian subgroup C\textsubscript{1} No p 1

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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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Stoichiometry  C48H33N5
Framework group  C1[X(C48H33N5)]
Deg. of freedom  252
Full point group  C1

Largest Abelian subgroup  C1
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Stoichiometry C48H33N5

Framework group C1[X(C48H33N5)]

Deg. of freedom 252

Full point group C1

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Largest concise Abelian subgroup C1  NOp  1

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\( \text{N}_8\text{SAPPh18} \) (Energy = \(-2.122.69815924\))

\text{Stoichiometry} \quad \text{C48H33N5}

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\text{Deg. of freedom} \quad 252

\text{Full point group} \quad \text{C1}

\text{Largest Abelian subgroup} \quad \text{C1} \quad \text{NOP} \quad 1

\text{Largest concise Abelian subgroup} \quad \text{C1} \quad \text{NOP} \quad 1

\text{Standard orientation:}

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**N₅SAPPh1** (Energy = −2123.14412552)

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$N_8SAPPh_2$ (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

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**N₆SAPPh₃** (Energy = -2123.1482290)

**Stoichiometry**  C₄₀H₃₄N₅(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:**
N$_8$SAPPh$_4$ $^\circledR$ (Energy = $-2123.14006537$)

Stoichiometry  C$_{48}$H$_{34}$N$_5$(1+)
Framework group  C$_1[X(C48H34N5)]$
Deg. of freedom  255
Full point group  C$_1$
Largest Abelian subgroup  C$_1$  NOp  1
Largest concise Abelian subgroup  C$_1$  NOp  1

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Deg. of freedom: 255
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Largest Abelian subgroup: C₁
Largest concise Abelian subgroup: C₁

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**Deg. of freedom**  255

**Full point group**  C₁

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**Largest concise Abelian subgroup**  C₁  NOp 1

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### Cartesian coordinates for the optimized structures of normal *meso*-tetrphenyl-sapphryns (dication)

\(N_2\text{SAPPh}^2\) (Energy = \(-2123.46581760\))

**Stoichiometry**  \(\text{C}_{48}\text{H}_{35}\text{N}_{5}(2+)\)

**Framework group**  \(\text{C1}[\text{X(C48H35N5)}]\)

**Deg. of freedom**  258

**Full point group**  \(\text{C1}\)

**Largest concise Abelian subgroup**  \(\text{C1} \quad \text{NOp} \quad 1\)

**Largest Abelian subgroup**  \(\text{C1} \quad \text{NOp} \quad 1\)

**Stoichiometry**  \(\text{C}_{48}\text{H}_{35}\text{N}_{5}(2+)\)

**Framework group**  \(\text{C1}[\text{X(C48H35N5)}]\)

**Deg. of freedom**  258

**Full point group**  \(\text{C1}\)

**Largest concise Abelian subgroup**  \(\text{C1} \quad \text{NOp} \quad 1\)

**Largest Abelian subgroup**  \(\text{C1} \quad \text{NOp} \quad 1\)

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Largest concise Abelian subgroup  C₁  NOP  1

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\( \text{N}_4\text{SAPPh1} \)\(^\circ\) (Energy = \(-2123.14019416\))

Stoichiometry \ C48H34N5\((1^+)\) 
Framework group \ C1\[X(C48H34N5)] \nDeg. of freedom \ 255 
Full point group \ C1 

Largest Abelian subgroup \ C1 \ NOp 1 
Largest concise Abelian subgroup \ C1 \ NOp 1 

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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

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Stoichiometry C$_{48}$H$_{34}$N$_{5}$(1+)
Framework group C$_1$[X(C$_{48}$H$_{34}$N$_{5}$)]
Deg. of freedom 255
Full point group C$_1$
Largest Abelian subgroup C$_1$ NOp 1
Largest concise Abelian subgroup C$_1$ NOp 1

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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

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Deg. of freedom 255
Full point group C₁
Largest Abelian subgroup C₁ NOp 1
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Deg. of freedom 255
Full point group C1
Largest Abelian subgroup C1 No. 1
Largest concise Abelian subgroup C1 No. 1

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Deg. of freedom  255

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Deg. of freedom  255
Full point group  C1
Largest Abelian subgroup  C1 NOp 1
Largest concise Abelian subgroup  C1 NOp 1

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Deg. of freedom  255
Full point group  C₁
Largest Abelian subgroup  C₁  NOp  1
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## Cartesian coordinates for the optimized structures of N-confused meso-tetraphenyl-sapphyrins (dication)

\( N_4SAPPh^{2+} \) (Energy = \(-2123.45257857\))

**Stoichiometry** C48H35N5(2+)

**Framework group** C1[X(C48H35N5)]

**Deg. of freedom** 258

**Full point group** C1

**Largest Abelian subgroup** C1

**Largest concise Abelian subgroup** C1

**Stoichiometry** C48H35N5(2+)

### N-sapphyrins (dication)

![N-sapphyrin structure](attachment:image.png)

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N$_2$SAPPh$_2^{2+}$ (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

N$_2$SAPPh$_2^{2+}$
| 76 | 1 | 0 | 7.155313 | -5.455712 | -0.033478 |
| 77 | 1 | 0 | 8.757252 | -4.289898 | 1.467378 |
| 78 | 6 | 0 | -5.243642 | -2.752019 | -0.824066 |
| 79 | 6 | 0 | -6.123626 | -2.127771 | -1.728286 |
| 80 | 6 | 0 | -5.652989 | -3.936961 | -0.188381 |
| 81 | 6 | 0 | -7.369588 | -2.687313 | -2.003059 |
| 82 | 1 | 0 | -5.815946 | -1.217734 | -2.235457 |
| 83 | 6 | 0 | -6.904631 | -4.489224 | -0.458138 |
| 84 | 1 | 0 | -5.003497 | -4.411888 | 0.542789 |
| 85 | 6 | 0 | -7.762985 | -3.868241 | -1.368950 |
| 86 | 1 | 0 | -8.031574 | -2.204205 | -2.715325 |
| 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.