

# Supporting Information

## for

# Aromaticity and Antiaromaticity in the Excited States of Porphyrin Nanorings

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## Contents

S1	Computational Chemistry	S3
S1.1	Summary of NICS values, and discussion of spin densities	S3
S1.2	NICS grids for $S_0$ ground states	S5
S1.3	NICS grids for $T_1$ excited states	S6
S1.4	Spin densities for $T_1$ excited states	S9
S1.5	NICS grids for a porphyrin monomer in neutral and $-1$ oxidation states	S10
S1.6	HOMO–LUMO gaps of porphyrin nanorings	S11
S2	Synthesis	S11
S2.1	<b>c-P6-T6</b>	S12
S2.2	Free-base <b>c-P6 [H<sub>2</sub>]<sub>6</sub>-c-P6</b>	S13
S2.3	<b>c-P6</b>	S14
S2.4	Removal of templates from larger rings	S14
S2.5	<b>c-P8</b>	S14
S2.6	<b>c-P9</b>	S15
S2.7	<b>c-P10</b>	S15
S2.8	<b>c-P11</b>	S15
S2.9	<b>c-P12</b>	S15
S2.10	<b>c-P13</b>	S15
S2.11	<b>c-P16</b>	S15
S2.12	GPC retention times of THS porphyrin oligomers	S16
S3	Photophysical measurements	S16
S3.1	Statistical analysis	S17
S4	Cartesian coordinates	S20
S4.1	<b>c-P5</b> $S_0$	S20

S4.2	<b>c-P5</b> T <sub>1</sub>	.....	S21
S4.3	<b>c-P6</b> S <sub>0</sub>	.....	S22
S4.4	<b>c-P6</b> T <sub>1</sub>	.....	S23
S4.5	<b>c-P7</b> S <sub>0</sub>	.....	S24
S4.6	<b>c-P7</b> T <sub>1</sub>	.....	S26
S4.7	<b>c-P8</b> S <sub>0</sub>	.....	S28
S4.8	<b>c-P8</b> T <sub>1</sub>	.....	S29
S4.9	<b>P1</b> S <sub>0</sub>	.....	S31
S4.10	<b>P1</b> 1-	.....	S31

# S1 Computational Chemistry

DFT geometry optimizations were performed using the B3LYP functional and the 6-31G\* all-electron basis set,<sup>S1-S5</sup> as implemented in Gaussian09/D.01 and Gaussian16/A.03.<sup>S6,S7</sup> 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<sup>S8</sup> 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.<sup>S9-S12</sup> 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  $1 \text{ \AA}$  spacing.

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

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

	$\pi$ -electron count	$S_0$		$T_1$	
		NICS(0) <sub>iso</sub>	NICS(0) <sub>zz</sub>	NICS(0) <sub>iso</sub>	NICS(0) <sub>zz</sub>
<b>c-P5</b>	70	-2.5	-0.1	1.6	10.3
<b>c-P6</b>	84	-1.4	1.1	-5.4	-12.2
<b>c-P7</b>	98	-1.2	0.5	0.4	2.1
<b>c-P8</b>	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<sup>S13</sup> in MATLAB. The total spin density is normalized to 1.

The angular deviation ( $\Gamma_{\text{trip}}$ ) 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:

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

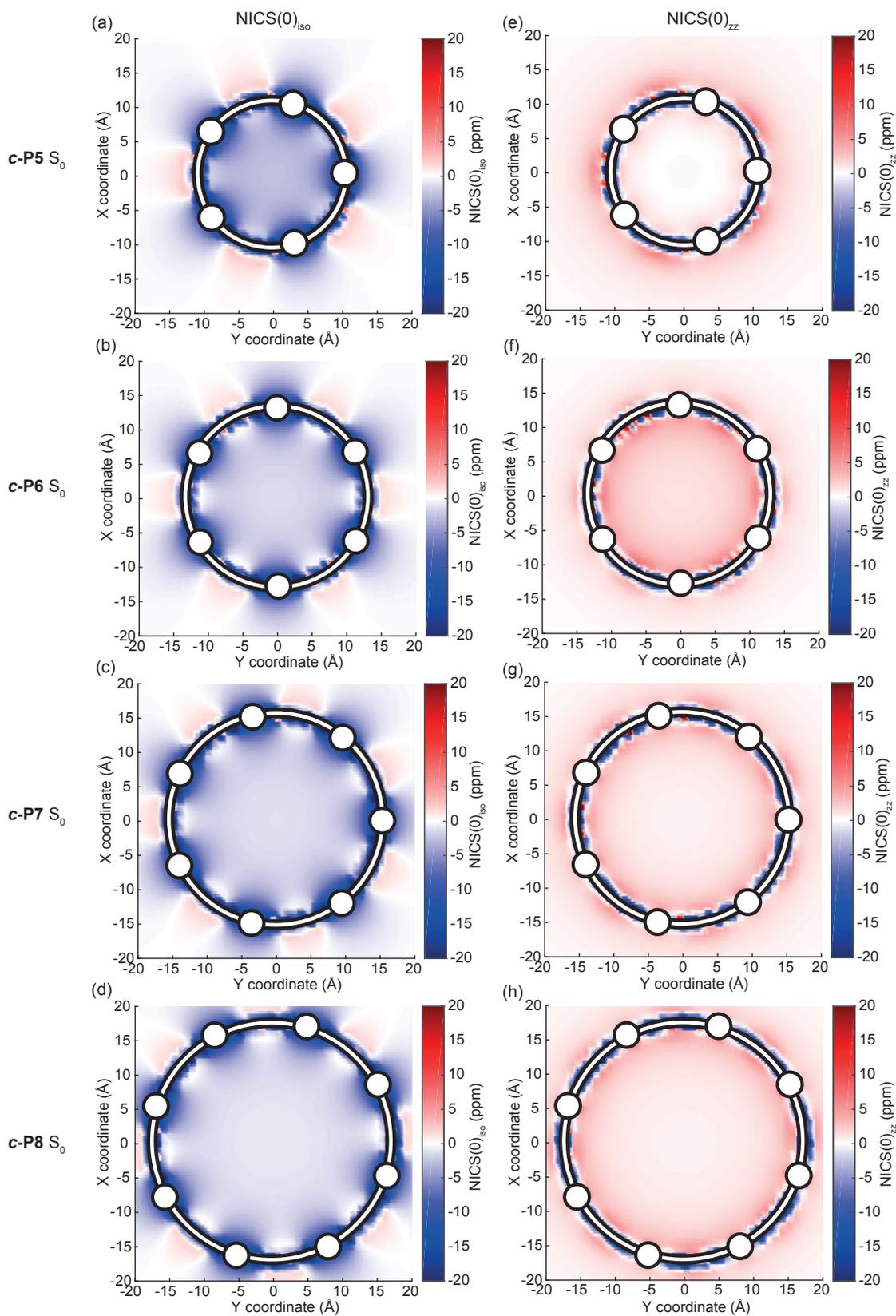
**Table S2:** NICS(0)<sub>iso</sub> and NICS(0)<sub>zz</sub> (all units ppm) at the center of **c-P5** in its T<sub>1</sub> state for different DFT functionals.

Functional	$\Gamma_{\text{trip}}$	NICS(0) <sub>iso</sub>	NICS(0) <sub>zz</sub>
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- $\omega$ HPBE//B3LYP ( $\omega = 0.05$ )	0.834	2.7	13.3
LC- $\omega$ HPBE//B3LYP ( $\omega = 0.1$ )	0.671	-0.6	3.4
LC- $\omega$ HPBE//B3LYP ( $\omega = 0.2$ )	0.579	-1.4	1.5

**Table S3:** NICS(0)<sub>iso</sub> and NICS(0)<sub>zz</sub> (all units ppm) at the center of **c-P6** in its T<sub>1</sub> state for different DFT functionals.

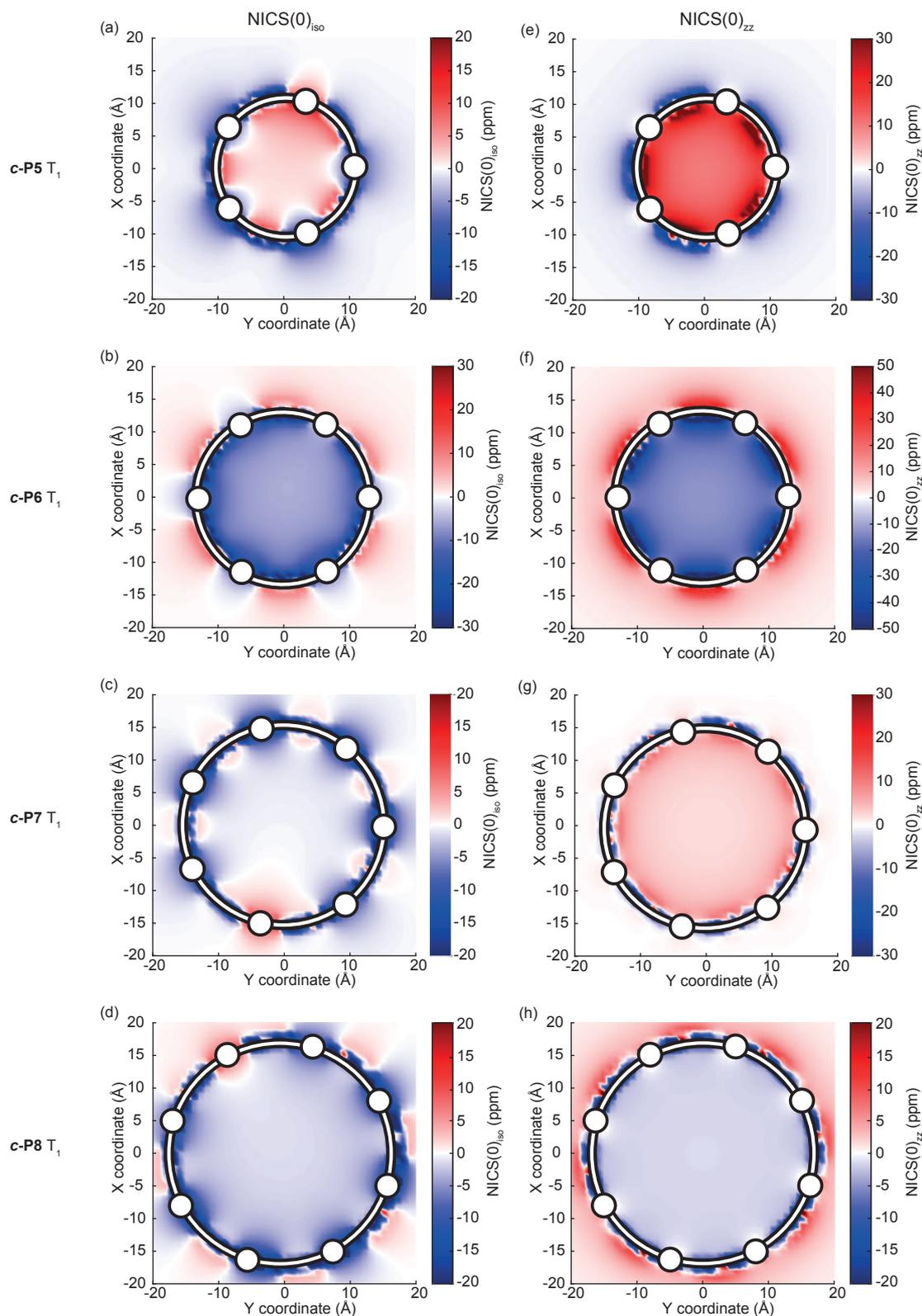
Functional	$\Gamma_{\text{trip}}$	NICS(0) <sub>iso</sub>	NICS(0) <sub>zz</sub>
B3LYP//B3LYP	0.941	-5.4	-12.2
M06-2X//M06-2X	0.490	-1.3	0.4
M06-L//B3LYP	1.414	-9.2	-23.6
M06-2X//B3LYP	0.548	-1.4	0.1
CAM-B3LYP//B3LYP	0.540	-1.1	0.6
LC- $\omega$ HPBE//B3LYP ( $\omega = 0.05$ )	0.873	-4.2	-8.9
LC- $\omega$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

## S1.2 NICS grids for $S_0$ ground states

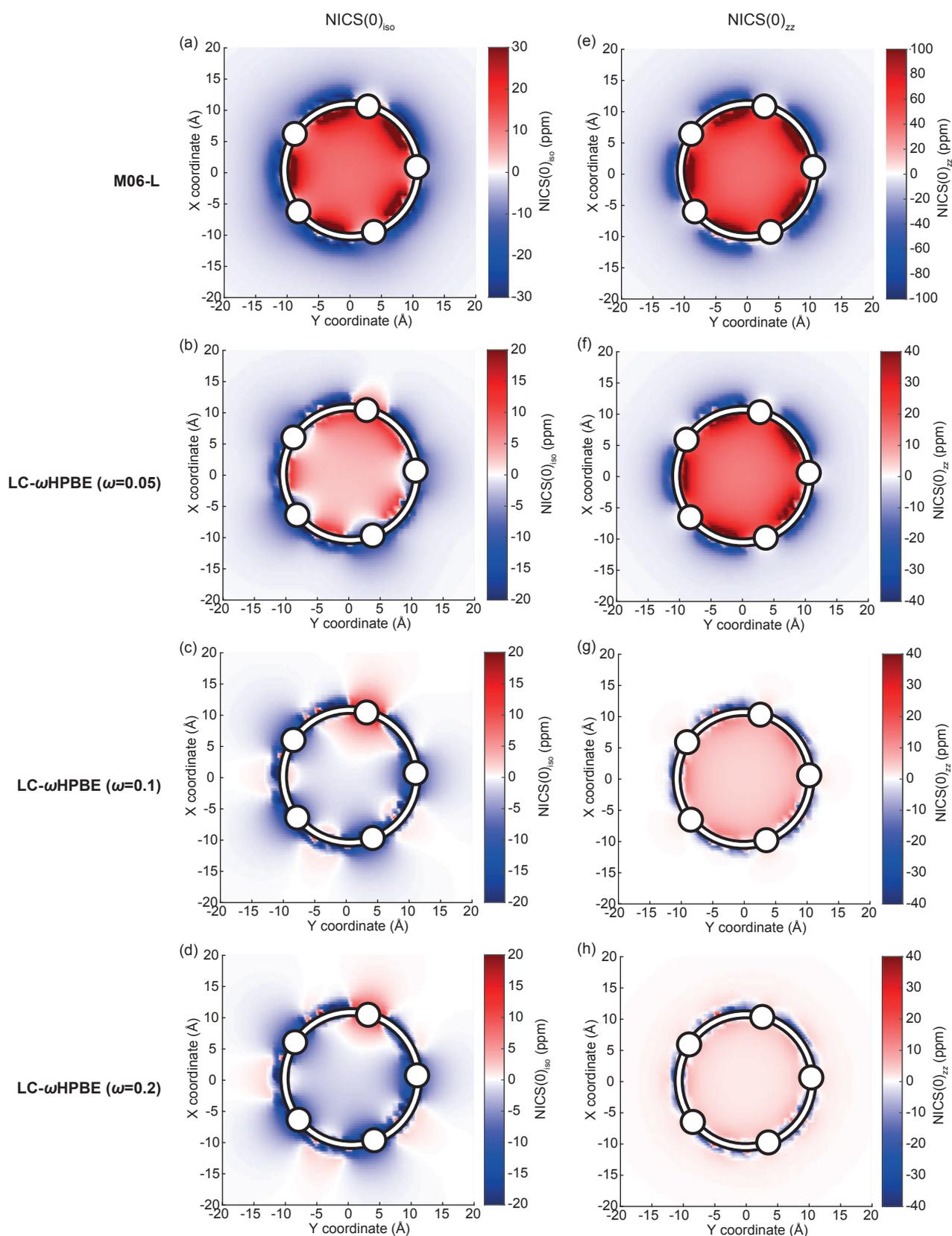


**Figure S1:** NICS(0)<sub>iso</sub> (left column) and NICS(0)<sub>zz</sub> (right column) for *c*-P5, *c*-P6, *c*-P7, and *c*-P8, in their  $S_0$  singlet ground states, calculated at the B3LYP/6-31G\* level of theory. White circles indicate the positions of porphyrin units.

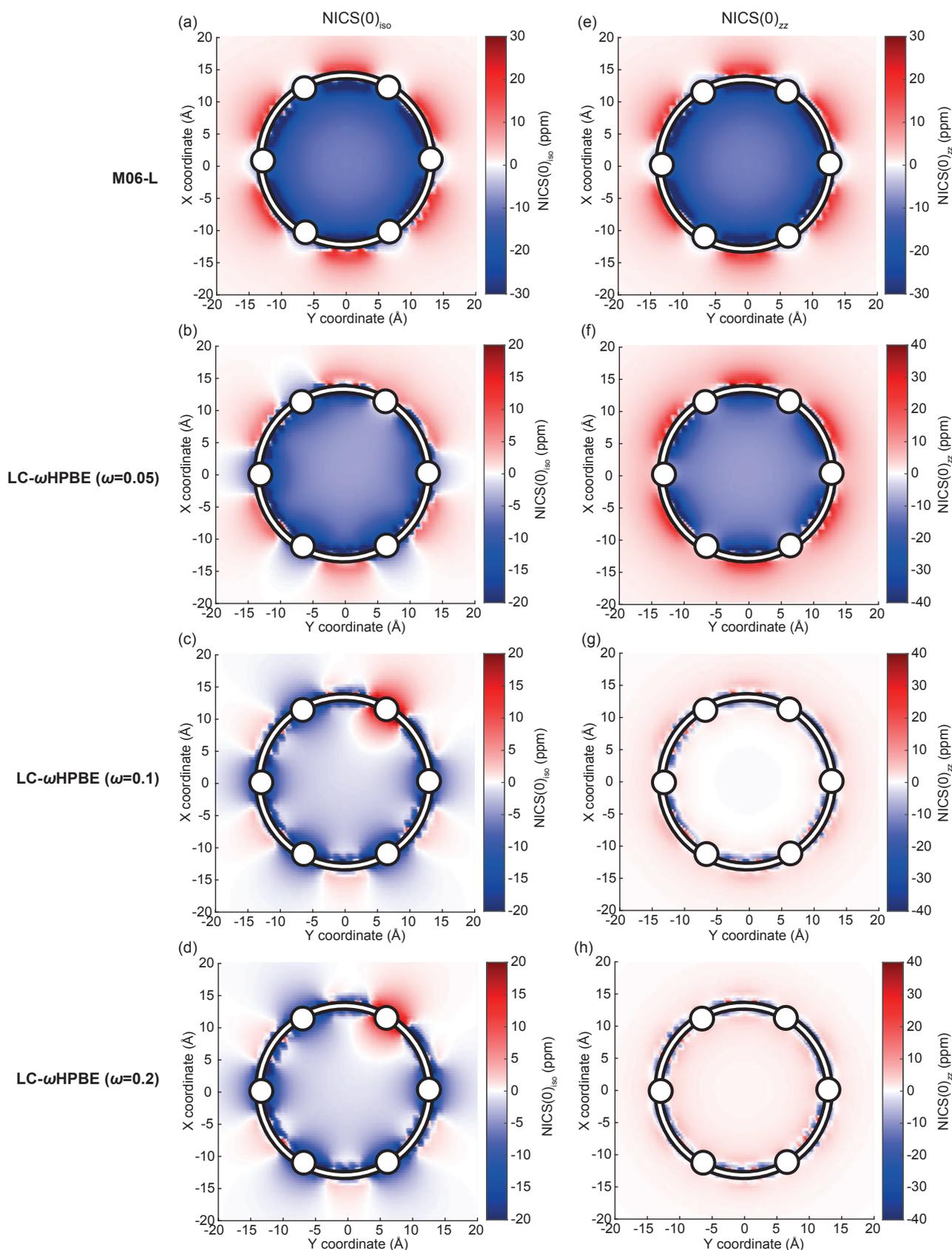
### S1.3 NICS grids for $T_1$ excited states



**Figure S2:** NICS(0)<sub>iso</sub> (left column) and NICS(0)<sub>zz</sub> (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.

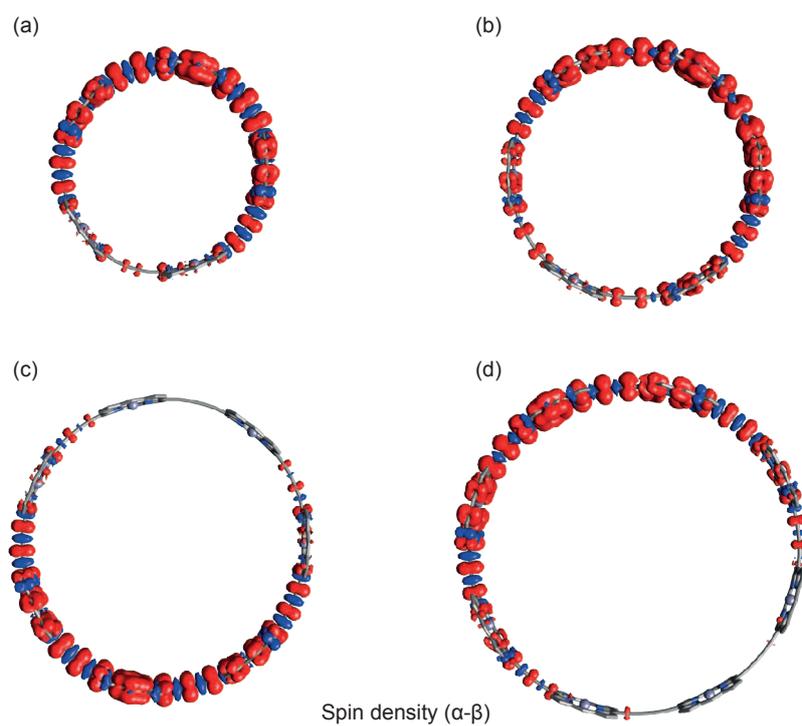


**Figure S3:** NICS(0)<sub>iso</sub> (left column) and NICS(0)<sub>zz</sub> (right column) for *c*-P5 in its T<sub>1</sub> state, calculated using the functionals M06-L and LC- $\omega$ HPBE ( $\omega = 0.05$ ,  $\omega = 0.1$ , and  $\omega = 0.2$ ), and the 6-31G\* basis set. White circles indicate the positions of porphyrin units.



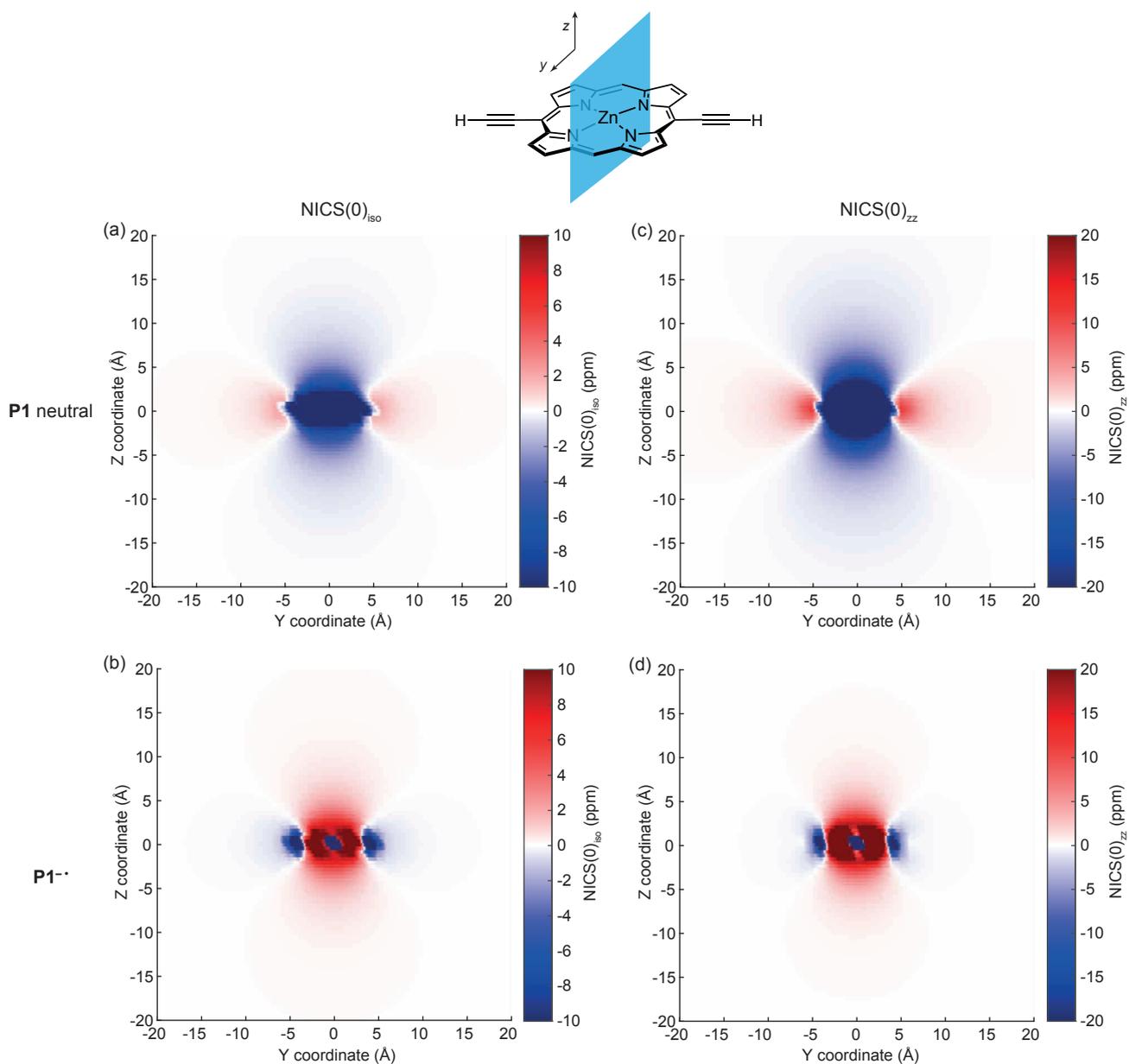
**Figure S4:**  $\text{NICS}(0)_{\text{iso}}$  (left column) and  $\text{NICS}(0)_{\text{zz}}$  (right column) for *c*-P6 in its  $T_1$  state, calculated using the functionals M06-L and LC- $\omega$ HPBE ( $\omega = 0.05$ ,  $\omega = 0.1$ , and  $\omega = 0.2$ ), and the 6-31G\* basis set. White circles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

## S1.4 Spin densities for $T_1$ excited states



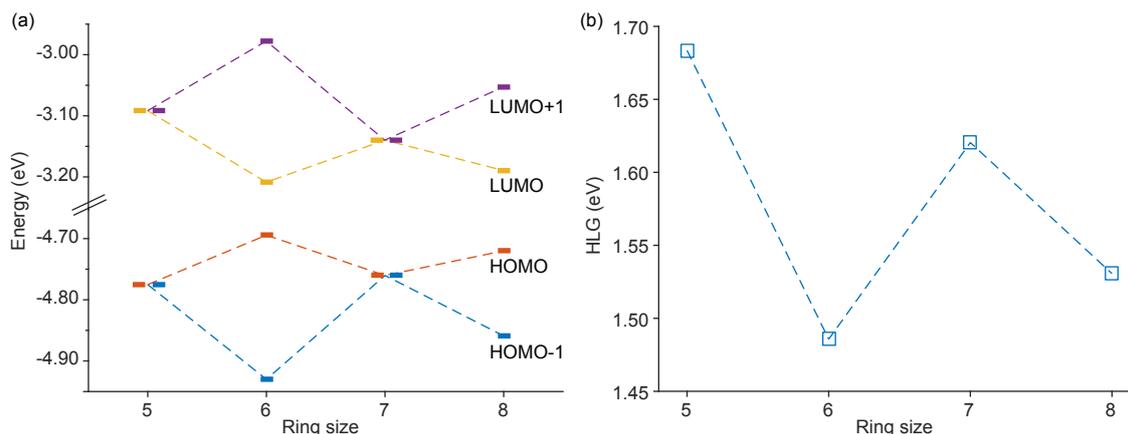
**Figure S5:** Calculated spin densities ( $\alpha - \beta$ ) for (a) *c-P5*, (b) *c-P6*, (c) *c-P7*, and (d) *c-P8* in their  $T_1$  states at the B3LYP/6-31G\* level of theory.

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



**Figure S6:**  $\text{NICS}(0)_{\text{iso}}$  (left column) and  $\text{NICS}(0)_{zz}$  (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

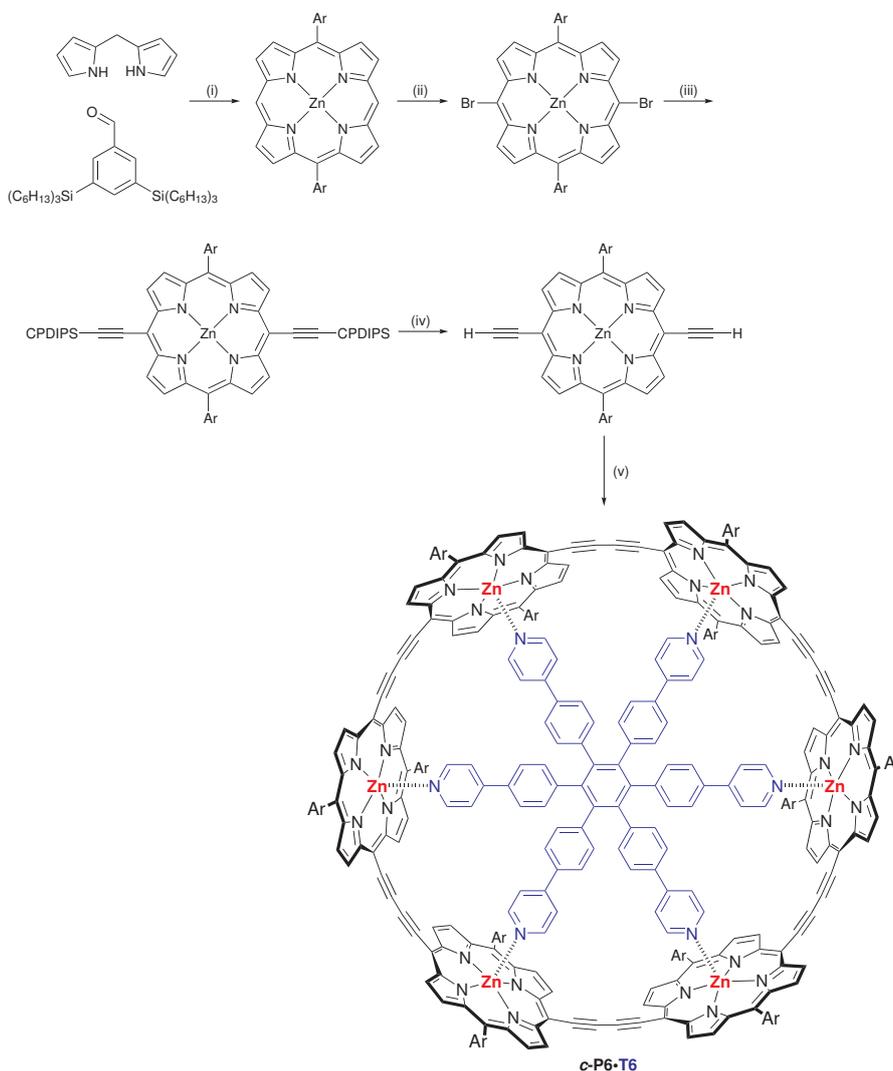
Unless stated otherwise, all reagents were obtained from commercial sources and used as received without further purification. Diethyl ether (Et<sub>2</sub>O), chloroform (CHCl<sub>3</sub>), tetrahydrofuran (THF), and toluene were dried by passing through activated alumina columns using a positive pressure of dry N<sub>2</sub> in an MBraun MB-SPS-5 benchtop solvent purification system (H<sub>2</sub>O content < 20 ppm, determined by Karl-Fischer titration). Diisopropylamine (DIPA) was dried by distillation from CaH<sub>2</sub>. Analytical gel permeation chromatography (GPC) was performed on a JAIGEL H-P precolumn, a JAIGEL 3H-A (8 mm × 500 mm) and a JAIGEL 4H-A column (8 mm × 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 × 600 mm) and a JAIGEL 4H column (20 mm × 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, ~150 mesh, 58 Å) 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).<sup>S14–S16</sup> 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<sub>2</sub> figure-of-eight complex,<sup>S17</sup> instead favoring a less-crowded *c*-P10·T6<sub>2</sub> complex in which two pyridine units (one per template) are unbound.

## S2.1 c-P6•T6

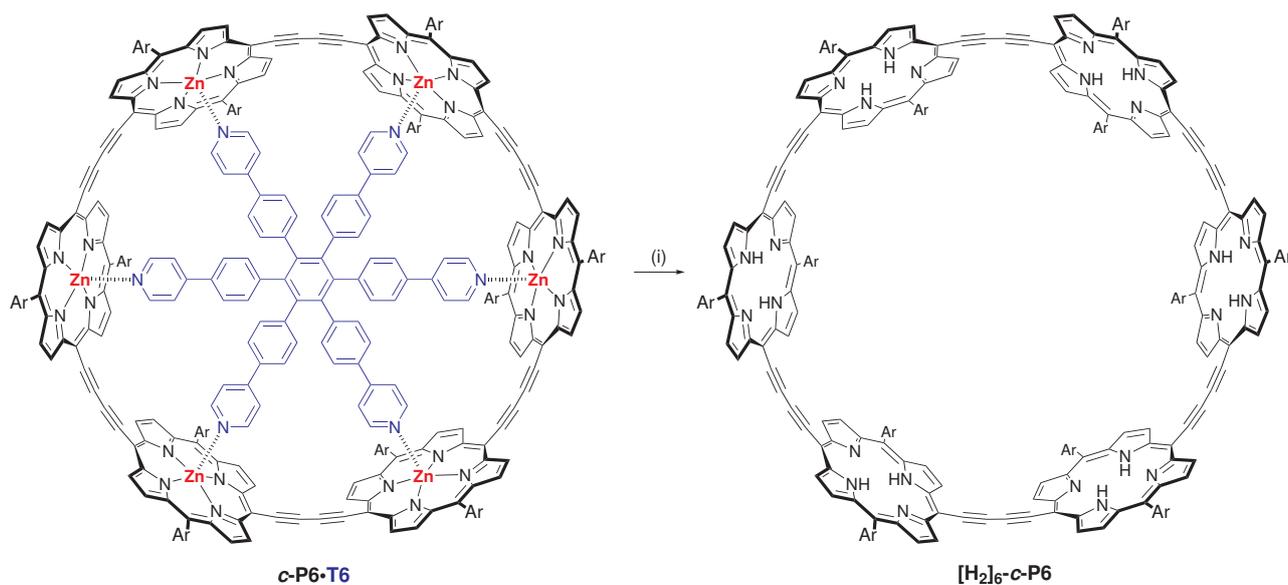
The overall route to **c-P6•T6** is shown in Scheme S1. Steps (i) to (v) are described elsewhere.<sup>S15</sup>



**Scheme S1:** (i) TFA, CH<sub>2</sub>Cl<sub>2</sub>, then DDQ, then Et<sub>3</sub>N; (ii) Zn(OAc)<sub>2</sub> · 2H<sub>2</sub>O, CHCl<sub>3</sub>, MeOH; (iii) *N*-bromosuccinimide, CH<sub>2</sub>Cl<sub>2</sub>; (iv) CPDIPS-acetylene, Pd(PPh<sub>3</sub>)<sub>2</sub>Cl<sub>2</sub>, CuI, THF, DIPA; (v) TBAF, CH<sub>2</sub>Cl<sub>2</sub>; (vi) **T6**, Pd(PPh<sub>3</sub>)<sub>2</sub>Cl<sub>2</sub>, CuI, 1,4-benzoquinone, CHCl<sub>3</sub>, 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 CHCl<sub>3</sub> (133 mL) by sonication for 2 h. A solution of Pd(PPh<sub>3</sub>)<sub>2</sub>Cl<sub>2</sub> (27 mg, 39 μmol), copper(I) iodide (37 mg, 0.19 mmol) and 1,4-benzoquinone (89 mg, 0.80 mmol) in CHCl<sub>3</sub> (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 (CHCl<sub>3</sub>). 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. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ<sub>H</sub>, 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<sup>+</sup> for C<sub>720</sub>H<sub>1068</sub>N<sub>30</sub>Si<sub>24</sub>Zn<sub>6</sub>: 11211; found: 11207. UV-vis (CH<sub>2</sub>Cl<sub>2</sub>) λ<sub>max</sub> [nm] (log ε [M<sup>-1</sup> cm<sup>-1</sup>]): 850 (5.61), 808 (5.70), 772 (5.57), 612 (4.59), 482 (5.76).

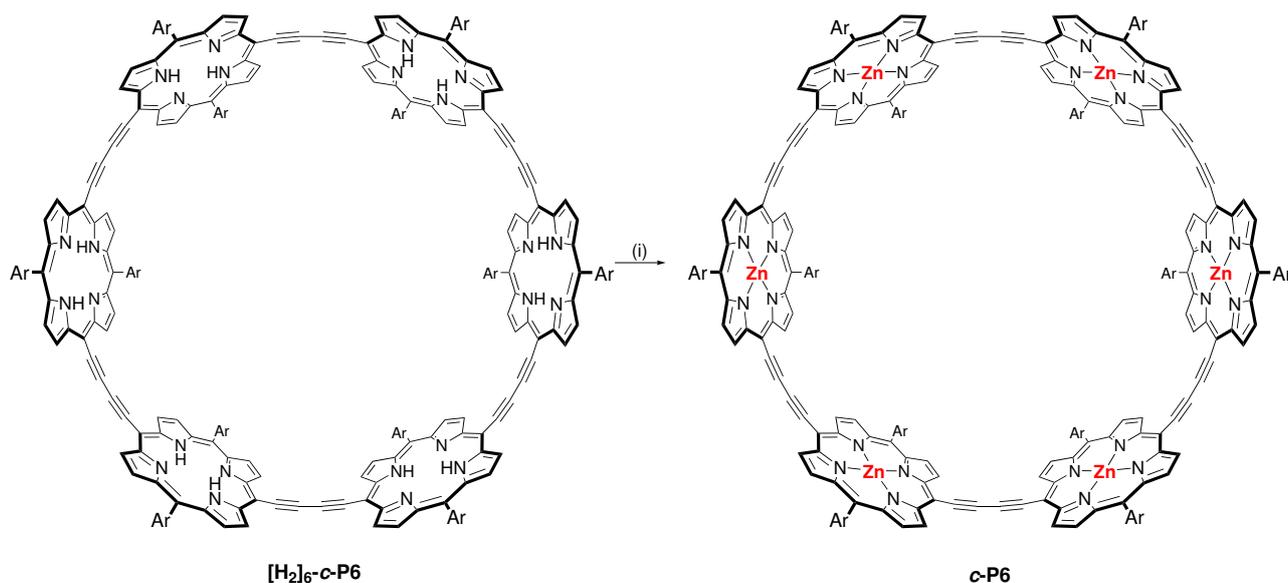
## S2.2 Free-base *c*-P6 [H<sub>2</sub>]<sub>6</sub>-*c*-P6



Scheme S2: (i) TFA, CHCl<sub>3</sub>, 20 °C, 5 min, 79–100%.

Trifluoroacetic acid (95  $\mu$ L, 1.24 mmol) was added to a solution of **c-P6·T6** (23 mg, 2.078  $\mu$ mol) in CHCl<sub>3</sub> (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 (CHCl<sub>3</sub> + 1% pyridine). Removing the solvent yielded **FB-c-P6** (16 mg, 79%) as a green solid. Yields varied from 79% to 100%. <sup>1</sup>H (400 MHz, CDCl<sub>3</sub>)  $\delta_{\text{H}}$ , 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<sup>+</sup> for C<sub>648</sub>H<sub>1032</sub>N<sub>24</sub>Si<sub>24</sub>: 9834; found: 9836; UV-vis (CH<sub>2</sub>Cl<sub>2</sub>)  $\lambda_{\text{max}}$  [nm] ( $\log \epsilon$  [M<sup>-1</sup> cm<sup>-1</sup>]): 791 (5.47), 771 (5.49), 659 (5.30), 466 (5.72).

## S2.3 c-P6



Scheme S3: (i)  $\text{Zn}(\text{OAc})_2 \cdot 2\text{H}_2\text{O}$ ,  $\text{CHCl}_3$ ,  $\text{MeOH}$ ,  $40^\circ\text{C}$ , 70 min, quant. Over two steps (with Scheme S2), 73%.

**[H<sub>2</sub>]<sub>6</sub>-c-P6** (43.9 mg, 4.5  $\mu\text{mol}$ ) was dissolved in  $\text{CHCl}_3$  (6 mL) and a solution of  $\text{Zn}(\text{OAc})_2 \cdot 2\text{H}_2\text{O}$  (8.8 mg, 219  $\mu\text{mol}$ ) in methanol (0.6 mL) was added. The mixture was stirred at  $40^\circ\text{C}$  for 70 min, at which time UV-vis indicated reaction completion. The mixture was then filtered through a short column of silica gel ( $\text{CH}_2\text{Cl}_2$  + 1% pyridine) to afford **c-P6** (46 mg, quant.) as a brown solid.  $^1\text{H}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta_{\text{H}}$ , 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  $\text{C}_{648}\text{H}_{1020}\text{N}_{24}\text{Si}_{24}\text{Zn}_6$ : 10214; found: 10211; UV-vis ( $\text{CH}_2\text{Cl}_2$ )  $\lambda_{\text{max}}$  [nm] ( $\log \epsilon$  [ $\text{M}^{-1}\text{cm}^{-1}$ ]): 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  $\text{CHCl}_3$  + 20% pyridine, and passed through a SEC column (eluting with  $\text{CHCl}_3$  + 20% pyridine). The absence of template was confirmed by  $^1\text{H}$  NMR spectroscopy. Residual pyridine could be removed by washing a  $\text{CH}_2\text{Cl}_2$  solution of nanoring with a saturated aqueous solution of potassium hydrogen phthalate (three times), then with water (twice) before passage over a  $\text{SiO}_2$  plug ( $\text{CHCl}_3$ ) 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%).  $^1\text{H}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta_{\text{H}}$ , 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  $\text{C}_{864}\text{H}_{1360}\text{N}_{32}\text{Si}_{32}\text{Zn}_8$ : 13615; found: 13786; UV-vis ( $\text{CH}_2\text{Cl}_2$ )  $\lambda_{\text{max}}$  [nm] ( $\log \epsilon$  [ $\text{M}^{-1}\text{cm}^{-1}$ ]): 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%).  $^1\text{H}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta_{\text{H}}$ , 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.  $\text{M}^+$  for  $\text{C}_{972}\text{H}_{1530}\text{N}_{36}\text{Si}_{36}\text{Zn}_9$ : 15317; found: 15550; UV-vis ( $\text{CH}_2\text{Cl}_2$ )  $\lambda_{\text{max}}$  [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%).  $^1\text{H}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta_{\text{H}}$ , 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.  $\text{M}^+$  for  $\text{C}_{1080}\text{H}_{1700}\text{N}_{40}\text{Si}_{40}\text{Zn}_{10}$ : 17019; found: 17241; UV-vis ( $\text{CH}_2\text{Cl}_2$ )  $\lambda_{\text{max}}$  [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%).  $^1\text{H}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta_{\text{H}}$ , 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.  $\text{M}^+$  for  $\text{C}_{1188}\text{H}_{1870}\text{N}_{44}\text{Si}_{44}\text{Zn}_{11}$ : 18721; found: 19016; UV-vis ( $\text{CH}_2\text{Cl}_2$ )  $\lambda_{\text{max}}$  [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%).  $^1\text{H}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta_{\text{H}}$ , 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.  $\text{M}^+$  for  $\text{C}_{1296}\text{H}_{2040}\text{N}_{48}\text{Si}_{48}\text{Zn}_{12}$ : 20423; found: 20657; UV-vis ( $\text{CH}_2\text{Cl}_2$ )  $\lambda_{\text{max}}$  [nm] ( $\log \epsilon$  [ $\text{M}^{-1} \text{cm}^{-1}$ ]): 821 (5.88), 596 (4.88), 488 (6.06), 472 (6.07).

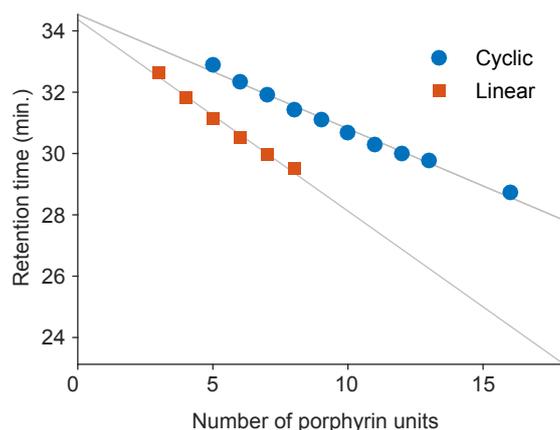
## S2.10 c-P13

**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%).  $^1\text{H}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta_{\text{H}}$ , 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.  $\text{M}^+$  for  $\text{C}_{1404}\text{H}_{2210}\text{N}_{52}\text{Si}_{52}\text{Zn}_{13}$ : 22125; found: 22530; UV-vis ( $\text{CH}_2\text{Cl}_2$ )  $\lambda_{\text{max}}$  [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%).  $^1\text{H}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta_{\text{H}}$ , 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.  $\text{M}^+$  for  $\text{C}_{1728}\text{H}_{2720}\text{N}_{64}\text{Si}_{64}\text{Zn}_{16}$ : 27230; found: 27686; UV-vis ( $\text{CH}_2\text{Cl}_2$ )  $\lambda_{\text{max}}$  [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  $1 \text{ mL min}^{-1}$  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

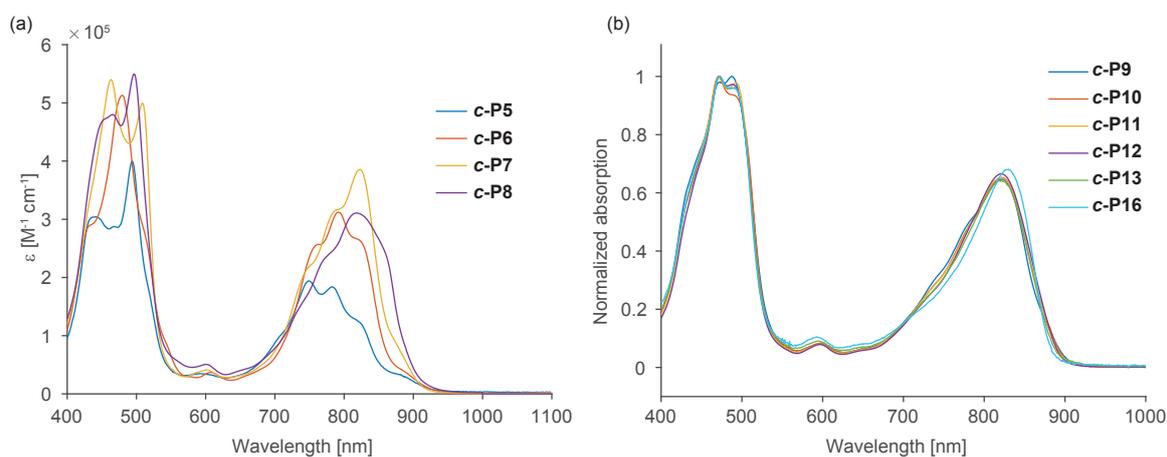
Nanoring samples were prepared at a concentration of  $\sim 1 \mu\text{M}$  in toluene + 1% pyridine (the latter to suppress aggregation). Fluorescence quantum yields ( $\Phi_F$ ) were measured relative to that of **I-P6**, using the technique reported previously, with excitation at 500 nm.<sup>S18,S19</sup> Excited state lifetimes ( $\tau$ ) 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.

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

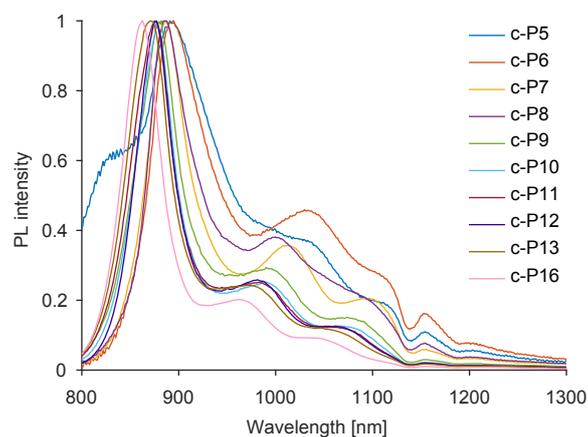
$$k_{\text{tot}} = k_R + k_{\text{NR}} \quad (\text{S3})$$

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

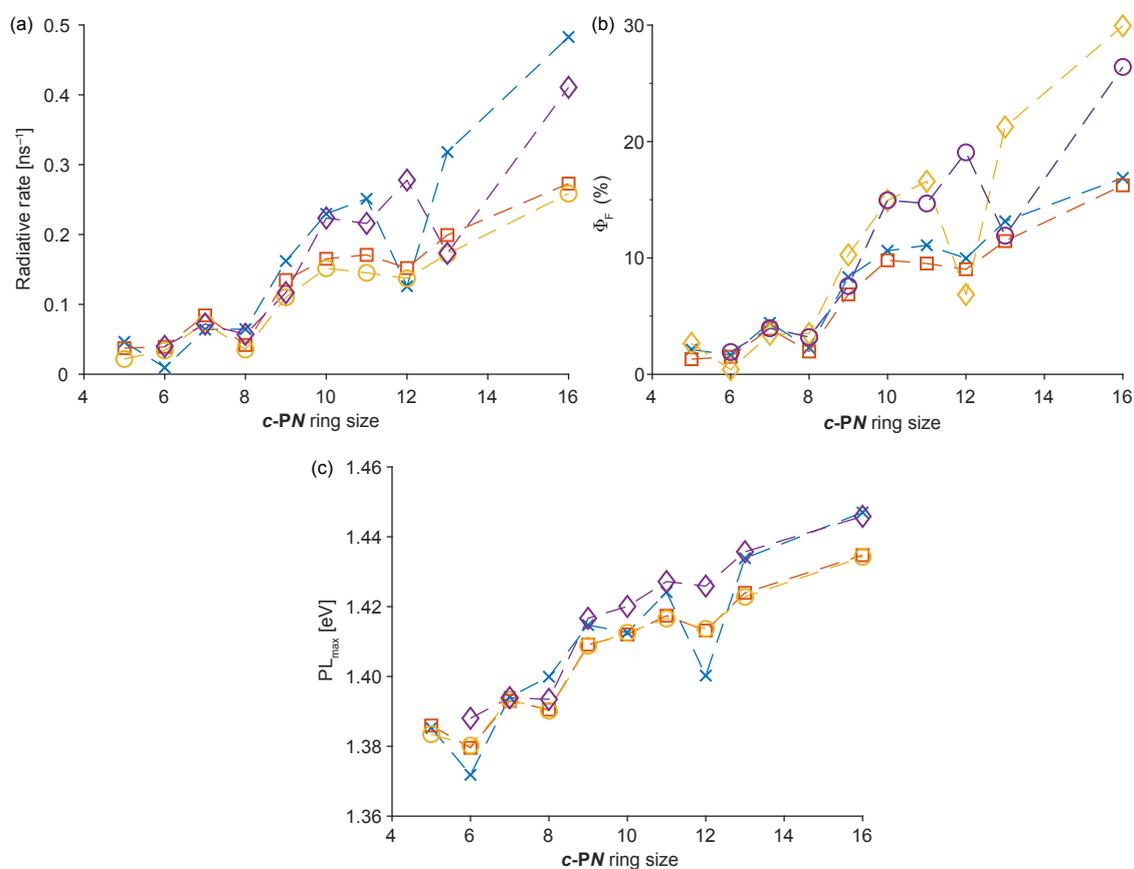
$$k_R = \Phi k_{\text{tot}} \quad (\text{S5})$$



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



**Figure S10:** Normalized photoluminescence spectra of porphyrin nanorings,  $\lambda_{\text{ex}}$  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  $\text{PL}_{\text{max}}$  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.<sup>S20</sup>

Model A,  $Y \sim N$ , states that  $Y$  (radiative rate,  $\text{PL}_{\text{max}}$ , 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)<sup>S21</sup> 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  $\Delta\text{AIC}$ , 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.

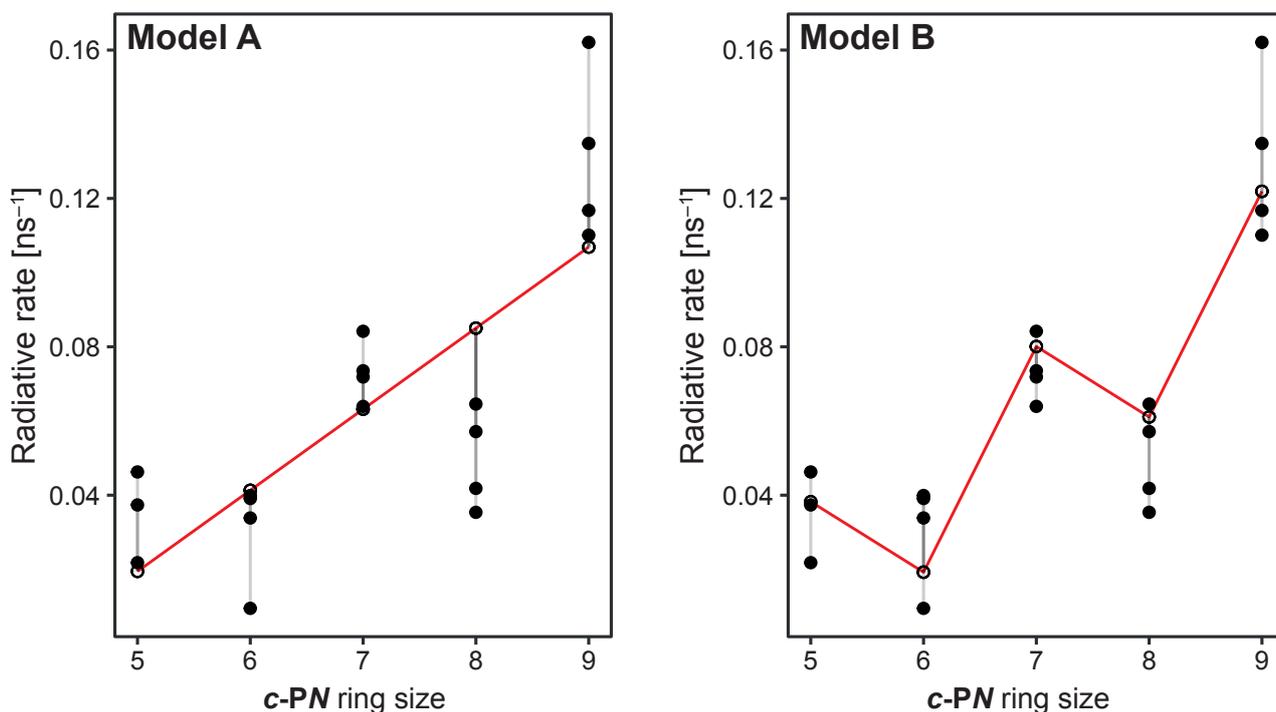
The AIC revealed that model B (including odd-even effects) fit the data better (Table S4) for nanorings from **c-P5** to **c-P9**. When the whole dataset was fit (i.e. **c-P5** to **c-P16**), model B was no better than model A for both radiative rates and quantum yields.

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

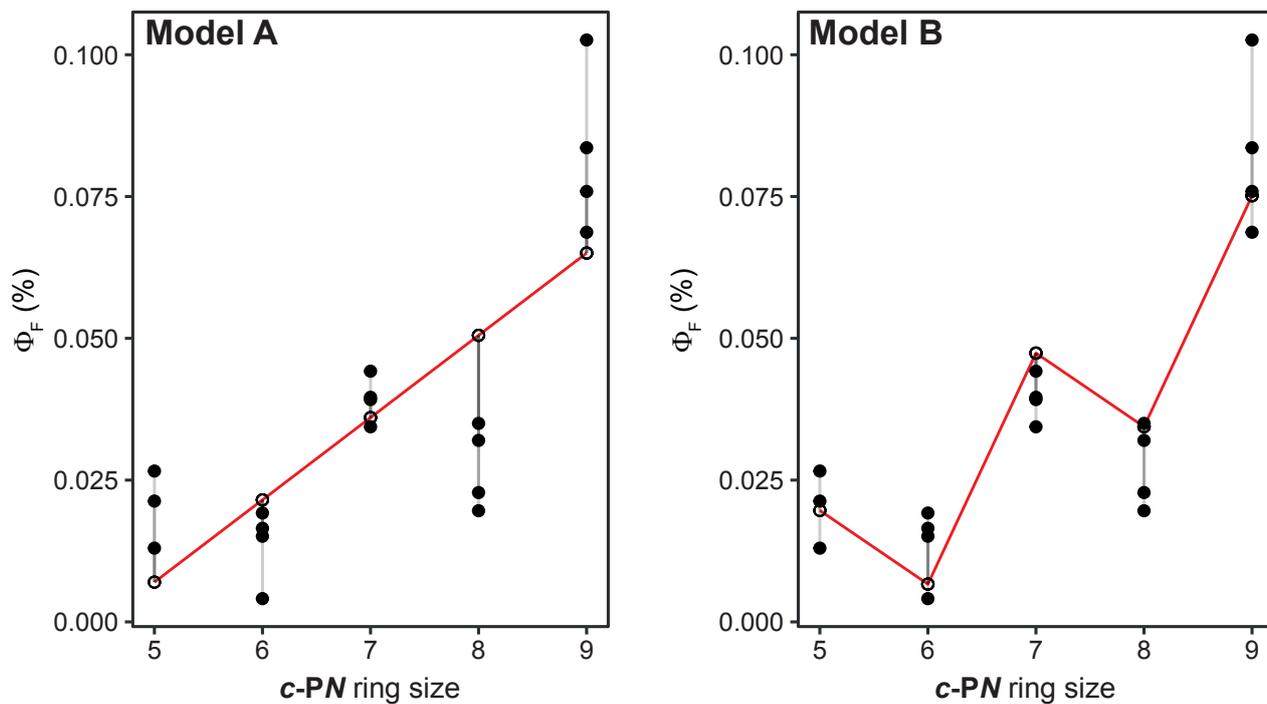
$Y$	$\Delta\text{AIC}$ for $5 \leq N \leq 16$	$\Delta\text{AIC}$ for $5 \leq N \leq 9$
Radiative rates	2	-16
Quantum yield ( $\Phi_F$ )	1	-17
$\text{PL}_{\text{max}}$	-12	-15

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

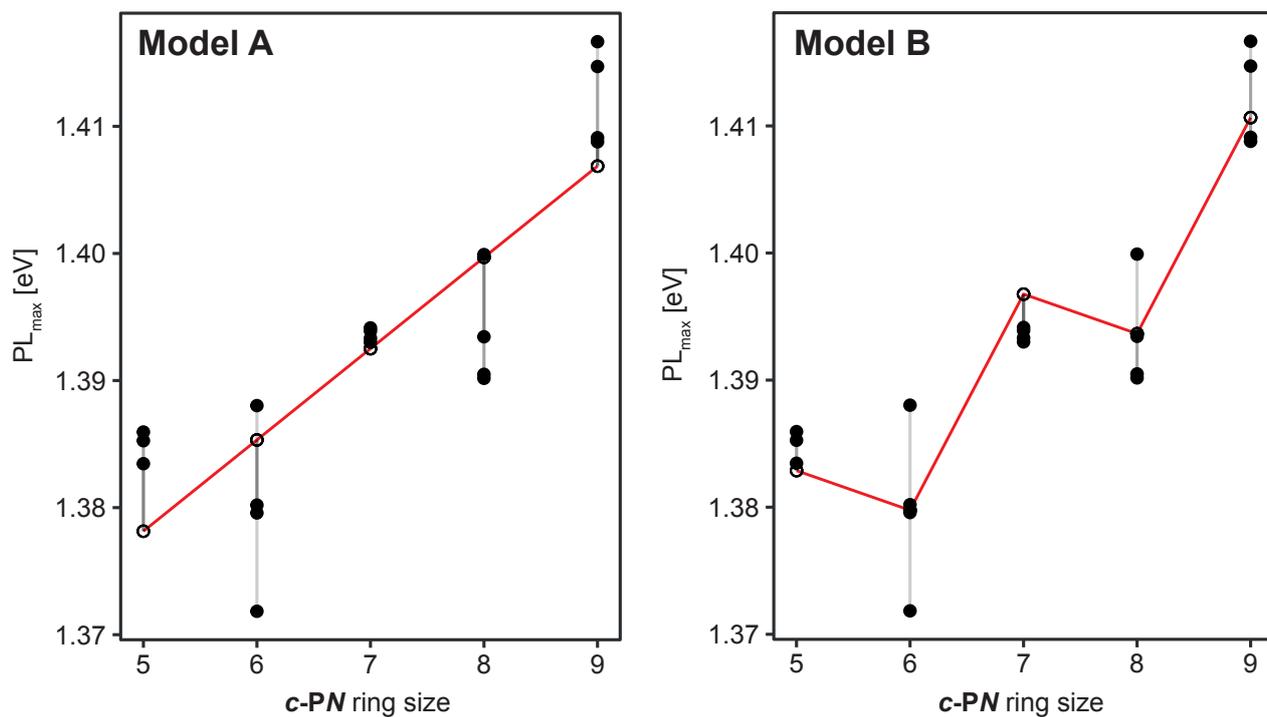
In conclusion, a model including odd-even behaviour is better able to describe the experimental photophysical data than a model without, but only for nanorings smaller than **c-P10**.



**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 S<sub>0</sub>

195

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

C	-1.248070842749	10.713934967178	2.788248274287	C	8.273874619545	-7.119901875992	-3.481152695826
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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
C	-2.797002856590	10.423120075879	-1.255893284110	C	-9.048654849825	5.881029034870	-1.255893284110
C	-3.468302642315	10.4231036401515	-2.532670154300	C	-8.839230115319	6.518829179578	-2.532670154300
C	-2.508731856339	10.623383095792	-3.481152695826	C	-9.328196938055	5.668751698259	-3.481152695826
C	0.000000002674	10.797222843464	-3.404764367996	C	-10.268769142789	3.336525352901	-3.404764367996
C	1.248070848057	10.713934966560	2.788248274287	C	-10.575232766739	2.123802073366	2.788248274287
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C	-2.797002856590	10.423120075879	1.255893284110	C	-9.048654849825	5.881029034870	1.255893284110
C	-3.468302642315	10.4231036401515	2.532670154300	C	-8.839230115319	6.518829179578	2.532670154300
C	-2.508731856339	10.623383095792	3.481152695826	C	-9.328196938055	5.668751698259	3.481152695826
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C	1.248070848057	10.713934966560	-2.788248274287	C	-10.777297684741	0.560813444675	-1.255893284110
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C	0.000000000000	10.797222843464	0.000000000000	N	-7.411658011639	-7.728749734130	1.430424178924
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C	-3.468302642315	10.4231036401515	2.532670154300	C	-7.307203493904	-7.934157827124	-2.788248274287
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C	-2.797002856590	10.423120075879	1.255893284110	C	-4.214661207329	-10.069093050217	3.481152695826
C	-3.468302642315	10.4231036401515	2.532670154300	C	-3.248009192510	-10.318018829906	0.000000000000
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C	0.000000000000	10.797222843464	0.000000000000	C	-8.931247293126	-6.392178400615	-2.532670154300
C	1.248070848057	10.713934966560	-2.788248274287	C	-8.273874623072	-7.119901871894	-3.481152695826
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C	-2.508731856339	10.623383095792	3.481152695826	N	-9.640806079102	4.660590635078	-1.430424178924
C	0.000000000000	10.797222843464	0.000000000000	C	-9.803882563324	4.497773893811	-2.788248274287
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C	-2.508731856339	10.623383095792	3.481152695826	C	10.136204848154	-4.005214351244	0.000000000000
C	0.000000000000	10.797222843464	0.000000000000	C	5.846156057525	9.198198196482	0.000000000000
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N	1.453312170552	10.609153154325	1.430424178924	C	-0.676925650915	-10.877782972314	0.000000000000
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C	-2.797002856590	10.423120075879	1.255893284110	H	2.634322087842	10.686172889642	4.554734107845
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## S4.2 c-P5 T<sub>1</sub>

195

CP5 T1 UB3LYP/6-31G\* E(au): -14593.4562255

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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	10.204516447797	8.594822451648	2.670445088502
H	-9.941352773439	-5.744969163863	-2.6725567611455	H	8.722184484941	9.840719155577	4.556815491321
H	-8.599188146635	-7.144249074204	-4.556493211934	C	4.161220537768	12.473992918242	4.556815491321
H	0.043934973589	10.675399588312	-4.489060714944	C	-10.939152170491	7.097468671114	0.000000000000
H	10.709016998287	3.478180556805	4.481975969126	C	-11.616164256994	5.924849339952	0.000000000000
H	10.710411653333	3.477887876564	-4.47782319080	C	-10.224281854676	8.093952097271	0.000000000000
H	6.306496597509	-8.613490518269	4.490294925556	C	-12.121709060589	4.807511772966	0.000000000000
H	6.308317932321	-8.613141613620	-4.487904147935	C	-9.241546543577	9.111556052248	0.000000000000
H	-10.440421863218	3.269031571855	4.487644644185	C	-12.511612281041	3.447636050870	0.000000000000
H	-10.439225018404	3.269553729983	-4.491225149353	C	-8.753439932530	9.556843976474	-1.255817326326
H	-6.528022190740	-8.779695198863	4.487879060643	C	-8.753439932530	9.556843976474	1.255817326326
H	-6.525890587473	-8.779002552773	-4.490990748594	C	-12.653189629896	2.802279363835	-1.255817326326
H	0.042435155354	10.676031656374	4.489138998477	C	-12.653189629896	2.802279363835	1.255817326326
				C	-9.334967270050	9.222210411522	-2.532960715949
				N	-7.665331111632	10.367181946203	-1.431029608907
				C	-9.334967270050	9.222210411522	2.532960715949
				N	-7.665331111632	10.367181946203	1.431029608907
				N	-12.810908486884	1.454780497991	-1.431029608907
				C	-12.654152130448	3.473213593599	-2.532960715949
				N	-12.810908486884	1.454780497991	1.431029608907
				C	-12.654152130448	3.473213593599	2.532960715949
				C	-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
				H	-8.587187480511	9.854264502471	3.482632209072
				H	-10.204516447797	8.594822451648	2.670445088502
				C	-7.532149936999	10.549935973971	2.789634986275
				C	-12.902587530258	1.248065203569	-2.789634986275
				Zn	-12.818609138434	0.000000000000	0.000000000000
				C	-12.827637135007	2.509590253946	-3.482632209072
				N	-12.810908486884	1.454780497991	1.431029608907
				H	-12.654152130448	3.473213593599	2.532960715949
				C	-12.883405022708	2.633273762665	4.556815491321
				C	-12.653189629896	2.802279363835	1.255817326326
				H	-12.545592808042	4.539959251304	2.670445088502
				C	-12.511612281041	3.447636050870	0.000000000000
				C	-12.653189629896	2.802279363835	-1.255817326326
				C	-12.654152130448	3.473213593599	-2.532960715949
				N	-12.810908486884	1.454780497991	-1.431029608907
				C	-12.827637135007	2.509590253946	-3.482632209072
				H	-12.545592808042	4.539959251304	3.406820644400
				C	-12.902587530258	1.248065203569	-3.406820644400
				H	-12.883405022708	2.633273762665	-4.556815491321
				N	-12.810908486884	1.454780497991	-1.431029608907
				C	-12.974592816329	0.000000000000	-3.406820644400
				C	-12.902587530258	-1.248065203569	-2.789634986275
				C	-12.827637135007	-2.509590253946	-3.482632209072
				N	-12.810908486884	-1.454780497991	-1.431029608907
				H	-12.883405022708	-2.633273762665	-4.556815491321
				C	-12.974592816329	0.000000000000	-3.406820644400
				C	-12.902587530258	-1.248065203569	-2.789634986275
				C	-12.827637135007	-2.509590253946	-3.482632209072
				N	-12.810908486884	-1.454780497991	-1.431029608907
				H	-12.883405022708	-2.633273762665	-4.556815491321

### S4.3 c-P6 S<sub>0</sub>

234

cP6 SO B3LYP/6-31G* E(au):	-17512.2110304		
C	12.653189629896	-2.802279363835	1.255817326326
C	12.654152130448	-3.473213593599	2.532960715949
C	12.827637135007	-2.509590253946	3.482632209072
C	12.902587530258	-1.248065203569	2.789634986275
N	12.810908486884	-1.454780497991	1.431029608907
H	12.545592808042	-4.539959251304	2.670445088502
H	12.883405022708	-2.633273762665	4.556815491321
C	12.974592816329	0.000000000000	3.406820644400
C	12.902587530258	1.248065203569	2.789634986275
C	12.827637135007	2.509590253946	3.482632209072
N	12.810908486884	1.454780497991	1.431029608907
C	12.654152130448	3.473213593599	2.532960715949
H	12.883405022708	2.633273762665	4.556815491321
C	12.653189629896	2.802279363835	1.255817326326
H	12.545592808042	4.539959251304	2.670445088502
C	12.511612281041	3.447636050870	0.000000000000
C	12.653189629896	2.802279363835	-1.255817326326
C	12.654152130448	3.4732135	

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
C	-12.654152130448	-3.473213593599	-2.532960715949	H	-6.516748992453	11.287340355103	-4.491712610839
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
H	-2.341076360245	13.134781702952	2.670445088502	H	6.516748992453	11.287340355103	4.491712610839
H	-12.883405022708	-2.633273762665	-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	-2.633273762665	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				
N	-7.665331111632	-10.367181946203	-1.431029608907				
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				
H	-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				
C	3.899749697366	-12.359123340309	-1.255817326326				
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 T<sub>1</sub>

234

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

C	12.6654658779465	-2.802462253263	1.260567024131
C	12.667290816422	-3.473535271791	2.534854850567
C	12.846940654423	-2.508278364498	3.484583690232
C	12.915086813761	-1.249394742250	2.792177242288
N	12.811594105922	-1.457323774551	1.431946819003
N	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	1.431946806701
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	-0.000003024970
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
C	5.144300481418	11.825913224261	-1.431993266564
C	8.595979500118	9.873243634407	-3.484605994809
N	7.668245371272	10.368345572374	-1.431989875136
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			

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C	-12.846943635134	2.508276143585	3.484583940993	C	2.349725600928	-13.152017277786	2.673438328803
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## S4.5 c-P7 S<sub>0</sub>

273

cP7 S0 B3LYP/6-31G\* E(a.u): -20430.9248371

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273  
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C	-15.107449661091	-2.139226304184	2.793056060662	Zn	6.519527089361	-13.433141655363	-0.002118038751
C	-15.243803361162	0.095925254253	-0.002124130298	Zn	11.781356861198	9.321571457495	-0.002114865089
C	-13.960108133358	-6.036397213350	-1.262930882956	Zn	14.731144940449	-3.334700097798	-0.002122988520
C	-13.822704931304	-6.692476743593	-2.536634966908	Zn	-11.781328133277	9.321555258813	-0.002119613596
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C	-13.027942056150	-7.883792966070	-0.002124164545	H	2.632174150645	14.961545053604	-4.561108549387
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C	-5.425657629321	-14.041223866949	2.789271715936	H	8.735928188415	12.702707932750	2.670949117693
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C	-3.320702161744	-14.801155551550	-2.535441184097	H	14.953291716505	-3.386350013883	4.490103741365
C	-4.260352889951	-14.525012183331	-3.486277033391	H	13.491421268279	-7.712072832612	-2.674922270985
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C	-8.996364151928	-12.107305832382	1.256710122750	H	15.552115455221	1.140390629332	-2.677343964167
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C	-8.797030461488	-12.379504106970	3.483637631993	H	13.491418605732	-7.712070319203	2.670679139659
C	-1.899502952723	-14.956907206146	-0.002121441366	H	14.229756773980	-5.919492528429	4.557335839411
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C	1.899475089430	-14.956896851072	-0.002120185426	H	-13.514406881584	7.340460736728	4.557926858198
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C	8.996332727301	-12.107285086009	-1.260948191598	H	-13.491451210221	-7.712095732520	-2.674924232046
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H	8.930691651014	-12.375408715769	-4.562350595569	C	1.872311756973	-17.198713068461	0.000000000000
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## S4.7 c-P8 S<sub>0</sub>

312

cP8 SO B3LYP/6-31G* E(a.u.):	-23349.6372778						
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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
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C	5.643663205960	16.438052278298	3.484457456736	C	13.85250978241	-10.837402298540	0.000000000000
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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
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C	3.321870708192	17.022504202555	0.000000000000	H	3.733339888748	17.178106377370	2.670061524636
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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
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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
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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
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C	17.325130008580	-0.761354105615	0.000000000000	C	-9.010280465607	-14.766354136622	2.791293534575
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1.888938232669	-17.315092170713	2.535020172893	C	-5.314784722658	-16.450416329645	-1.259335316750	
2.854303706782	-17.151311102137	3.486288706714	C	-4.723603177183	-16.766120545584	-2.535020385489	
1.866468307083	-17.190526708308	-0.000003057470	C	-5.648685135495	-16.445236085578	-3.486295937183	
7.873590126552	-15.389251386212	-1.259337678065	C	-12.776580576160	-11.697832717754	0.000002049551	
8.514860171070	-15.194505983959	-2.535026030248	C	-11.917756329551	-12.573502645500	0.000002542256	
7.633792839833	-15.621673251223	-3.486298447974	C	-3.321582730468	-17.006716328248	-0.000001637651	
N	15.939412146241	-6.569876824599	-1.432460802693	C	-2.106450271910	-17.194969345147	-0.000002988958
C	14.770007818056	-9.013266095111	-2.793466865110	C	-16.055141080112	-6.449485404887	-2.793443141409
N	14.603172268273	-9.16299583029	-1.432457400105	C	-16.491615128506	-5.277697690423	-3.408834004340
C	13.877781576654	-10.307636872965	-1.259340624086	C	-16.804553917900	-3.846355773590	1.432426506205
C	13.579639950903	-10.907868458981	-2.535027237440	C	-16.055091109302	-6.449465892760	2.793453979079
C	14.146656620385	-10.109602337255	-3.486304838080	N	-15.915345385800	-6.624751908099	1.432445017599
C	15.394216017139	-7.929777814219	-3.408873793413	C	-15.389239522748	-7.873592528923	1.259337586458
C	15.272596393935	-7.867079805769	-0.000003885816	C	-15.194475533007	-8.514856357321	2.535026238709
C	17.006711552283	-3.321576508097	-0.000004007550	C	-15.621627771734	-7.633783999557	3.486300609562
C	15.914277880430	-6.792619689174	2.793464912002	C	-16.491553986359	-5.277673884320	3.408845501870
C	15.939398534787	-6.569871340155	1.432454424251	Zn	-16.361150055642	-5.235950124320	0.000004396086
C	16.450394795991	-5.314770854596	1.259334232817	C	-16.816614253359	-4.070236108080	-2.793430770236
C	16.766083764519	-4.723581450634	2.535019576027	N	-16.804579522017	-3.846365689591	-1.432419387511
C	16.445187238069	-5.648657229412	3.486296975915	C	-17.101356079981	-2.529423730070	-1.259329241469
C	15.914304490942	-6.792630461049	-2.793470668441	C	-17.315132029570	-1.888958011426	-2.535020927448
C	16.646874376166	-4.680874377246	-0.000003484934	C	-17.151366249572	-2.854328316516	-3.486287080606
N	14.603158660789	-1.62994001063	1.432448323170	C	-16.816564146880	-4.070216650234	2.793439660179
C	13.877769626673	-10.307631963875	1.259329058990	C	-17.190528698773	-1.866475840146	0.000000836645
C	13.579615860298	-10.907858614192	2.535015170921	N	-15.915370900344	-6.624761902567	-1.432434440757
C	14.146623411621	-10.109588776555	3.486295072480	C	-15.389261899634	-7.873601311223	-1.259327725819
C	13.475682346024	-10.835612810962	-0.000006691209	C	-15.194520716593	-8.514874038154	-2.535015380750
C	16.450406768059	-5.314775661448	-1.259340596724	C	-15.621690118207	-7.633808369545	-3.486288268593
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C	-0.763106264024	-17.306493422398	-0.000003755875	C	-17.315086603245	-1.888940398021	2.535023546149
C	0.466435012458	-17.321182529818	-0.000003924325	C	-17.151303639753	-2.854304037236	3.486293487683
C	11.697824191114	-12.776573505783	-0.000008824781	C	-13.647418965240	-10.668925280744	0.000002009539
C	12.577827701050	-11.917749476535	-0.000008443286	C	-14.373374509705	-9.676466904836	0.000002562581
C	9.676457558364	-14.373366397833	-0.000007905102	C	-17.321183340912	-0.466441915547	-0.000003168100
C	10.668915913995	-13.647410678902	-0.000008628159	C	-17.306492635706	0.763099073037	-0.000004950788
C	17.194965362705	-2.106444357505	-0.000003537576	C	-14.769971774059	9.013252795163	2.793457854044
H	11.821473684177	13.018527198113	-2.672593506752	C	-15.394172279122	7.929757929877	3.408867111896
H	10.240899064858	14.135602188525	-4.560967689408	C	-4.070215639585	16.816567308969	2.793432480314
H	3.736364648786	17.184322298024	2.672590635398	C	-5.277673606778	16.491556708203	3.408836749113
H	5.563442058296	16.545673540576	4.560979549034	N	-6.624751759081	15.915364862476	-1.432444712598
H	11.821452871281	13.018495539010	2.672609097336	C	-4.070224334436	16.816607992629	-2.793437591767
H	10.240863446398	14.135547881806	4.560984209018	N	-3.846356810015	16.804576402046	-1.432425824868
H	3.736385394013	17.184354149826	-2.672588410420	C	-2.524116279596	17.101354479946	-1.432444710552
H	5.563477594356	16.545728016675	-4.560970790317	C	-1.888947106586	17.315128348315	-2.535024444849
H	14.79220998371	9.508684302834	2.672592974820	C	-2.854315194790	17.151359585852	-3.486292183622

C	-5.277684302735	16.491606436834	-3.408842805974	H	-15.441432765805	7.954101337061	-4.494233825655
Zn	-5.235943520207	16.361148337533	-0.000004081946	H	-5.293859203143	16.542120771852	4.494197917181
C	-6.449463944857	16.055091661652	-2.793443463437	H	-5.293873330303	16.542186419111	-4.494203191238
N	-6.624747226005	15.915344030690	1.432434481733	H	7.954077106912	15.441380951754	4.494237999984
C	-7.873587069086	15.389236276064	1.259325269754	H	7.954112202049	15.441434603200	-4.494223750946
C	-8.514853060746	15.194473291743	2.535013235813				
C	-7.633782964487	15.621627633673	3.486288584405				
C	-6.449472748000	16.055132380545	-2.793452215813				
C	-8.460768767577	15.079965576807	-0.000008343372				
N	-3.846352407868	16.804555633420	1.432419843837				
C	-2.524112438436	17.101336217993	1.259327614014				
C	-1.888939289416	17.315091559120	2.535019784147				
C	-2.854304368612	17.151308813313	3.486288138941				
C	-1.866470199123	17.190530265065	-0.000003288253				
C	-7.873591064567	15.3893254569128	-1.25933259810				
C	-8.514861064767	15.194510175319	-2.535028044077				
C	-7.633793980746	15.621678465217	-3.486299946520				
N	-15.939416193431	6.569877185834	-1.432461235940				
C	-14.770015204990	9.013271334376	-2.793467284624				
N	-14.603175824137	9.162999403016	-1.432458224003				
C	-13.877784361050	10.307363437056	-1.259341852384				
C	-13.579646232428	10.907869638680	-2.535028650145				
C	-14.146665615031	10.109604903771	-3.486305621547				
C	-15.394225412309	7.929780559308	-3.408873999021				
Zn	-15.27259268192	7.867078028351	-0.000004639287				
C	-17.006712602882	3.321575322303	-0.000005733006				
C	-15.914268811946	6.792614089877	2.793464470749				
N	-15.939393898564	6.569867754504	1.432453821313				
C	-16.450391003146	5.314767626497	1.259333754060				
C	-16.766076064038	4.723576463005	2.535018898280				
C	-16.445176201881	5.648650648681	3.486296565189				
C	-15.914312365619	6.792632584824	-2.793470806285				
C	-16.646874815719	4.680873094867	-0.000004479414				
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	-2.672612207642				
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 S<sub>0</sub>

41

l-P1 neut SO 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-

41

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
H	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
H	-2.506966031112	-3.494545033615	0.000000000000
H	-2.625899691848	-4.572267034287	0.000000000000
C			

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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