

Supporting Information

for

Aromaticity and Antiaromaticity in the Excited States of Porphyrin Nanorings

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S1 Computational Chemistry

DFT geometry optimizations were performed using the B3LYP functional and the 6-31G* all-electron basis set,^{S1-S5} as implemented in Gaussian09/D.01 and Gaussian16/A.03.^{S6,S7} The *meso*-aryl groups on the nanorings were truncated to -H. Nanorings **c-P5**, **c-P6**, **c-P7** and **c-P8** were optimized in their S_0 state with the highest possible symmetry (D_{Nh}). The geometries converged as follows: **c-P5** (D_{5h}), **c-P6** (D_{6h}), **c-P7** (C_{7h}) and **c-P8** (C_{8h}). Triplet states were then optimized and converged to non-symmetric (C_1) geometries. The stability of the triplet wavefunctions was checked, confirming that they corresponded to the T_1 state and not some higher energy state. There was no excessive spin contamination ($\langle S^2 \rangle = 2$). NICS shieldings^{S8} were calculated using the GIAO method using either B3LYP, LC-wHPBE ($w = 0.05, 0.1$ or 0.2), M06-L, M06-2X, or CAM-B3LYP, at the B3LYP/6-31G* geometry.^{S9-S12} Additionally, M06-2X NMR shieldings were calculated at the M06-2X/6-31G*//M06-2X/6-31G* level. NICS surfaces were calculated with a $20 \text{ \AA} \times 20 \text{ \AA}$ grid of ghost atoms with 1 \AA spacing.

S1.1 Summary of NICS values, and discussion of spin densities

Table S1: NICS(0)_{iso} and NICS(0)_{zz} (all units ppm) at the centers of porphyrin nanorings in their S_0 and T_1 states. Level of theory: B3LYP/6-31G*.

	π -electron count	S_0		T_1	
		NICS(0) _{iso}	NICS(0) _{zz}	NICS(0) _{iso}	NICS(0) _{zz}
c-P5	70	-2.5	-0.1	1.6	10.3
c-P6	84	-1.4	1.1	-5.4	-12.2
c-P7	98	-1.2	0.5	0.4	2.1
c-P8	112	-0.9	0.5	-1.3	-1.5

The Mulliken spin populations of the constituent atoms for each porphyrin were summed, affording the spin per porphyrin subunit. These spin densities were then represented as N equally spaced radial vectors (r_i) around a circle, with length (weight) proportional to their spin density. The spin density delocalization was quantified as the angular deviation of these vectors, calculated using the CircStat toolbox^{S13} in MATLAB. The total spin density is normalized to 1.

The angular deviation (Γ_{trip}) takes a range of values from 0 to $\sqrt{2}$, where a higher value corresponds to increased delocalization. It is calculated from the length of the normalized mean resultant vector ($R = \|\bar{r}\|$, where $\bar{r} = \sum r_i$) of the distribution, using:

$$\Gamma_{\text{trip}} = \sqrt{2(1 - R)} \quad (\text{S1})$$

Table S2: NICS(0)_{iso} and NICS(0)_{zz} (all units ppm) at the center of **c-P5** in its T₁ state for different DFT functionals.

Functional	Γ_{trip}	NICS(0) _{iso}	NICS(0) _{zz}
B3LYP//B3LYP	0.777	1.6	10.3
M06-2X//M06-2X	0.572	-1.5	1.7
M06-L//B3LYP	0.926	11.1	38.3
M06-2X//B3LYP	0.655	-1.2	2.5
CAM-B3LYP//B3LYP	0.609	-1.4	1.6
LC- ω HPBE//B3LYP ($\omega = 0.05$)	0.834	2.7	13.3
LC- ω HPBE//B3LYP ($\omega = 0.1$)	0.671	-0.6	3.4
LC- ω HPBE//B3LYP ($\omega = 0.2$)	0.579	-1.4	1.5

Table S3: NICS(0)_{iso} and NICS(0)_{zz} (all units ppm) at the center of **c-P6** in its T₁ state for different DFT functionals.

Functional	Γ_{trip}	NICS(0) _{iso}	NICS(0) _{zz}
B3LYP//B3LYP	0.941	-5.4	-12.2
M06-2X//M06-2X	0.490	-1.3	0.4
M06-L//B3LYP	1.414	-9.2	-23.6
M06-2X//B3LYP	0.548	-1.4	0.1
CAM-B3LYP//B3LYP	0.540	-1.1	0.6
LC- ω HPBE//B3LYP ($\omega = 0.05$)	0.873	-4.2	-8.9
LC- ω HPBE//B3LYP ($\omega = 0.1$)	0.573	-1.3	-0.3
LC- ω HPBE//B3LYP ($\omega = 0.2$)	0.487	-1.1	0.6

S1.2 NICS grids for S_0 ground states

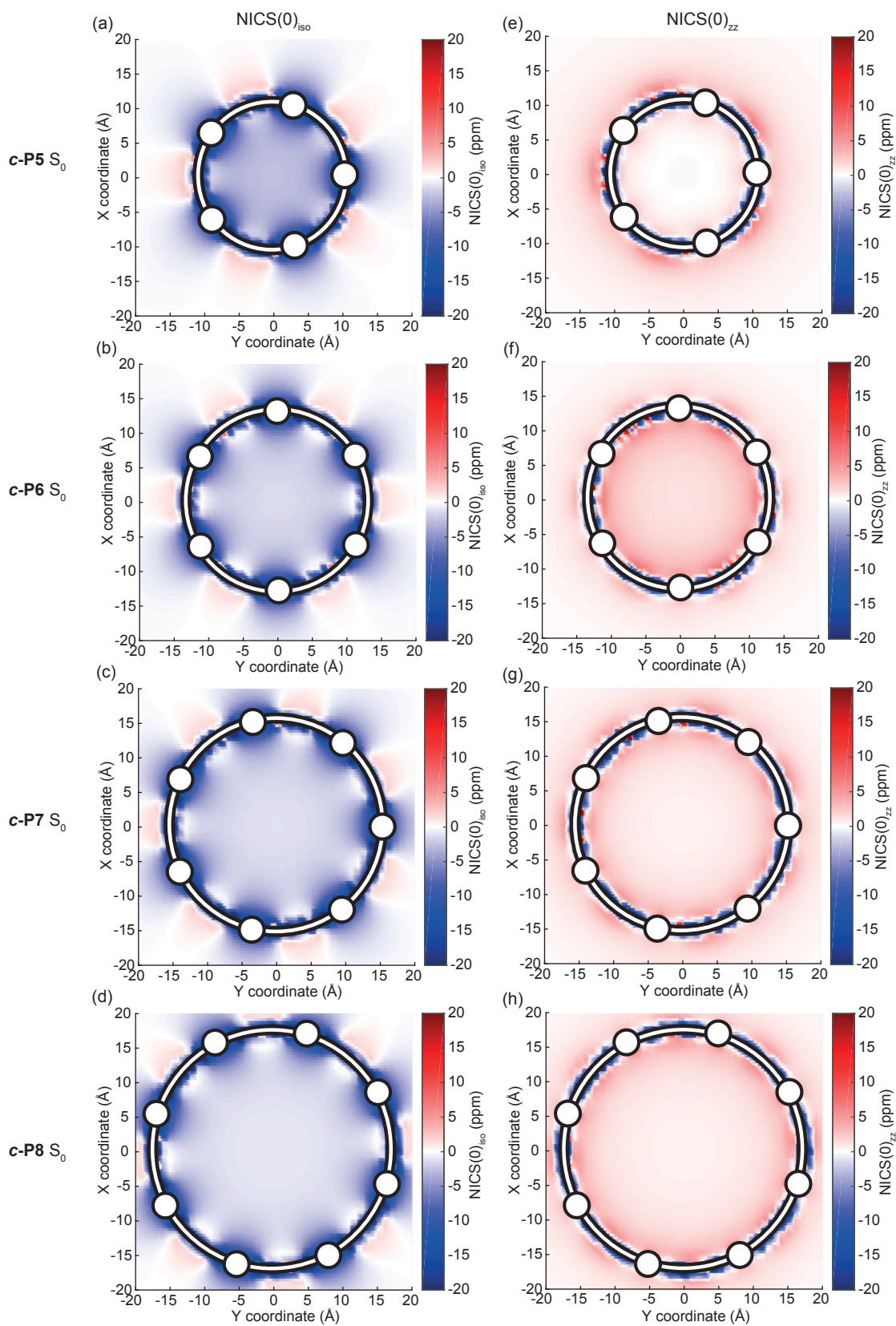


Figure S1: NICS(0)_{iso} (left column) and NICS(0)_{zz} (right column) for *c*-P5, *c*-P6, *c*-P7, and *c*-P8, in their S_0 singlet ground states, calculated at the B3LYP/6-31G* level of theory. White circles indicate the positions of porphyrin units.

S1.3 NICS grids for T_1 excited states

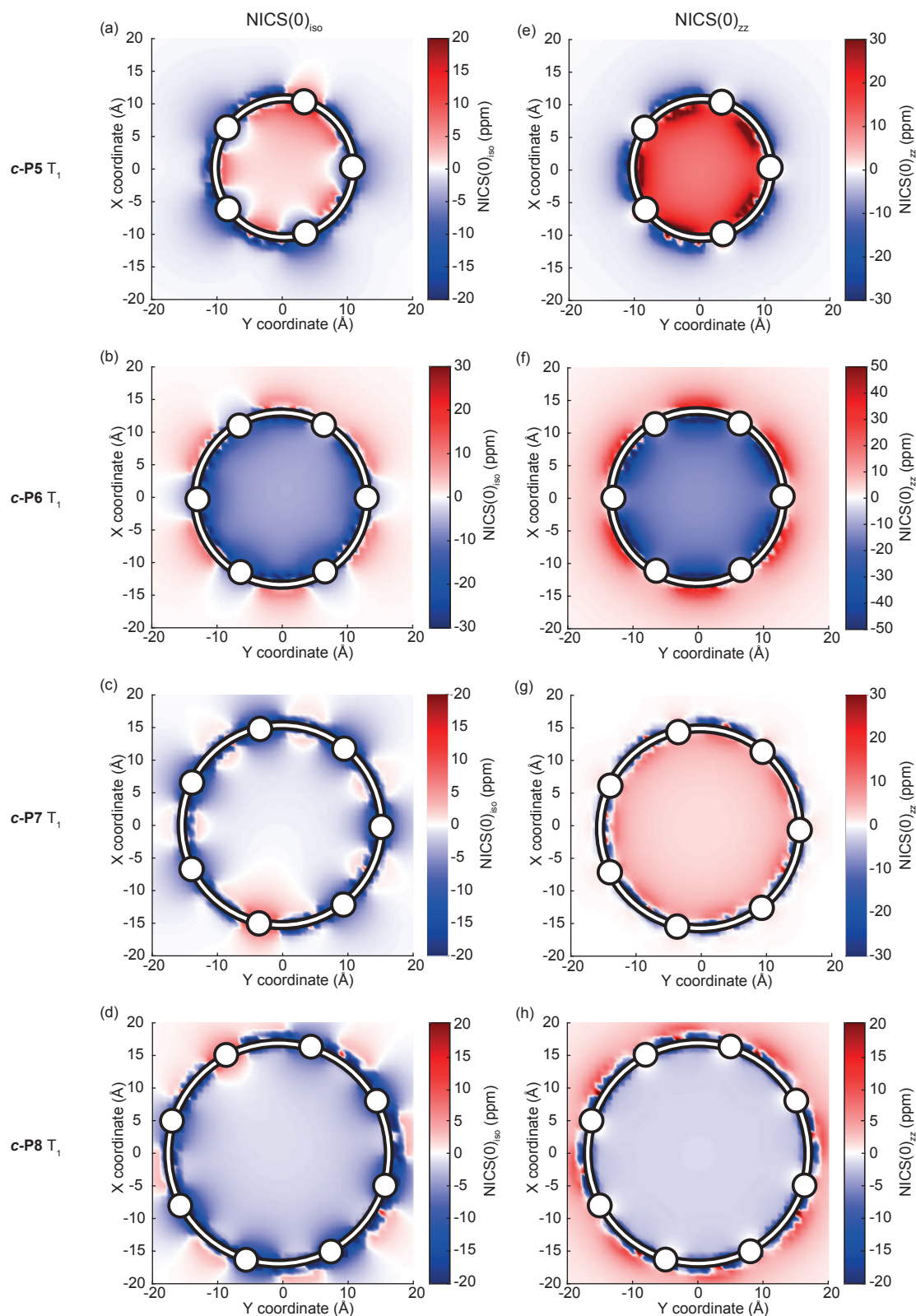


Figure S2: NICS(0)_{iso} (left column) and NICS(0)_{zz} (right column) for **c-P5**, **c-P6**, **c-P7**, and **c-P8**, in their T_1 states, calculated at the B3LYP/6-31G* level of theory. White circles indicate the positions of porphyrin units.

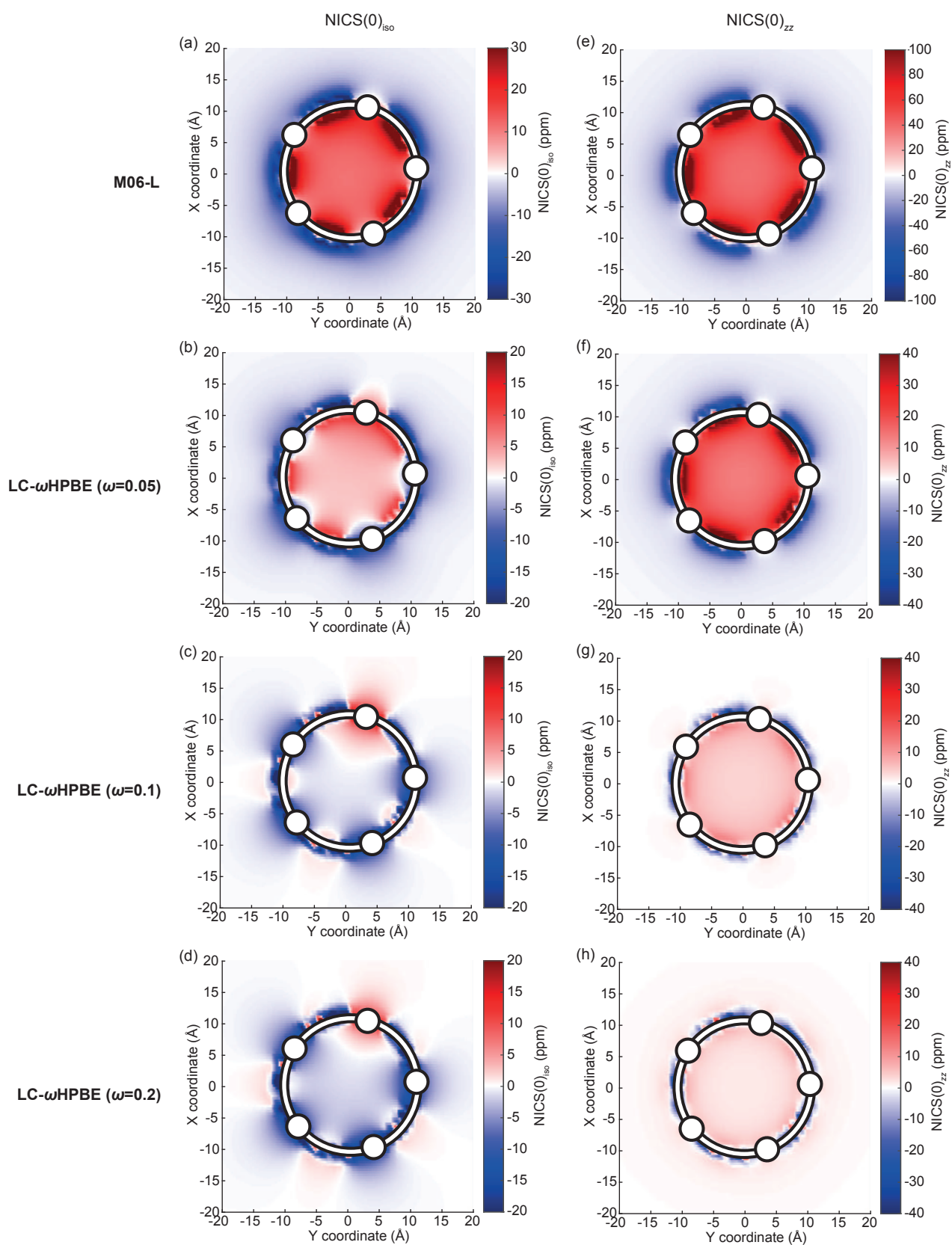


Figure S3: $\text{NICS}(0)_{\text{iso}}$ (left column) and $\text{NICS}(0)_{zz}$ (right column) for *c*-P5 in its T_1 state, calculated using the functionals M06-L and LC- ω HPBE ($\omega = 0.05$, $\omega = 0.1$, and $\omega = 0.2$), and the 6-31G* basis set. White circles indicate the positions of porphyrin units.

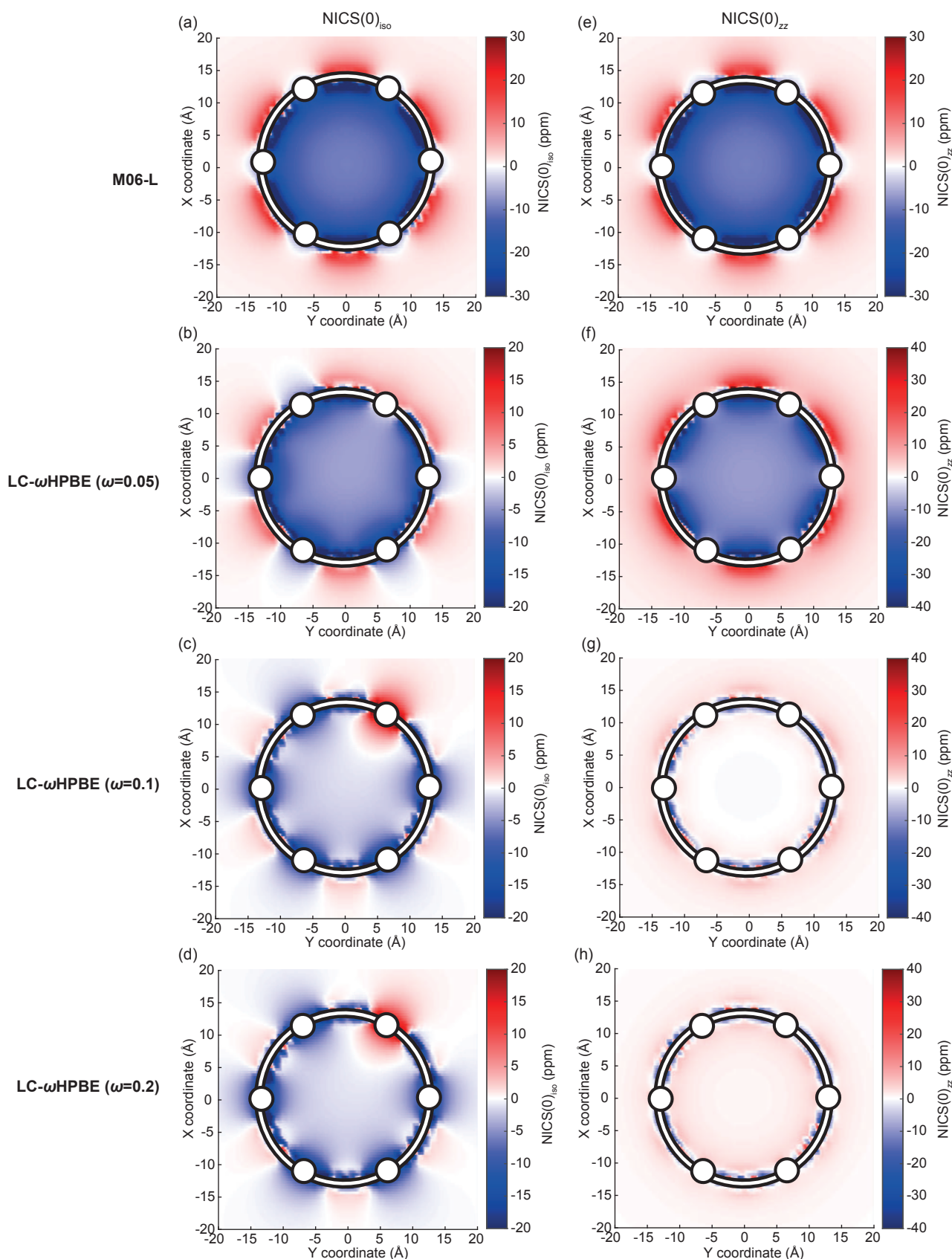


Figure S4: $\text{NICS}(0)_{\text{iso}}$ (left column) and $\text{NICS}(0)_{\text{zz}}$ (right column) for *c*-P6 in its T_1 state, calculated using the functionals M06-L and LC- ω HPBE ($\omega = 0.05$, $\omega = 0.1$, and $\omega = 0.2$), and the 6-31G* basis set. White circles indicate the positions of porphyrin units.

S1.4 Spin densities for T_1 excited states

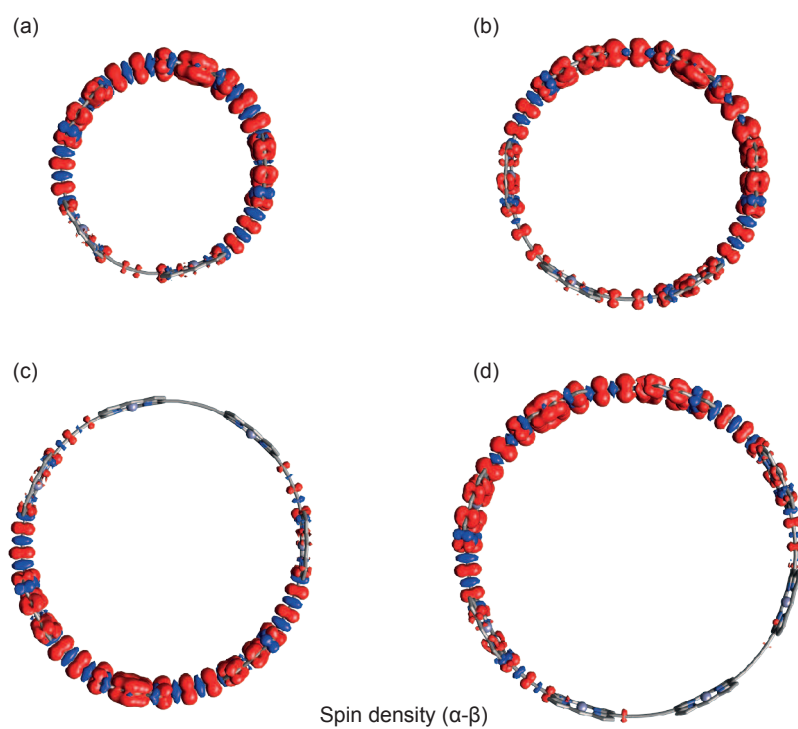


Figure S5: Calculated spin densities ($\alpha - \beta$) for (a) *c-P5*, (b) *c-P6*, (c) *c-P7*, and (d) *c-P8* in their T_1 states at the B3LYP/6-31G* level of theory.

S1.5 NICS grids for a porphyrin monomer in neutral and -1 oxidation states

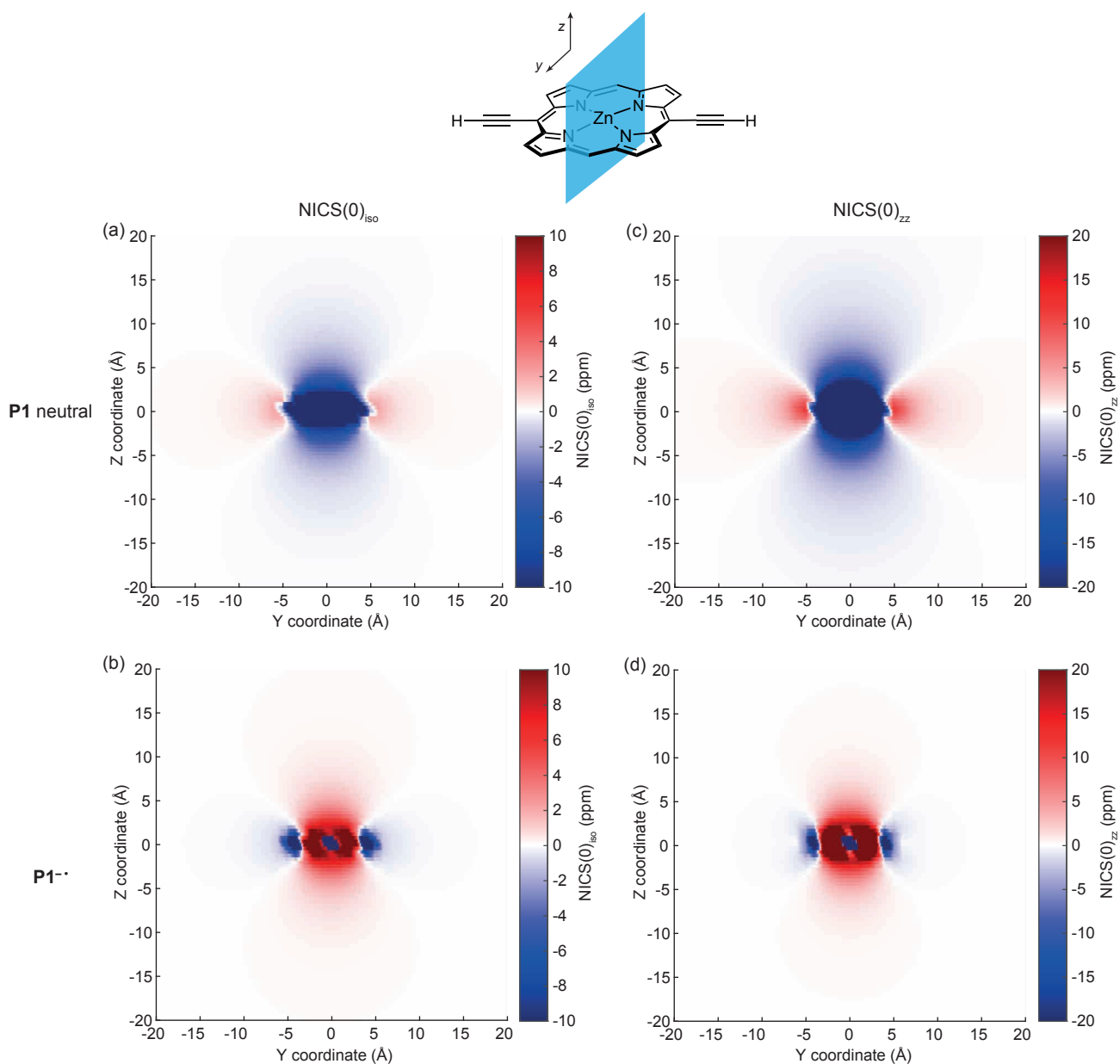


Figure S6: NICS(0)_{iso} (left column) and NICS(0)_{zz} (right column) for P1 in its neutral and radical anion states, calculated using at the B3LYP/6-31G* level of theory.

S1.6 HOMO–LUMO gaps of porphyrin nanorings

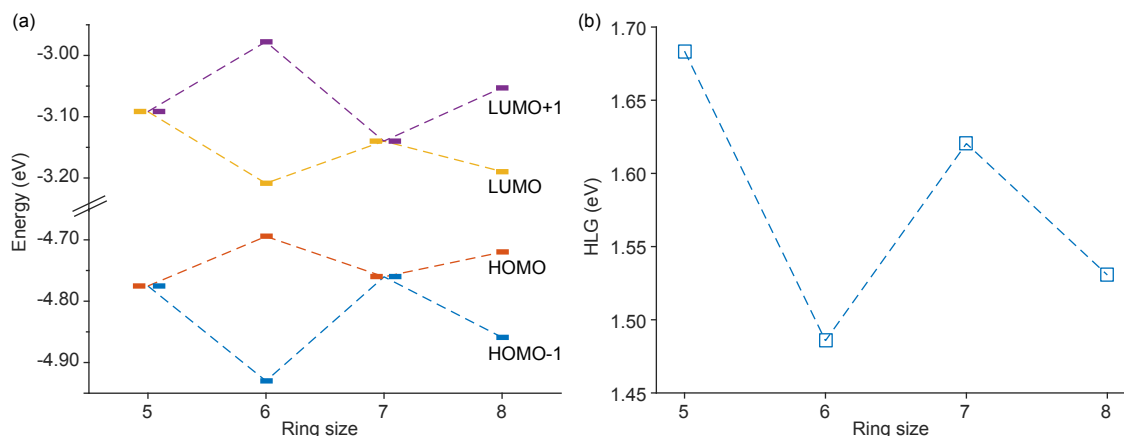


Figure S7: (a) Frontier molecular orbital energies for *c-P5*–*c-P8* (B3LYP/6-31G*) in the S_0 state. (b) HOMO–LUMO gaps for *c-P5*–*c-P8* in the S_0 state (B3LYP/6-31G*).

S2 Synthesis

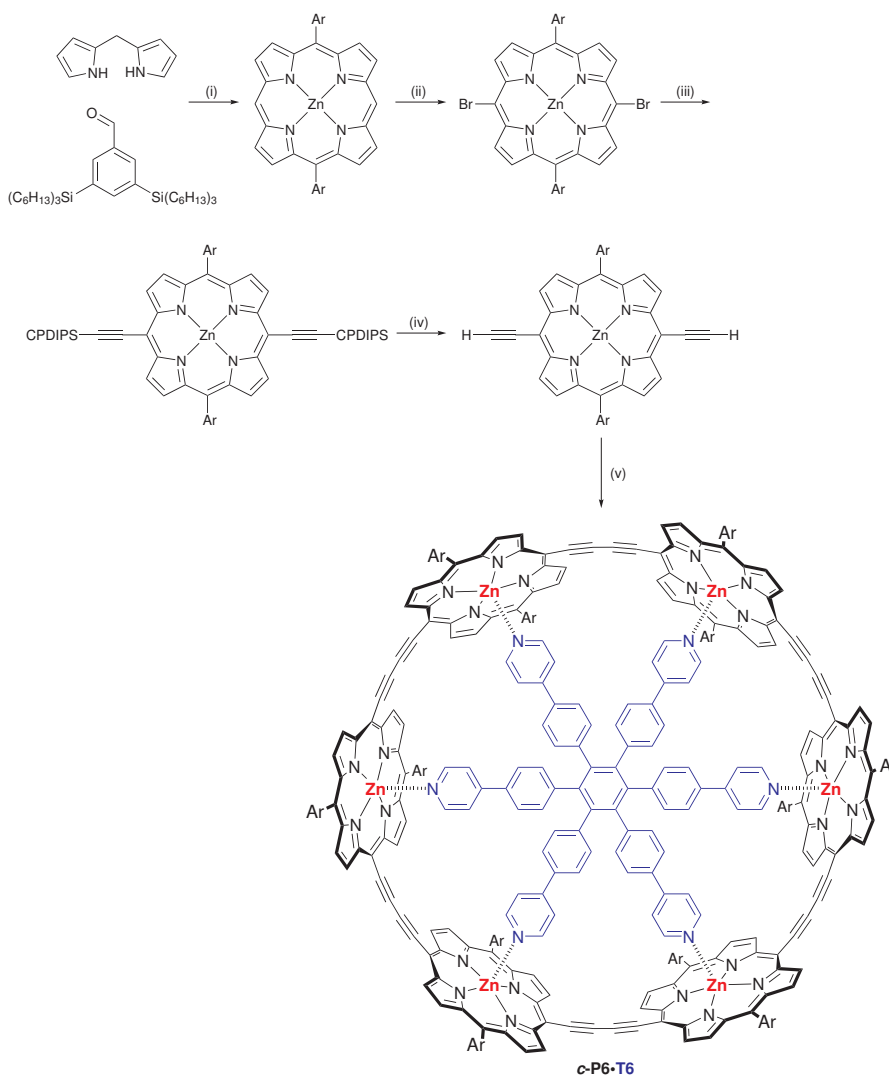
Unless stated otherwise, all reagents were obtained from commercial sources and used as received without further purification. Diethyl ether (Et_2O), chloroform (CHCl_3), tetrahydrofuran (THF), and toluene were dried by passing through activated alumina columns using a positive pressure of dry N_2 in an MBraun MB-SPS-5 benchtop solvent purification system (H_2O content < 20 ppm, determined by Karl-Fischer titration). Diisopropylamine (DIPA) was dried by distillation from CaH_2 . Analytical gel permeation chromatography (GPC) was performed on a JAIGEL H-P precolumn, a JAIGEL 3H-A (8 mm \times 500 mm) and a JAIGEL 4H-A column (8 mm \times 500 mm) in series with THF:pyridine 100:1 as eluent. Preparative recycling gel permeation chromatography was performed on a JAIGEL H-P precolumn, a JAIGEL 3H (20 mm \times 600 mm) and a JAIGEL 4H column (20 mm \times 600 mm) in series with toluene:pyridine 100:1 as eluent. Flash column chromatography was performed on Merck silica gel 60 (40–63 μm). Alumina columns were performed using aluminium oxide (activated, basic, Brockmann I, standard grade, \sim 150 mesh, 58 \AA) from Sigma Aldrich (purchased before 2017). For TLC, Merck silica gel 60 F254 aluminium-backed sheets were used. Size exclusion chromatography (SEC) was carried out using Bio-Beads SX-1, 200–400 mesh (Bio Rad).

NMR spectra were recorded on Bruker AVII400, Bruker AVIII400, Bruker AVII500 and Bruker AVIII500 spectrometers. The residual solvent peak was used as internal reference. Multiplicities (s = singlet, d = doublet, t = triplet, q = quartet, and m = multiplet) and coupling constant(s) are reported wherever possible. MALDI-TOF-MS spectra were measured using a Waters MALDI Micro MX. UV-vis absorption spectra were recorded at ambient temperature with a Perkin-Elmer Lambda 20 using quartz 1 cm cuvettes.

All porphyrin oligomers bore bulky trihexylsilyl (THS) solubilizing groups on the *meso*-aryl groups, to inhibit aggregation. *c-P5*, *c-P6*, and *c-P7* were prepared using template-directed synthesis followed by removal of the template (see below and refs).^{S14–S16} The larger nanorings were all produced as side-products in the large-scale synthesis of *c-P6* and were isolated by recycling GPC. Notably, the yield of *c-P10* (2.3%) is much higher than that of *c-P12* (0.1%), presumably because the bulky THS sidechains disfavour the formation of the *c-P12*· T6_2 figure-of-eight complex,^{S17} instead favoring a less-crowded *c-P10*· T6_2 complex in which two pyridine units (one per template) are unbound.

S2.1 c-P6•T6

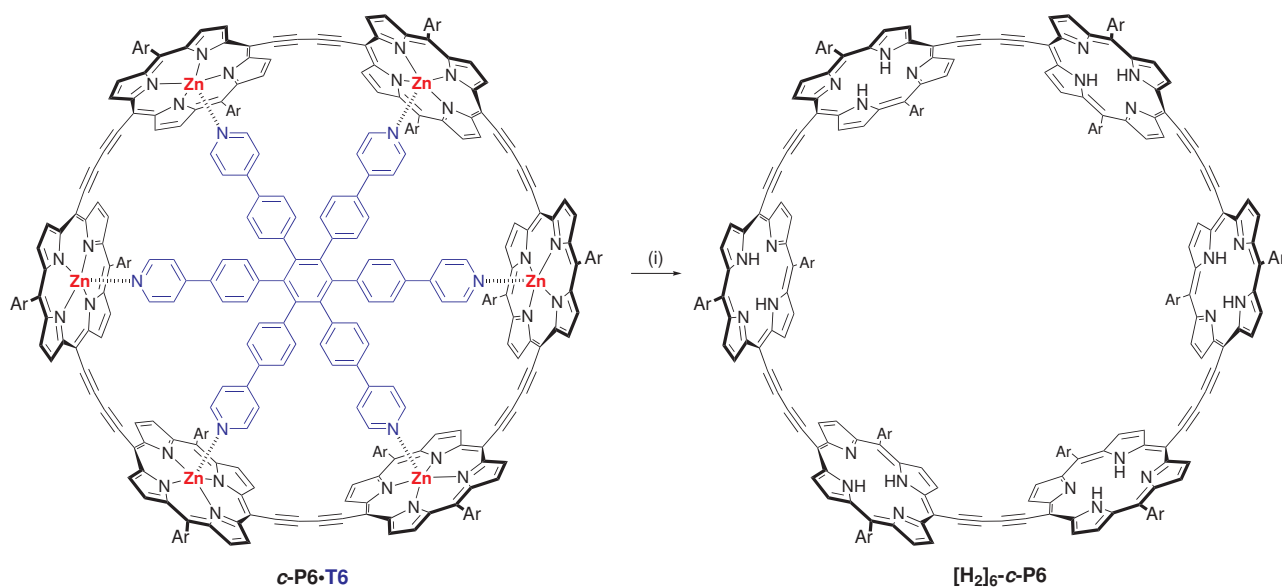
The overall route to **c-P6•T6** is shown in Scheme S1. Steps (i) to (v) are described elsewhere.^{S15}



Scheme S1: (i) TFA, CH₂Cl₂, then DDQ, then Et₃N; (ii) Zn(OAc)₂ · 2H₂O, CHCl₃, MeOH; (iii) *N*-bromosuccinimide, CH₂Cl₂; (iv) CPDIPS-acetylene, Pd(PPh₃)₂Cl₂, CuI, THF, DIPA; (v) TBAF, CH₂Cl₂; (vi) **T6**, Pd(PPh₃)₂Cl₂, CuI, 1,4-benzoquinone, CHCl₃, DIPA, 20 °C, 16 h, 20–36%. Yields and full experimental procedures for steps (i)–(v) reported in ref. [S15].

{H,H}-P1 (200 mg, 0.12 mmol) and template **T6** (26 mg, 29 μmol) were dissolved in CHCl₃ (133 mL) by sonication for 2 h. A solution of Pd(PPh₃)₂Cl₂ (27 mg, 39 μmol), copper(I) iodide (37 mg, 0.19 mmol) and 1,4-benzoquinone (89 mg, 0.80 mmol) in CHCl₃ (18 mL) and DIPA (0.25 mL) was added to the porphyrin mixture at 20 °C. The mixture was stirred at 20 °C overnight, open to air. The reaction mixture was partially concentrated and passed over a plug of alumina (CHCl₃). Purification by SEC (toluene) and preparative recycling GPC (toluene + 1% pyridine) afforded **c-P6•T6** (78 mg, 36%) as a brown solid. On a larger scale (800 mg **{H,H}-P1**), the yield was only 20% due to apparent co-absorption of polymer and product to alumina and glass frits during purification, and consequent mechanical losses. ¹H NMR (500 MHz, CDCl₃) δ_H, ppm: 9.54 (d, *J* = 4.2 Hz, 24H), 8.72 (d, *J* = 4.2 Hz, 24H), 8.30 (bs, 12H), 7.98 (bs, 12H), 7.97 (bs, 12H), 5.52 (d, *J* = 8.5 Hz, 12H), 5.45 (d, *J* = 8.5 Hz, 12H), 4.98 (d, *J* = 6.1 Hz, 12H), 2.41 (d, *J* = 5.8 Hz, 12H), 1.54–1.41 (m, 144H), 1.41–1.17 (m, 432H), 0.98–0.77 (m, 360H); MS (MALDI-TOF) *m/z*: calcd. M⁺ for C₇₂₀H₁₀₆₈N₃₀Si₂₄Zn₆: 11211; found: 11207. UV-vis (CH₂Cl₂) λ_{max} [nm] (log ε [M⁻¹ cm⁻¹]): 850 (5.61), 808 (5.70), 772 (5.57), 612 (4.59), 482 (5.76).

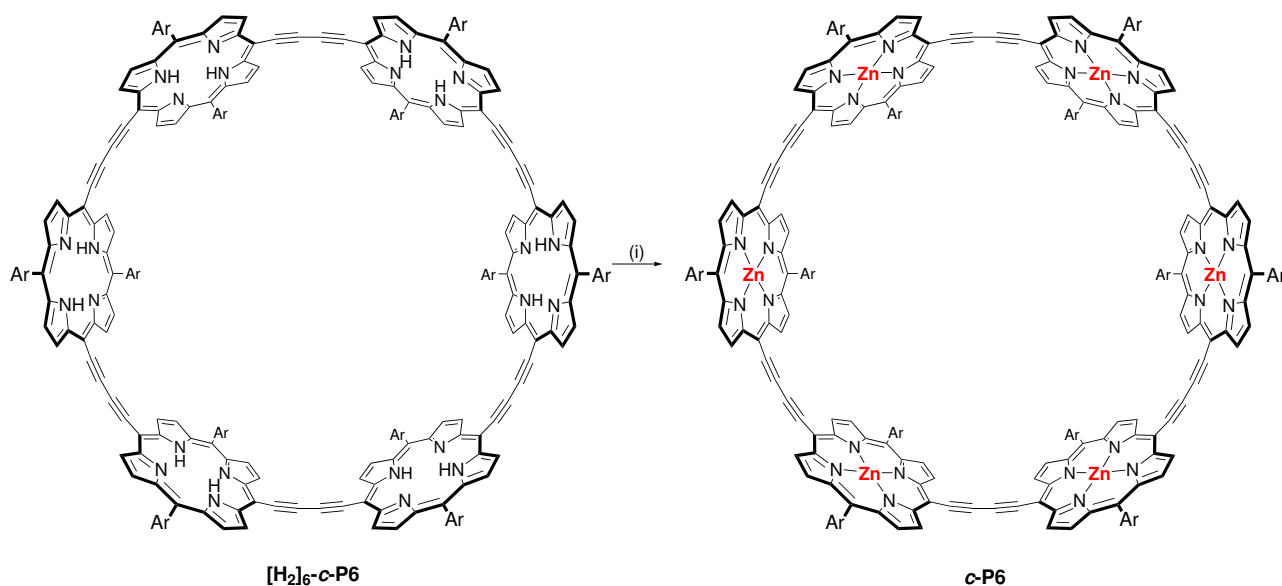
S2.2 Free-base *c*-P6 [H₂]₆-*c*-P6



Scheme S2: (i) TFA, CHCl₃, 20 °C, 5 min, 79–100%.

Trifluoroacetic acid (95 μ L, 1.24 mmol) was added to a solution of **c-P6·T6** (23 mg, 2.078 μ mol) in CHCl₃ (2 mL). The mixture was stirred at 20 °C until UV-vis indicated complete conversion of starting material (typically 5 min), then pyridine (0.2 mL) was added and the mixture was immediately filtered over a short column of silica gel (CHCl₃ + 1% pyridine). Removing the solvent yielded **FB-c-P6** (16 mg, 79%) as a green solid. Yields varied from 79% to 100%. ¹H (400 MHz, CDCl₃) δ_{H} , ppm: 9.56 (d, $J = 4.7$ Hz, 24H), 8.71 (d, $J = 4.7$ Hz, 24H), 8.15 (bs, 24H), 7.96 (bs, 12H), 1.52–1.36 (m, 144H), 1.36–1.14 (m, 432H), 1.07–0.94 (m, 144H), 0.94–0.85 (m, 216H), –1.29 (s, 12H); MS (MALDI-TOF) m/z : calcd. M⁺ for C₆₄₈H₁₀₃₂N₂₄Si₂₄: 9834; found: 9836; UV-vis (CH₂Cl₂) λ_{max} [nm] ($\log \epsilon$ [M⁻¹ cm⁻¹]): 791 (5.47), 771 (5.49), 659 (5.30), 466 (5.72).

S2.3 c-P6



Scheme S3: (i) Zn(OAc)₂ · 2H₂O, CHCl₃, MeOH, 40 °C, 70 min, quant. Over two steps (with Scheme S2), 73%.

[H₂]₆-c-P6 (43.9 mg, 4.5 μmol) was dissolved in CHCl₃ (6 mL) and a solution of Zn(OAc)₂ · 2H₂O (8.8 mg, 219 μmol) in methanol (0.6 mL) was added. The mixture was stirred at 40 °C for 70 min, at which time UV-vis indicated reaction completion. The mixture was then filtered through a short column of silica gel (CH₂Cl₂ + 1% pyridine) to afford **c-P6** (46 mg, quant.) as a brown solid. ¹H (400 MHz, CDCl₃) δ_H, ppm: 9.67 (d, *J* = 4.6 Hz, 24H), 8.81 (d, *J* = 4.6 Hz, 24H), 8.16 (m, 24H), 7.91 (m, 12H), 1.50–1.37 (m, 144H), 1.37–1.12 (m, 432H), 0.94–0.84 (m, 144H), 0.84–0.72 (m, 216H); MS (MALDI-TOF) *m/z*: calcd. M⁺ for C₆₄₈H₁₀₂₀N₂₄Si₂₄Zn₆: 10214; found: 10211; UV-vis (CH₂Cl₂) λ_{max} [nm] (log ε [M⁻¹ cm⁻¹]): 772 (5.45), 748 (5.49), 593 (4.62), 473 (5.71).

In another example, the two-step preparation of **c-P6** from **c-P6·T6** had an overall yield of 73%.

S2.4 Removal of templates from larger rings

The template, **T6**, was removed from rings larger than **c-P6** by displacement with pyridine. A sample of ring was dissolved in CHCl₃ + 20% pyridine, and passed through a SEC column (eluting with CHCl₃ + 20% pyridine). The absence of template was confirmed by ¹H NMR spectroscopy. Residual pyridine could be removed by washing a CH₂Cl₂ solution of nanoring with a saturated aqueous solution of potassium hydrogen phthalate (three times), then with water (twice) before passage over a SiO₂ plug (CHCl₃) to remove water and phthalate residues. An alternative method of removing pyridine is to repeatedly dissolve the sample in tetrahydrofuran, and remove the solvents by evaporation. The phthalate wash is much more reliable.

S2.5 c-P8

c-P8 was isolated as a by-product in the synthesis of **c-P6·T6** (from 0.8 g **{H,H}-P1**) as a brown solid (3.2 mg, 0.4%). ¹H (400 MHz, CDCl₃) δ_H, ppm: 9.74 (d, *J* = 4.5 Hz, 32H), 8.85 (d, *J* = 4.5 Hz, 32H), 8.21 (s, 32H), 7.97 (s, 16H), 1.76–0.72 (m, 1248H); MS (MALDI-TOF) *m/z*: calcd. M⁺ for C₈₆₄H₁₃₆₀N₃₂Si₃₂Zn₈: 13615; found: 13786; UV-vis (CH₂Cl₂) λ_{max} [nm] (log ε [M⁻¹ cm⁻¹]): 818 (5.54), 597 (4.62), 495 (5.74), 469 (5.68).

S2.6 c-P9

c-P9 was isolated as a by-product in the synthesis of **c-P6•T6** (from 0.8 g **{H,H}-P1**) as a brown solid (2.9 mg, 0.4%). ^1H (400 MHz, CDCl_3) δ_{H} , ppm: 9.83 (d, $J = 4.6$ Hz, 36H), 8.93 (d, $J = 4.6$ Hz, 36H), 8.26 (s, 36H), 8.00 (s, 18H), 1.52–0.80 (m, 1404H); MS (MALDI-TOF) m/z : calcd. M^+ for $\text{C}_{972}\text{H}_{1530}\text{N}_{36}\text{Si}_{36}\text{Zn}_9$: 15317; found: 15550; UV-vis (CH_2Cl_2) λ_{max} [nm] ($\log \epsilon$ [$\text{M}^{-1} \text{cm}^{-1}$]): 821 (5.60), 600 (4.66), 487 (5.78), 472 (5.77).

S2.7 c-P10

c-P10 was isolated as a by-product in the synthesis of **c-P6•T6** (from 0.8 g **{H,H}-P1**) as a brown solid (19.2 mg, 2.3%). ^1H (400 MHz, CDCl_3) δ_{H} , ppm: 9.80 (d, $J = 4.6$ Hz, 40H), 8.88 (d, $J = 4.6$ Hz, 40H), 8.25 (s, 40H), 7.99 (s, 20H), 1.60–0.79 (m, 1560H); MS (MALDI-TOF) m/z : calcd. M^+ for $\text{C}_{1080}\text{H}_{1700}\text{N}_{40}\text{Si}_{40}\text{Zn}_{10}$: 17019; found: 17241; UV-vis (CH_2Cl_2) λ_{max} [nm] ($\log \epsilon$ [$\text{M}^{-1} \text{cm}^{-1}$]): 821 (5.73), 598 (4.81), 495 (5.89, sh.), 471 (5.92).

S2.8 c-P11

c-P11 was isolated as a by-product in the synthesis of **c-P6•T6** (from 0.8 g **{H,H}-P1**) as a brown solid (2.1 mg, 0.3%). ^1H (400 MHz, CDCl_3) δ_{H} , ppm: 9.90 (d, $J = 4.7$ Hz, 44H), 8.98 (d, $J = 4.6$ Hz, 40H), 8.31 (s, 40H), 8.02 (s, 20H), 1.60–0.80 (m, 1716H); MS (MALDI-TOF) m/z : calcd. M^+ for $\text{C}_{1188}\text{H}_{1870}\text{N}_{44}\text{Si}_{44}\text{Zn}_{11}$: 18721; found: 19016; UV-vis (CH_2Cl_2) λ_{max} [nm] ($\log \epsilon$ [$\text{M}^{-1} \text{cm}^{-1}$]): 820 (5.70), 596 (4.79), 493 (5.88), 471 (5.89).

S2.9 c-P12

c-P12 was isolated as a by-product in the synthesis of **c-P6•T6** (from 0.8 g **{H,H}-P1**) as a brown solid (1.2 mg, 0.1%). ^1H (400 MHz, CDCl_3) δ_{H} , ppm: 9.68 (d, $J = 4.5$ Hz, 48H), 8.80 (d, $J = 4.5$ Hz, 48H), 8.17 (s, 48H), 7.95 (s, 24H), 1.74–0.63 (m, 1872H); MS (MALDI-TOF) m/z : calcd. M^+ for $\text{C}_{1296}\text{H}_{2040}\text{N}_{48}\text{Si}_{48}\text{Zn}_{12}$: 20423; found: 20657; UV-vis (CH_2Cl_2) λ_{max} [nm] ($\log \epsilon$ [$\text{M}^{-1} \text{cm}^{-1}$]): 821 (5.88), 596 (4.88), 488 (6.06), 472 (6.07).

S2.10 c-P13

c-P13 was isolated as a by-product in the synthesis of **c-P6•T6** (from 0.8 g **{H,H}-P1**) as a brown solid (1.9 mg, 0.2%). ^1H (400 MHz, CDCl_3) δ_{H} , ppm: 9.93 (d, $J = 0.45$ Hz, 52H), 9.00 (d, $J = 0.45$ Hz, 52H), 8.33 (s, 52H), 8.04 (s, 52H), 1.62–0.82 (m, 2028H); MS (MALDI-TOF) m/z : calcd. M^+ for $\text{C}_{1404}\text{H}_{2210}\text{N}_{52}\text{Si}_{52}\text{Zn}_{13}$: 22125; found: 22530; UV-vis (CH_2Cl_2) λ_{max} [nm] ($\log \epsilon$ [$\text{M}^{-1} \text{cm}^{-1}$]): 821 (5.75), 595 (4.83), 490 (5.91), 472 (5.93).

S2.11 c-P16

c-P16 was isolated as a by-product in the synthesis of **c-P6•T6** (from 0.8 g **{H,H}-P1**) as a brown solid (2.4 mg, 0.3%). ^1H (400 MHz, CDCl_3) δ_{H} , ppm: 10.00 (d, $J = 4.4$ Hz, 64H), 9.07 (d, $J = 4.4$ Hz, 64H), 8.39 (s, 64H), 8.08 (s, 32H), 1.60–0.86 (m, 2496H); MS (MALDI-TOF) m/z : calcd. M^+ for $\text{C}_{1728}\text{H}_{2720}\text{N}_{64}\text{Si}_{64}\text{Zn}_{16}$: 27230; found: 27686; UV-vis (CH_2Cl_2) λ_{max} [nm] ($\log \epsilon$ [$\text{M}^{-1} \text{cm}^{-1}$]): 829 (5.89), 594 (4.97), 491 (6.03), 473 (6.05).

S2.12 GPC retention times of THS porphyrin oligomers

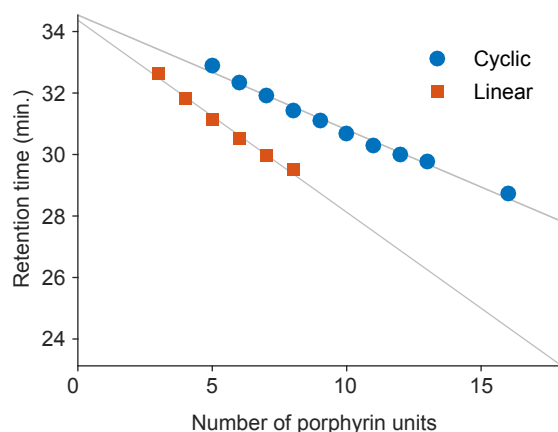


Figure S8: Analytical GPC retention times for THS porphyrin oligomers. Using two JIAGEL-H columns in series (3H-A then 4H-A), with THF:1% pyridine eluent and a 1 mL min^{-1} flow rate. The lines show linear regression fits: $RT = m \cdot N + c$ where RT is retention time and N is oligomer length. For cyclic oligomers, $m = -0.373 \text{ min}$ and $c = 34.54 \text{ min}$. For linear oligomers, $m = -0.625 \text{ min}$ and $c = 34.37 \text{ min}$. For both fits, $R^2 = 0.989$.

S3 Photophysical measurements

Nanoring samples were prepared at a concentration of $\sim 1 \mu\text{M}$ in toluene + 1% pyridine (the latter to suppress aggregation). Fluorescence quantum yields (Φ_F) were measured relative to that of **I-P6**, using the technique reported previously, with excitation at 500 nm.^{S18,S19} Excited state lifetimes (τ) were measured by time-correlated single-photon counting (TCSPC) spectroscopy, and the radiative rate (k_R) was calculated. In Figure S11 and Main Text Figure 5, the dotted lines connect measurements within the same experimental replicate: i.e. measurements taken on the same day, with the same solvent stocks, with identical instrument configuration, and at the same temperature.

$$\tau = \frac{1}{k_{\text{tot}}} \quad (\text{S2})$$

$$k_{\text{tot}} = k_R + k_{\text{NR}} \quad (\text{S3})$$

$$\Phi = \frac{k_R}{k_R + k_{\text{NR}}} \quad (\text{S4})$$

$$k_R = \Phi k_{\text{tot}} \quad (\text{S5})$$

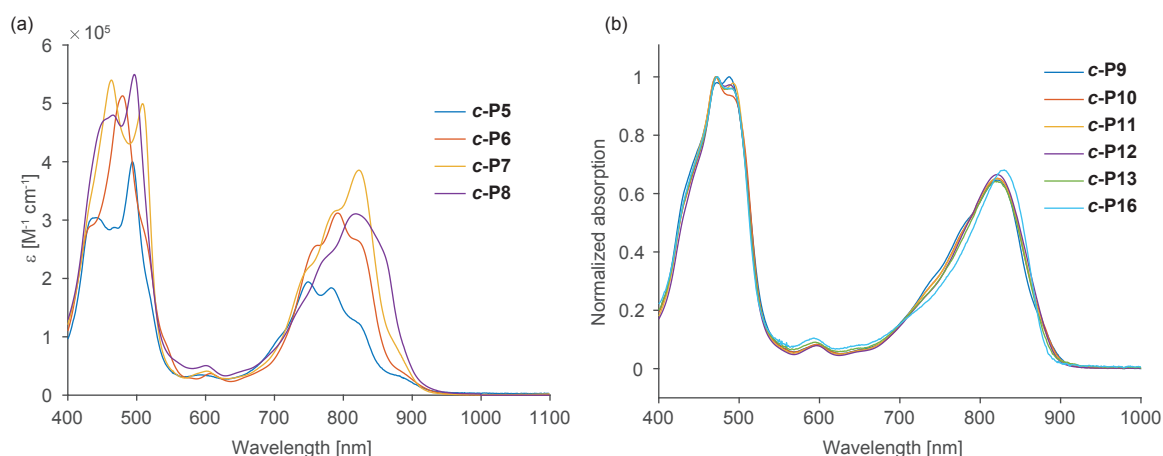


Figure S9: UV-Vis spectra of nanorings in toluene/1% pyridine.

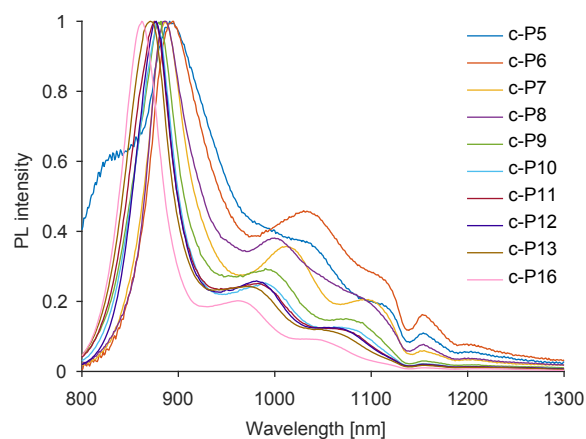


Figure S10: Normalized photoluminescence spectra of porphyrin nanorings, λ_{ex} 500 nm, in toluene/1% pyridine.

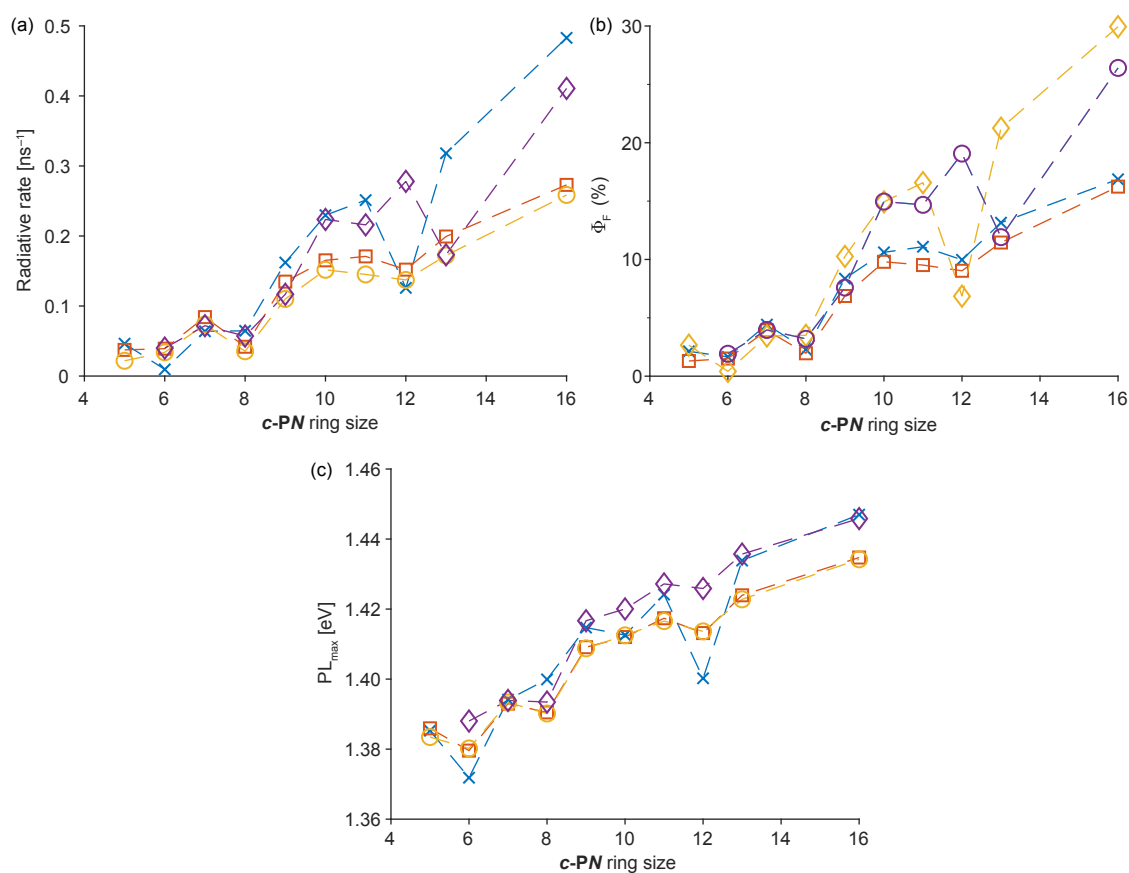


Figure S11: (a) Radiative rates; (b) quantum yields and (c) energy of maximum intensity peak in PL spectra, for **c-P5** to **c-P16**. $\lambda_{\text{ex}} = 500$ nm, in toluene/1% pyridine. Lines connect measurements from the same experimental replicate. The PL maxima are calibrated based on measurements of **I-P6**, for which PL_{max} is taken as 1.47 eV.

S3.1 Statistical analysis

We compare two linear models in their ability to describe the experimental data for **c-P5** to **c-P9**, inclusive.^{S20}

Model A, $Y \sim N$, states that Y (radiative rate, PL_{max} , or quantum yield) only depends on oligomer length (N).

In model B, $Y \sim N + O$, Y also depends on whether the oligomer is odd ($O = 1$) or even ($O = -1$).

$$\text{Model A: } Y \sim N$$

$$\text{Model B: } Y \sim N + O$$

The R package (v. 3.2.1)^{S21} was used to compare the fits of the model. A linear model was employed, assuming Gaussian distribution of errors in measurements. The data from all four runs was analyzed together. The AIC (Akaike information criterion) statistic was used to evaluate the best model. Essentially, AIC tests (and compares) the suitability of models. A lower AIC score (hence a negative ΔAIC , where $\Delta\text{AIC} = \text{AIC}_{\text{model B}} - \text{AIC}_{\text{model A}}$) corresponds to a better model. The AIC score is increased by the presence of additional parameters, and by a poor fit to the data.

The AIC revealed that model B (including odd-even effects) fit the data better (Table S4) for nanorings from **c-P5** to **c-P9**. When the whole dataset was fit (i.e. **c-P5** to **c-P16**), model B was no better than model A for both radiative rates and quantum yields.

Table S4: Comparison of calculated ΔAIC (defined as $\Delta\text{AIC} = \text{AIC}_{\text{model B}} - \text{AIC}_{\text{model A}}$) for different experimental measurements (Y).

Y	ΔAIC for $5 \leq N \leq 16$	ΔAIC for $5 \leq N \leq 9$
Radiative rates	2	-16
Quantum yield (Φ_F)	1	-17
PL_{max}	-12	-15

The difference between models A and B is clearly illustrated by plots of the fits to all three experimental datasets (Figures S12 to S14).

In conclusion, a model including odd-even behaviour is better able to describe the experimental photophysical data than a model without, but only for nanorings smaller than **c-P10**.

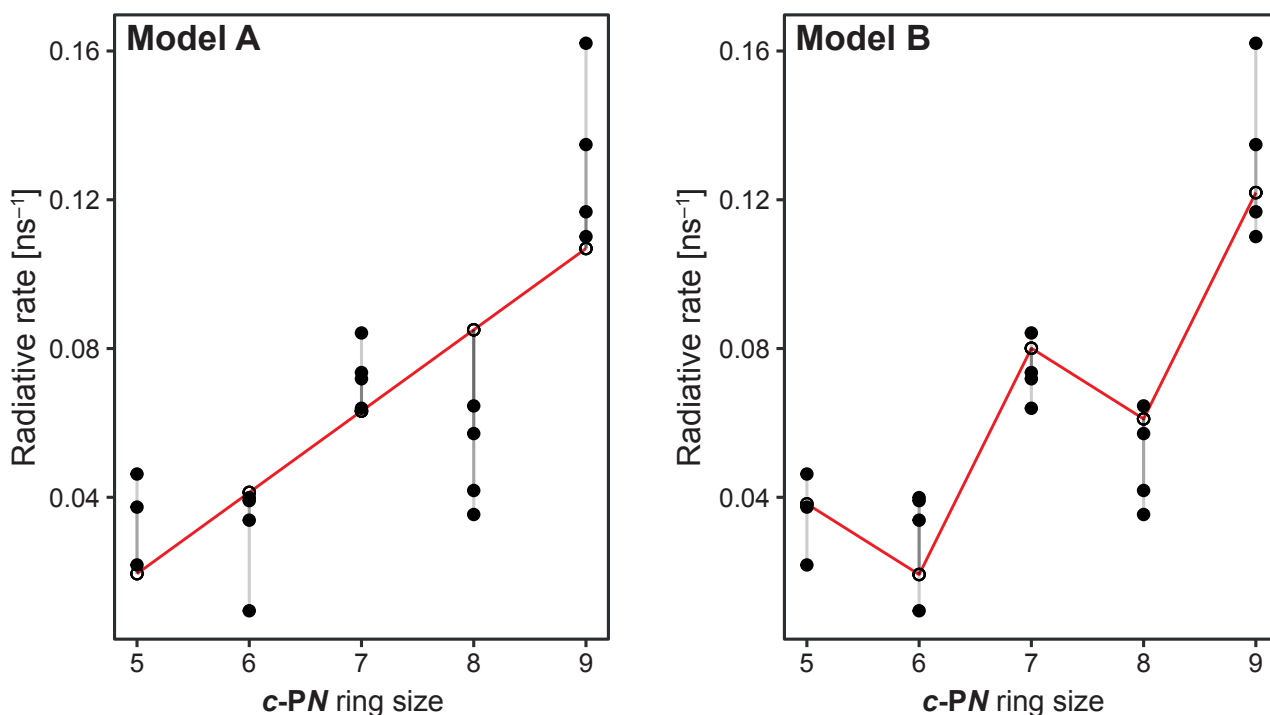


Figure S12: Comparison of fit (red line and open circles) and data (filled black circles) for radiative rates of **c-P5** to **c-P9**. (a) model A, which depends only on N ; (b) model B, which depends on N and whether the ring is odd or even. In model B, $\text{RR} = 0.02092 \cdot N + 0.03992 \cdot \text{odd} - 0.10627$

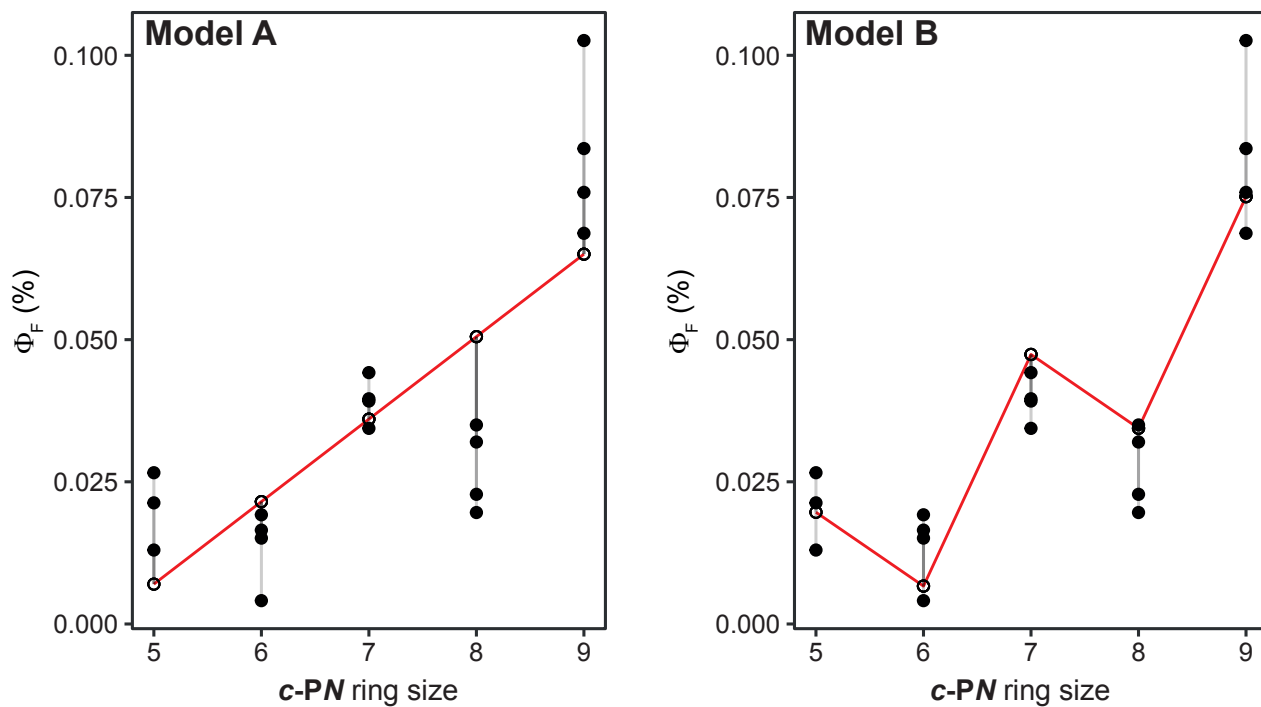


Figure S13: Comparison of fit (red line and open circles) and data (filled black circles) for QY of *c*-P5 to *c*-P9. (a) model A, which depends only on *N*; (b) model B, which depends on *N* and whether the ring is odd or even. In model B, $\Phi_F = 0.1388 \cdot N + 0.2686 \cdot \text{odd} - 0.7659$

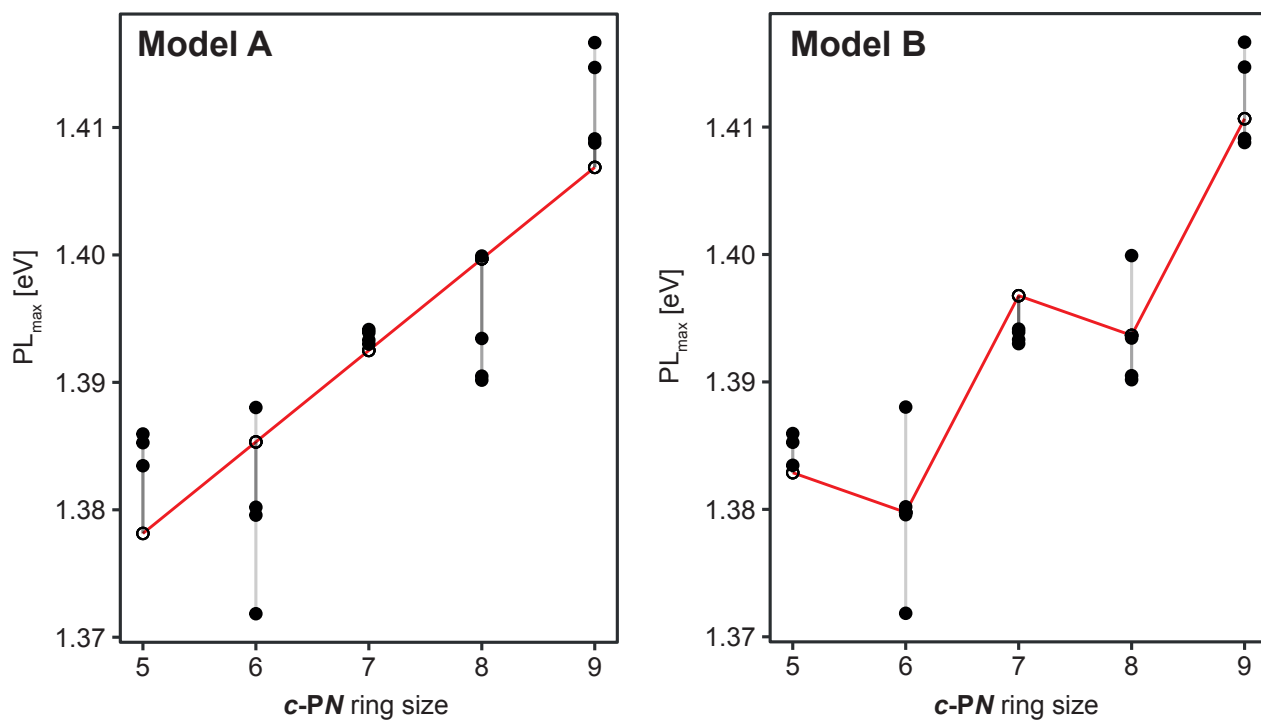


Figure S14: Comparison of fit (red line and open circles) and data (filled black circles) for PL_{\max} of *c*-P5 to *c*-P9. (a) model A, which depends only on *N*; (b) model B, which depends on *N* and whether the ring is odd or even. In model B, $PL_{\max} = 0.006945 \cdot N + 0.010057 \cdot \text{odd} + 1.338092$

S4 Cartesian coordinates

The Cartesian coordinates listed below are also available in the native XYZ file format in a separate ZIP archive, with the Supporting Information online.

S4.1 c-P5 S₀

195

cP5 SO B3LYP/6-31G* E(a.u): -14593.4950447

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C	-1.248070842749	10.713934967178	-2.788248274287	C	-10.268769142789	3.336525352901	3.404764367996
N	-1.453312170552	10.609153154325	-1.430424178924	N	-10.539002399075	1.896226610273	-1.430424178924
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C	-3.468302642315	10.4231036401515	-2.532670154300	C	-8.839230115319	6.518829179578	-2.532670154300
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N	1.453312170552	10.609153154325	1.430424178924	C	-4.214661207329	-10.069093050217	3.481152695826
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H	8.387728040715	7.491352633661	-2.670921658216	C	11.215518195098	1.007581057231	3.485881164509
H	9.349104070475	5.807598210433	-4.554734107845	C	11.004280970151	-0.0022726064942	0.002227432622
H	2.382507925623	-10.990814436093	-2.670921658216	C	9.301195248489	5.957918659384	-1.270546947122
H	4.149963490535	-10.193711146424	-4.554734107845	C	9.142650089594	6.616422609915	-2.534380151867
H	9.716650247333	-5.662248135703	2.670921658216	C	9.668410514401	5.774580241422	-3.481825552768
H	8.412386162462	-7.096879804548	4.554734107845	C	5.200852755617	-9.211706056666	2.790267106677
H	2.382507925623	-10.990814436093	2.670921658216	C	6.265923781813	-8.554449164698	3.406003261606
H	4.149963490535	-10.193711146424	4.554734107845	N	7.340605863344	-7.550858985313	-1.430392816522
H	9.716650247333	-5.662248135703	-2.670921658216	C	5.201980031964	-9.211482166047	-2.788372027285
H	8.412386162462	-7.096879804548	-4.554734107845	N	4.971966885363	-9.243086233430	-1.429942950083
H	-8.387728037004	7.491352637816	-2.670921658216	C	3.774284364907	-9.878703851636	-1.256910154933
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H	-11.189121127199	-1.130448749768	2.670921658216	C	4.128666232448	-9.875357881260	-3.481160813974
H	-10.977204654805	0.796819845178	4.554734107845	C	6.267305256754	-8.554184367363	-3.403624376705
H	-8.387728037004	7.491352637816	2.670921658216	Zn	6.158909887204	-8.402398028688	0.001173434738
H	-9.349104067598	5.807598215065	4.554734107845	C	7.235813483472	-7.762989853602	-2.793244827556
H	-11.189121127199	-1.130448749768	-2.670921658216	N	7.340022808530	-7.550968018948	1.433285221244
H	-10.977204654805	0.796819845178	-4.554734107845	C	8.331948103764	-6.629826044037	1.263403524931
H	-2.382507931068	-10.990814434913	-2.670921658216	C	8.885816280383	-6.250101594070	2.537246495473
H	-4.149963495585	-10.193711144368	-4.554734107845	C	8.216334188053	-6.969782414147	3.485865163185
H	-9.716650250138	-5.662248130889	2.670921658216	C	7.236951884642	-7.762780628073	-2.790410472760
H	-8.412386165978	-7.096879800380	4.554734107845	C	8.756671375957	-6.114111682530	0.001789056253
H	-2.382507931068	-10.990814434913	2.670921658216	N	4.971387308821	-9.243198276349	1.431742630162
H	-4.149963495585	-10.193711144368	4.554734107845	C	3.773776706761	-9.878805108376	1.258174560167
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H	-8.412386165978	-7.096879800380	-4.554734107845	C	4.127261942521	-9.875643428671	3.482567941167
H	0.000000002691	0.863870541667	-4.489221914243	C	3.155862131490	-10.118111956441	0.000497733746
H	10.332154872119	3.357120619179	4.489221914243	C	8.332466167961	-6.629736884686	-1.260037584006
H	10.332154872119	3.357120619179	-4.489221914243	C	8.886863611205	-6.249926433198	-2.533625892547
H	6.385622885306	-8.789055895333	4.489221914243	C	8.217763801251	-6.969532081949	-3.482570971558
H	6.385622885306	-8.789055895333	-4.489221914243	C	1.806486435023	-10.532935012888	0.000205629028
H	-10.332154870456	3.357120624298	4.489221914243	C	-9.878741726073	4.394119595266	2.786900524342
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H	-6.385622889660	-8.789055892169	-4.489221914243	C	-9.083766721968	5.755393934798	-1.257660501420
H	0.000000002691	10.863870541667	4.489221914243	C	-8.855713648744	6.386910842633	-2.534324873505
H				C	-9.368382999271	5.551081598600	-3.482955440348
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H				C	-10.690506156809	1.816178799050	1.428411986135
H				C	-10.963973039444	0.487484861327	1.253684650502
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H				C	-11.056579212484	0.825659634716	3.478964366100
H				C	-10.719048779925	2.044348378052	-2.790060130604
H				C	-11.018476112292	-0.171465989062	-0.002067556918
H				C	-9.710889340817	4.582919249712	1.428219249712
H				C	-9.084096210217	5.755246161888	1.254731039751
H				C	-8.856371772866	6.386609373162	2.531530254350
H				C	-9.369293611524	5.506929593218	3.4779927244389
H				C	-8.712222042330	6.302561864470	-0.001383781986
H				C	-10.963635329239	0.487628958291	-1.257728782211
H				C	-11.185867575078	-0.145907783491	-2.534479762861
H				C	-11.055639534180	0.826060429650	-3.482994428527
H				C	-9.847200981232	-5.189242200103	-0.002071628302
H				C	-7.831863836307	7.408828780486	-0.001204800191
H				C	-11.017193690754	-1.586584329050	-0.002143045294
H				C	-5.412318443817	-9.360024021183	2.787213920066
H				C	-6.490179283407	-8.725198599946	3.403403068877
H				N	-7.583033195287	-7.750632536931	-1.432047701107
H				C	-5.410992031986	-9.359589925435	-2.789886124247
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H				C	-3.968831708486	-9.994282706515	-1.257238196795
H				C	-3.413125132411	-10.371247699720	-2.533867079405
H				C	-4.318968031590	-9.996070938635	-3.482667158132
H				C	-6.488561073019	-8.724631954266	-3.406488681015
H				Zn	-6.390423535561	-8.580761922539	-0.001508605843
H				C	-7.473670711343	-7.9852495531462	2.530394658965
H				N	-7.583713712185	-7.750855892269	1.428592915581
H				C	-8.585646319761	-6.836347758258	1.253811927375
H				C	-9.138190197076	-6.454404681153	2.530394658965
H				C	-8.462098150787	-7.164503121943	3.479088851350
H				C	-7.472346425108	-7.952064252664	-2.789877989145
H				C	-9.016793824222	-6.335097480186	-0.001958417487
H				N	-5.183385015191	-9.389393760690	1.429256005755
H				C	-3.969429688536	-9.994478695941	1.255153324126
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H				C	-3.346818085083	-10.218809336904	-0.000911573288
H				C	-8.585051962877	-6.836155820422	-1.257601417439
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H				Zn	-1.984458311596	-10.596742318000	-0.000619916280
H				C	0.044271537687	10.604245282544	3.404858608424
H				C	0.046945094550	10.417794411376	0.000058276640
H				C	-9.710509115348	4.552534392449	-1.432158249222
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H				Zn	-10.212659531628	3.188815050217	-0.001764624379
H				C	-6.914122688217	8.223736672756	-0.001041775736
H				C	-5.806879599015	9.000807079344	-0.000857134556
H				C	10.589807855060	-2.619024956854	0.002205059054

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cP5 T1 UB3LYP/6-31G* E(au): -14593.4562255

C	-1.203755419266	10.510215585922	2.789162591052	C	-10.719048779925	2.044348378052	-2.790060130604
C	7.974934670012	7.537794625632	0.001507377038	C	-11.018476112292	-0.171465989062	-0.002067556918
N	1.503452562303	10.422806967018	-1.431538034257	C	-9.710889340817	4.582919249712	1.428219249712
C	-1.202823200505	10.509828206529	-2.789476853990	C	-9.084096210217	5.755246161888	1.254731039751
N	-1.407489434239	10.400471004639	-1.431026500024	C	-8.856371772866	6.386609373162	2.531530254350
C	-2.750095060460	10.211146125537	-1.257937090244	C	-9.369293611524	5.506929593218	3.4779927244389
C	-3.421318943143	10.210010925279	-2.533529882225	C	-8.712222042330	6.302561864470	-0.001383781986
C	-2.4614111067688	10.416308695452	-3.482226463942	C	-10.963635329239	0.487628958291	-1.257728782211
C	0.045409188237	10.603786858789	-3.404769437111	C	-11.185867575078	-0.145907783491	-2.534479762861
C	1.294103696270	10.533560634408	2.792086144718	C	-11.055639534180	0.826060429650	-3.482994428527
N	1.502973750344	10.423001190222	1.432140173870	C	-9.847200981232	-5.189242200103	-0.002071628302
C	2.846840240639	10.260395331178	1.262257362532	C	-7.831863836307	7.408828780486	-0.001204800191
C	3.518157199569	10.278757380223	2.536083663348	C	-11.017193690754	-1.586584329050	-0.002143045294
C	2.553592226965	10.467919191233	3.484691329418	C	-5.412318443817	-9.360024021183	2.787213920066
C	1.295036344294	10.533170379235	-2.791569516311	C	-6.490179283407	-8.725198599946	3.403403068877
C	3.493501520597	10.092421907939	0.000656541047	N	-7.583033195287	-7.750632536931	-1.432047701107
N	-1.407967630625	10.400667482501	1.430659279122	C	-5.410992031986	-9.359589925435	-2.789886124247
C	-2.750514994024	10.211316386195	1.257147857010	N	-5.182701956690	-9.389166944890	-1.431824196294
C	-3.422165160067	10.210357047633	2.532516189816	C	-3.968831708486	-9.994282706515	-1.257238196795
C	-2.462574731653	10.416790126705	3.481503752170	C	-3.413125132411	-10.371247699720	-2.533867079405
C	-3.391154964996	10.041715120455	-0.000489822238	C	-4.318968031590	-9.996070938635	-3.482667158132
C	2.847261997870	10.2602225					

C	10.121416649172	-3.871383719688	0.002113950013	C	12.654152130448	-3.473213593599	-2.532960715949
C	5.915539200145	9.079458544899	0.001114546462	H	12.883405022708	-2.633273762665	-4.556815491321
C	0.589501306230	-10.695177437868	-0.000058641651	C	12.653189629896	-1.255817326326	-1.255817326326
C	-0.763034039353	-10.716938071106	-0.000353121257	H	12.545592808042	-4.539959251304	-2.670445088502
C	7.030372183630	8.341259366873	0.001327235822	C	12.511612281041	-3.447636050870	0.000000000000
C	-10.371217709397	-4.080000112138	-0.002130028095	Zn	12.818609138434	0.000000000000	0.000000000000
C	-10.789487278463	-2.792055966236	-0.002154882781	C	12.121709060589	-4.807511772966	0.000000000000
H	-4.485480960700	10.079527033349	-2.672260441851	C	11.616164256994	-5.924849339952	0.000000000000
H	-2.587276695049	10.480986461741	-4.555682207120	C	12.121709060589	4.807511772966	0.000000000000
H	4.584808565907	10.171117712481	2.675390380707	C	11.616164256994	5.924849339952	0.000000000000
H	2.678441390987	10.539040172249	4.557831643456	C	6.487296408164	11.236326982700	-3.406820644400
H	-4.486373681828	10.079891741685	2.670907916497	C	5.370437593259	11.798001177540	-2.789634986275
H	-2.588799634052	10.481617954353	4.554909250659	C	7.532149936999	10.549935973971	-2.789634986275
H	4.585701230201	10.170737704913	-2.673725373615	C	4.20449654496	12.363854756418	-3.482632209072
H	2.679962435371	10.538392449714	-4.556854207203	N	5.145577375251	11.821962444194	-1.431029608907
H	11.503432104917	-1.032172640134	-2.674810789184	C	8.587187480511	9.854264502471	-3.482632209072
H	11.359108011059	0.915388314514	-4.550914128015	N	7.665331111632	10.367181946203	-1.431029608907
H	8.701319339588	7.593767306297	2.678769285139	C	3.319184860398	12.695424005120	-2.532960715949
H	9.728327378042	5.932863142099	4.555000443668	H	4.161220537768	12.473992918242	-4.556815491321
H	11.502581929714	-1.032001774801	2.679486158605	C	3.899749697366	12.359123340309	-1.255817326326
H	11.357673513251	0.915681899301	4.555418172993	Zn	6.409304569217	11.101241155067	0.000000000000
H	8.702135638262	7.593584482683	-2.675528334657	C	9.334967270050	9.222210411522	-2.532960715949
H	9.729726554421	5.932558961306	-4.551333035438	H	8.722184484941	9.840719155577	-4.556815491321
H	2.292841432764	-10.791970770889	-2.671289835716	C	8.753439932530	9.556843976474	-1.255817326326
H	4.064933089743	-10.001767859358	-4.554610057846	C	2.341076360245	13.134781702952	-2.670445088502
H	9.685680706720	-5.536275989864	2.676556753462	C	3.270065737464	12.559192103118	0.000000000000
H	8.359026830381	-6.953848888498	4.559019585417	N	7.665331111632	10.367181946203	1.431029608907
H	2.291766620195	-10.792195174885	2.671878064994	H	5.145577375251	11.821962444194	1.431029608907
H	4.063095960199	-10.002143390700	4.555980767323	N	10.204516447797	8.594822451648	-2.670445088502
H	9.686791974352	-5.536099006808	-2.672558917478	C	9.241546543577	9.111556052248	0.000000000000
H	8.360896960358	-6.953253045574	-4.555665610760	C	3.899749697366	12.359123340309	1.255817326326
H	-8.376538616151	7.346107754767	-2.672484711784	C	1.897427205913	12.901463870237	0.000000000000
H	-9.384765640302	5.690248039726	-4.556570295977	C	8.753439932530	9.556843976474	1.255817326326
H	-11.420889077440	-1.192571306630	2.668254999116	C	7.532149936999	10.549935973971	2.789634986275
H	-11.157658767228	0.728040933157	4.552536915002	C	5.370437593259	11.798001177540	2.789634986275
H	-8.377226050735	7.345786569693	2.669929427652	C	10.224281854676	8.093952097271	0.000000000000
H	-9.385953566083	5.689707531686	4.553554506856	C	3.319184860398	12.695424005120	2.532960715949
H	-11.420159598536	-1.192266330363	-2.672615863124	C	0.677012086503	13.022318011066	0.000000000000
H	-11.156427780092	0.728566013978	-4.556605637516	C	9.334967270050	9.222210411522	2.532960715949
H	-2.461796142186	-10.865878342665	-2.671958903863	C	8.587187480511	9.854264502471	3.482632209072
H	-4.250354156472	-10.118256119842	-4.556181379863	C	6.487296408164	11.236326982700	3.406820644400
H	-9.942611341564	-5.745371203189	2.668302675625	C	4.20449654496	12.363854756418	3.482632209072
H	-8.601346173953	-7.144945883353	4.552649236441	C	10.939152170491	7.097468671114	0.000000000000
H	-2.463063910289	-10.866288900276	2.670455306030	H	10.204516447797	8.594822451648	2.670445088502
H	-4.252516361123	-10.118957895146	4.553943354771	H	8.722184484941	9.840719155577	4.556815491321
H	-9.941352773439	-5.744969163863	-2.6725567611455	H	4.161220537768	12.473992918242	4.556815491321
H	-8.599188146635	-7.144249074204	-4.556493211934	C	-10.939152170491	7.097468671114	0.000000000000
H	0.043934973589	10.675399588312	-4.489060714944	C	-11.616164256994	5.924849339952	0.000000000000
H	10.709016998287	3.478180566805	4.481975969126	C	-10.224281854676	8.093952097271	0.000000000000
H	10.710411653333	3.477887876564	-4.47782319080	C	-12.121709060589	4.807511772966	0.000000000000
H	6.306496597509	-8.613490518269	4.490294925556	C	-9.241546543577	9.111556052248	0.000000000000
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H	-10.440421863218	3.269031571855	4.487644644185	C	-8.753439932530	9.556843976474	-1.255817326326
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H	0.042435155354	10.676031656374	4.489138998477	C	-9.334967270050	9.222210411522	-2.532960715949

S4.3 c-P6 S₀

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cP6 SO B3LYP/6-31G* E(au): -17512.2110304							
C	12.653189629896	-2.802279363835	1.255817326326	C	-12.654152130448	3.473213593599	2.532960715949
C	12.654152130448	-3.473213593599	2.532960715949	C	-12.827637135007	-2.509590253946	3.482632209072
C	12.827637135007	-2.509590253946	3.482632209072	C	12.902587530258	-1.248065203569	2.789634986275
C	12.902587530258	-1.248065203569	2.789634986275	N	12.810908486884	-1.454780497991	1.431029608907
N	12.810908486884	-1.454780497991	1.431029608907	H	12.545592808042	-4.539959251304	2.670445088502
H	12.545592808042	-4.539959251304	2.670445088502	H	12.883405022708	-2.633273762665	4.556815491321
H	12.883405022708	-2.633273762665	4.556815491321	C	12.974592816329	0.000000000000	3.406820644400
C	12.974592816329	0.000000000000	3.406820644400	C	12.902587530258	1.248065203569	2.789634986275
C	12.902587530258	1.248065203569	2.789634986275	C	12.827637135007	2.509590253946	3.482632209072
C	12.827637135007	2.509590253946	3.482632209072	Zn	12.810908486884	1.454780497991	1.431029608907
N	12.810908486884	1.454780497991	1.431029608907	N	12.654152130448	3.473213593599	2.532960715949
H	12.654152130448	3.473213593599	2.532960715949	C	12.883405022708	2.633273762665	4.556815491321
H	12.883405022708	2.633273762665	4.556815491321	C	12.653189629896	2.802279363835	1.255817326326
C	12.653189629896	2.802279363835	1.255817326326	H	12.545592808042	4.539959251304	2.670445088502
H	12.545592808042	4.539959251304	2.670445088502	H	12.511612281041	3.447636050870	0.000000000000
C	12.511612281041	3.447636050870	0.000000000000	H	12.653189629896	2.802279363835	-1.255817326326
H	12.653189629896	2.802279363835	-1.255817326326	C	12.654152130448	3.473213593599	-2.532960715949
C	12.654152130448	3.473213593599	-2.532960715949	N	12.810908486884	1.454780497991	-1.431029608907
N	12.810908486884	1.454780497991	-1.431029608907	H	12.827637135007	-2.509590253946	3.482632209072
H	12.827637135007	-2.509590253946	3.482632209072	H	12.545592808042	4.539959251304	2.670445088502
H	12.545592808042	4.539959251304	2.670445088502	C	12.902587530258	1.248065203569	-2.789634986275
C	12.902587530258	1.248065203569	-2.789634986275	H	12.883405022708	2.633273762665	-4.556815491321
H	12.883405022708	2.633273762665	-4.556815491321	N	12.974592816329	0.000000000000	-3.406820644400
C	12.974592816329	0.000000000000	-3.406820644400	C	12.902587530258	-1.248065203569	-2.789634986275
C	12.902587530258	-1.248065203569	-2.789634986275	C	12.827637135007	-2.509590253946	-3.482632209072
C	12.827637135007	-2.509590253946	-3.482632209072	N	12.810908486884	-1.454780497991	-1.431029608907
N	12.810908486884	-1.454780497991	-1.431029608907	H	12.654152130448	3.473213593599	2.532960715949
H	12.654152130448	3.473213593599	2.532960715949	H	12.883405022708	2.633273762665	4.556815491321
H	12.883405022708	2.633273762665	4.556815491321	C	12.653189629896	2.802279363835	1.255817326326
C	12.653189629896	2.802279363835	1.255817326326	H	12.545592808042	4.539959251304	2.670445088502
H	12.545592808042	4.539959251304	2.670445088502	H	12.511612281041	3.447636050870	0.000000000000
C	12.511612281041	3.447636050870	0.000000000000	H	12.653189629896	2.802279363835	-1.255817326326
H	12.653189629896	2.802279363835	-1.255817326326	C	12.654152130448	3.473213593599	-2.532960715949
C	12.654152130448	3.473213593599	-2.532960715949	N	12.810908486884	1.454780497991	-1.431029608907
N	12.810908486884	1.454780497991	-1.431029608907	H	12.827637135007	-2.509590253946	3.482632209072
H	12.827637135007	-2.509590253946	3.482632209072	H	12.545592808042	4.539959251304	2.670445088502
H	12.						

C	-5.370437593259	11.798001177540	-2.789634986275	C	8.753439932530	-9.556843976474	-1.255817326326
C	-3.899749697366	12.359123340309	-1.255817326326	C	7.532149936999	-10.549935973971	-2.789634986275
C	-5.370437593259	11.798001177540	2.789634986275	C	8.587187480511	-9.854264502471	3.482632209072
C	-3.899749697366	12.359123340309	1.255817326326	C	9.334967270050	-9.222210411522	2.532960715949
C	-12.902587530258	-1.248065203569	-2.789634986275	C	9.241546543577	-9.111556052248	0.000000000000
C	-12.653189629896	-2.802279363835	-1.255817326326	C	9.334967270050	-9.222210411522	-2.532960715949
C	-12.653189629896	-2.802279363835	1.255817326326	C	8.587187480511	-9.854264502471	-3.482632209072
C	-12.902587530258	-1.248065203569	2.789634986275	H	8.722184484941	-9.840719155577	4.556815491321
C	-4.240449654496	12.363854756418	-3.482632209072	H	10.204516447797	-8.594822451648	2.670445088502
C	-3.319184860398	12.695424005120	-2.532960715949	C	10.224281854676	-8.093952097271	0.000000000000
C	-3.270065737464	12.559192103118	0.000000000000	H	10.204516447797	-8.594822451648	-2.670445088502
C	-4.240449654496	12.363854756418	3.482632209072	H	8.722184484941	-9.840719155577	-4.556815491321
C	-3.319184860398	12.695424005120	2.532960715949	C	10.939152170491	-7.097468671114	0.000000000000
C	-12.827637135007	-2.509590253946	-3.482632209072	H	6.516748992453	11.287340355103	-4.491712610839
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C	-12.511612281041	-3.447636050870	0.000000000000	H	-13.033497984907	0.000000000000	-4.491712610839
C	-12.654152130448	-3.473213593599	2.532960715949	H	-6.516748992453	-11.287340355103	-4.491712610839
C	-12.827637135007	-2.509590253946	3.482632209072	H	6.516748992453	-11.287340355103	-4.491712610839
H	-4.161220537768	12.473992918242	-4.556815491321	H	13.033497984907	0.000000000000	-4.491712610839
H	-2.341076360245	13.134781702952	-2.670445088502	H	-6.516748992453	11.287340355103	4.491712610839
C	-1.897427205913	12.901463870237	0.000000000000	H	-13.033497984907	0.000000000000	4.491712610839
H	-4.161220537768	12.473992918242	4.556815491321	H	-6.516748992453	11.287340355103	4.491712610839
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H	-12.883405022708	-2.632373762665	-4.556815491321	H	13.033497984907	0.000000000000	4.491712610839
H	-12.545592808042	-4.539959251304	-2.670445088502	H	6.516748992453	-11.287340355103	4.491712610839
C	-12.121709060589	-4.807511772966	0.000000000000				
H	-12.545592808042	-4.539959251304	2.670445088502				
H	-12.883405022708	-2.632373762665	4.556815491321				
C	-0.677012086503	13.022318011066	0.000000000000				
C	-11.616164256994	-5.924849339952	0.000000000000				
C	-10.939152170491	-7.097468671114	0.000000000000				
C	-10.224281854676	-8.093952097271	0.000000000000				
C	-9.241546543577	-9.111556052248	0.000000000000				
C	-8.753439932530	-9.556843976474	1.255817326326				
C	-8.753439932530	-9.556843976474	-1.255817326326				
C	-9.334967270050	-9.222210411522	2.532960715949				
N	-7.665331111632	-10.367181946203	1.431029608907				
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C	-9.334967270050	-9.222210411522	-2.532960715949				
H	-8.587187480511	-9.854264502471	3.482632209072				
H	-10.204516447797	-8.594822451648	2.670445088502				
C	-7.532149936999	-10.549935973971	2.789634986275				
Zn	-6.409304569217	-11.101241155067	0.000000000000				
C	-7.532149936999	-10.549935973971	-2.789634986275				
C	-8.587187480511	-9.854264502471	-3.482632209072				
H	-10.204516447797	-8.594822451648	-2.670445088502				
H	-8.722184484941	-9.840719155577	4.556815491321				
C	-6.487296408165	-11.236326982700	3.406820644400				
N	-5.145577375251	-11.821962444194	1.431029608907				
N	-5.145577375251	-11.821962444194	-1.431029608907				
C	-6.487296408165	-11.236326982700	-3.406820644400				
H	-8.722184484941	-9.840719155577	-4.556815491321				
C	-5.370437593259	-11.798001177540	2.789634986275				
C	-3.899749697366	-12.359123340309	1.255817326326				
C	-3.899749697366	-12.359123340309	-1.255817326326				
C	-5.370437593259	-11.798001177540	-2.789634986275				
C	-4.240449654496	-12.363854756418	3.482632209072				
C	-3.319184860398	-12.695424005120	2.532960715949				
C	-3.270065737464	-12.559192103118	0.000000000000				
C	-3.319184860398	-12.695424005120	-2.532960715949				
C	-4.240449654496	-12.363854756418	-3.482632209072				
C	-4.161220537768	-12.473992918242	4.556815491321				
H	-2.341076360245	-13.134781702952	2.670445088502				
C	-1.897427205913	-12.901463870237	0.000000000000				
C	-2.341076360245	-13.134781702952	-2.670445088502				
H	-4.161220537768	-12.473992918242	-4.556815491321				
C	-0.677012086503	-13.022318011066	0.000000000000				
C	-0.677012086503	-13.022318011066	0.000000000000				
C	1.897427205913	-12.901463870237	0.000000000000				
C	3.270065737464	-12.559192103118	0.000000000000				
C	3.899749697366	-12.359123340309	1.255817326326				
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C	3.319184860398	-12.695424005120	2.532960715949				
N	5.145577375251	-11.821962444194	1.431029608907				
N	5.145577375251	-11.821962444194	-1.431029608907				
C	3.319184860398	-12.695424005120	-2.532960715949				
C	4.240449654496	-12.363854756418	3.482632209072				
H	2.341076360245	-13.134781702952	2.670445088502				
C	5.370437593259	-11.798001177540	2.789634986275				
Zn	6.409304569217	-11.101241155067	0.000000000000				
C	5.370437593259	-11.798001177540	-2.789634986275				
C	4.240449654496	-12.363854756418	-3.482632209072				
H	2.341076360245	-13.134781702952	-2.670445088502				
H	4.161220537768	-12.473992918242	4.556815491321				
C	6.487296408164	-11.236326982700	3.406820644400				
N	7.665331111632	-10.367181946203	1.431029608907				
N	7.665331111632	-10.367181946203	-1.431029608907				
C	6.487296408164	-11.236326982700	-3.406820644400				
H	-4.161220537768	-12.473992918242	-4.556815491321				
C	7.532149936999	-10.549935973971	2.789634986275				
C	8.753439932530	-9.556843976474	1.255817326326				

S4.4 c-P6 T₁

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cP6 T1 UB3LYP/6-31G* E(au): -17512.1692341

C	12.6654658779465	-2.802462253263	1.260567024131
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C	12.846940654423	-2.508278364498	3.484583690232
C	12.915086813761	-1.249394742250	2.792177242288
C	12.811594105922	-1.457323774551	1.431946819003
H	12.562672029251	-4.540515183635	2.67345868014
H	12.911817052209	-2.632679173513	4.58190461866
C	12.990599767462	-0.000000472097	3.405851709283
C	12.915084780247	1.249393356764	2.792176640654
C	12.846936635288	2.508277208468	3.484582440515
N	12.811591715357	1.457321570018	1.431946806070
C	12.667285298494	3.473533356070	2.534851005040
H	12.911812827709	2.632678670052	4.558189147057
C	12.654654283540	2.802459669390	1.260565651333
H	12.562664841739	4.540513165847	2.673456383908
C	12.501322356041	3.450425418527	-0.000003256472
C	12.654650727230	2.802458999973	-1.260572246790
C	12.667278121685	3.473532017509	-2.534860075277
N	12.811587655110	1.457320818974	-1.431952427135
C	12.846926740746	2.508275369646	-3.484589406308
C	12.562657282270	4.540511755223	-2.673463618996
C	12.915076842367	1.249391892872	-2.792183148521
H	12.911799877034	2.632676270335	-4.558196351898
C	12.990590059882	-0.000002320249	-3.405857775163
C	12.915078848663	-1.249396161329	-2.792182459680
C	12.846930689508	-2.508280121602	-3.484588066886
N	12.811590023701	-1.457324499094	-1.431951656126
C	12.667283554642	-3.473536546549	-2.534858241727
C	12.911804146655	-2.632681474463	-4.558194950674
H	12.654655183936	-2.802462884160	-1.260570726234
H	12.562664355343	-4.540516525371	-2.673461217949
C	12.501327912910	-3.45042829080	-0.000001472102
Zn	12.814417535447	-0.000001473336	-0.000002795117
C	12.102624681982	-4.795732402551	-0.00000540619
C	11.590822732743	-5.915755763979	0.00000585317
C	12.102617259485	4.795728171133	-0.000003204970
C	11.590814198930	5.915751154007	-0.000002542302
C	6.495709069677	11.251994978345	-3.405922334886
C	5.376034204126	11.811465074243	-2.792234349578
C	7.539917288770	10.561862587231	-2.792225958256
C	4.251735937743	12.381916718373	-3.484611066444
N	5.144300481418	11.825913224261	-1.431993266564
C	8.595979500118	9.873243634407	-3.484605994809
N	7.668245371272	10.368345572374	-1.43198875136
C	3.326045926297	12.709087374166	-2.534855020374
H	4.176391584209	12.500230478269	-4.558222697165
C	3.900942596441	12.362648369210	-1.260577946710
Zn	6.407719042564	11.099640221056	-0.00000634110
C	9.342028267618	9.234996552419	-2.534853931739
H</			

C	4.828236812005	14.402332874419	-0.001835968654	C	-9.455939627684	11.987224073878	2.531125461911
C	-1.248074386673	15.079070589997	-2.792799944157	C	-10.177424983507	11.326685326471	3.481500707469
C	0.000000000000	15.142022696504	-3.410439496954	C	-14.270553675513	5.204840125708	-0.001835968654
C	-1.248074404210	15.082605841315	2.788344665069	C	-7.193610433468	13.377289265062	-0.001780166257
C	-2.805730187458	14.863610059041	1.253719486525	C	-14.642621606091	4.036524699786	-0.001780166257
C	-3.476307243567	14.866863259869	2.531125461911	C	-15.115620084654	1.502362272183	-0.001835968654
C	-2.510038493908	15.019104052449	3.481500707469	C	-14.423284129857	-4.572191427025	-2.792799944157
C	0.000000000000	15.146335313094	3.405903900992	C	-14.762380573791	-3.369417032513	-3.410439496954
C	1.248074386673	15.079070589997	-2.792799944157	C	-14.426730741142	-4.572978111548	-2.788344665069
C	2.805719073675	14.862009648291	-1.257890792699	C	-13.866614620682	-6.042849066203	1.253719486525
C	3.476304181367	14.863664041271	-2.535298291123	C	-13.720568824157	-6.697337260759	2.531125461911
C	2.510041041890	15.014710897990	-3.485869699019	C	-14.084007646844	-5.789171649399	3.481500707469
C	1.248074404210	15.082605841315	2.788344665069	C	-14.766585064079	-3.370376679984	3.405903900992
C	3.454480804334	14.739746213924	-0.002006571138	C	-14.978729486196	-2.138626314931	-2.792799944157
C	-2.805719073675	14.862009648291	-1.257890792699	C	-15.113719266007	-0.571734468837	-1.257890792699
C	-3.476304181367	14.863664041271	-2.535298291123	C	-15.264551404361	0.081669573074	-2.535298291123
C	-2.510041041890	15.014710897990	-3.485869699019	C	-15.196797424780	-0.893978419743	-3.485869699019
C	-3.454480804334	14.739746213924	-0.002006571138	C	-14.982176105286	-2.139412965259	-2.788344665069
C	2.805730187458	14.863610059041	1.253719486525	C	-15.138884297424	0.087967664341	-0.002006571138
C	3.476307243567	14.866863259869	2.531125461911	C	-13.865056808620	-6.042482106171	-1.257890792699
C	2.510038493908	15.019104052449	3.481500707469	C	-13.717450498053	-6.69622382225	-2.535298291123
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S4.6 c-P7 T₁

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 C -11.058908166224 -10.344697387661 2.79105192522
 C -9.388674277864 11.829550039928 -0.002116222446
 C -13.448609712202 7.060420047663 -1.263097444154

H	10.532556745806	-11.288211132824	-2.674934672125	C	2.850962168297	-17.144222590106	3.484461909906
H	8.930691651014	-12.375408715769	-4.562350595569	C	1.872311756973	-17.198713068461	0.000000000000
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S4.7 c-P8 S₀

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cP8 SO B3LYP/6-31G* E(a.u.):	-23349.6372778						
C	9.010280465607	14.766354136622	2.791293534575		15.388099545132	-7.926630533582	-3.409223278575
C	7.926630533582	15.388099545132	3.409223278575	Zn	15.276970723533	-7.869374643667	0.000000000000
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C	9.010280465607	14.766354136622	-2.791293534575	C	15.909573825236	-6.791319885461	2.791296221111
N	9.162251816966	14.606242067047	-1.431702825126	N	15.940365929431	-6.572733040066	1.431706335487
C	10.308456602016	13.880029847017	-1.255795933120	C	16.451976930501	-5.315979659641	1.255796133637
C	10.905824804313	13.575848341732	-2.533386438230	C	16.761767577218	-4.721497317444	2.533382738837
C	10.106861369527	14.138730733744	-3.484461909906	C	16.438052278298	-5.643663205960	3.484457456736
C	7.926630533582	15.388099545132	-3.409223278575	C	15.909573825236	-6.791319885461	-2.791296221111
Zn	7.869374643667	15.276970723533	0.000000000000	C	16.653399614537	-4.687445797263	0.000000000000
C	6.791319885461	15.909573825236	2.791296221111	N	14.606242067047	-9.162251816966	1.431702825126
C	6.572733040066	15.940365929431	1.431706335487	C	13.880029847017	-10.308456602016	1.255795933120
C	5.315979659641	16.451976930501	1.255796133637	C	13.575848341732	-10.905824804313	2.533386438230
C	4.721497317444	16.761767577218	2.533382738837	C	14.138730733744	-10.106861369527	3.484461909906
C	5.643663205960	16.438052278298	3.484457456736	C	13.85250978241	-10.837402298540	0.000000000000
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C	4.687445797263	16.653399614537	0.000000000000	C	16.761767577218	-4.721497317444	-2.533382738837
N	9.162251816966	14.606242067047	1.431702825126	C	16.438052278298	-5.643663205960	-3.484457456736
C	10.308456602016	13.880029847017	1.255795933120	C	-0.761354105615	-17.325130008580	0.000000000000
C	10.905824804313	13.575848341732	2.533386438230	C	0.464536388380	-17.337248380645	0.000000000000
C	10.106861369527	14.138730733744	3.484461909906	C	11.712358263041	-12.789075564970	0.000000000000
C	10.837402298540	13.485250978241	0.000000000000	C	12.587762727401	-11.930809066738	0.000000000000
C	5.315979659641	16.451976930501	-1.255796133637	C	9.687810850416	-14.385645458391	0.000000000000
C	4.721497317444	16.761767577218	-2.533382738837	C	10.678822882232	-13.663947503609	0.000000000000
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C	12.789075564970	11.712358263041	0.000000000000	H	11.818492388318	13.012975854621	-2.670090965232
C	11.930809066738	12.587762727401	0.000000000000	H	10.235424918666	14.123031152719	-4.559396616219
C	3.321870708192	17.022504202555	0.000000000000	H	3.733339888748	17.178106377370	2.670061524636
C	2.110801862463	17.212938012696	0.000000000000	H	5.56252418542	16.533642380774	4.559391096876
C	16.051955881829	6.447579193396	-2.791296221111	H	11.818492388318	13.012975854621	2.670090965232
C	16.486003740192	5.276055335680	-3.409223278575	H	10.235424918666	14.123031152719	4.559396616219
N	16.806863203977	3.849482422546	1.431702825126	H	3.733339888748	17.178106377370	-2.670061524636
C	16.051955881829	6.447579193396	2.791296221111	H	5.56252418542	16.533642380774	-4.559391096876
N	15.919164946855	6.623916739736	1.431706335487	H	14.786625459190	9.506885555575	2.670061524636
C	15.392269717464	7.874339185501	1.255796133637	H	15.619914408294	7.762186882024	4.559391096876
C	15.190962289042	8.513756748005	2.533382738837	H	17.558499581400	0.844627359038	-2.670090965232
C	15.614130759151	7.632785711816	3.484457456736	H	17.224029467311	2.748952730682	-4.559396616219
C	16.486003740192	5.276055335680	3.409223278575	H	14.786625459190	9.506885555575	-2.670061524636
Zn	16.366937768833	5.237961420364	0.000000000000	H	15.619914408294	7.762186882024	-4.559391096876
C	16.812619561031	4.070158725784	-2.791293534575	H	17.558499581400	0.844627359038	2.670090965232
N	16.806863203977	3.849482422546	-1.431702825126	H	17.224029467311	2.748952730682	4.559396616219
C	17.103842794750	2.525483661045	-1.255795933120	H	0.844627359038	-17.558499581400	-2.670090965232
C	17.311157096361	1.887991749236	-2.533386438230	H	2.748952730682	-17.224029467311	-4.559396616219
C	17.144222590106	2.850962168297	-3.484461909906	H	9.506885555575	-14.786625459190	2.670061524636
C	16.812619561031	4.070158725784	2.791293534575	H	7.762186882024	-15.619914408294	4.559391096876
C	17.198713068461	1.872311756973	0.000000000000	H	0.844627359038	-17.558499581400	2.670090965232
N	15.919164946855	6.623916739736	-1.431706335487	H	2.748952730682	-17.224029467311	4.559396616219
C	15.392269717464	7.874339185501	-1.255796133637	H	9.506885555575	-14.786625459190	-2.670061524636
C	15.190962289042	8.513756748005	-2.533382738837	H	7.762186882024	-15.619914408294	-4.559391096876
C	15.614130759151	7.632785711816	-3.484457456736	H	13.012975854621	-11.818492388318	-2.670090965232
C	15.090256506938	8.461207087560	0.000000000000	H	14.235424918666	-10.235424918666	-4.559396616219
C	17.103842794750	2.525483661045	1.255795933120	H	17.178106377370	-3.733339888748	2.670061524636
C	17.311157096361	1.887991749236	2.533386438230	H	16.533642380774	-5.56252418542	4.559391096876
C	17.144222590106	2.850962168297	3.484461909906	H	13.012975854621	-11.818492388318	2.670090965232
C	13.663947503609	10.678822882232	0.000000000000	H	14.235424918666	-10.235424918666	4.559396616219
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C	17.337248380645	0.464536388380	0.000000000000	H	16.533642380774	-5.56252418542	-4.559391096876
C	17.325130008580	-0.761354105615	0.000000000000	C	-9.010280465607	-14.766354136622	2.791293534575
C	14.766354136622	-9.010280465607	2.791293534575	C	-7.926630533582	-15.388099545132	3.409223278575
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N	6.623916739736	-15.919164946855	-1.431706335487	C	-10.308456602016	-13.880029847017	-1.255795933120
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N	-14.603153659140	9.162999914238	1.432447197444				
C	-13.877764913683	10.307628107732	1.259327112084				
C	-13.579606952746	10.907852857266	2.535013265717				
C	-14.146611426446	10.109581747960	3.486293751126				
C	-13.475681867536	10.835610735014	-0.0000086767038				
C	-16.450410627680	5.314775906568	-1.259341159113				
C	-16.766115612035	4.723593213253	-2.535025669821				
C	-16.445230636492	5.648673739467	-3.486302219475				
C	0.763105250477	17.306496151993	-0.000003709821				
C	-0.466435555340	17.321186482769	-0.000004050359				
C	-11.697824004374	12.776572228365	-0.000012854198				
C	-12.577827054611	11.917748246515	-0.000011679571				
C	-9.676458921751	14.373367372184	-0.000011122223				
C	-10.668916068496	13.647410659208	-0.000012425573				
C	-17.194966935022	2.106443369155	-0.000005771020				
H	-11.821476186141	-13.018531553620	-2.672596563266				
H	-10.240901728524	-14.135608677043	-4.560969746954				
H	-3.736364187577	-17.184317305623	2.672590883444				
H	-5.563441403572	-16.545666600441	4.560979500609				
H	-11.821453246053	-13.018492374975	2.672606523347				
H	-10.240862632844	-14.135541746753	4.560982511016				
H	-3.736386660518	-17.184355961698	-2.672588903025				
H	-5.563480034809	-16.545733015046	-4.560971368448				
H	-14.792202968820	-9.508683742711	2.672591382739				
H	-15.632446333857	-7.765089064093	4.560976367592				
H	-17.564649815366	-0.846243314751	-2.672610308112				
H	-17.236406700860	-2.753708852264	-4.560963455627				
H	-14.792250551629	-9.508702380716	-2.672580758914				
H	-15.632527994822	-7.765120960733	-4.560962917989				
H	-17.564601925000	-0.846224762752	2.672610159881				
H	-17.236324712014	-2.753677043662	4.560970679814				
H	-0.846232299951	17.564646728967	-2.672612207647				
H	-2.753693563172	17.236397727145	-4.560968563384				
H	-9.508680246803	14.792199711501	2.672577088548				
H	-7.765089963322	15.632447366758	4.560964121241				
H	-0.846224085092	17.564607979041	2.672607958972				
H	-2.753679360095	17.236331227696	4.560965442609				
H	-9.508688684802	14.792238552712	-2.672594611322				
H	-7.765104369697	15.632513914753	-4.560974915271				
H	-13.018522261358	11.821463822086	-2.672610288186				
H	-14.135600243514	10.240887833383	-4.560981510573				
H	-17.184310022701	3.736359198380	2.672586254007				
H	-16.545656534273	5.563437264059	4.560972889974				
H	-13.018480893445	11.821446137911	2.672592263525				
H	-14.135529264126	10.240857515094	4.560970336817				
H	-17.184351716159	3.736376839345	-2.672593015769				
H	-16.545727789575	5.563467518259	-4.560977545204				
H	16.542133196871	5.293860997325	4.494206768149				
H	16.542185340668	5.293884331696	-4.494194273076				
H	15.441420346918	-7.954097158918	-4.494233799652				
H	15.441377433279	-7.954079716088	4.494228038176				
H	5.293858664356	-16.542125164801	4.494198750756				
H	5.293872153996	-16.542179556887	-4.494202383814				
H	-7.954114418500	-15.441439652419	-4.494224669841				
H	-7.954076100453	-15.441373884548	4.494237034514				
H	-16.542116863364	-5.293857521511	4.494206723299				
H	-16.542197586780	-5.293888946597	-4.494194211673				
H	-15.441362627790	7.954071452098	4.494227829454				

S4.9 P1 S₀

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l-P1 neut S0 B3LYP/6-31G* E(au): -2919.8722989

Zn	0.000000000000	0.000000000000	0.000000000000
N	1.457132561991	1.432284129385	0.000000000000
N	-1.457132561991	1.432284129385	0.000000000000
N	-1.457132561991	-1.432284129385	0.000000000000
N	1.457132561991	-1.432284129385	0.000000000000
C	2.815993219404	1.252027617555	0.000000000000
C	3.485975005226	2.531576103856	0.000000000000
H	4.558500016096	2.664495613437	0.000000000000
C	2.512645950560	3.485116019551	0.000000000000
H	2.631163472533	4.561377980962	0.000000000000
C	1.247680186634	2.792340691593	0.000000000000
C	0.000000000000	3.413074780407	0.000000000000
C	-1.247680186634	2.792340691593	0.000000000000
C	-2.512645950560	3.485116019551	0.000000000000
H	-2.631163472533	4.561377980962	0.000000000000
C	-3.485975005226	2.531576103856	0.000000000000
H	-4.558500016096	2.664495613437	0.000000000000
C	-2.815993219404	1.252027617555	0.000000000000
C	-3.470706479031	0.000000000000	0.000000000000
C	-2.815993219404	-1.252027617555	0.000000000000
C	-3.485975005226	-2.531576103856	0.000000000000
H	-4.558500016096	-2.664495613437	0.000000000000
C	-2.512645950560	-3.485116019551	0.000000000000
H	-2.631163472533	-4.561377980962	0.000000000000
C	-1.247680186634	-2.792340691593	0.000000000000
C	0.000000000000	-3.413074780407	0.000000000000
C	1.247680186634	-2.792340691593	0.000000000000
C	2.512645950560	-3.485116019551	0.000000000000
C	2.631163472533	-4.561377980962	0.000000000000
C	3.485975005226	-2.531576103856	0.000000000000
H	4.558500016096	-2.664495613437	0.000000000000
C	2.815993219404	-1.252027617555	0.000000000000
C	3.470706479031	0.000000000000	0.000000000000
C	-4.899442700377	0.000000000000	0.000000000000
C	-6.110779241909	0.000000000000	0.000000000000
C	4.899442700377	0.000000000000	0.000000000000
C	6.110779241909	0.000000000000	0.000000000000
H	0.000000000000	4.499497746060	0.000000000000
H	0.000000000000	-4.499497746060	0.000000000000
H	-7.177070388066	0.000000000000	0.000000000000
H	7.177070388066	0.000000000000	0.000000000000

S4.10 P1 1-

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l-P1 1- UB3LYP/6-31G* E(au): -2919.9232003

Zn	0.000000000000	0.000000000000	0.000000000000
N	1.468732486567	1.435177013511	0.000000000000
N	-1.468732486567	1.435177013511	0.000000000000
N	-1.468732486567	-1.435177013511	0.000000000000
N	1.468732486567	-1.435177013511	0.000000000000
C	2.824718425744	1.259142819900	0.000000000000
C	3.488445984862	2.537502415825	0.000000000000
H	4.561413336927	2.671814341518	0.000000000000
C	2.506966031112	3.494545033615	0.000000000000
H	2.625899691848	4.572267034287	0.000000000000
C	1.251117871003	2.808070248681	0.000000000000
C	0.000000000000	3.419597703255	0.000000000000
C	-1.251117871003	2.808070248681	0.000000000000
C	-2.506966031112	3.494545033615	0.000000000000
C	-2.625899691848	4.572267034287	0.000000000000
C	-3.488445984862	2.537502415825	0.000000000000
H	-4.561413336927	2.671814341518	0.000000000000
C	-4.561413336927	-1.259142819900	0.000000000000
C	-2.506966031112	-3.494545033615	0.000000000000
H			

C	3.491133110091	0.000000000000	0.000000000000	H	0.000000000000	4.507960562295	0.000000000000
C	-4.911957240195	0.000000000000	0.000000000000	H	0.000000000000	-4.507960562295	0.000000000000
C	-6.128681699253	0.000000000000	0.000000000000	H	-7.193289518343	0.000000000000	0.000000000000
C	4.911957240195	0.000000000000	0.000000000000	H	7.193289518343	0.000000000000	0.000000000000
C	6.128681699253	0.000000000000	0.000000000000				

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