

Supporting Information

Discrimination between alkyl and aryl substituents of chiral monoamines by *m*-phthalic diamide-linked zinc bisporphyrinates

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Experimental section

Materials and methods

All reagents and solvents were purchased from commercial sources and used as received unless otherwise noted. Triethylamine (Et₃N) was distilled over potassium hydroxide and methylene dichloride was treated with CaH₂ before use. The synthesis of the bisporphyrin [Zn₂-1] is accomplished by following the literature method.¹

Elemental analyses (C, H and N) were performed with an ElementarVario EL III analytical instrument. ¹H NMR titration and ¹H NMR spectra were obtained at room temperature, using a Bruker AVANCE 400 MHz spectrometer in CDCl₃ with tetramethylsilane (TMS) as the internal standard; chemical shifts are expressed in ppm relative to TMS (0 ppm). Two-dimensional NMR spectra were recorded on Agilent 600MHz NMR instrument. Mass spectra were taken with Finnigan Accurate-Mass LCQ™. CD spectra were measured on an AVIV Model 410 spectropolarimeter. Scanning conditions were as follows: wavelength step=0.50 nm, bandwidth=2 nm, response time=0.1 s, averaging time=1.00 seconds, settling time=0.333 seconds.

General procedure for CD measurement

The background spectrum was taken from 390 nm to 440 nm with a scan rate of 100 nm/min at 295 K. Zinc bisporphyrinate solution (1.00 to 2.00×10⁻⁶ M, 2.50 mL) was injected into a 1 cm quartz cuvette. Then 1500 equivalents of the optically active monoamines were added into the above solution to form the corresponding complex. The CD spectra were measured after several minutes (minimum of 4 accumulations). The resultant ECCD spectra recorded in millidegrees were normalized based on the zinc bisporphyrinate concentration.

¹H NMR and CD titrations

The CD titration experiments were carried out as follows. Measurements have been performed by adding different aliquots of the optically active monoamines solution to the zinc-bisporphyrin solution in DCM at room temperature. Then the CD spectra were taken after each addition. The resultant ECD spectra recorded in millidegrees were normalized based on the zinc bisporphyrinate concentration.

¹H NMR titration experiments were done as follows. Portions of a solution of the chiral monoamine in CDCl₃ were added to the solution of bisporphyrin (0.50 mL) in CDCl₃ in a 5 mm o.d. NMR tube and ¹H NMR spectra were taken after each addition.

Preparation of free base bisporphyrin 2

A solution of 5-methylisophthalic acid (0.080 g, 0.44 mmol) in thionyl chloride (8 mL) was refluxed under nitrogen for four hours, followed by the removal of excess reagent under reduced pressure. The residual white solid was redissolved in CH₂Cl₂ (30 mL), and Et₃N (150 μL, 1.07 mmol) was added to the above solution and stirred for 10 minutes in an ice bath. 5-(2-aminophenyl)-10,15,20-triphenyl-porphyrinate (0.50 g, 0.78 mmol) was added to the solution under nitrogen atmosphere overnight in an ice bath. Then the mixture was washed by water for three times, dried with Na₂SO₄, purified by silica gel chromatography (pure CH₂Cl₂) to give the pure product (0.394 g, yield 72%). ¹H NMR (400 MHz, CDCl₃): δ 8.84 (4H, d), 8.79 (4H, d), 8.65 (4H, d), 8.56 (4H, d), 8.27 (2H, d), 8.21 (2H, d), 8.17 (2H, d), 8.09 (4H, s), 7.99 (2H, d), 7.93 (4H, d), 7.82 (2H, m), 7.78 (4H, t), 7.69 (10H, m), 7.51 (4H, s), 7.46 (2H, t), 7.08 (2H, s), 6.29 (1H, s), 5.09 (2H, s), -0.36 (3H, s), -2.28 (4H, s). Anal. Calcd for C₉₇H₆₆N₁₀O₂: C, 83.00; H, 4.74; N, 9.98. Found: C, 83.31; H, 4.71; N, 9.99. MS (ESI) m/z (C₉₇H₆₆N₁₀O₂): Calc. [M+H]⁺: 1404.54, Found [M+H]⁺: 1404.83.

Preparation of zinc bisporphyrinate [Zn₂-2]

The free base bisporphyrin **2** (0.394 g, 0.28 mmol) was dissolved in CHCl_3 (150 mL) and CH_3OH (50 mL). $\text{Zn}(\text{CH}_3\text{COO})_2$ (0.25 g, 1.4 mmol) was added to the above solution and refluxed for two hours. Then it was washed by water, and the organic layer was evaporated to dryness under vacuum. The purple solid was obtained and purified by silica gel chromatography ($\text{CH}_2\text{Cl}_2:\text{CH}_3\text{OH}=50:1$) (0.411 g, yield 96%). ^1H NMR (400 MHz, $\text{DMSO}-d_6$): δ 8.74 (4H, d), 8.68 (4H, d), 8.60 (4H, d), 8.53 (4H, d), 8.16 (2H, d), 8.07 (8H, m), 7.89 (2H, d), 7.81 (11H, m), 7.70 (11H, m), 7.58 (2H, d), 7.44 (4H, d), 6.68 (1H, s), 5.10 (2H, s), -0.21 (3H, s). Anal. Calcd for $\text{C}_{97}\text{H}_{62}\text{N}_{10}\text{O}_2\text{Zn}_2\cdot\text{H}_2\text{O}$: C, 75.24; H, 4.17; N, 9.05. Found: C, 75.27; H, 4.15; N, 9.07. MS (ESI) m/z ($\text{C}_{97}\text{H}_{62}\text{N}_{10}\text{O}_2\text{Zn}_2$): Calc. $[\text{M}+\text{H}]^+$: 1531.36, Found $[\text{M}+\text{H}]^+$: 1531.25.

Preparation of copper bisporphyrinate [$\text{Cu}_2\text{-2}$]

The free base bisporphyrin **2** (0.394 g, 0.28 mmol) was dissolved in CHCl_3 (150 mL) and CH_3OH (50 mL). $\text{Cu}(\text{CH}_3\text{COO})_2$ (0.25 g, 1.4 mmol) was added to the above solution and refluxed for two hours. Then it was washed by water, and the organic layer was evaporated to dryness under the vacuum. The purple solid was obtained and purified by silica gel chromatography ($\text{CH}_2\text{Cl}_2:\text{CH}_3\text{OH}=50:1$) (0.402 g, yield 94%). Anal. Calcd for $\text{C}_{97}\text{H}_{62}\text{Cu}_2\text{N}_{10}\text{O}_2\cdot 2\text{H}_2\text{O}$: C, 74.55; H, 4.26; N, 8.96. Found: C, 74.53; H, 4.27; N, 8.99. MS (ESI) m/z $\text{C}_{97}\text{H}_{62}\text{Cu}_2\text{N}_{10}\text{O}_2$: Calc. $[\text{M}+\text{H}]^+$: 1527.37, Found $[\text{M}+\text{H}]^+$: 1527.33. [$\text{Cu}_2\text{-2}$] was dissolved in CH_2Cl_2 and transferred into 8 mm \times 250 mm glass tubes, and layered by *n*-hexane. X-ray quality crystals were obtained after two months.

Preparation of free base bisporphyrin 3

A solution of 5-tertiary butyl isophthalic acid (0.080 g, 0.36 mmol) in thionyl chloride (8 mL) was refluxed under nitrogen for four hours, followed by the removal of excess reagent under reduced pressure. The residual white solid was redissolved in CH_2Cl_2 (30 mL), and Et_3N (150 μL , 1.07 mmol) was added

to the above solution and stirred for 10 minutes in an ice bath. 5-(2-aminophenyl)-10,15,20-triphenyl-porphyrinate (0.50 g, 0.78 mmol) was added to the solution under nitrogen atmosphere overnight in an ice bath. Then the mixture was washed by water for three times, dried with Na₂SO₄, purified by silica gel chromatography (pure CH₂Cl₂) to give the pure product (0.271 g, yield 48%). ¹H NMR (400 MHz, CDCl₃): δ 8.82 (4H, d), 8.78 (4H, d), 8.64 (4H, d), 8.52 (4H, d), 8.27 (2H, d), 8.18 (4H, d), 8.07 (4H, d), 7.97 (6H, m), 7.74 (16H, m), 7.60 (4H, t), 7.44 (2H, t), 7.03 (2H, s), 6.27 (1H, s), 5.14 (2H, s), -1.86 (9H, s), -2.93 (4H, s). Anal. Calcd for C₁₀₀H₇₂N₁₀O₂: C, 83.08; H, 5.02; N, 9.69. Found: C, 83.07; H, 4.99; N, 9.71. MS (ESI) m/z (C₁₀₀H₇₂N₁₀O₂): Calc. [M+H]⁺: 1446.59, Found [M+H]⁺: 1446.92.

Preparation of zinc bisporphyrinate [Zn₂-3]

The free base bisporphyrin **3** (0.271 g, 0.19 mmol) was dissolved in CHCl₃ (150 mL) and CH₃OH (50 mL). Zn(CH₃COO)₂ (0.25 g, 1.4 mmol) was added to the above solution and refluxed for two hours. Then it was washed by water, and the organic layer was evaporated to dryness under vacuum. The purple solid was obtained and purified by silica gel chromatography (CH₂Cl₂:CH₃OH=50:1) (0.284 g, yield 95%). ¹H NMR (400 MHz, CDCl₃): δ 8.98 (4H, d), 8.93 (4H, d), 8.72 (4H, d), 8.49 (4H, d), 8.26 (2H, s), 8.13 (6H, m), 7.99 (2H, d), 7.92 (4H, d), 7.74 (14H, m), 7.57 (6H, d), 7.45 (2H, t), 7.08 (2H, d), 6.94 (2H, s), 5.25 (2H, s), 3.89 (1H, s), -1.48 (9H, s). Anal. Calcd for C₁₀₀H₆₈N₁₀O₂Zn₂·2H₂O: C, 74.67; H, 4.51; N, 8.71. Found: C, 74.65; H, 4.49; N, 8.74. MS (ESI) m/z (C₁₀₀H₆₈N₁₀O₂Zn₂): Calc. [M+H]⁺: 1573.41, Found [M+H]⁺: 1573.58. [Zn₂-3] was dissolved in CH₂Cl₂ and transferred into 8 mm×250 mm glass tubes, layered by *n*-heptane. X-ray quality crystals were obtained after three weeks.

X-ray structure determination

The measurements of a single crystal of [Cu₂-**2**] were made on Agilent Xcalibur diffractometer with an Atlas (Gemini Ultra Cu) detector by using graphite monochromated Cu Ka ($\lambda=0.154178$ nm) at 220(2) K. The measurements of a single crystal of [Zn₂-**3**] were made on a Bruker APEX-II CCD X-ray diffractometer by using graphite monochromated Mo Ka ($\lambda=0.071073$ nm) at 220(2) K. Both structures were solved by direct methods and refined on F^2 using full matrix least-squares methods with SHELXTL version 97.² All non-hydrogen atoms were refined anisotropically. In the asymmetric unit, all the hydrogen atoms were theoretically added and riding on their parent atoms. Complete crystallographic details, atomic coordinates, anisotropic thermal parameters, and fixed hydrogen atom coordinates are given in the CIF file. For [Cu₂-**2**], the asymmetric unit contains a half molecule of compound **2** and badly disorder solvent molecules. While SQUEEZE³ was used to model all disordered solvate. Electron counts within the interporphyrin voids of 399 e (corresponding to roughly to 2 molecules of CH₂Cl₂ and 2 molecules of H₂O per compound **2**). One phenyl ring was found disordered over two positions. The final refinement gave the occupancy of the major component of 60%. For [Zn₂-**3**], the asymmetric unit contains two molecules of compound **3** and badly disorder solvent molecules. While SQUEEZE¹² was used to model all disordered solvate. Electron counts within the interporphyrin voids of 1831 e (corresponding to roughly to 3 molecules of CH₂Cl₂ and 2 molecules of C₇H₁₆ per compound **3**). Details of the crystal parameters, data collection, and refinements are summarized in Table S1.

Computation methods.

Firstly, we performed DFT calculations on the free host [Zn₂-**1**] based on the crystal structure of [Zn₂-**1**]. Due to the asymmetric arrangement, the host molecules exist as a pair of enantiomers, conformers I and II as shown in Fig. S31. Then we did calculations on the corresponding host-guest complexes

formed between [Zn₂-1] (both conformers I and II) and chiral monoamine **1S** or **5S**.

Full optimizations on all conformations of possible complexes studied were performed at the semi-empirical Parameterized Model (PM6) with Gaussian09 programs.⁴ Some relatively stable minima's by PM6 were then subjected to geometry optimization at the B3LYP/6-31G* (gas phase) level of theory. The local minima with lowest energy at the level of B3LYP/6-31G* are reported in the current communication. We employed the density functional theory (DFT) with no symmetry constraints to investigate the optimized geometries. To confirm that each structure was a true minimum, vibrational analyses were performed.

References

- (1) J. Jiang, X. Fang, B. Liu and C. Hu, *Inorg. Chem.* 2014, **53**, 3298
- (2) G. M. Sheldrick, *Acta Crystallogr. Sect.A* 2008, **64**, 112.
- (3) A. L. Spek, *J. Appl. Crystallogr.* 2003, **36**, 7.
- (4) M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian 09, Revision C.01, Gaussian, Inc., Wallingford CT, 2010.

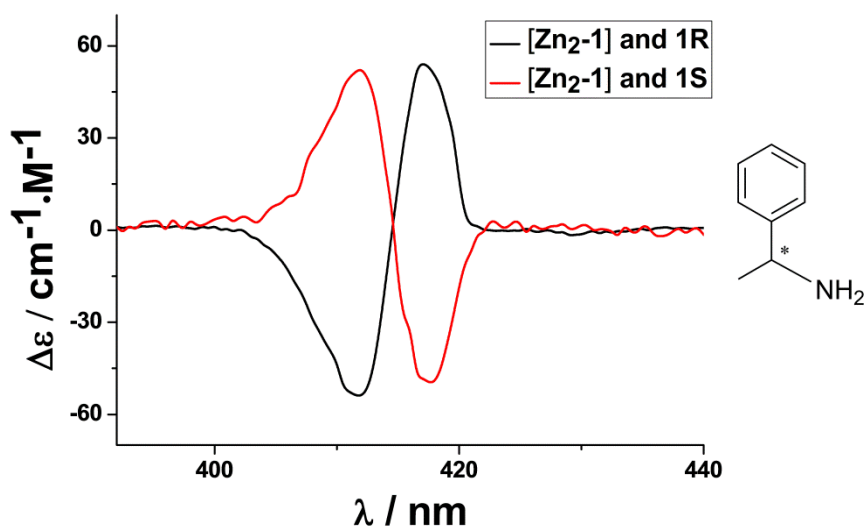


Fig. S1. Circular dichroism spectra of a solution of [Zn₂-1] (1.63×10^{-6} M) and 1500 equivalents of **1R** (black) and **1S** (red) in CH₂Cl₂ at 295 K

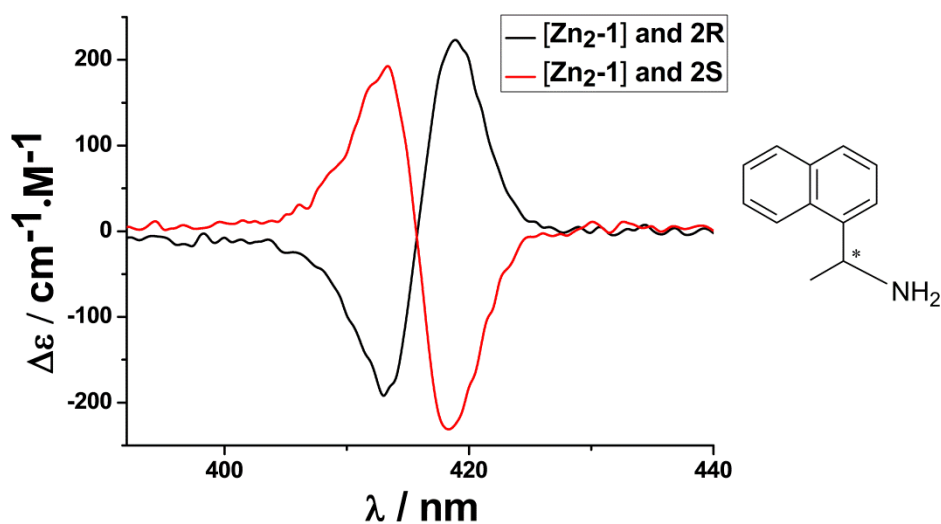


Fig. S2. Circular dichroism spectra of a solution of [Zn₂-1] (1.63×10^{-6} M) and 1500 equivalents of **2R** (black) and **2S** (red) in CH₂Cl₂ at 295 K

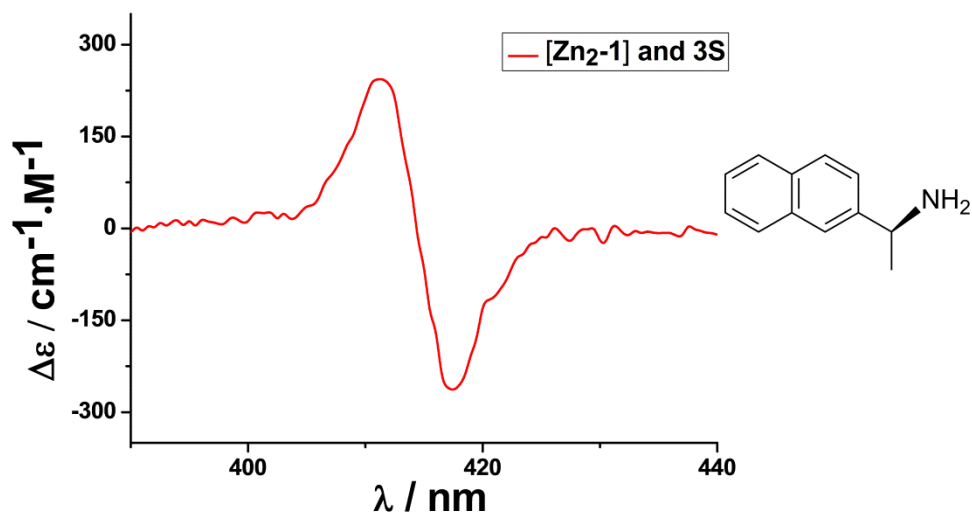


Fig. S3. Circular dichroism spectrum of a solution of $[Zn_2-1]$ (1.63×10^{-6} M) and 1500 equivalents of **3S** in CH_2Cl_2 at 295 K

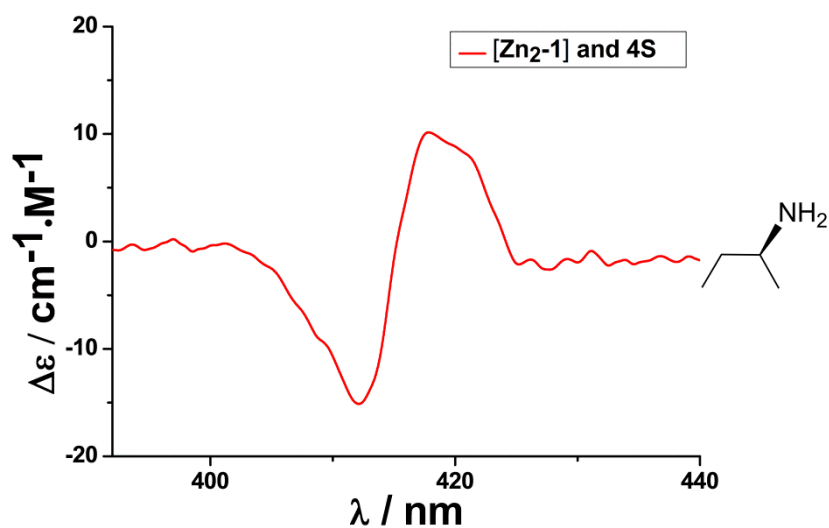


Fig. S4. Circular dichroism spectrum of a solution of $[Zn_2-1]$ (1.63×10^{-6} M) and 1500 equivalents of **4S** in CH_2Cl_2 at 295 K

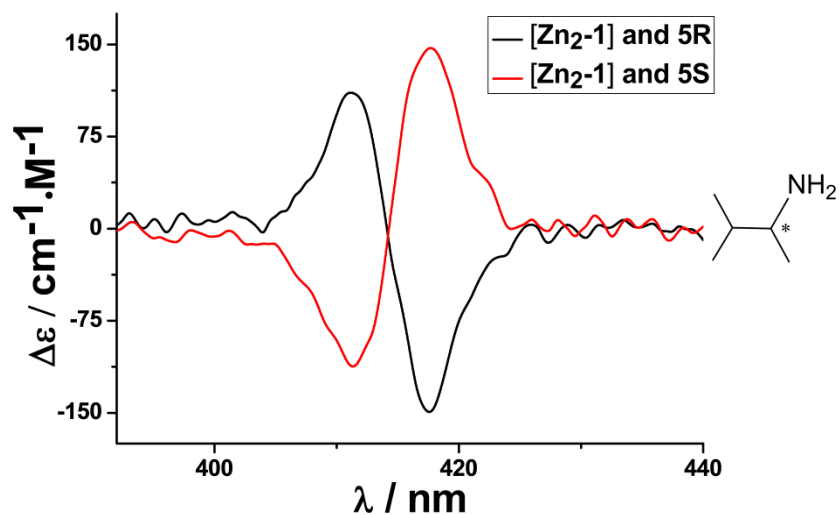


Fig. S5. Circular dichroism spectra of a solution of [Zn₂-1] (1.63×10^{-6} M) and 1500 equivalents of **5R** (black) and **5S** (red) in CH₂Cl₂ at 295 K

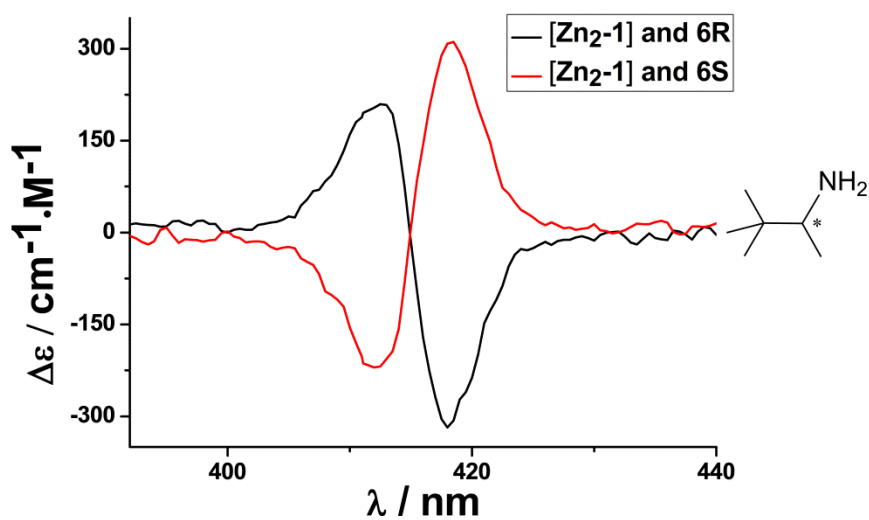


Fig. S6. Circular dichroism spectra of a solution of [Zn₂-1] (1.63×10^{-6} M) and 1500 equivalents of **6R** (black) and **6S** (red) in CH₂Cl₂ at 295 K

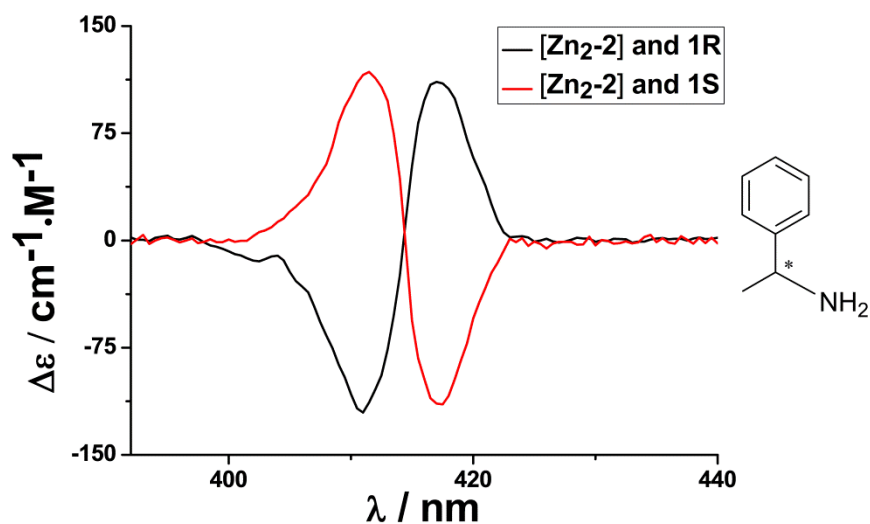


Fig. S7. Circular dichroism spectra of a solution of [Zn₂-2] (1.61×10^{-6} M) and 1500 equivalents of **1R** (black) and **1S** (red) in CH₂Cl₂ at 295 K.

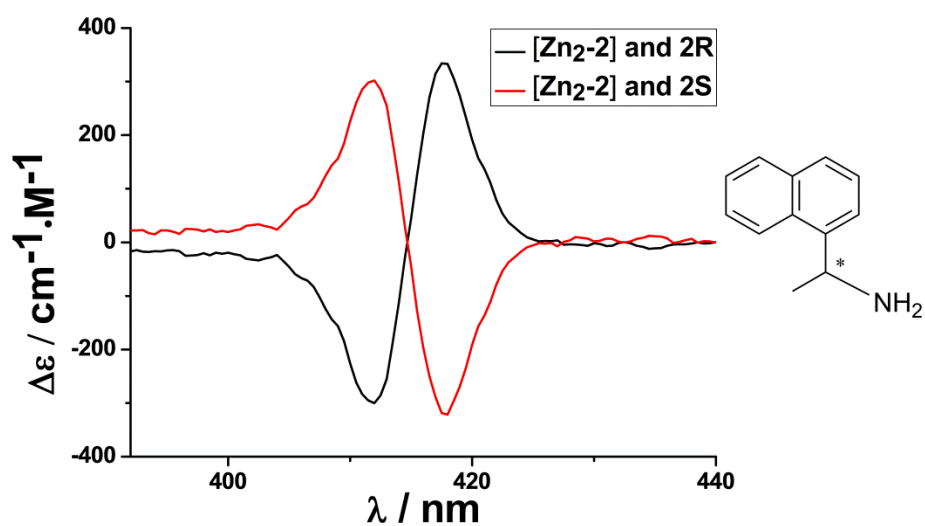


Fig. S8. Circular dichroism spectra of a solution of [Zn₂-2] (1.61×10^{-6} M) and 1500 equivalents of **2R** (black) and **2S** (red) in CH₂Cl₂ at 295 K.

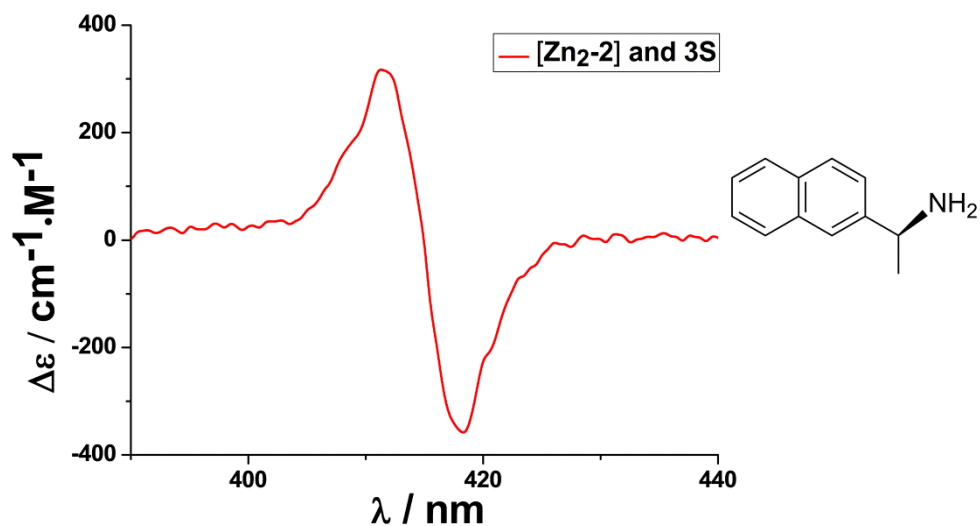


Fig. S9. Circular dichroism spectrum of a solution of $[Zn_2-2]$ (1.61×10^{-6} M) and 1500 equivalents of **3S** in CH_2Cl_2 at 295 K.

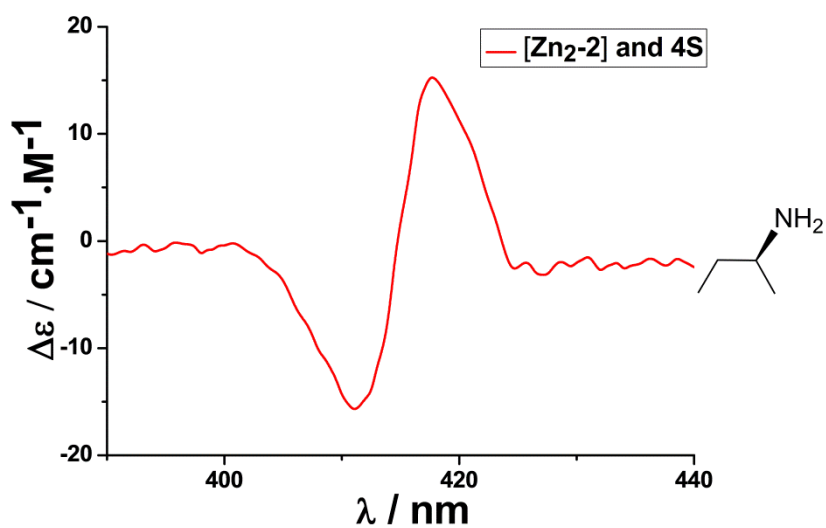


Fig. S10. Circular dichroism spectrum of a solution of $[Zn_2-2]$ (1.61×10^{-6} M) and 1500 equivalents of **4S** in CH_2Cl_2 at 295 K.

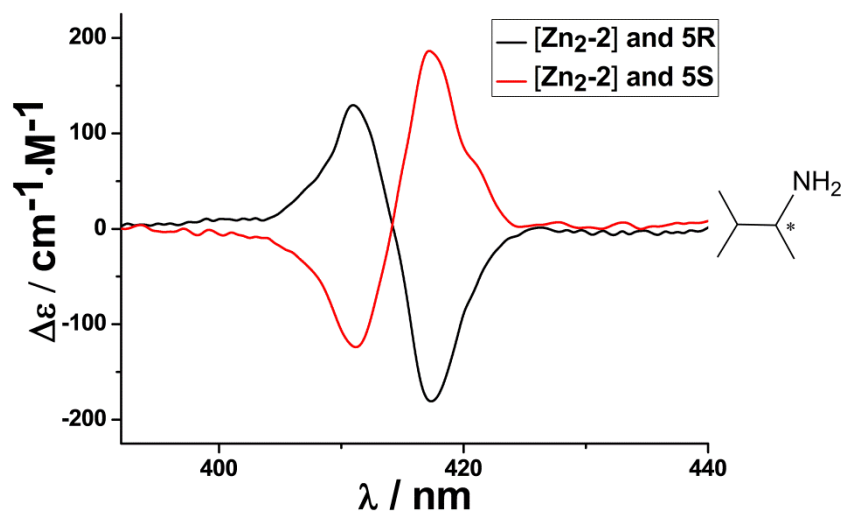


Fig. S11. Circular dichroism spectra of a solution of [Zn₂-2] (1.61×10^{-6} M) and 1500 equivalents of **5R** (black) and **5S** (red) in CH₂Cl₂ at 295 K.

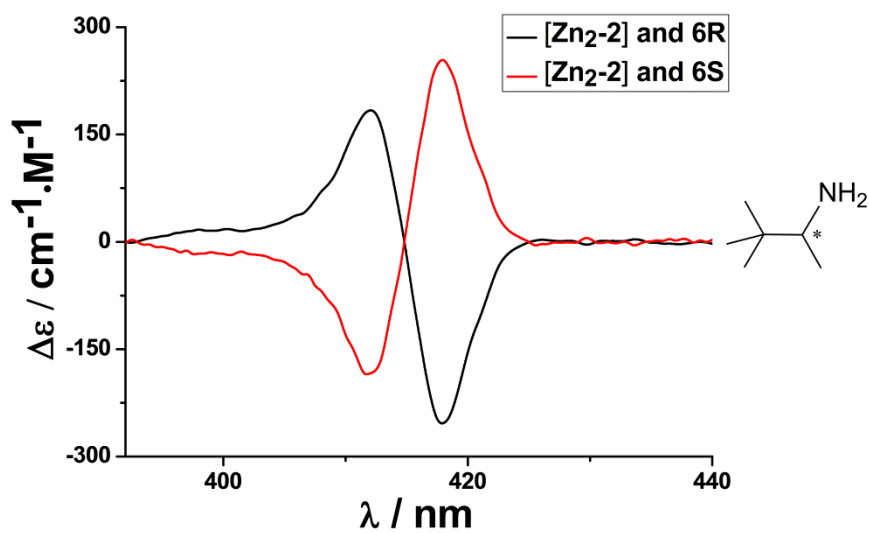


Fig. S12. Circular dichroism spectra of a solution of [Zn₂-2] (1.61×10^{-6} M) and 1500 equivalents of **6R** (black) and **6S** (red) in CH₂Cl₂ at 295 K.

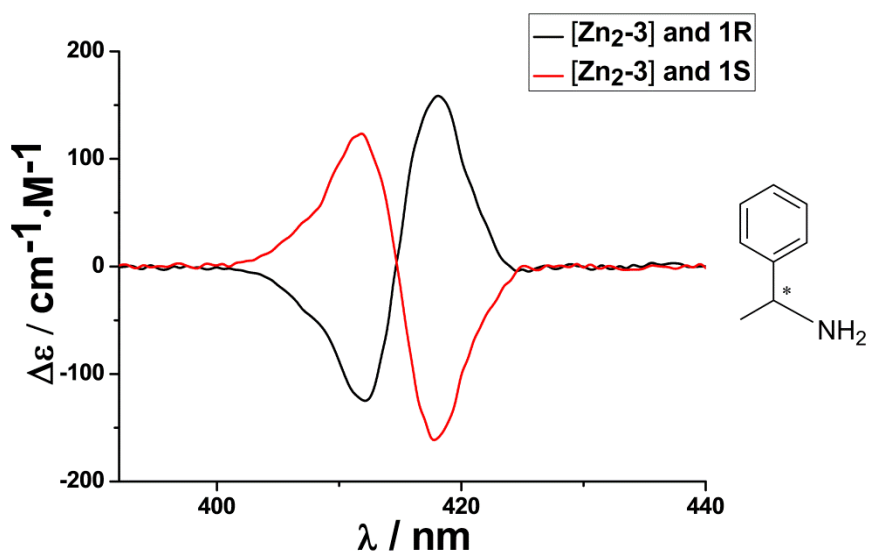


Fig. S13. Circular dichroism spectra of a solution of [Zn₂-3] (1.57×10^{-6} M) and 1500 equivalents of **1R** (black) and **1S** (red) in CH₂Cl₂ at 295 K.

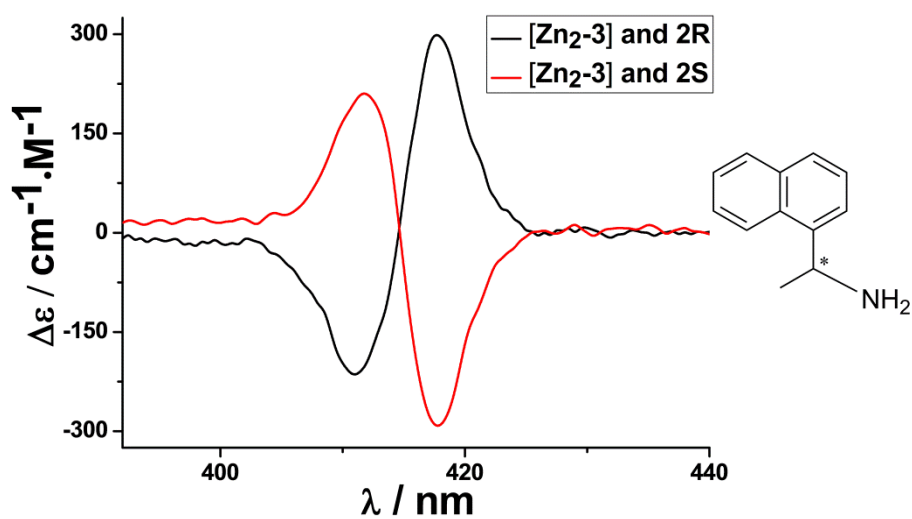


Fig. S14. Circular dichroism spectra of a solution of [Zn₂-3] (1.57×10^{-6} M) and 1500 equivalents of **2R** (black) and **2S** (red) in CH₂Cl₂ at 295 K.

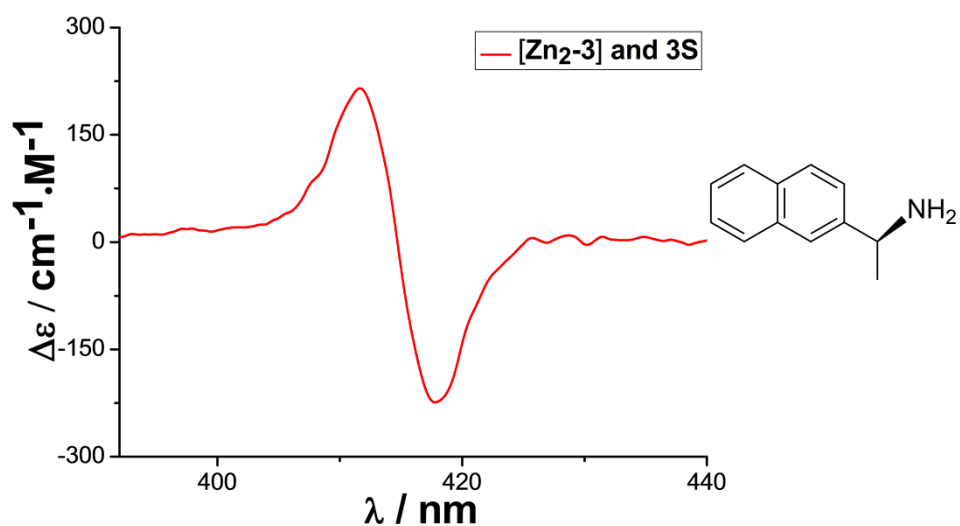


Fig. S15. Circular dichroism spectrum of a solution of $[Zn_2-3]$ (1.57×10^{-6} M) and 1500 equivalents of **3S** in CH_2Cl_2 at 295 K.

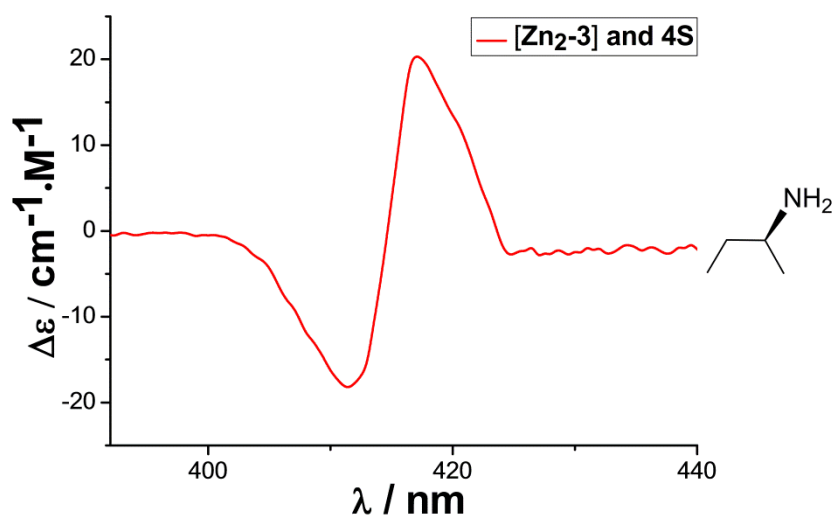


Fig. S16. Circular dichroism spectrum of a solution of $[Zn_2-3]$ (1.57×10^{-6} M) and 1500 equivalents of **4S** in CH_2Cl_2 at 295 K.

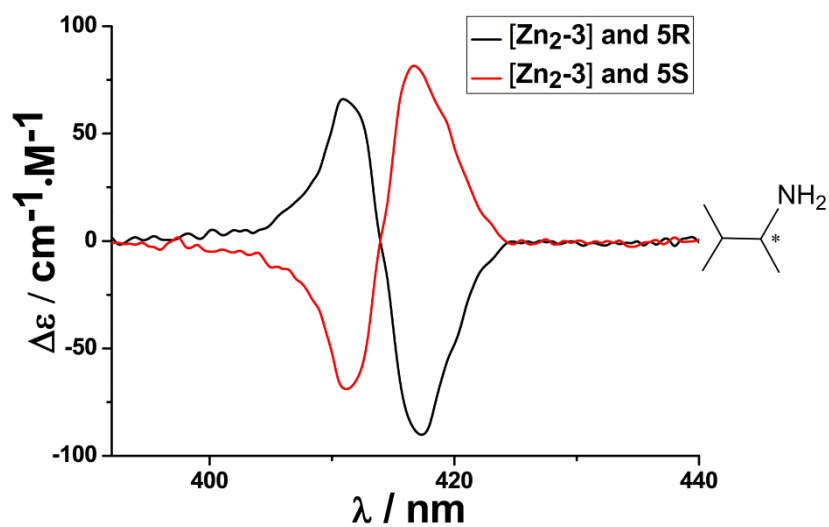


Fig. S17. Circular dichroism spectra of a solution of [Zn₂-3] (1.57×10^{-6} M) and 1500 equivalents of **5R** (black) and **5S** (red) in CH₂Cl₂ at 295 K.

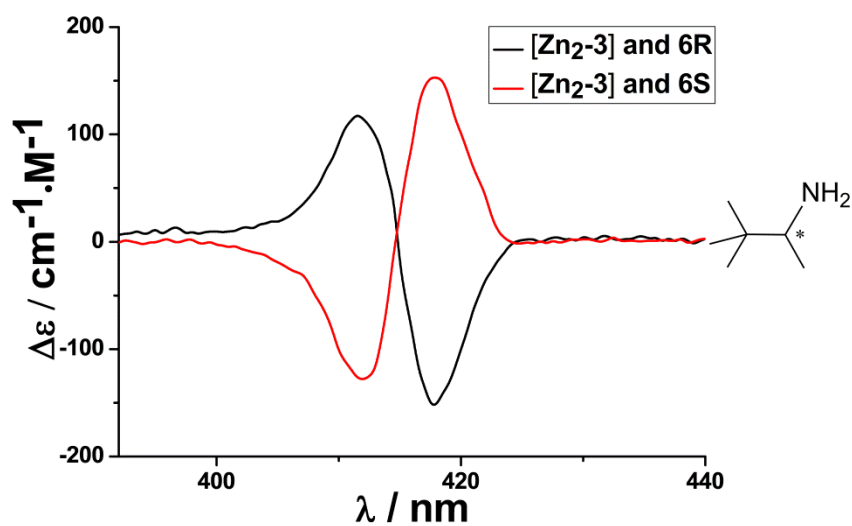


Fig. S18. Circular dichroism spectra of a solution of [Zn₂-3] (1.57×10^{-6} M) and 1500 equivalents of **6R** (black) and **6S** (red) in CH₂Cl₂ at 295 K.

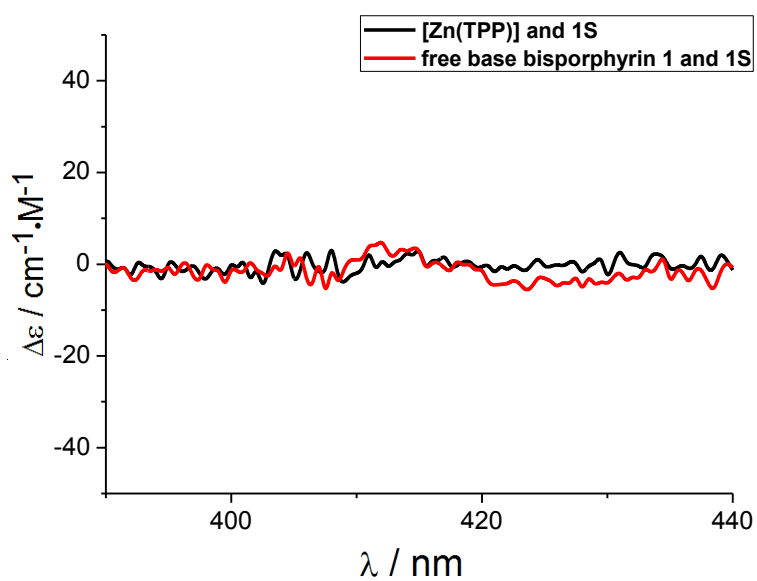


Fig. S19. Circular dichroism spectrum of a solution of [Zn(TPP)] (1.42×10^{-6} M) and 1500 equivalents of **1S** in CH_2Cl_2 at 295 K.(black). Circular dichroism spectrum of a solution of free base bisporphyrin **1**(1.35×10^{-6} M) and 1500 equivalents of **1S** in CH_2Cl_2 at 295 K.(red).

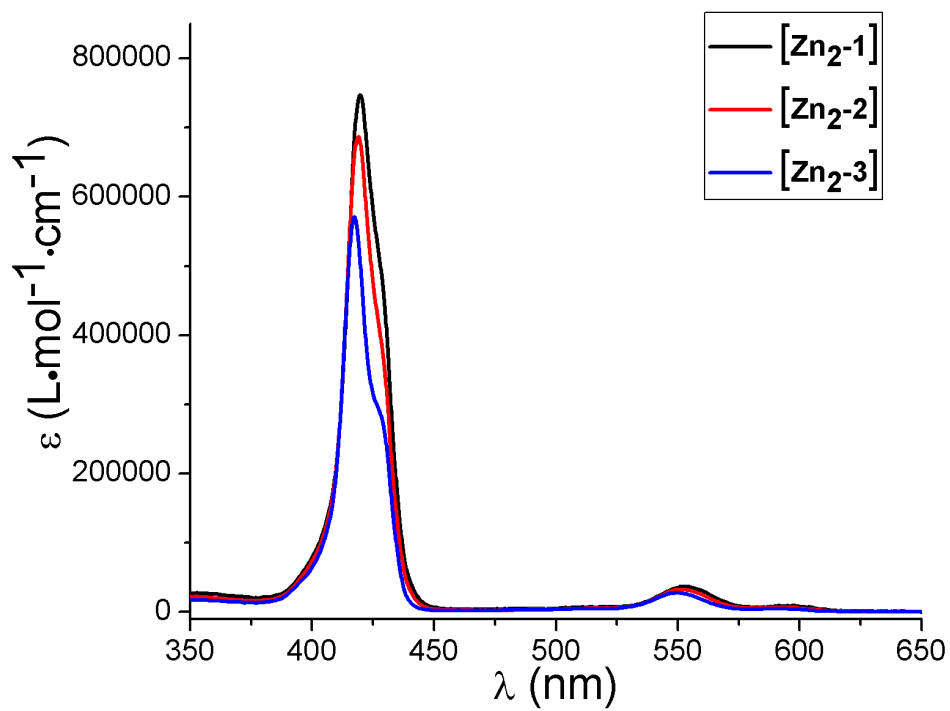


Fig. S20. The UV-vis spectra of [Zn₂-1] (1.63×10^{-6} M), [Zn₂-2] (1.61×10^{-6} M), [Zn₂-3] (1.57×10^{-6} M) in methylene dichloride.

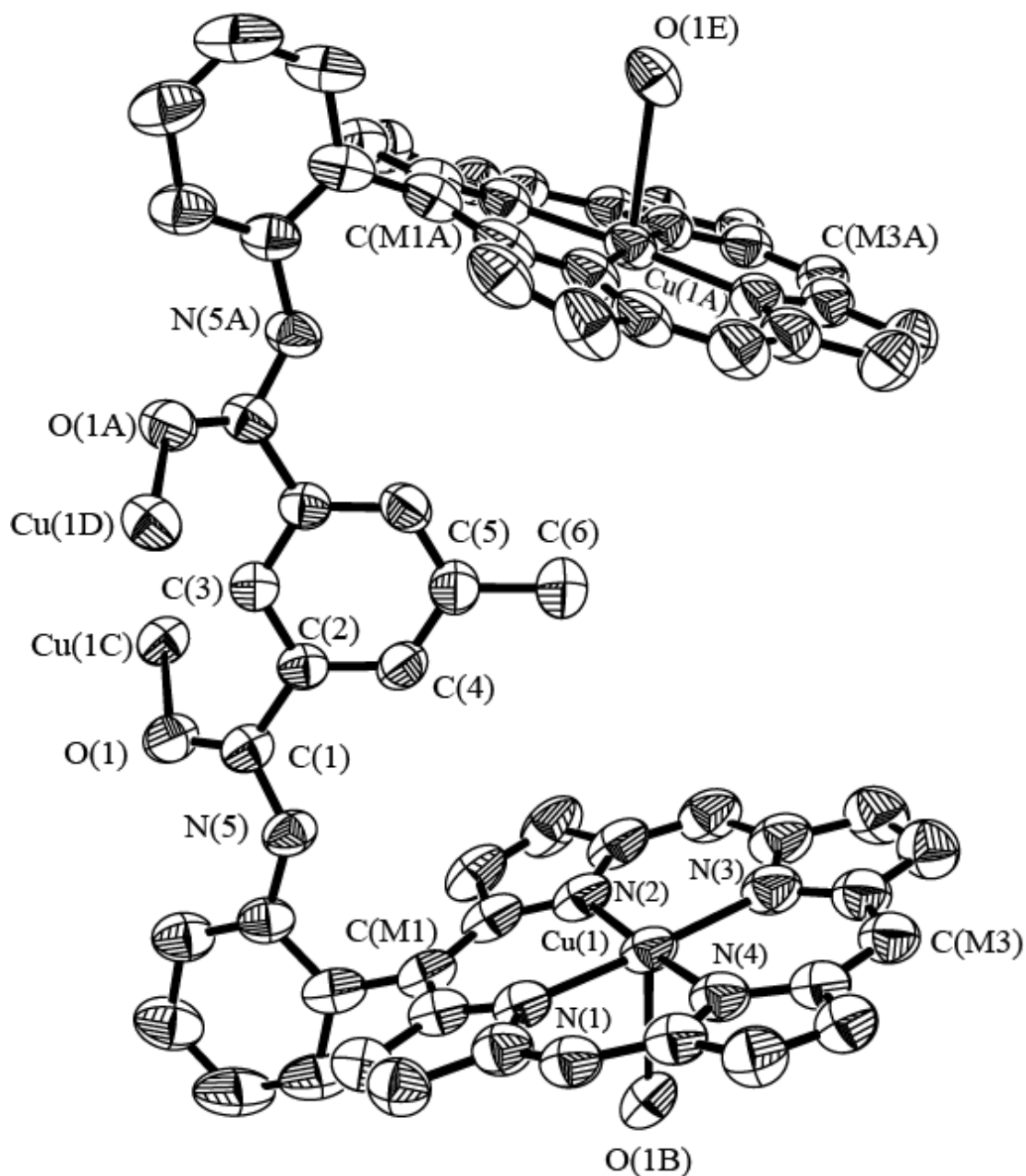


Fig. S21. ORTEP diagram of $[\text{Cu}_2\text{-2}]$. 50% probability ellipsoids are depicted. $\text{Cu}(1)\text{-O}(1\text{B})=2.653(3)$ Å, $\text{Cu}(1)\text{-N}(1)=1.995(2)$ Å, $\text{Cu}(1)\text{-N}(2)=2.006(3)$ Å, $\text{Cu}(1)\text{-N}(3)=2.014(3)$ Å, $\text{Cu}(1)\text{-N}(4)=2.012(3)$ Å. (symmetry code A: $1-X, -Y, Z$, B: $1/2+Y, 1-X, -1/4+Z$, C: $1-Y, -1/2+X, 1/4+z$, D: $Y, 1/2-X, 1/4+Z$, E: $1/2-Y, -1+X, -1/4+Z$). Some phenyl groups at *meso*-positions and all hydrogen atoms are omitted for clarity.

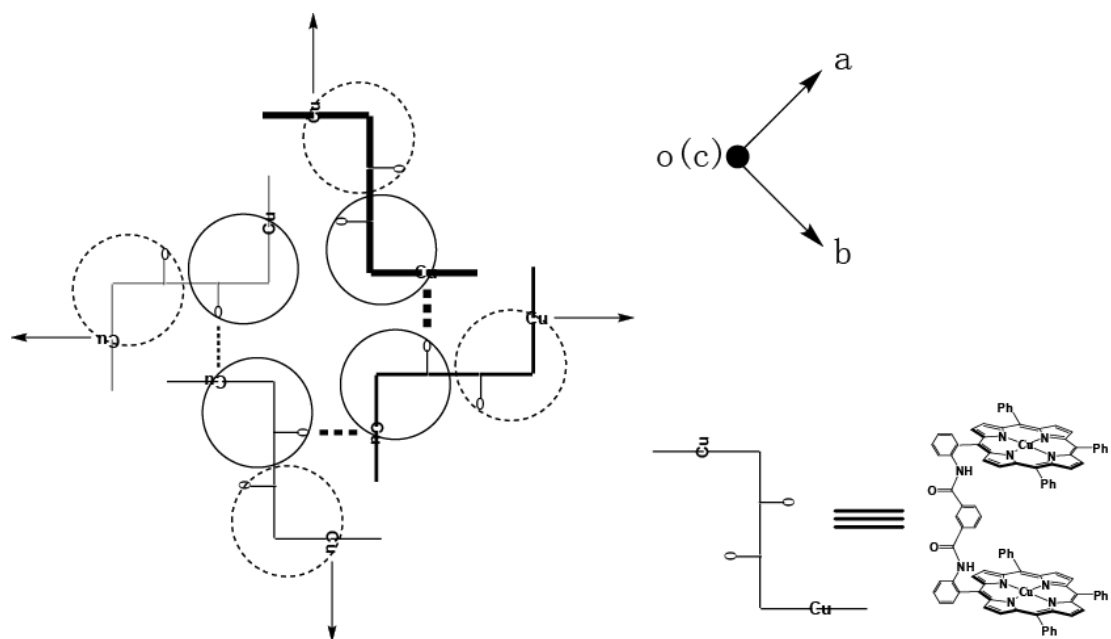


Fig. S22. Illustration of the packing structure of $[\text{Cu}_2\text{-2}]$ in the solid state with cell axes labeled. The unit in thicker lines is facing the reader, and the unit in narrower lines is away from the reader.

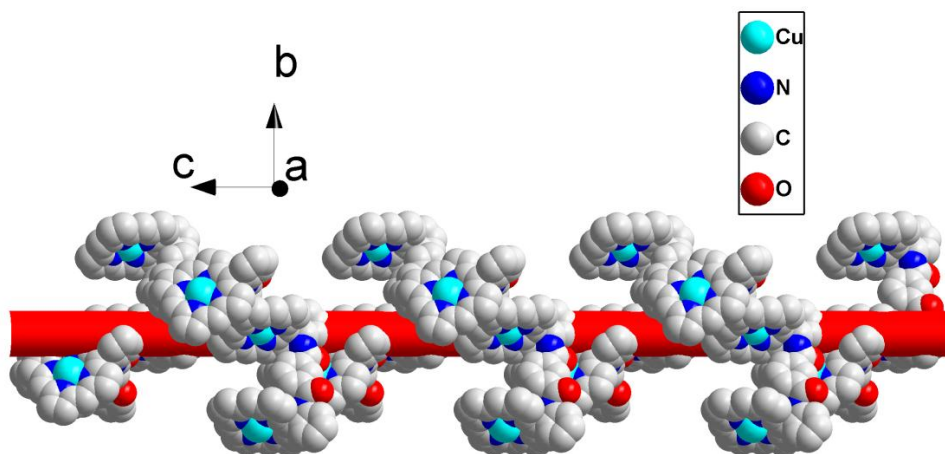


Fig. S23. The space-filling representation of the helical chain with P configuration of $[\text{Cu}_2\text{-2}]$ formed by Cu-O coordination bonds along c axis.

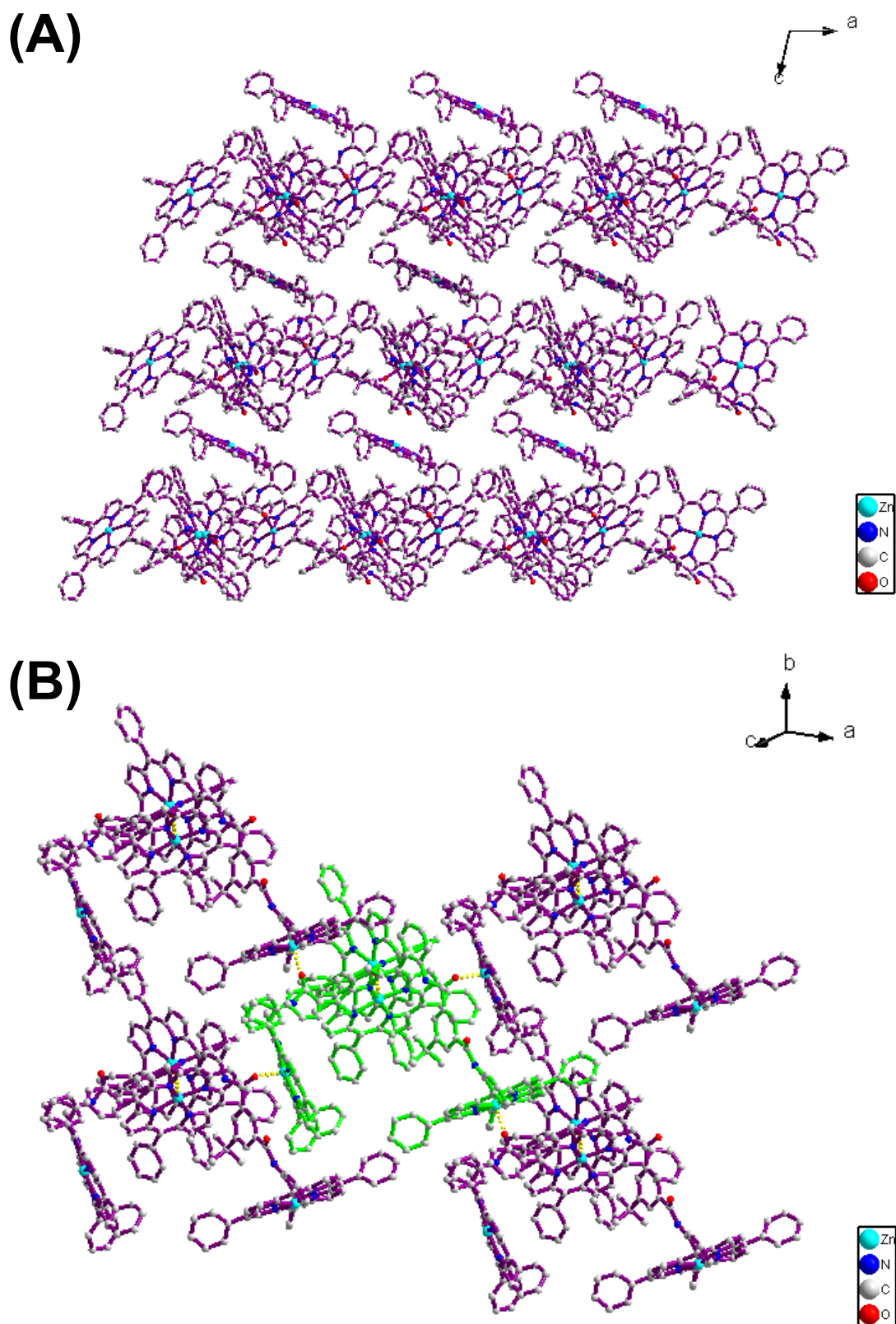


Fig. S24. Diagram illustrating the packing of [Zn₂-3] in the unit cell (H-atoms and the uncoordinated solvent molecules present in crystal lattice have been omitted for clarity). (A) view along *b* axis, (B) view along another orientation showing the two dimensional binding network.

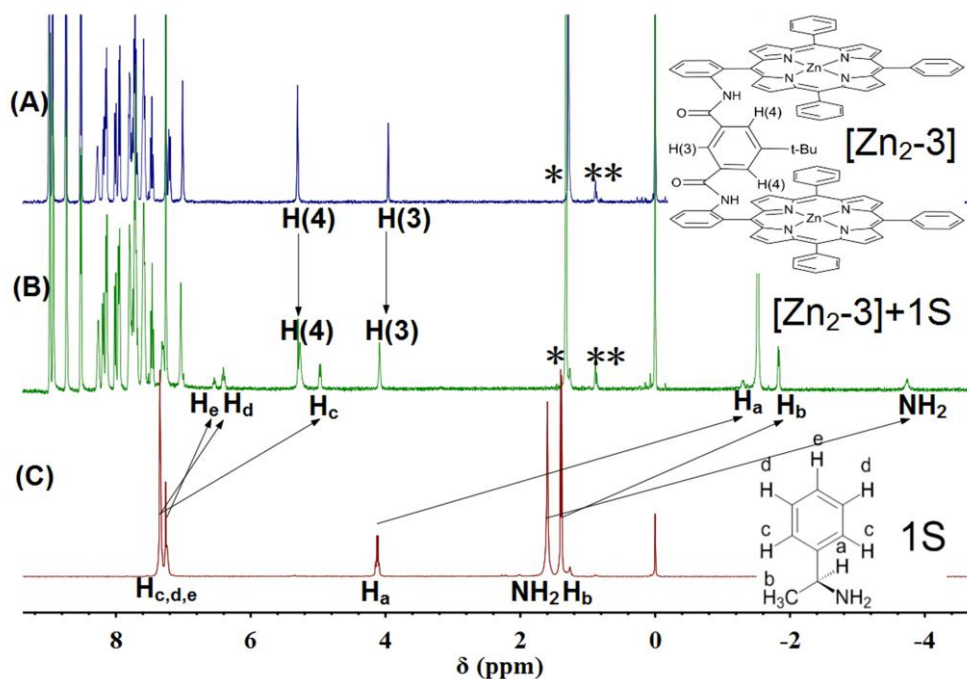


Fig. S25. ¹H NMR spectra in CDCl₃ (at 295 K) of (A) [Zn₂-3] (6.36 × 10⁻³ M), (B) the mixture of [Zn₂-3] (6.36 × 10⁻³ M) and 1S (0.5 eq.), (C) 1S. Inset shows the proton numbering scheme of [Zn₂-3] and 1S. *: Impurity from water; **: Impurity from petroleum ether.

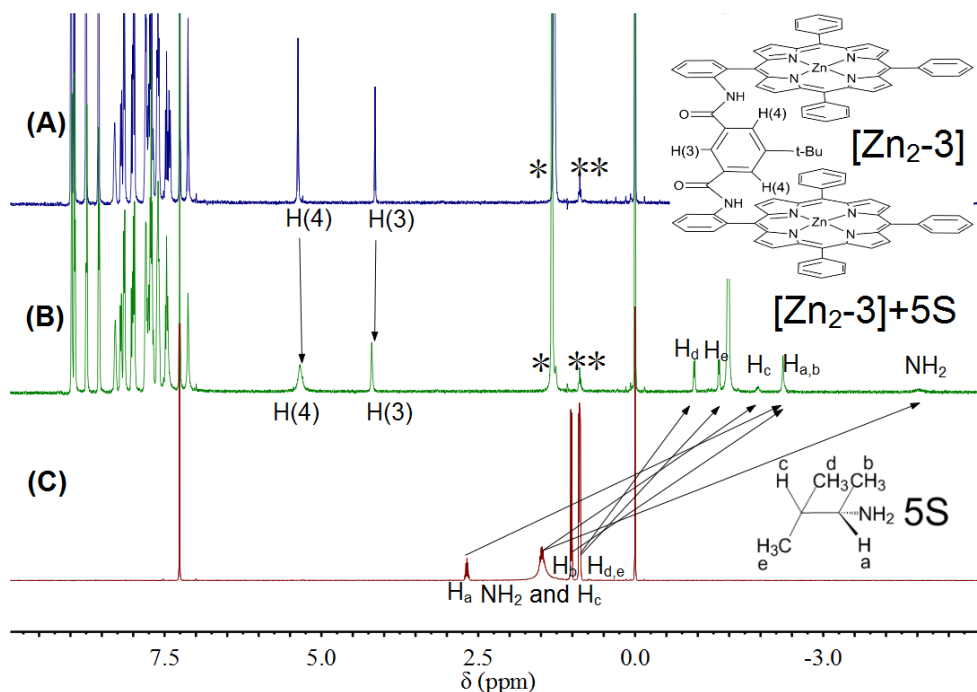


Fig. S26. ¹H NMR spectra in CDCl₃ (at 295 K) of (A) [Zn₂-3] (6.36 × 10⁻³ M), (B) the mixture of [Zn₂-3] (6.36 × 10⁻³ M) and 5S (0.5 eq.), (C) 5S. Inset shows the proton numbering scheme of [Zn₂-3] and 5S. *: Impurity from water; **: impurity from petroleum ether.

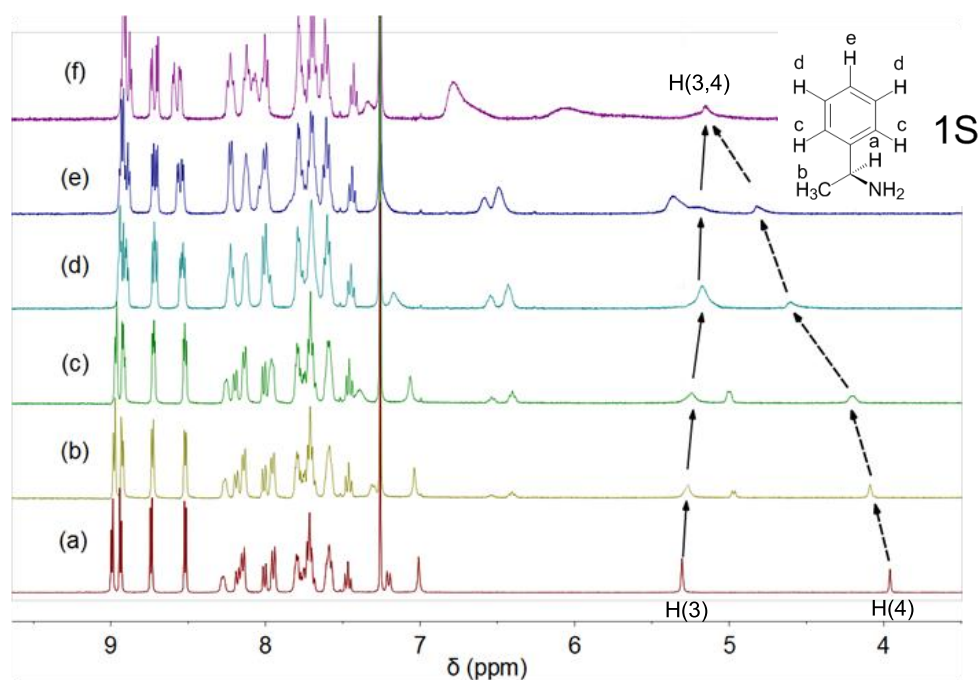


Fig. S27. ^1H NMR spectral changes of $[\text{Zn}_2\text{-3}]$ (6.36×10^{-3} M) upon addition of **1S** in CDCl_3 at 295 K as the host-guest molar ratio: (a) 1:0, (b) 1:0.26, (c) 1:0.52, (d) 1:0.78, (e) 1:1.12, (f) 1:1.53. Inset shows the proton numbering scheme of **1S**.

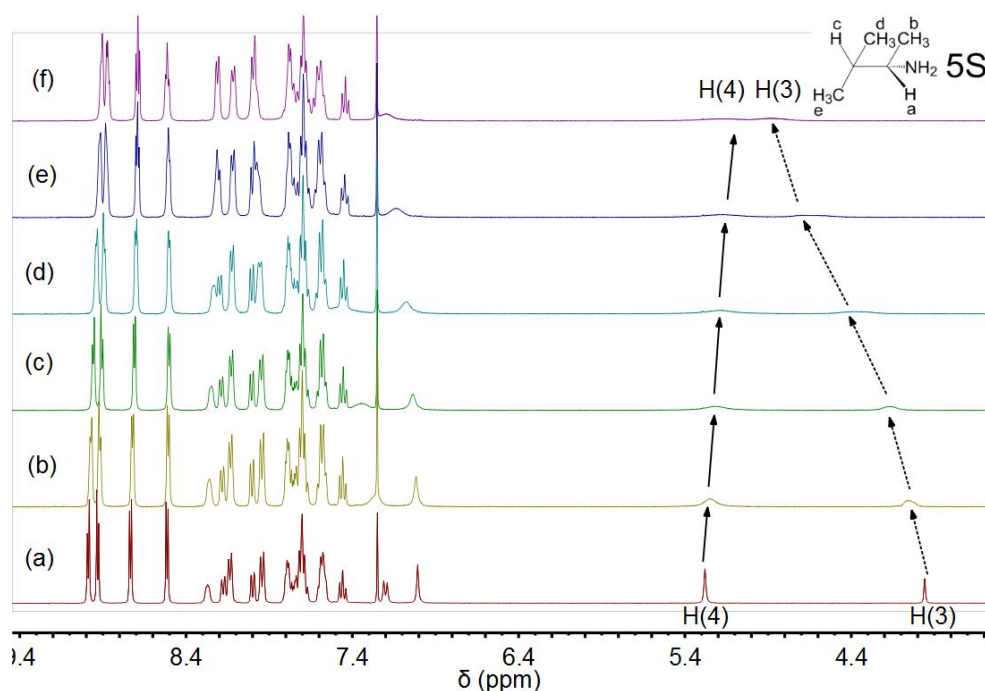


Fig. S28. ^1H NMR spectral changes of $[\text{Zn}_2\text{-3}]$ (6.36×10^{-3} M) upon addition of **5S** in CDCl_3 at 295 K as the host-guest molar ratio: (a) 1:0, (b) 1:0.26, (c) 1:0.52, (d) 1:0.78, (e) 1:1.12, (f) 1:1.53. Inset shows the proton numbering scheme of **5S**.

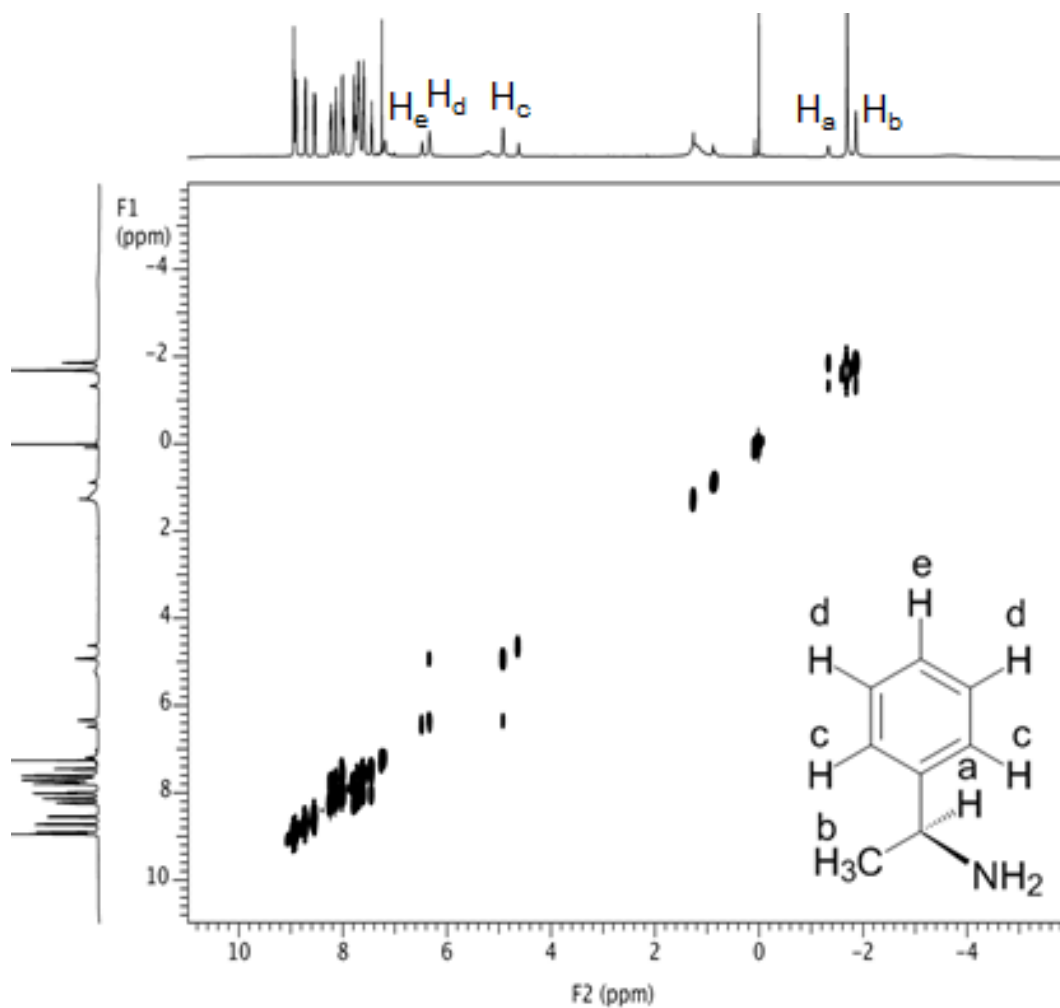


Fig. S29. ^1H - ^1H gCOSY spectrum of the mixture of $[\text{Zn}_2\text{-3}]$ (6.36×10^{-3} M) and **1S** (0.5 equiv) in CDCl_3 at 295K. Inset shows the proton numbering scheme of **1S**.

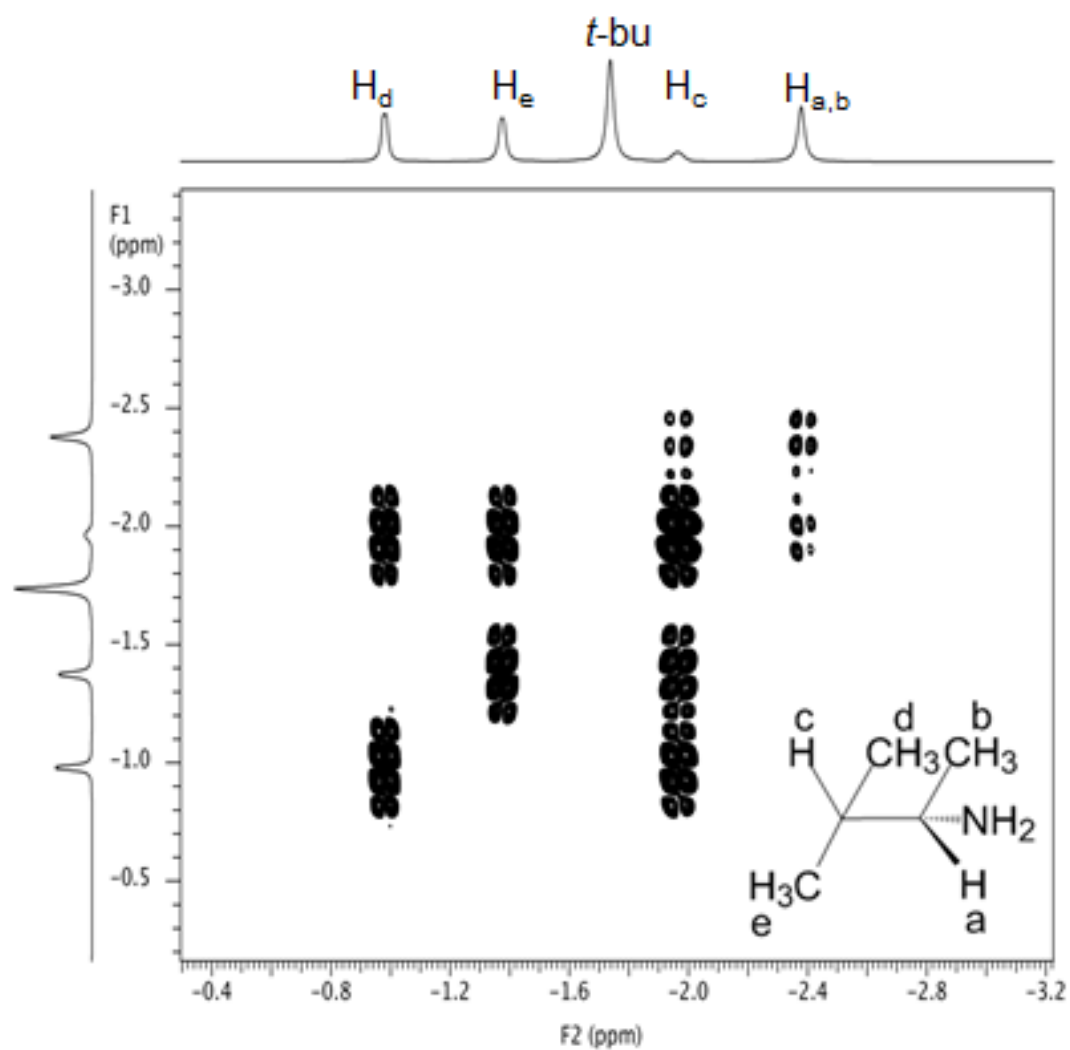


Fig. S30. ^1H - ^1H GDQCOSY spectrum of the mixture of $[\text{Zn}_2\text{-3}]$ (6.36×10^{-3} M) and **5S** (0.5 equiv) in CDCl_3 at 295K (selected proton only). Inset shows the proton numbering scheme of **5S**.

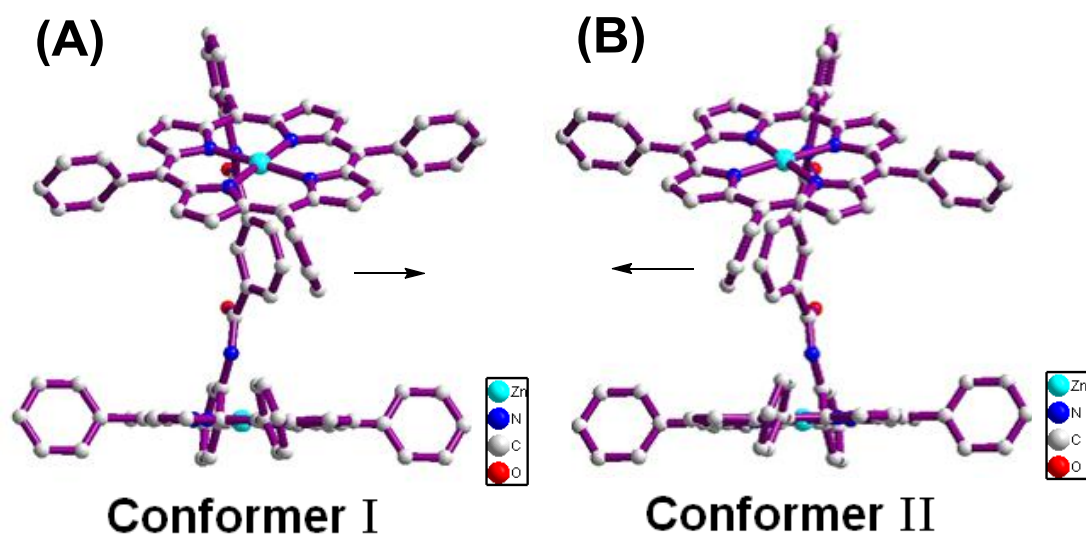


Fig. S31. DFT B3LYP/6-31G* optimized structure of [Zn₂-1]. It exists as a pair of enantiomers, named **Conformer I** and **Conformer II**. For clarity, the outside binding ligand, some phenyl rings at *meso*-positions and all hydrogen atoms are omitted.

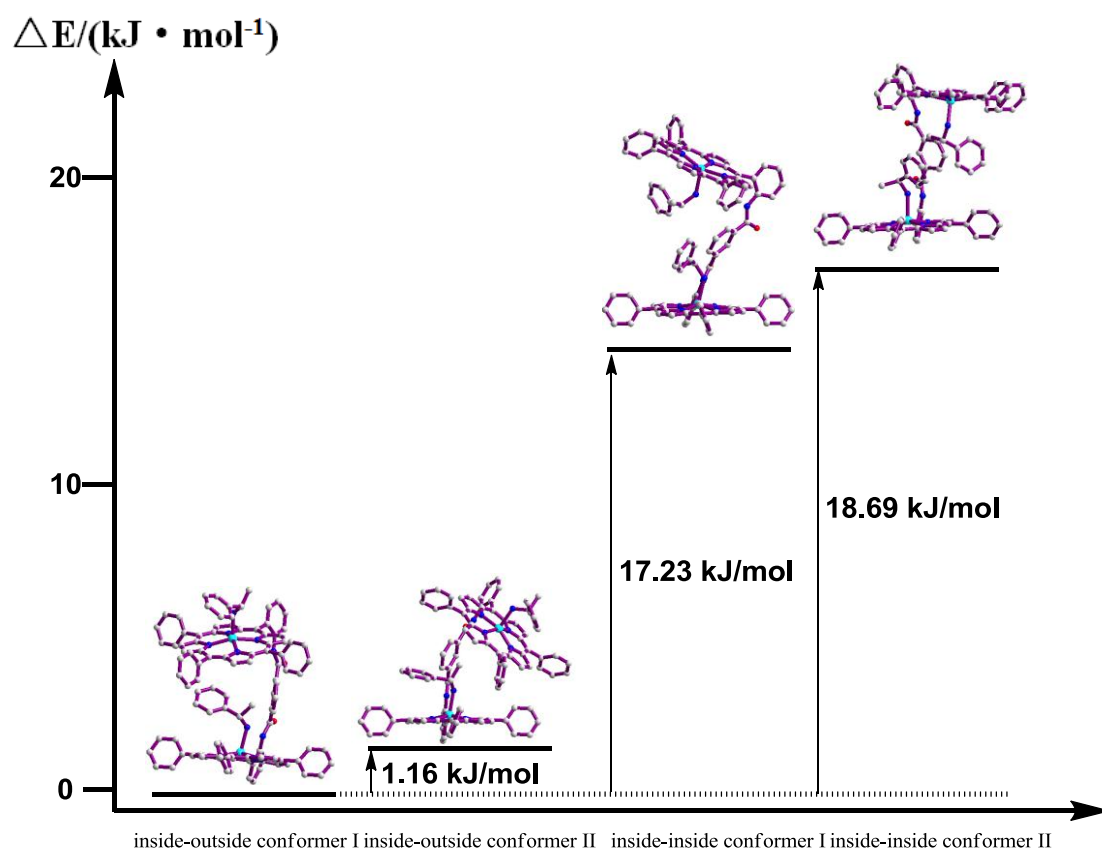


Fig. S32. Relative energies of DFT-optimized “inside-inside” and “inside-outside” conformers of $[Zn_2-1] \cdot 1S$.

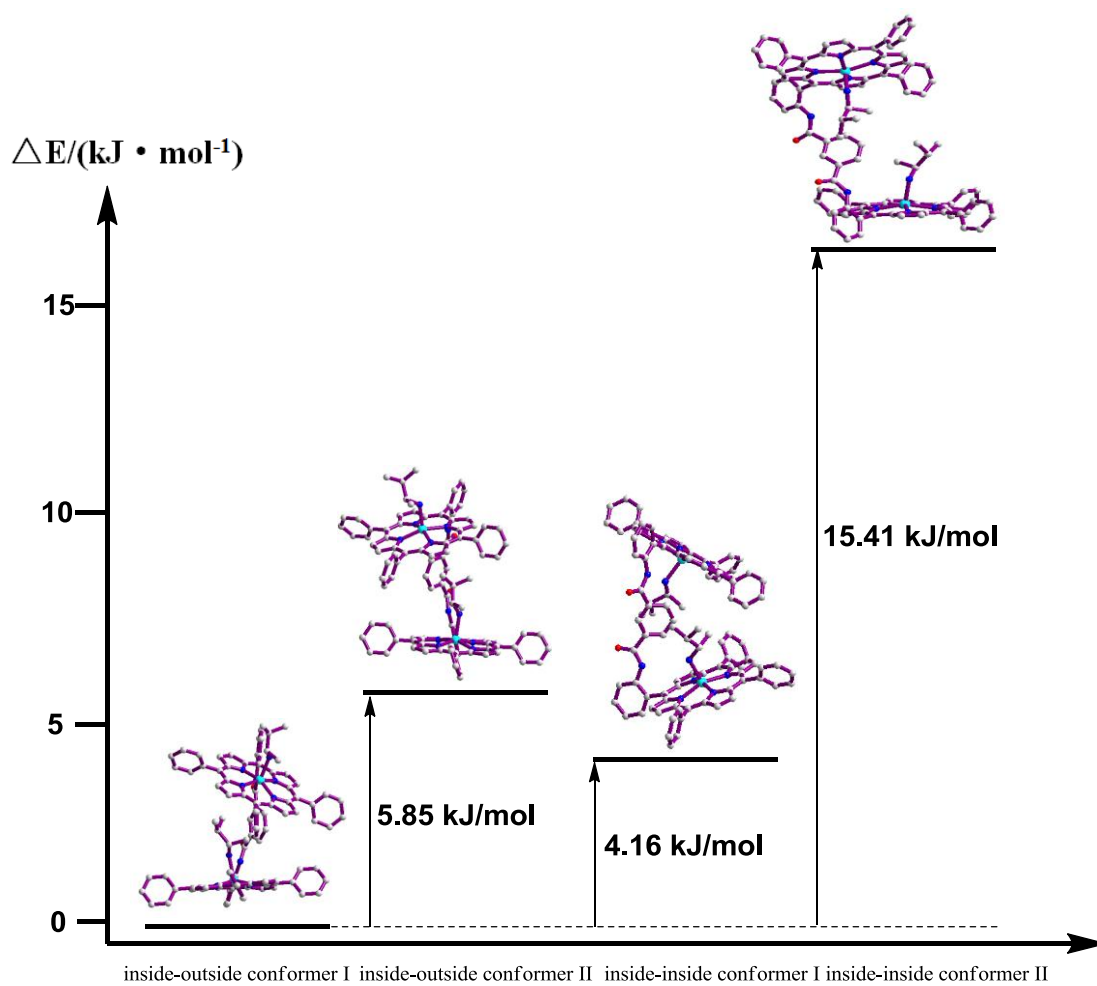


Fig. S33. Relative energies of DFT-optimized “inside-inside” and “inside-outside” conformers of $[Zn_2-1] \cdot 5S$.

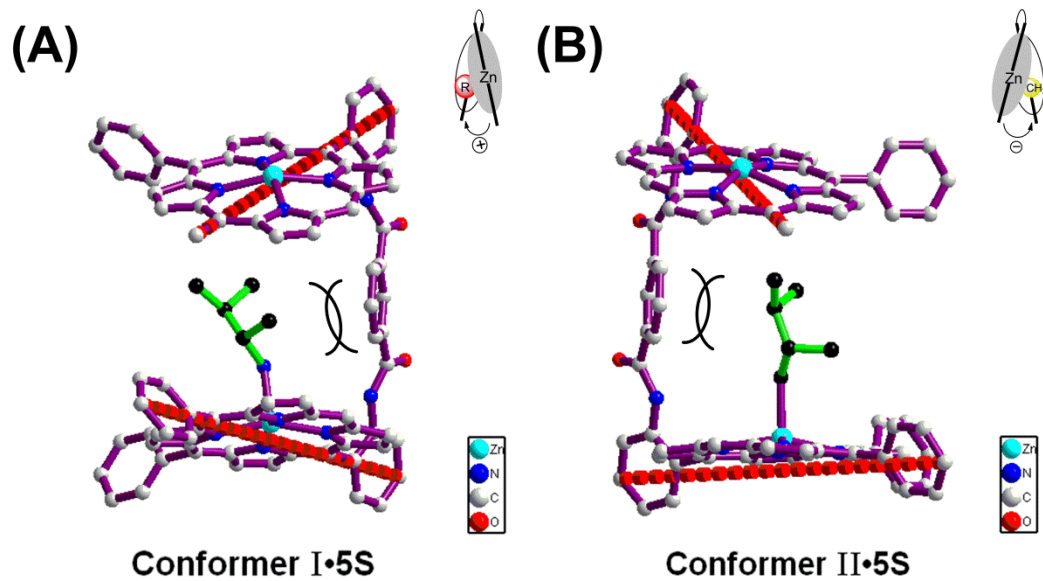


Fig. S34. DFT B3LYP/6-31G* optimized structures of the corresponding complex formed between [Zn₂-1] and **5S**: (A) **Conformer I·5S** and (B) **conformer II·5S**. For clarity, the outside binding ligand, some phenyl rings at *meso*-positions and most hydrogen atoms are omitted.

Table S1. Crystal data and structural refinements of [Cu₂-2] and [Zn₂-3]

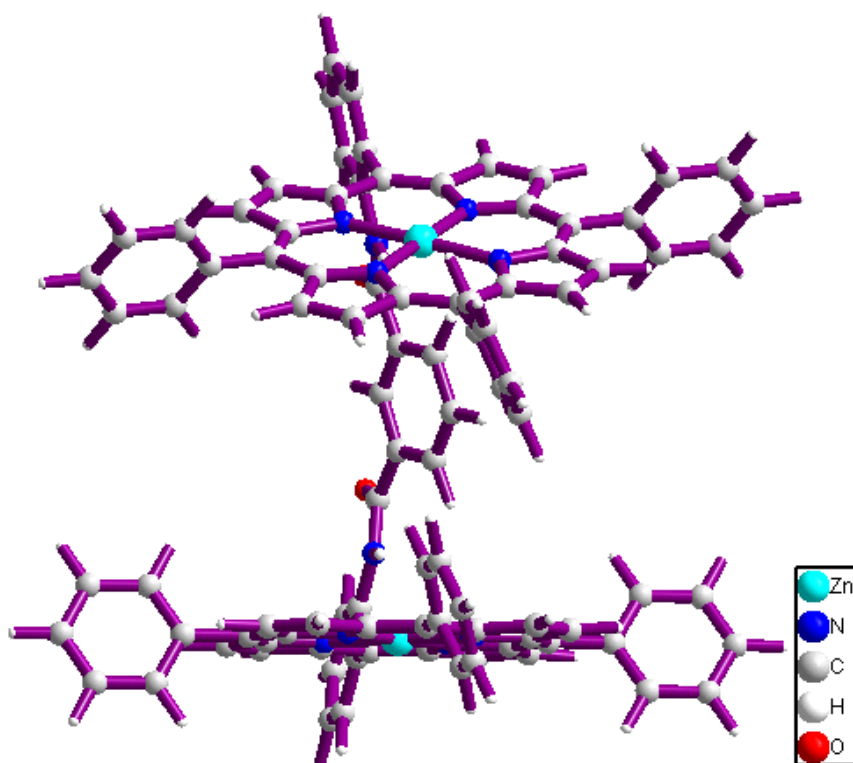
Crystal	[Cu ₂ -2]	[Zn ₂ -3]
Chemical formula	C ₉₇ H ₆₂ Cu ₂ N ₁₀ O ₂	C ₂₀₀ H ₁₃₆ N ₂₀ O ₄ Zn ₄
Formula weight	1526.65	3144.77
Wavelength (Å)	1.54178	0.71073
Temperature	220(2) K	220(2) K
Crystal system	Tetragonal	Monoclinic
Space group	<i>I</i> 4 ₁	C _c
a (Å)	17.8413(2)	31.160(3)
b (Å)	17.8413(2)	19.409(2)
c (Å)	27.0941(5)	32.877(4)
α (deg)	90	90
β (deg)	90	103.566(2)
γ (deg)	90	90
V (Å ³)	8624.4(2)	19329(4)
Z	4	4
Density (Mg/m ³)	1.176	1.081
Absorption coefficient (mm ⁻¹)	1.022	0.545
F(000)	3152	6512
Data collection θ range	2.97-73.44°	2.06-25.00°
Index ranges	-19<=h<=21, -21<=k<=21, -33<=l<=33	-37<=h<=37, -23<=k<=23, -38<=l<=38
Reflections collected	20873	127275
R _{int}	0.0447	0.0785
Independent reflections	8083	32530
Data / restraints / parameters	8083 / 109 / 527	32530 / 260 / 2024
GOF on F ²	1.034	1.049
R1 ^a [<i>I</i> > 2σ(<i>I</i>)]	0.0479	0.0940
wR2	0.1279	0.2260
Residual peak/hole (e/Å ⁻³)	0.339/-0.191	1.546/-0.989
Flack parameter	-0.01(2)	0.179(12)

$$^a R_1 = (F_0 - F_c) / F_0, wR2 = w(F_0^2 - F_c^2) / w(F_0^2)^{1/2}$$

Table S2. Selected bond distances for [Zn₂-3]

Zn(1)-N(11)	2.019(7) Å	Zn(2)-N(23)	2.027(7) Å	Zn(4)-N(41)	2.099(7) Å
Zn(1)-N(12)	2.080(6) Å	Zn(2)-N(24)	2.011(7) Å	Zn(4)-N(42)	2.034(6) Å
Zn(1)-N(13)	2.060(7) Å	Zn(3)-N(31)	2.064(7) Å	Zn(4)-N(43)	2.053(7) Å
Zn(1)-N(14)	2.052(7) Å	Zn(3)-N(32)	2.048(7) Å	Zn(4)-N(44)	2.048(7) Å
Zn(1)-O(601A)	2.143(6) Å	Zn(3)-N(33)	2.048(7) Å	Zn(4)-O(501B)	2.183(6) Å
Zn(2)-N(21)	2.050(6) Å	Zn(3)-N(34)	2.054(7) Å		
Zn(2)-N(22)	2.045(7) Å	Zn(3)-O(502)	2.166(5) Å		

symmetry code A: -1+X, -1-Y, 1/2+Z, B: X, -1-Y, 1/2+Z, C: -1+X, -Y, 1/2+Z, D:
1/2+X, 1/2+Y, Z



Conformer I

$$\Delta H^\circ = -7950.83352331 \text{ hartree}$$

Cartesian coordinates for Geometry Optimized **Conformer I**

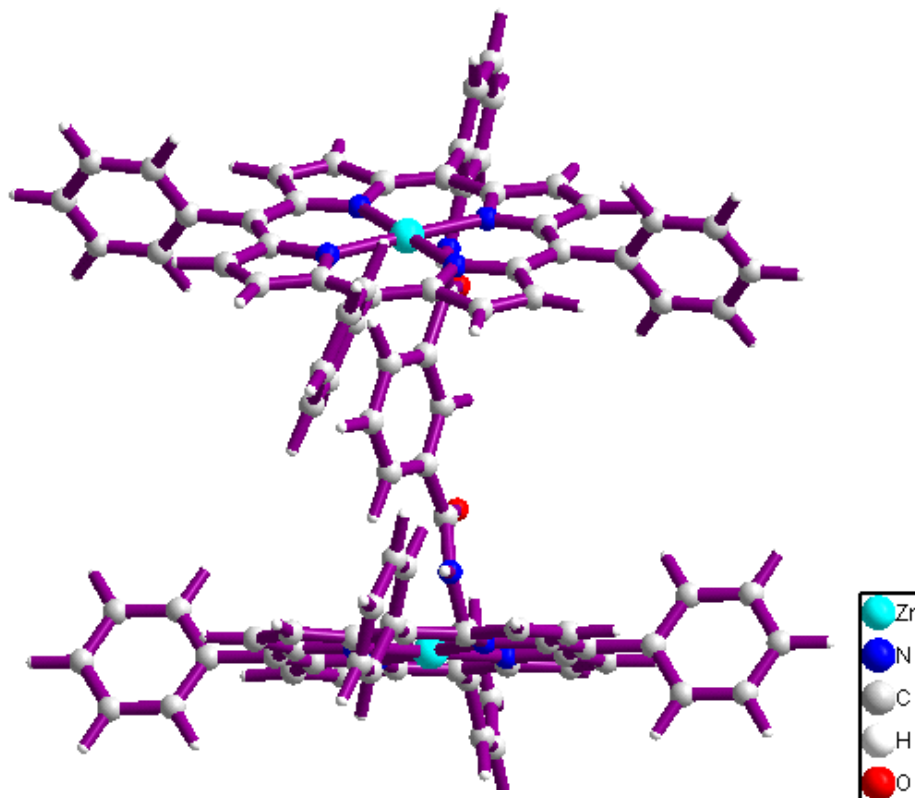
Atoms	x	y	z
Zn	-4.61128500	0.56466200	0.27358400
N	-4.65958600	-0.60408800	1.94759900
N	-5.12684200	-1.04929900	-0.86902700
N	-4.51958000	1.71944900	-1.40778400
N	-4.07716400	2.17214500	1.41233400
C	-4.40188000	-0.20464800	3.24079200
C	-5.00692500	-1.93493900	2.01300000
C	-5.42483100	-2.31505800	-0.41495400
C	-5.33985600	-1.06337200	-2.23068700
C	-4.79815600	1.32375100	-2.69700200
C	-4.18369400	3.05381200	-1.47186400
C	-3.77221600	3.43610800	0.95759000
C	-3.85708300	2.18140600	2.77137400
C	-4.59846200	-1.31758400	4.14285400
H	-4.47827100	-1.27837100	5.21556900
C	-4.96405100	-2.38630600	3.38512100

H	-5.19584600	-3.38805800	3.71718000
C	-5.83282600	-3.14961100	-1.52193700
H	-6.13163100	-4.18515800	-1.44261100
C	-5.78406800	-2.37667500	-2.64074000
H	-6.03697100	-2.66110100	-3.65167300
C	-4.62583400	2.43996200	-3.59742300
H	-4.76914500	2.40549000	-4.66745600
C	-4.25695600	3.50909500	-2.84094700
H	-4.05210500	4.51542700	-3.17561400
C	-3.33953400	4.25975400	2.06286300
H	-3.02184400	5.28930300	1.98624400
C	-3.39204200	3.48632500	3.18104400
H	-3.12450900	3.76394500	4.19003600
C	-5.36150100	-2.74855900	0.92219600
C	-5.18298900	0.03089200	-3.09806800
C	-3.83021200	3.86697500	-0.37993700
C	-4.01955000	1.08695200	3.64130200
C	-5.71910300	-4.18145700	1.20747900
C	-7.01124100	-4.50626100	1.63376100
H	-7.73427400	-3.70350500	1.75005800
C	-7.37729900	-5.82506200	1.90177400
H	-8.38697800	-6.05513000	2.22961300
C	-6.43281500	-6.83850400	1.74173600
H	-6.70063000	-7.87159900	1.94691800
C	-5.13580500	-6.54926100	1.32177500
H	-4.39815800	-7.32997900	1.20291900
C	-4.76992100	-5.22100700	1.05151400
C	-5.45560900	-0.19313600	-4.55553200
C	-6.59628900	0.35375800	-5.16340900
H	-7.28692000	0.94048400	-4.56394600
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H	-7.74262800	0.57189400	-6.97157600
C	-5.96970900	-0.61491700	-7.29043400
H	-6.16842100	-0.77814100	-8.34625000
C	-4.83158100	-1.16415600	-6.69728700
H	-4.13806500	-1.75445300	-7.29041800
C	-4.57739900	-0.95524400	-5.34102400
H	-3.68857600	-1.38030600	-4.88281600
C	-3.48217100	5.29744300	-0.66281500
C	-4.33255000	6.33597600	-0.25249100
H	-5.25298100	6.09206700	0.27082500
C	-4.01152600	7.66807800	-0.51685200
H	-4.68535300	8.45806400	-0.19566800
C	-2.83333700	7.98465100	-1.19571800

H	-2.58451900	9.02191700	-1.40373000
C	-1.97794400	6.96073700	-1.60809500
H	-1.05521600	7.19594200	-2.13146500
C	-2.29995900	5.62847900	-1.34300000
H	-1.62964800	4.83467700	-1.66092200
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H	-1.95272500	0.14372900	5.14013000
C	-2.39774500	0.96102500	7.08450300
H	-1.52246700	0.51738800	7.55171600
C	-3.27392000	1.74331000	7.83896200
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C	-4.39211400	2.31266800	7.22696600
H	-5.08187200	2.91971800	7.80747000
C	-4.63204300	2.10116900	5.86862300
H	-5.50575600	2.54082500	5.39544500
C	-2.38608300	-5.65927900	0.36990700
C	-1.17782800	-4.92816700	-0.15762100
C	0.06633600	-5.53828900	0.02836200
H	0.12047900	-6.49987500	0.52591400
C	-1.24655400	-3.71007300	-0.85162700
H	-2.20447300	-3.24309700	-1.06524600
C	-0.08276200	-3.11044100	-1.33125200
H	-0.14445500	-2.18146800	-1.89076900
O	-2.36140800	-6.86973400	0.56178600
Zn	4.60507200	0.62641400	-0.22091600
N	4.86712900	-0.88476800	-1.57131700
N	5.04809900	-0.65790000	1.30430700
N	4.28616400	2.12010400	1.13172300
N	4.15807900	1.90663000	-1.74856800
C	4.76585900	-0.79461300	-2.94291700
C	5.27764600	-2.16995200	-1.29397600
C	5.41092900	-1.98099800	1.18813400
C	5.08168000	-0.36119400	2.64925600
C	4.42268900	2.03731400	2.49911800
C	3.90229300	3.41354800	0.85404100
C	3.76667200	3.22166300	-1.62819000
C	4.09865700	1.60193300	-3.09017500
C	5.12481700	-2.06069100	-3.54161400
H	5.14884200	-2.26429000	-4.60215000
C	5.43734300	-2.90962200	-2.52482200
H	5.76330200	-3.93768400	-2.59443000
C	5.67647200	-2.53357800	2.49695100
H	5.98084500	-3.55179000	2.69175500

C	5.48169900	-1.53264900	3.39690200
H	5.60087800	-1.57606300	4.46958900
C	4.10981300	3.31423600	3.09833100
H	4.12638100	3.52670100	4.15722300
C	3.79838900	4.16521600	2.08357100
H	3.52147800	5.20672100	2.15609500
C	3.44428800	3.75516500	-2.93117500
H	3.09245400	4.75809500	-3.12400400
C	3.64886300	2.75659500	-3.83267900
H	3.49448800	2.78903000	-4.90125900
C	5.52078200	-2.70214300	-0.01396600
C	4.79325800	0.88870200	3.22286100
C	3.65450400	3.94182200	-0.42511100
C	4.39497500	0.35225100	-3.66623900
C	5.94921600	-4.14118300	0.07437000
C	7.30481700	-4.45741500	0.21356700
H	8.02384400	-3.64362200	0.25122200
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H	8.79485300	-6.00305000	0.40651600
C	6.79519000	-6.80770100	0.24899800
H	7.11385900	-7.84451600	0.31656600
C	5.43673300	-6.52773000	0.11343800
H	4.70255500	-7.32011300	0.08211600
C	5.00408400	-5.19500000	0.02403100
C	4.89060500	1.00859500	4.71448300
C	5.93315000	1.73694700	5.30780500
H	6.67635800	2.21199800	4.67329100
C	6.02588100	1.84812800	6.69579600
H	6.84301000	2.41270100	7.13718600
C	5.07698200	1.23254100	7.51406700
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C	4.03517200	0.50529200	6.93557100
H	3.29031500	0.02486200	7.56460000
C	3.94298400	0.39438100	5.54743300
H	3.12831900	-0.16804800	5.09955700
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H	5.08789400	6.04993100	-1.37408800
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H	4.39596400	8.42474600	-1.51983400
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H	2.13709300	9.11562900	-0.73886000
C	1.56739400	7.11704000	-0.15698300
H	0.57597200	7.40648500	0.18040900

C	1.96016500	5.77989400	-0.07597400
H	1.27667700	5.03691200	0.32582900
C	4.30756000	0.23572500	-5.15787500
C	3.30313700	-0.53788200	-5.76006500
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H	4.08372800	-0.07153900	-9.04128300
C	5.14997100	0.78673900	-7.37315700
H	5.87640500	1.30160900	-7.99641100
C	5.22925700	0.89723900	-5.98436600
H	6.01540900	1.49411700	-5.53028600
C	2.53619200	-5.65543900	-0.17330800
C	1.24026200	-4.92709400	-0.42169000
C	1.15781200	-3.70843100	-1.11287900
H	2.04844300	-3.24143700	-1.52540400
O	2.56291100	-6.87122300	-0.02056400
N	3.64813200	-4.84311600	-0.12592100
N	-3.47922300	-4.85859900	0.61817900
H	3.47855600	-3.84648200	-0.14511800
H	-3.33933100	-3.86150000	0.52630000



Conformer II

$$\Delta H^\circ = -7950.83352331 \text{ hartree}$$

Cartesian coordinates for Geometry Optimized **Conformer II**

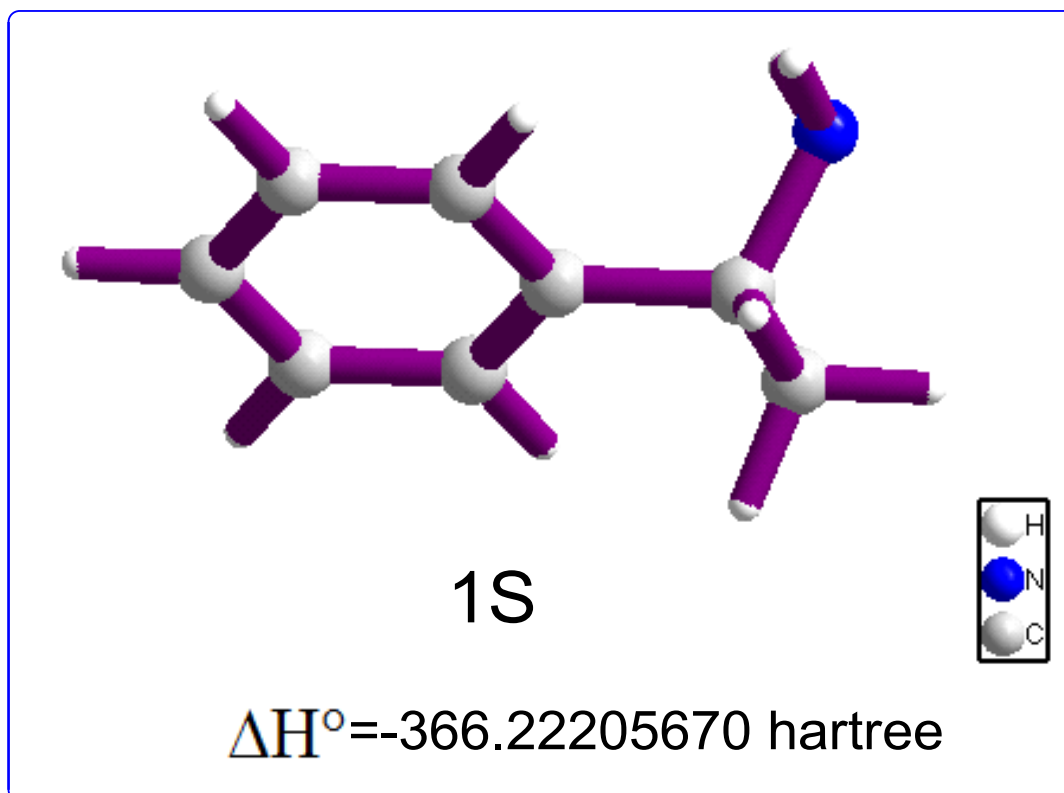
Atoms	x	y	z
Zn	4.61128500	0.56466200	0.27358400
N	4.65958600	-0.60408800	1.94759900
N	5.12684200	-1.04929900	-0.86902700
N	4.51958000	1.71944900	-1.40778400
N	4.07716400	2.17214500	1.41233400
C	4.40188000	-0.20464800	3.24079200
C	5.00692500	-1.93493900	2.01300000
C	5.42483100	-2.31505800	-0.41495400
C	5.33985600	-1.06337200	-2.23068700
C	4.79815600	1.32375100	-2.69700200
C	4.18369400	3.05381200	-1.47186400
C	3.77221600	3.43610800	0.95759000
C	3.85708300	2.18140600	2.77137400
C	4.59846200	-1.31758400	4.14285400
H	4.47827100	-1.27837100	5.21556900
C	4.96405100	-2.38630600	3.38512100

H	5.19584600	-3.38805800	3.71718000
C	5.83282600	-3.14961100	-1.52193700
H	6.13163100	-4.18515800	-1.44261100
C	5.78406800	-2.37667500	-2.64074000
H	6.03697100	-2.66110100	-3.65167300
C	4.62583400	2.43996200	-3.59742300
H	4.76914500	2.40549000	-4.66745600
C	4.25695600	3.50909500	-2.84094700
H	4.05210500	4.51542700	-3.17561400
C	3.33953400	4.25975400	2.06286300
H	3.02184400	5.28930300	1.98624400
C	3.39204200	3.48632500	3.18104400
H	3.12450900	3.76394500	4.19003600
C	5.36150100	-2.74855900	0.92219600
C	5.18298900	0.03089200	-3.09806800
C	3.83021200	3.86697500	-0.37993700
C	4.01955000	1.08695200	3.64130200
C	5.71910300	-4.18145700	1.20747900
C	7.01124100	-4.50626100	1.63376100
H	7.73427400	-3.70350500	1.75005800
C	7.37729900	-5.82506200	1.90177400
H	8.38697800	-6.05513000	2.22961300
C	6.43281500	-6.83850400	1.74173600
H	6.70063000	-7.87159900	1.94691800
C	5.13580500	-6.54926100	1.32177500
H	4.39815800	-7.32997900	1.20291900
C	4.76992100	-5.22100700	1.05151400
C	5.45560900	-0.19313600	-4.55553200
C	6.59628900	0.35375800	-5.16340900
H	7.28692000	0.94048400	-4.56394600
C	6.85162000	0.14438900	-6.51926100
H	7.74262800	0.57189400	-6.97157600
C	5.96970900	-0.61491700	-7.29043400
H	6.16842100	-0.77814100	-8.34625000
C	4.83158100	-1.16415600	-6.69728700
H	4.13806500	-1.75445300	-7.29041800
C	4.57739900	-0.95524400	-5.34102400
H	3.68857600	-1.38030600	-4.88281600
C	3.48217100	5.29744300	-0.66281500
C	4.33255000	6.33597600	-0.25249100
H	5.25298100	6.09206700	0.27082500
C	4.01152600	7.66807800	-0.51685200
H	4.68535300	8.45806400	-0.19566800
C	2.83333700	7.98465100	-1.19571800

H	2.58451900	9.02191700	-1.40373000
C	1.97794400	6.96073700	-1.60809500
H	1.05521600	7.19594200	-2.13146500
C	2.29995900	5.62847900	-1.34300000
H	1.62964800	4.83467700	-1.66092200
C	3.75954000	1.31531100	5.09988900
C	2.63898600	0.74837500	5.72658700
H	1.95272500	0.14372900	5.14013000
C	2.39774500	0.96102500	7.08450300
H	1.52246700	0.51738800	7.55171600
C	3.27392000	1.74331000	7.83896200
H	3.08670300	1.90812400	8.89665200
C	4.39211400	2.31266800	7.22696600
H	5.08187200	2.91971800	7.80747000
C	4.63204300	2.10116900	5.86862300
H	5.50575600	2.54082500	5.39544500
C	2.38608300	-5.65927900	0.36990700
C	1.17782800	-4.92816700	-0.15762100
C	-0.06633600	-5.53828900	0.02836200
H	-0.12047900	-6.49987500	0.52591400
C	1.24655400	-3.71007300	-0.85162700
H	2.20447300	-3.24309700	-1.06524600
C	0.08276200	-3.11044100	-1.33125200
H	0.14445500	-2.18146800	-1.89076900
O	2.36140800	-6.86973400	0.56178600
Zn	-4.60507200	0.62641400	-0.22091600
N	-4.86712900	-0.88476800	-1.57131700
N	-5.04809900	-0.65790000	1.30430700
N	-4.28616400	2.12010400	1.13172300
N	-4.15807900	1.90663000	-1.74856800
C	-4.76585900	-0.79461300	-2.94291700
C	-5.27764600	-2.16995200	-1.29397600
C	-5.41092900	-1.98099800	1.18813400
C	-5.08168000	-0.36119400	2.64925600
C	-4.42268900	2.03731400	2.49911800
C	-3.90229300	3.41354800	0.85404100
C	-3.76667200	3.22166300	-1.62819000
C	-4.09865700	1.60193300	-3.09017500
C	-5.12481700	-2.06069100	-3.54161400
H	-5.14884200	-2.26429000	-4.60215000
C	-5.43734300	-2.90962200	-2.52482200
H	-5.76330200	-3.93768400	-2.59443000
C	-5.67647200	-2.53357800	2.49695100
H	-5.98084500	-3.55179000	2.69175500

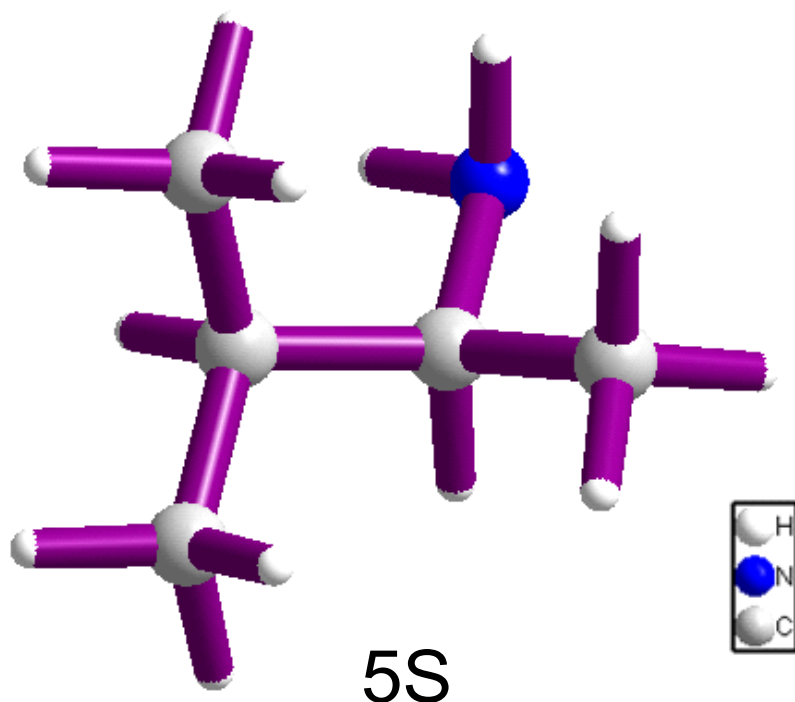
C	-5.48169900	-1.53264900	3.39690200
H	-5.60087800	-1.57606300	4.46958900
C	-4.10981300	3.31423600	3.09833100
H	-4.12638100	3.52670100	4.15722300
C	-3.79838900	4.16521600	2.08357100
H	-3.52147800	5.20672100	2.15609500
C	-3.44428800	3.75516500	-2.93117500
H	-3.09245400	4.75809500	-3.12400400
C	-3.64886300	2.75659500	-3.83267900
H	-3.49448800	2.78903000	-4.90125900
C	-5.52078200	-2.70214300	-0.01396600
C	-4.79325800	0.88870200	3.22286100
C	-3.65450400	3.94182200	-0.42511100
C	-4.39497500	0.35225100	-3.66623900
C	-5.94921600	-4.14118300	0.07437000
C	-7.30481700	-4.45741500	0.21356700
H	-8.02384400	-3.64362200	0.25122200
C	-7.73699300	-5.78049100	0.30057600
H	-8.79485300	-6.00305000	0.40651600
C	-6.79519000	-6.80770100	0.24899800
H	-7.11385900	-7.84451600	0.31656600
C	-5.43673300	-6.52773000	0.11343800
H	-4.70255500	-7.32011300	0.08211600
C	-5.00408400	-5.19500000	0.02403100
C	-4.89060500	1.00859500	4.71448300
C	-5.93315000	1.73694700	5.30780500
H	-6.67635800	2.21199800	4.67329100
C	-6.02588100	1.84812800	6.69579600
H	-6.84301000	2.41270100	7.13718600
C	-5.07698200	1.23254100	7.51406700
H	-5.14929500	1.31837200	8.59494900
C	-4.03517200	0.50529200	6.93557100
H	-3.29031500	0.02486200	7.56460000
C	-3.94298400	0.39438100	5.54743300
H	-3.12831900	-0.16804800	5.09955700
C	-3.23134000	5.37761800	-0.51377200
C	-4.09924300	6.34870700	-1.03662700
H	-5.08789400	6.04993100	-1.37408800
C	-3.70802400	7.68589100	-1.11710800
H	-4.39596400	8.42474600	-1.51983400
C	-2.44098700	8.07396900	-0.67751400
H	-2.13709300	9.11562900	-0.73886000
C	-1.56739400	7.11704000	-0.15698300
H	-0.57597200	7.40648500	0.18040900

C	-1.96016500	5.77989400	-0.07597400
H	-1.27667700	5.03691200	0.32582900
C	-4.30756000	0.23572500	-5.15787500
C	-3.30313700	-0.53788200	-5.76006500
H	-2.57951300	-1.04972200	-5.13164000
C	-3.22204400	-0.64736000	-7.14882100
H	-2.43451200	-1.24787300	-7.59646600
C	-4.14573600	0.01437900	-7.95979000
H	-4.08372800	-0.07153900	-9.04128300
C	-5.14997100	0.78673900	-7.37315700
H	-5.87640500	1.30160900	-7.99641100
C	-5.22925700	0.89723900	-5.98436600
H	-6.01540900	1.49411700	-5.53028600
C	-2.53619200	-5.65543900	-0.17330800
C	-1.24026200	-4.92709400	-0.42169000
C	-1.15781200	-3.70843100	-1.11287900
H	-2.04844300	-3.24143700	-1.52540400
O	-2.56291100	-6.87122300	-0.02056400
N	-3.64813200	-4.84311600	-0.12592100
N	3.47922300	-4.85859900	0.61817900
H	-3.47855600	-3.84648200	-0.14511800
H	3.33933100	-3.86150000	0.52630000



Cartesian coordinates for Geometry Optimized **1S**

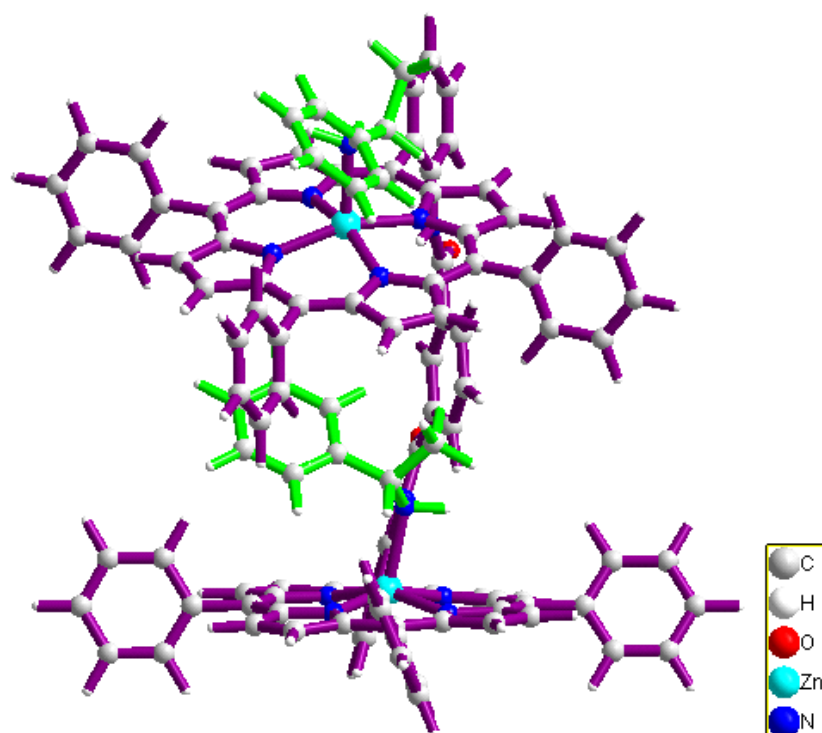
Atoms	x	y	z
H	6.56054021	0.82429791	2.51965342
N	6.28729410	1.21306114	1.61571963
C	6.82734571	2.52065973	1.57359946
H	6.86284665	0.74018264	0.91842367
C	8.30404129	2.82668814	1.38420963
H	6.27020803	3.02808849	0.78038733
C	6.29440672	3.01975784	2.92521001
C	9.26967808	2.30927814	2.26171187
C	8.72620278	3.65440703	0.33782289
H	6.43622086	4.10055402	3.02144761
H	5.22075455	2.81220165	3.01502173
H	6.81185064	2.53902418	3.76373316
C	10.62138221	2.61575372	2.09724737
H	8.97334102	1.66243754	3.08494384
C	10.07687905	3.97284084	0.17717432
H	7.99485246	4.04458938	-0.36524155
H	11.35567684	2.20344160	2.78392708
C	11.02804025	3.45477310	1.05633779
H	10.38347497	4.62407603	-0.63614111
H	12.07756071	3.70717549	0.93623940



$$\Delta H^\circ = -366.22205670 \text{ hartree}$$

Cartesian coordinates for Geometry Optimized **5S**

Atoms	x	y	z
H	6.91812500	-0.58495700	-0.63862600
N	6.70165500	0.03626300	0.14291800
C	7.57450100	1.24145900	0.07869900
H	6.90545800	-0.49970100	0.98750700
C	9.03557300	0.89135500	-0.31277800
H	7.16215600	1.85597300	-0.73100700
C	7.42962300	2.01910500	1.38824100
C	9.77233500	0.04050800	0.73349200
C	9.84264100	2.15128000	-0.66206000
H	8.96114000	0.29175500	-1.23455900
H	6.38321300	2.28386600	1.56071300
H	7.77389900	1.43075500	2.24755100
H	8.01314700	2.94419800	1.36183800
H	9.94409400	0.60014200	1.66013200
H	9.22131300	-0.87272800	0.98890700
H	10.75163100	-0.26928800	0.35225300
H	9.32331700	2.76639500	-1.40673500
H	10.02239500	2.77360500	0.22221500
H	10.82050400	1.88079400	-1.07588900



“inside-outside” **Conformer I•1S**

$\Delta H^\circ = -8683.32447956$ hartree

Cartesian coordinates for Geometry Optimized “inside-outside” **Conformer I•1S**

Atoms	x	y	z
C	5.26175100	4.87925300	-0.55392200
C	6.58770100	5.31524600	-0.65511900
H	7.37661200	4.56782300	-0.66649100
C	6.90796200	6.66984300	-0.73482800
H	7.94537300	6.98246800	-0.81255400
C	5.88044900	7.61212900	-0.70815800
H	6.10982100	8.67293600	-0.76375200
C	4.54888700	7.21431300	-0.60834500
H	3.75076000	7.94199200	-0.57256000
C	4.22909300	5.84881600	-0.53491300
C	1.73858200	6.11357000	-0.30933300
C	0.47318500	5.30017300	-0.39713200
C	-0.64623500	5.77460100	0.29319800
H	-0.57198300	6.68562100	0.87611200
C	0.35562800	4.15105700	-1.19284400

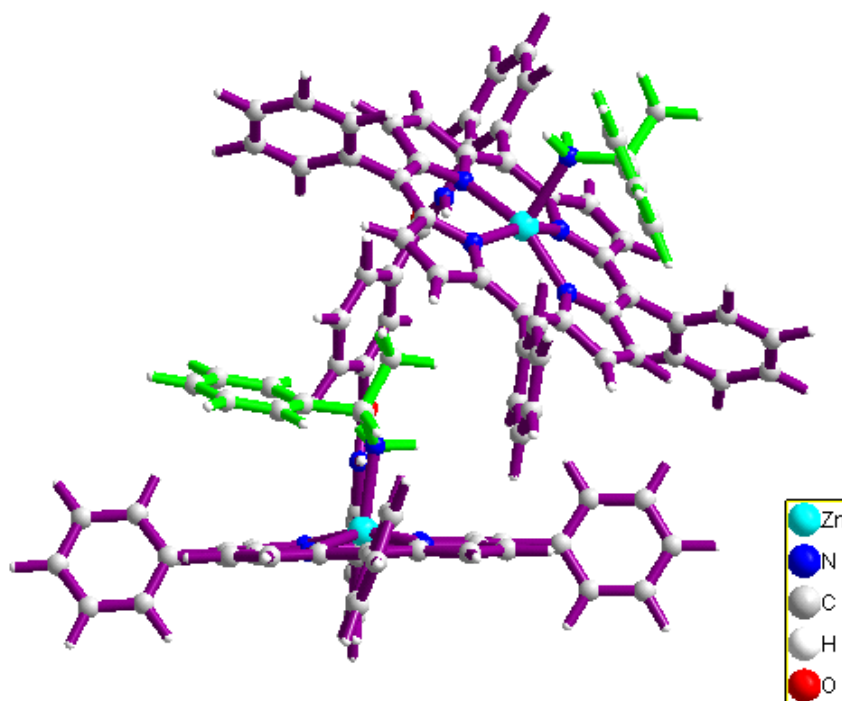
H	1.19746500	3.79505200	-1.78105700
C	-0.87207800	3.49464700	-1.28991800
H	-0.97148600	2.63429700	-1.94645200
O	1.70020200	7.32359500	-0.12002300
Zn	-4.88740900	-0.54443900	0.22698400
N	-5.68036300	1.23627600	-0.55725400
N	-5.14826400	0.25428100	2.11987400
N	-4.85427400	-2.43489200	1.07530100
N	-5.40185100	-1.45760500	-1.60015900
C	-5.97268200	1.49705800	-1.87514300
C	-5.94125900	2.39102800	0.13858900
C	-5.41836100	1.56210300	2.43875000
C	-4.88994800	-0.39299800	3.30401900
C	-4.67932100	-2.71470900	2.40787500
C	-4.82106400	-3.63772800	0.41037100
C	-5.22327600	-2.78463700	-1.90632500
C	-5.62928000	-0.80700900	-2.78833700
C	-6.42906400	2.86582000	-2.01279900
H	-6.75052900	3.32901700	-2.93430900
C	-6.41327900	3.41626100	-0.76878400
H	-6.71445100	4.41383400	-0.48163500
C	-5.29848300	1.75353300	3.86985900
H	-5.46011400	2.68672700	4.39000600
C	-4.97399900	0.54585100	4.40376800
H	-4.82336600	0.30146800	5.44541600
C	-4.52461300	-4.14143100	2.59156100
H	-4.37792600	-4.63776900	3.53999300
C	-4.62467100	-4.71306700	1.35990300
H	-4.58600400	-5.76478600	1.11573600
C	-5.31255800	-2.97323600	-3.33888300
H	-5.19392400	-3.91406800	-3.85655400
C	-5.55815100	-1.75081400	-3.88443000
H	-5.67818800	-1.50864000	-4.93031400
C	-5.79522900	2.57158700	1.53057000
C	-4.65536000	-1.77119100	3.45468100
C	-4.96912400	-3.81779500	-0.97991900
C	-5.90200200	0.57118200	-2.93567700
C	-6.13279800	3.92480500	2.09454300
C	-7.35545200	4.11712400	2.74811200
H	-8.03320400	3.27214600	2.83149600
C	-7.71180500	5.35721700	3.27712900
H	-8.66822200	5.48220700	3.77679700
C	-6.82894800	6.42932900	3.15265600
H	-7.09036600	7.40284800	3.55896700

C	-5.60123400	6.27326500	2.51180300
H	-4.90982700	7.09847400	2.41784600
C	-5.24633900	5.02368100	1.98006000
C	-4.39579700	-2.27940200	4.84257900
C	-5.38919800	-2.96814800	5.55502500
H	-6.35829000	-3.13010800	5.09094200
C	-5.14540800	-3.43645000	6.84704200
H	-5.92820600	-3.96473800	7.38525400
C	-3.90371600	-3.22210300	7.44831200
H	-3.71404100	-3.58532900	8.45494700
C	-2.90792100	-2.53741900	6.74935300
H	-1.93776000	-2.36749100	7.20941600
C	-3.15175300	-2.06945700	5.45689700
H	-2.37343400	-1.54390800	4.91052300
C	-4.86321500	-5.21427000	-1.51334400
C	-5.98360100	-5.85919700	-2.06152200
H	-6.93429200	-5.33424800	-2.08897800
C	-5.88914600	-7.16013600	-2.55729100
H	-6.77011700	-7.64304000	-2.97215600
C	-4.67111200	-7.84112300	-2.51571800
H	-4.59717500	-8.85416100	-2.90213500
C	-3.54873200	-7.21184100	-1.97435300
H	-2.59441700	-7.73136200	-1.94245200
C	-3.64505000	-5.91129800	-1.47779200
H	-2.76741100	-5.42302600	-1.06287900
C	-6.17715500	1.08432200	-4.31581900
C	-5.31807600	2.01726700	-4.91865700
H	-4.44254700	2.36020700	-4.37402700
C	-5.57262500	2.50290200	-6.20172200
H	-4.89229500	3.22226900	-6.65014500
C	-6.69498800	2.06535000	-6.90696400
H	-6.89544800	2.44407300	-7.90563300
C	-7.56024800	1.14054600	-6.31909800
H	-8.44149400	0.80012700	-6.85662100
C	-7.30370800	0.65517300	-5.03644500
H	-7.98460100	-0.05629600	-4.57798600
C	-3.01125000	5.68270200	1.02719200
C	-1.86758600	5.09758600	0.23499000
C	-1.97877600	3.95862300	-0.57869900
H	-2.93686900	3.46138800	-0.70983500
O	-2.99929000	6.85824900	1.37598400
N	-4.02067200	4.79719200	1.32126100
N	2.89956800	5.38702600	-0.46186300
H	-3.87543700	3.83323100	1.05439300

H	2.80576700	4.37963200	-0.46096300
H	1.45801100	0.31678300	2.35859900
C	0.72326500	-0.44847700	2.12573300
C	-0.06873700	-0.32347700	0.98449300
C	0.58581100	-1.56500100	2.95376700
C	-1.00743000	-1.31125500	0.64970600
H	0.06075200	0.54864800	0.34718800
C	-0.35292500	-2.54775800	2.63762000
H	1.21679400	-1.67306200	3.83124200
C	-1.14454100	-2.42009300	1.49333300
H	-0.47272600	-3.41667400	3.27898000
H	-1.87919200	-3.18559500	1.25822200
C	-1.85148500	-1.19593400	-0.60892000
H	-2.43105000	-2.11755300	-0.71535100
C	-1.00578700	-1.01750000	-1.87886000
H	-0.29668100	-1.84409700	-1.99142800
H	-1.65192400	-0.99963400	-2.76559200
H	-0.42782300	-0.08650200	-1.85155000
N	-2.85731800	-0.09507600	-0.45882900
H	-2.44172300	0.68422700	0.05201700
H	-3.10416900	0.26639400	-1.38128400
H	3.48355300	2.50521800	-4.72332200
C	3.79532300	2.39342000	-3.69485400
C	3.77302200	1.15693800	-2.93967700
C	4.26717600	3.36020500	-2.85991800
N	4.21800500	1.38711900	-1.65996100
C	3.31949300	-0.07831500	-3.44449600
C	4.52037100	2.72502500	-1.58287400
H	4.42319700	4.40732200	-3.07931400
C	3.21336800	-1.26663300	-2.69080000
C	2.90080300	-0.12469600	-4.88353800
C	4.97015800	3.40863100	-0.43315500
N	3.55680400	-1.41490200	-1.36862700
C	2.72551200	-2.52695700	-3.21138600
C	3.84967200	0.00539300	-5.91005600
C	1.55338600	-0.29295900	-5.24007500
C	5.15276100	2.82322300	0.83663800
C	3.28726700	-2.71930700	-1.03287900
C	2.76749400	-3.42228200	-2.18548000
H	2.39681900	-2.70093600	-4.22576100
H	4.89695300	0.13339600	-5.64994100
C	3.46485500	-0.03301400	-7.25085900
C	1.16661000	-0.33135000	-6.58033800
H	0.80630800	-0.38769600	-4.45684100

N	4.98850300	1.49421700	1.14123800
C	5.51237500	3.56152400	2.03017500
C	3.49831200	-3.30999000	0.22833900
H	2.47920200	-4.46342800	-2.20493400
H	4.21624800	0.06591600	-8.02995500
C	2.12139000	-0.20153900	-7.59053400
H	0.11752600	-0.45833500	-6.83459400
C	5.23510100	1.36765100	2.48724700
H	5.68323800	4.62748200	2.07719500
C	5.55997800	2.66303400	3.04994100
C	3.99679800	-2.64211700	1.36204700
C	3.14469400	-4.76002700	0.38160300
H	1.82062300	-0.23093600	-8.63432500
C	5.15209000	0.17519200	3.23210000
H	5.77438400	2.85672600	4.09104300
N	4.36969100	-1.32161300	1.41882300
C	4.14564400	-3.24892400	2.66753300
C	1.80361600	-5.16530600	0.46172100
C	4.14910300	-5.73743100	0.45209100
C	4.73624000	-1.07065700	2.71794200
C	5.50679200	0.24490000	4.68758500
C	4.61144200	-2.28147200	3.50330200
H	3.91453800	-4.27650700	2.90817000
H	1.01984700	-4.41378000	0.42519400
C	1.47580800	-6.51453800	0.60583200
C	3.82024600	-7.08648000	0.59625500
H	5.19012300	-5.43396400	0.38400700
C	4.51828300	0.13650400	5.67819400
C	6.83854300	0.42658000	5.09157700
H	4.84298900	-2.37209300	4.55466600
H	0.43197300	-6.81084500	0.67218900
C	2.48277300	-7.47931800	0.67291400
H	4.61055300	-7.83123500	0.64668900
H	3.48147300	0.00748000	5.37997500
C	4.85128000	0.20422500	7.03163300
C	7.17363400	0.49338000	6.44464400
H	7.61438500	0.51131900	4.33542600
H	2.22709300	-8.52956000	0.78624500
H	4.07012200	0.12375900	7.78303700
C	6.18064500	0.38168100	7.41937600
H	8.21158000	0.63065400	6.73657600
H	6.44033600	0.43479200	8.47322800
Zn	4.64183900	-0.07917900	-0.21519400
N	6.76316000	-0.19624900	-0.71364500

C	7.25364800	-0.81296900	-1.98446500
H	7.27977400	-0.57599700	0.07999900
H	6.95923300	0.80581500	-0.72378200
C	7.45570000	-2.30850000	-1.79842300
H	6.45209800	-0.66665500	-2.71552200
C	8.51339300	-0.10692800	-2.50938100
C	8.47505400	-2.80385900	-0.97154200
C	6.62935200	-3.22150200	-2.46289900
H	8.83218700	-0.54596300	-3.46057600
H	8.31476400	0.95830800	-2.67923200
H	9.34819200	-0.18998000	-1.80403200
C	8.66381200	-4.17660400	-0.81444300
H	9.13748500	-2.11695700	-0.44832400
C	6.81909300	-4.59665200	-2.31281700
H	5.82510300	-2.85498100	-3.09495500
H	9.45960600	-4.54180400	-0.17077100
C	7.83737600	-5.07817900	-1.48921600
H	6.16518200	-5.28881800	-2.83586400
H	7.98825500	-6.14819600	-1.37385200



“inside-outside” **Conformer II•1S**

$\Delta H^\circ = -8683.32403656$ hartree

Cartesian coordinates for Geometry Optimized “inside-outside” **Conformer II•1S**

Atoms	x	y	z
Zn	-4.31284400	-0.30285400	-0.53873000
N	-4.60303700	1.45270400	0.58075000
N	-4.22810700	0.92093500	-2.25200400
N	-3.32165500	-1.75934900	-1.62834500
N	-3.64847600	-1.20679100	1.20479000
C	-4.69619100	1.53193200	1.94929500
C	-5.01981300	2.66589100	0.09037700
C	-4.69259700	2.21014200	-2.34799800
C	-3.96487800	0.50243700	-3.53430800
C	-3.13836300	-1.79297900	-2.98946100
C	-2.81618100	-2.93621000	-1.13158900
C	-3.11528100	-2.47014800	1.30705900
C	-3.85250900	-0.75864500	2.48801500
C	-5.20443900	2.83482000	2.33167900
H	-5.38676500	3.16477900	3.34390200

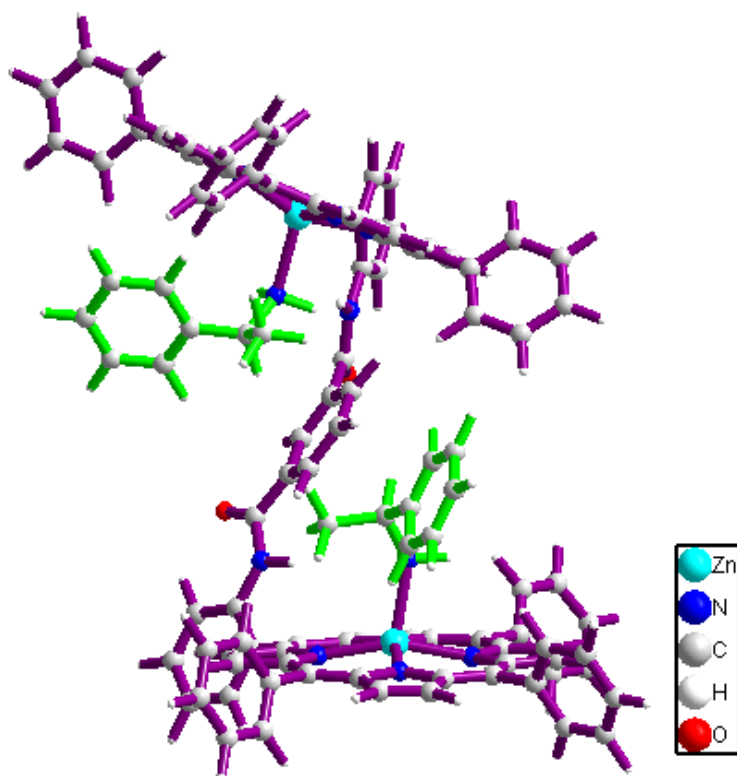
C	-5.39645200	3.53782800	1.18377700
H	-5.75856300	4.55060100	1.07902600
C	-4.73009900	2.61879700	-3.73671300
H	-5.06168700	3.58344300	-4.09508200
C	-4.28605500	1.56164300	-4.47022800
H	-4.18818800	1.49965300	-5.54430600
C	-2.49108400	-3.03251800	-3.36345600
H	-2.20282500	-3.30991900	-4.36698600
C	-2.29277000	-3.73814500	-2.21660100
H	-1.81432000	-4.70066400	-2.10869700
C	-2.98979700	-2.83420300	2.70162000
H	-2.59794800	-3.76939100	3.07348200
C	-3.43342800	-1.77369800	3.43080800
H	-3.45732300	-1.67981200	4.50666000
C	-5.07453200	3.03384500	-1.26925200
C	-3.46251400	-0.76277800	-3.89776100
C	-2.73939700	-3.29694300	0.22919000
C	-4.35882100	0.50717000	2.85475500
C	-5.54608200	4.42807700	-1.58119200
C	-6.90971200	4.69492200	-1.73988600
H	-7.61186000	3.86958800	-1.65575000
C	-7.37444200	5.98591000	-1.99110800
H	-8.43854200	6.17010600	-2.10828400
C	-6.45758700	7.03297600	-2.08189900
H	-6.80272800	8.04601500	-2.27066500
C	-5.09133400	6.80165400	-1.93405700
H	-4.37828200	7.61207600	-1.99167300
C	-4.62716900	5.49980400	-1.68935500
C	-3.22693400	-1.02800900	-5.35360800
C	-3.99185100	-1.98382900	-6.04104800
H	-4.76408700	-2.52906400	-5.50520200
C	-3.77616600	-2.23341400	-7.39685300
H	-4.38314300	-2.97400600	-7.91119500
C	-2.78858800	-1.53235800	-8.09120100
H	-2.61975400	-1.72648400	-9.14697700
C	-2.01796100	-0.58170500	-7.41951000
H	-1.24152100	-0.03579500	-7.94901200
C	-2.23531900	-0.33263100	-6.06388600
H	-1.62661300	0.40099200	-5.54281200
C	-2.20026000	-4.65874700	0.54785900
C	-2.92601100	-5.80735800	0.19191000
H	-3.88600900	-5.69281000	-0.30326300
C	-2.43414900	-7.08123100	0.48005700
H	-3.01302600	-7.95785900	0.20033100

C	-1.20686700	-7.22995200	1.12874500
H	-0.82404600	-8.22148200	1.35587300
C	-0.47534400	-6.09593200	1.48738500
H	0.48348400	-6.19905500	1.98718600
C	-0.96683400	-4.82150100	1.19882600
H	-0.38732400	-3.94621100	1.47928100
C	-4.53012100	0.78822300	4.31703000
C	-3.73179700	1.74402600	4.96654800
H	-2.97738900	2.27982100	4.39712400
C	-3.89518400	2.00764800	6.32797200
H	-3.26593100	2.75063300	6.81085100
C	-4.85956000	1.31836700	7.06619300
H	-4.98734000	1.52397200	8.12550900
C	-5.65929100	0.36519800	6.43343700
H	-6.41602700	-0.17343200	6.99787800
C	-5.49533200	0.10362800	5.07259000
H	-6.12473800	-0.63518100	4.58399600
C	-2.18694800	6.04924800	-1.42412800
C	-0.84963200	5.35617900	-1.39768200
C	0.17144200	5.93147000	-0.63621900
H	-0.01483600	6.84912600	-0.08954900
C	-0.58334100	4.20163200	-2.14795100
H	-1.35118100	3.76941600	-2.78401700
C	0.69097800	3.63517500	-2.12814700
H	0.90318300	2.77282500	-2.75361300
O	-2.28026400	7.26611500	-1.32097900
Zn	4.35019900	-0.36906200	0.87221400
N	5.64604000	1.10686500	0.19457700
N	3.83623500	0.92307700	2.45729800
N	3.62003800	-1.94442400	2.04931900
N	5.46281300	-1.76209900	-0.18414800
C	6.52412500	0.98677300	-0.85553200
C	5.71835700	2.41117100	0.61970200
C	4.16226100	2.25148700	2.57057500
C	3.02140300	0.62816800	3.52491900
C	2.82917800	-1.83971400	3.16729200
C	3.68551600	-3.27945700	1.73521500
C	5.24780800	-3.11930400	-0.21170200
C	6.33181900	-1.47966500	-1.20881900
C	7.15475300	2.26536700	-1.11378900
H	7.90022300	2.45240100	-1.87300100
C	6.65644500	3.14498500	-0.20392600
H	6.91277400	4.18757900	-0.07946200
C	3.51660700	2.82114000	3.73547200

H	3.61523100	3.84588400	4.06517800
C	2.80995100	1.81899700	4.32370300
H	2.22120000	1.86773000	5.22836200
C	2.36778300	-3.15297300	3.56476700
H	1.73473000	-3.36386400	4.41436000
C	2.90854000	-4.04374600	2.68815900
H	2.81591100	-5.12015200	2.69939700
C	5.99357100	-3.70884100	-1.30350100
H	5.99902300	-4.75685400	-1.56555200
C	6.66255500	-2.69654000	-1.91853200
H	7.31427900	-2.76260600	-2.77738900
C	5.02844600	2.96501800	1.71689900
C	2.52120200	-0.64640200	3.85425200
C	4.42052500	-3.84246000	0.67114300
C	6.83453900	-0.20428400	-1.53901400
C	5.33358100	4.39592800	2.07517500
C	6.44099600	4.67320100	2.88513900
H	7.04627400	3.84008900	3.23149900
C	6.77118800	5.97848000	3.24754400
H	7.63541500	6.16730400	3.87803900
C	5.97850000	7.03151300	2.79247900
H	6.21948700	8.05546600	3.06566100
C	4.86897500	6.79222600	1.98438600
H	4.24769500	7.60397000	1.63433200
C	4.54047200	5.47612100	1.62115400
C	1.64108500	-0.74946600	5.06479300
C	2.11638600	-1.33662100	6.24822500
H	3.13400200	-1.71623500	6.27890200
C	1.30229100	-1.42718400	7.37791900
H	1.69052700	-1.88127700	8.28607100
C	-0.00208600	-0.93025800	7.34444500
H	-0.63597400	-0.99890300	8.22468300
C	-0.48744600	-0.34312100	6.17465100
H	-1.50054500	0.04829600	6.13828700
C	0.32843700	-0.25431000	5.04525900
H	-0.05587200	0.19783400	4.13491400
C	4.32724600	-5.32588200	0.47780700
C	5.43603200	-6.15546300	0.71014100
H	6.36972300	-5.70930500	1.04082600
C	5.34679600	-7.53647400	0.53005500
H	6.21613800	-8.16083800	0.71964700
C	4.14590900	-8.11535400	0.11500700
H	4.07698600	-9.19090300	-0.02515400
C	3.03441700	-7.30307400	-0.11700600

H	2.09326800	-7.74038800	-0.44029200
C	3.12539200	-5.92202600	0.06307900
H	2.25565700	-5.29661300	-0.11879300
C	7.80648100	-0.11254800	-2.67618200
C	7.45717600	0.54281200	-3.86723900
H	6.46237900	0.96811100	-3.96238600
C	8.36423800	0.63665000	-4.92372900
H	8.07381900	1.14518200	-5.83965200
C	9.63803900	0.07717300	-4.80782600
H	10.34503900	0.15119700	-5.62994400
C	9.99824800	-0.57692700	-3.62815700
H	10.98972800	-1.01055800	-3.52577000
C	9.09060400	-0.67039000	-2.57233000
H	9.37676000	-1.17186100	-1.65197000
C	2.46481600	6.00842600	0.30425100
C	1.43453800	5.33607700	-0.56720400
C	1.69459700	4.18895600	-1.33314600
H	2.69313700	3.75781700	-1.35323900
O	2.39613600	7.20805300	0.54790400
N	3.44007000	5.16956500	0.79299300
N	-3.25750800	5.19339500	-1.56953200
H	3.31206700	4.17834200	0.63519800
H	-3.05846300	4.20610300	-1.46916700
H	1.84383100	0.02126800	0.68327100
N	2.44805100	-0.01081500	-0.13982000
C	1.85060100	-0.96137000	-1.12138400
H	2.42775600	0.93658500	-0.51866100
C	2.58733600	-0.92941800	-2.45116300
H	1.98818600	-1.95484000	-0.68202600
C	0.34412500	-0.71297200	-1.30732500
C	2.82793200	0.27130800	-3.13307200
C	2.97425400	-2.12790600	-3.06161800
H	-0.08794000	-1.43805500	-2.00380700
H	-0.19046100	-0.80497900	-0.35428200
H	0.15794100	0.29096900	-1.70780100
C	3.43357800	0.27454100	-4.39004000
H	2.54487000	1.22175200	-2.68685000
C	3.57842000	-2.13083300	-4.31939900
H	2.81082600	-3.06818900	-2.54168900
H	3.60840800	1.21772200	-4.90146000
C	3.80781100	-0.92939600	-4.98985800
H	3.87726800	-3.07328600	-4.76973300
H	4.27988100	-0.92923900	-5.96845100
H	-7.21710600	-6.69008900	0.10124200

C	-7.22135900	-5.60412400	0.14136700
C	-6.61355500	-4.93780200	1.20606700
C	-7.83711700	-4.86739200	-0.87298900
C	-6.62188600	-3.54219600	1.25718500
H	-6.12489600	-5.50132900	1.99594700
C	-7.84972800	-3.47431100	-0.81483400
H	-8.31358000	-5.37741800	-1.70597200
C	-7.24237700	-2.79339300	0.25113200
H	-6.13376000	-3.03131400	2.08284600
H	-8.34718000	-2.91687700	-1.60623800
C	-7.27036700	-1.27502000	0.32503600
N	-6.44653500	-0.68982400	-0.77812200
H	-6.78483900	-0.96962400	1.25725300
C	-8.69983000	-0.71090900	0.32572600
H	-6.75777200	0.26470300	-0.96424200
H	-6.60191200	-1.21075000	-1.64128300
H	-9.27357000	-1.11981400	1.16397900
H	-8.68211600	0.38073700	0.43056600
H	-9.23347100	-0.95749500	-0.59941300



“inside-inside” Conformer I•1S

$\Delta H^\circ = -8683.31791620$ hartree

Cartesian coordinates for Geometry Optimized “inside-inside” **Conformer I•1S**

Atoms	x	y	z
Zn	-5.64959900	0.67289000	-0.90310900
N	-6.80217600	-1.03912900	-0.56816700
N	-4.82082000	-0.34044600	-2.56509500
N	-5.02331000	2.44435700	-1.78798900
N	-7.02443000	1.75310300	0.19011400
C	-7.77402900	-1.16836200	0.39492400
C	-6.60949000	-2.29145000	-1.09940000
C	-4.91397800	-1.68498200	-2.83421600
C	-3.93619500	0.18286200	-3.47848100
C	-4.09650400	2.58158700	-2.79288200
C	-5.29900200	3.71128700	-1.33185100
C	-7.02908800	3.11550700	0.37124000
C	-7.98591200	1.23949800	1.02564200
C	-8.19606000	-2.55103300	0.48393600
H	-8.95478100	-2.93041800	1.15306200

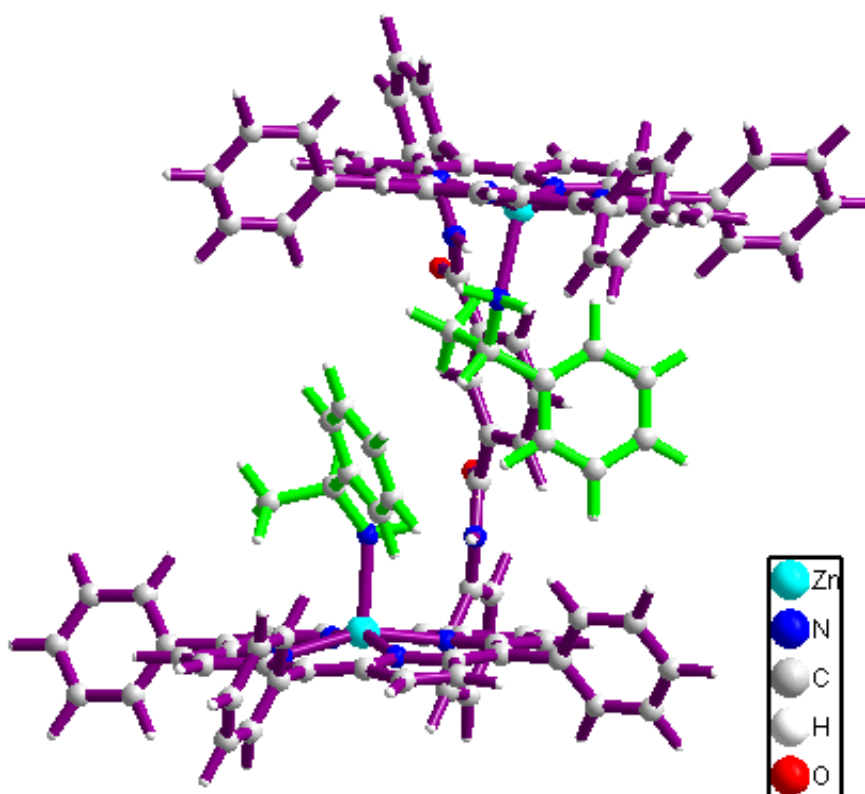
C	-7.47249300	-3.24625400	-0.43353100
H	-7.52387400	-4.30244100	-0.65479100
C	-4.04858300	-2.02480300	-3.94447700
H	-3.94199600	-3.01052100	-4.37552600
C	-3.43441100	-0.87345000	-4.33388300
H	-2.72329500	-0.74638500	-5.13715300
C	-3.77006700	3.98082100	-2.96936800
H	-3.08126300	4.37525800	-3.70223700
C	-4.50400800	4.67708200	-2.06016600
H	-4.51908600	5.74582600	-1.90386000
C	-8.02591400	3.47183900	1.35838400
H	-8.25590400	4.47725400	1.67987400
C	-8.60978000	2.31258300	1.76906700
H	-9.40210000	2.19200900	2.49361800
C	-5.72532900	-2.61427200	-2.14939400
C	-3.56891600	1.53916200	-3.58221300
C	-6.21920600	4.04149200	-0.31658600
C	-8.32717800	-0.12110200	1.15404300
C	-5.67991100	-4.04934700	-2.59888700
C	-6.73138000	-4.57437400	-3.35931300
H	-7.55371300	-3.91589600	-3.62459400
C	-6.73910500	-5.90683400	-3.77072800
H	-7.56711600	-6.29000000	-4.36020200
C	-5.67611500	-6.73651800	-3.41510000
H	-5.66887400	-7.77859200	-3.72330600
C	-4.61026400	-6.24687500	-2.66268500
H	-3.78850800	-6.88710100	-2.37392000
C	-4.60338500	-4.90401300	-2.25610400
C	-2.57076400	1.90637300	-4.63944100
C	-2.90581500	1.83572100	-6.00088700
H	-3.90677800	1.52169500	-6.28314200
C	-1.97401900	2.16784600	-6.98537000
H	-2.25509000	2.10985300	-8.03364000
C	-0.68842500	2.57672000	-6.62662100
H	0.03836100	2.83232200	-7.39293800
C	-0.34252200	2.65598100	-5.27640900
H	0.65890500	2.96539800	-4.98810400
C	-1.27693000	2.32605000	-4.29338000
H	-1.00778600	2.39280200	-3.24221900
C	-6.37399600	5.49008500	0.03909500
C	-6.97904000	6.38828800	-0.85405700
H	-7.33986600	6.02116500	-1.81084500
C	-7.12722200	7.73536800	-0.52140300
H	-7.60221000	8.41433400	-1.22480100

C	-6.67352700	8.20830300	0.71136000
H	-6.78910500	9.25730400	0.97064100
C	-6.07159500	7.32510400	1.60935500
H	-5.71269000	7.68432400	2.57037400
C	-5.92385600	5.97805000	1.27564800
H	-5.45145600	5.29380500	1.97529500
C	-9.38114800	-0.48032700	2.15993700
C	-9.02933700	-1.09087400	3.37340300
H	-7.98188600	-1.28920800	3.58334000
C	-10.00815200	-1.43167600	4.30855900
H	-9.71799300	-1.90264500	5.24425500
C	-11.35351400	-1.16771000	4.04524800
H	-12.11537500	-1.43441200	4.77293600
C	-11.71485700	-0.55974500	2.84149800
H	-12.76019600	-0.35372700	2.62647600
C	-10.73612700	-0.21903800	1.90648800
H	-11.01938200	0.24821600	0.96721400
C	-2.44691600	-4.95871400	-0.95321600
C	-1.48334600	-4.00566900	-0.29023300
C	-0.78061300	-4.46847000	0.82518000
H	-0.95513200	-5.47460000	1.18918600
C	-1.24113700	-2.70815800	-0.76781200
H	-1.73415100	-2.35266900	-1.66980300
C	-0.32573600	-1.88371100	-0.11134100
H	-0.14133600	-0.87817100	-0.48105600
O	-2.24374800	-6.16704800	-0.95640100
Zn	5.86885100	-0.19137600	0.54743000
N	5.47750100	-2.26589200	0.56602900
N	5.50432500	-0.18225100	2.58657100
N	6.90503600	1.58051800	0.76533900
N	6.88212600	-0.50138200	-1.25912800
C	5.66508000	-3.14838300	-0.47316400
C	5.01233200	-3.00641200	1.62742500
C	4.94298800	-1.18540000	3.33925800
C	5.61730600	0.91222100	3.41237400
C	6.85612800	2.42040000	1.85187000
C	7.59119900	2.24820000	-0.22100600
C	7.52411600	0.47569900	-1.98239000
C	6.76292100	-1.58990700	-2.08958000
C	5.29400800	-4.48400900	-0.05441500
H	5.36510600	-5.37294100	-0.66400600
C	4.89833200	-4.39783500	1.24397900
H	4.58484000	-5.20247800	1.89416100
C	4.65740600	-0.69581200	4.67174400

H	4.21255200	-1.27473300	5.46794500
C	5.07668900	0.59708700	4.71763800
H	5.04634900	1.27126400	5.56122100
C	7.53189600	3.66128900	1.53914500
H	7.64580500	4.49892800	2.21177900
C	7.99588400	3.54967900	0.26376600
H	8.56833200	4.27507900	-0.29608200
C	7.79032200	-0.00185400	-3.32206200
H	8.27068900	0.56668000	-4.10509000
C	7.31684700	-1.27571800	-3.39002800
H	7.33647900	-1.94126700	-4.24055500
C	4.71951300	-2.51323800	2.91666200
C	6.23258600	2.13569500	3.08415300
C	7.86893100	1.75793300	-1.51160300
C	6.20315500	-2.83672000	-1.73795100
C	4.27330200	-3.49837400	3.96286300
C	5.17906100	-3.85812400	4.97040100
H	6.17152400	-3.41748700	4.94724000
C	4.83725800	-4.75604400	5.97939600
H	5.56244600	-5.01817100	6.74442500
C	3.55859200	-5.31117000	5.98877700
H	3.27088800	-6.01287000	6.76709400
C	2.63218500	-4.97989300	5.00286500
H	1.64285500	-5.41330800	5.00201600
C	2.98100700	-4.07877400	3.98338100
C	6.26278700	3.20045800	4.13998200
C	7.46149200	3.53421500	4.78979700
H	8.37301600	3.00674000	4.52262500
C	7.48899300	4.52312100	5.77403600
H	8.42631600	4.76422700	6.26864900
C	6.31739600	5.19550800	6.12684600
H	6.33851400	5.96529800	6.89361500
C	5.11840200	4.87191700	5.48944000
H	4.20152300	5.39156300	5.75534700
C	5.09214900	3.88299800	4.50496800
H	4.15783600	3.63731900	4.00742300
C	8.59142200	2.67093800	-2.45694000
C	9.92565000	2.42432800	-2.81552500
H	10.43700700	1.56314100	-2.39430700
C	10.59680600	3.27464900	-3.69548500
H	11.63160300	3.07015900	-3.95774100
C	9.94398700	4.38523400	-4.23352500
H	10.46629800	5.04705500	-4.91927200
C	8.61609300	4.63997600	-3.88573400

H	8.09830700	5.49942000	-4.30389700
C	7.94577900	3.79062800	-3.00416800
H	6.90971900	3.98603100	-2.74065200
C	6.22141400	-3.92650200	-2.76502500
C	5.02209600	-4.45359200	-3.27068800
H	4.07599400	-4.05622800	-2.91337100
C	5.03265100	-5.47126600	-4.22515600
H	4.09273100	-5.86184100	-4.60619800
C	6.24499400	-5.98380900	-4.69002400
H	6.25428700	-6.77757000	-5.43213400
C	7.44537000	-5.47264200	-4.19280300
H	8.39418800	-5.87138800	-4.54220700
C	7.43354300	-4.45397200	-3.23959400
H	8.36921700	-4.06579900	-2.84726300
C	0.82689200	-4.22847700	2.69661500
C	0.14375100	-3.65041300	1.48271700
C	0.35798900	-2.34616800	1.01426800
H	1.03523100	-1.67815300	1.53936100
O	0.27946600	-5.10298000	3.35907400
N	2.07343000	-3.70976500	2.96488900
N	-3.54064200	-4.34445300	-1.51648600
H	2.47205300	-3.10312900	2.26011700
H	-3.64327800	-3.35507100	-1.33569700
H	-2.37526400	-1.01051500	3.51228600
C	-3.28775500	-0.46204500	3.73703700
C	-3.91159800	-0.63981100	4.97318500
C	-3.82009000	0.41246700	2.78072100
C	-5.08433500	0.05643500	5.26731400
H	-3.48123000	-1.32145000	5.70185400
C	-4.99954200	1.10592800	3.08617900
C	-5.62697300	0.92783700	4.31954200
H	-5.57295800	-0.07779600	6.22879100
H	-5.43688200	1.78135900	2.35850700
H	-6.54266900	1.47115800	4.53557500
H	3.47150500	5.99613200	-2.54665800
C	3.34244400	5.01171800	-2.10485200
C	2.27248300	4.20413600	-2.49156300
C	4.24318500	4.54879400	-1.14272400
C	2.11017000	2.94101600	-1.91896100
H	1.56059000	4.55650100	-3.23332400
C	4.07407000	3.28900600	-0.56668800
H	5.07900400	5.16821800	-0.82919400
C	3.00306000	2.46942700	-0.94871400
H	1.27750500	2.31298300	-2.22958400

H	4.77952700	2.94588500	0.18214000
C	2.77589500	1.10869600	-0.31142200
H	1.89466100	0.67084900	-0.80428600
C	-3.11623400	0.57727400	1.44422500
H	-2.17145500	0.01954500	1.51293700
C	-2.78200400	2.02987600	1.09494700
H	-2.13258000	2.46167200	1.86348100
H	-2.26099200	2.08853100	0.13203900
H	-3.68527600	2.64095300	1.01833100
C	2.48087500	1.20663200	1.18932400
H	1.57155000	1.79273200	1.35789300
H	2.33890900	0.21230700	1.62816100
H	3.30779700	1.68410900	1.72129700
N	-3.93142600	-0.02708900	0.34078700
H	-3.31005600	-0.21941600	-0.44687700
H	-4.27003100	-0.93986100	0.64932800
N	3.94221100	0.19874700	-0.53427700
H	3.62423500	-0.76767700	-0.44162000
H	4.25855300	0.28975500	-1.50063000



“inside-inside” Conformer II•1S
 $\Delta H^\circ = -8683.31736109$ hartree

Cartesian coordinates for Geometry Optimized “inside-inside” **Conformer II•1S**

Atoms	x	y	z
Zn	5.37427300	0.53025700	-0.61765100
N	6.36040700	-1.05213800	0.33854500
N	4.94535800	-0.80669400	-2.18598000
N	5.01985100	2.07919300	-1.94398700
N	6.47214000	1.83329400	0.55741700
C	7.07705800	-0.96788500	1.50925900
C	6.33703000	-2.38258300	-0.00946200
C	5.09703100	-2.17339100	-2.16951100
C	4.32664600	-0.49533900	-3.37441700
C	4.43410000	1.99477700	-3.18574600
C	5.24261300	3.41468100	-1.70193400
C	6.41207400	3.20538800	0.49557400
C	7.12258400	1.52030000	1.72646400
C	7.49858200	-2.29047200	1.92205300

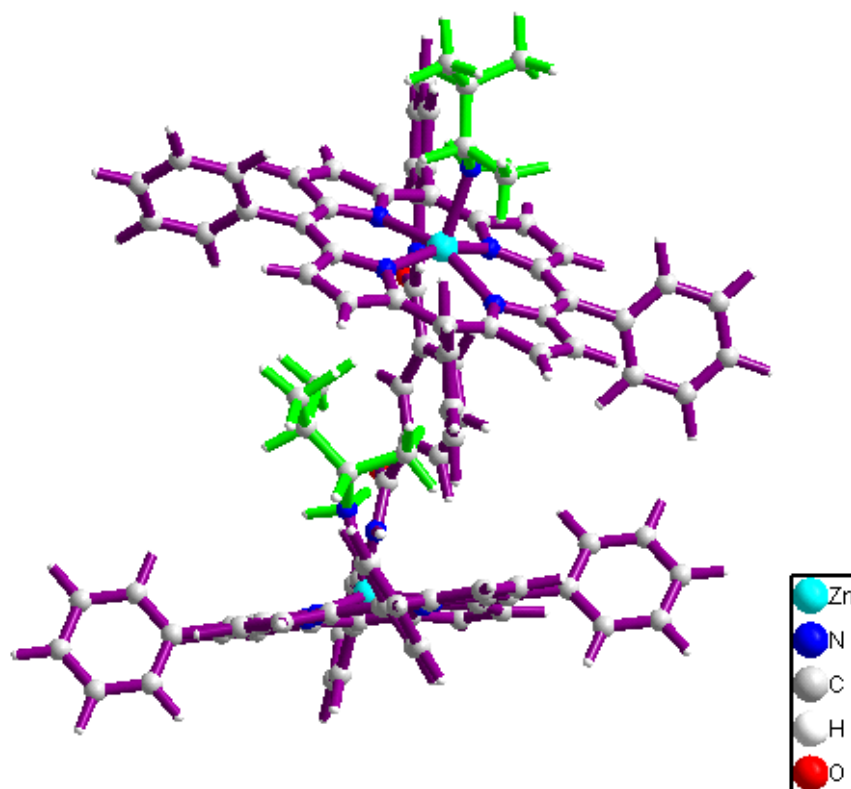
H	8.08754200	-2.51380000	2.79958000
C	7.03986100	-3.16375000	0.98632200
H	7.17315200	-4.23537000	0.95941500
C	4.52144400	-2.74590700	-3.36754900
H	4.51964700	-3.79760900	-3.61950400
C	4.02886200	-1.71098000	-4.10315800
H	3.53558700	-1.76278500	-5.06278800
C	4.29183700	3.32111200	-3.74673500
H	3.89430100	3.54713700	-4.72537800
C	4.78898200	4.19646100	-2.83032200
H	4.87267000	5.26979900	-2.92025100
C	7.01995900	3.77485400	1.67874000
H	7.09516500	4.82997900	1.89778100
C	7.45857600	2.73472500	2.43849400
H	7.95914800	2.78183300	3.39457200
C	5.74854200	-2.92396700	-1.16987600
C	4.06827200	0.80643300	-3.85099000
C	5.84919400	3.95855600	-0.55280000
C	7.41493800	0.22021700	2.18654300
C	5.94504400	-4.39859700	-1.39916300
C	7.19536900	-4.84602900	-1.84864500
H	7.96364200	-4.10524400	-2.05172600
C	7.46768200	-6.20135600	-2.02029600
H	8.44695100	-6.52145700	-2.36454800
C	6.47214400	-7.13671600	-1.73629300
H	6.66784500	-8.19889500	-1.85610900
C	5.21522000	-6.72432000	-1.30328200
H	4.44600000	-7.44827800	-1.07332800
C	4.93983700	-5.35695700	-1.14007700
C	3.40997700	0.94666400	-5.19022300
C	4.06282000	0.53569500	-6.36394100
H	5.06092300	0.11266500	-6.29414500
C	3.45081600	0.67701400	-7.60997500
H	3.97614800	0.35717300	-8.50609300
C	2.17398400	1.23357600	-7.70775200
H	1.69786300	1.34308700	-8.67840000
C	1.51491400	1.65130200	-6.55048100
H	0.52037600	2.08491800	-6.61418800
C	2.12914200	1.51130100	-5.30472100
H	1.61302300	1.84103200	-4.40724800
C	5.91437400	5.45228400	-0.44969900
C	7.14026600	6.12946100	-0.54505400
H	8.05070900	5.55770800	-0.70194500
C	7.19629500	7.52062300	-0.45048200

H	8.15422200	8.02764700	-0.53221900
C	6.02715900	8.25879100	-0.25706600
H	6.07089100	9.34212700	-0.18270600
C	4.80172000	7.59687500	-0.16021100
H	3.88699000	8.16312200	-0.00475300
C	4.74564400	6.20589200	-0.25705100
H	3.79214800	5.69155100	-0.17237100
C	8.17243600	0.09137700	3.47322900
C	7.56972800	-0.47181900	4.60909900
H	6.53874200	-0.80993400	4.54994000
C	8.27510800	-0.59588000	5.80665700
H	7.78845200	-1.03083700	6.67571900
C	9.59880000	-0.16030400	5.88926800
H	10.14921400	-0.25755800	6.82119500
C	10.21159900	0.39915400	4.76650500
H	11.24399000	0.73492100	4.81912200
C	9.50481300	0.52393100	3.56994400
H	9.98704700	0.95170000	2.69545400
C	2.67875500	-5.61337400	-0.09347700
C	1.34234300	-4.92720400	-0.00476300
C	0.52657400	-5.23666200	1.08728400
H	0.88457800	-5.91634700	1.85204400
C	0.85236700	-4.08379300	-1.01316000
H	1.45759300	-3.86180900	-1.88852600
C	-0.44535900	-3.57799900	-0.93197800
H	-0.84024900	-2.96412400	-1.73505500
O	2.85336600	-6.72508800	0.38907600
Zn	-5.39709900	0.30905600	0.63555100
N	-5.56970700	-1.75762300	0.56244200
N	-4.91258900	0.14819000	2.65188400
N	-5.92800600	2.31859600	1.01795800
N	-6.57110700	0.40787800	-1.07861900
C	-6.05112000	-2.50227800	-0.48876900
C	-5.26341400	-2.64809700	1.56570000
C	-4.61351600	-1.00589100	3.33332000
C	-4.65444400	1.19056200	3.51155400
C	-5.55478800	3.06038300	2.11203800
C	-6.48381600	3.19414300	0.11804700
C	-6.98604700	1.55860500	-1.70846900
C	-6.79778600	-0.62421400	-1.95748200
C	-6.02980000	-3.90791500	-0.14200400
H	-6.37774400	-4.71322600	-0.77200400
C	-5.55079800	-3.99715600	1.12757900
H	-5.43153500	-4.88790400	1.72763600

C	-4.11909700	-0.68162700	4.65457000
H	-3.81205500	-1.40061200	5.40021400
C	-4.14267600	0.67381400	4.76446800
H	-3.87071400	1.27007900	5.62320300
C	-5.88881600	4.45301000	1.89468900
H	-5.70487300	5.25912500	2.58979000
C	-6.47973000	4.53208700	0.67129700
H	-6.87596600	5.41245000	0.18631300
C	-7.45029700	1.24422100	-3.04217000
H	-7.81501900	1.96100600	-3.76336700
C	-7.32980300	-0.10190200	-3.19791400
H	-7.57349500	-0.68754200	-4.07206700
C	-4.78954200	-2.32120000	2.85321000
C	-4.92522700	2.55304300	3.26967000
C	-6.96949700	2.85807600	-1.16175900
C	-6.57266900	-1.99319500	-1.69524000
C	-4.61030400	-3.44305200	3.84048600
C	-5.55262400	-3.56844100	4.87142900
H	-6.36545700	-2.84904800	4.91163800
C	-5.47377700	-4.58493800	5.82052900
H	-6.22215900	-4.65859400	6.60439000
C	-4.42758500	-5.50278700	5.74331800
H	-4.34588000	-6.30399400	6.47304000
C	-3.47135000	-5.40930300	4.73525500
H	-2.65709600	-6.11625300	4.67529900
C	-3.55321500	-4.38501700	3.77630100
C	-4.54819900	3.53072200	4.34132400
C	-5.52902300	4.22138900	5.07092900
H	-6.57754700	4.03331700	4.85794300
C	-5.17132700	5.13275300	6.06530500
H	-5.94657600	5.65344300	6.62132000
C	-3.82555200	5.36925500	6.35181200
H	-3.54760300	6.07862400	7.12661000
C	-2.83942900	4.68518000	5.63893700
H	-1.78876900	4.86139500	5.85457700
C	-3.19914400	3.77497500	4.64431100
H	-2.42915000	3.24056000	4.09363900
C	-7.52458800	3.96781800	-2.00401600
C	-8.90100700	4.04229600	-2.26994400
H	-9.56179900	3.28788300	-1.85220200
C	-9.42324600	5.07277600	-3.05254200
H	-10.49246700	5.11512800	-3.24300600
C	-8.57759700	6.04783700	-3.58471200
H	-8.98372300	6.85022300	-4.19478600

C	-7.20684600	5.98585600	-3.32798600
H	-6.53998700	6.73819600	-3.74121300
C	-6.68606700	4.95540600	-2.54404700
H	-5.61784000	4.90843000	-2.35019400
C	-6.96066900	-2.98336500	-2.74901200
C	-5.99911600	-3.82651600	-3.33126900
H	-4.96409000	-3.75050000	-3.00997900
C	-6.35669500	-4.75367800	-4.31086700
H	-5.59528700	-5.39252700	-4.75067200
C	-7.68564300	-4.86025100	-4.72428600
H	-7.96543200	-5.58327700	-5.48570600
C	-8.65369100	-4.03504500	-4.14874900
H	-9.69309700	-4.11807000	-4.45541000
C	-8.29494900	-3.10687600	-3.17094500
H	-9.05397300	-2.47617400	-2.71722400
C	-1.54325700	-5.07581500	2.43136800
C	-0.75744300	-4.69418400	1.20174300
C	-1.24784100	-3.88221500	0.16769300
H	-2.27006900	-3.51480200	0.18201600
O	-1.21534900	-6.04948800	3.10136100
N	-2.60636100	-4.25375700	2.73740300
N	3.65429900	-4.90602100	-0.76713000
H	-2.74195400	-3.44049500	2.15279900
H	3.47198300	-3.92812800	-0.94852200
H	0.59006700	1.82107600	2.83462400
C	0.78472700	2.32877100	1.89200800
C	0.01472800	3.43558000	1.53689900
C	1.81053200	1.86238900	1.05480600
C	0.24929900	4.09284100	0.32514900
H	-0.76738300	3.78768800	2.20516300
C	2.03796900	2.52728600	-0.15543500
C	1.25997700	3.63279300	-0.51834600
H	-0.34976400	4.95545200	0.04585600
H	2.83419700	2.20197400	-0.81528400
H	1.45876300	4.13272400	-1.46261000
C	2.64372200	0.67558900	1.51782200
H	1.94222300	-0.06819600	1.92730500
C	3.61615200	1.06691100	2.63858000
H	3.06406600	1.44146600	3.50598900
H	4.20706600	0.20126300	2.95950200
H	4.30252500	1.84599100	2.29866000
N	3.40946700	0.04718600	0.40439000
H	3.75866700	-0.85152900	0.74030100
H	2.77420200	-0.17745400	-0.36319400

H	0.09017400	0.63469100	-1.87401900
C	-0.72000100	0.05842100	-2.31719100
C	-0.52647300	-0.57964200	-3.54311900
C	-1.94964300	-0.02214700	-1.64857900
C	-1.57292500	-1.29600100	-4.12922300
H	0.43331200	-0.50447900	-4.04628300
C	-2.99039400	-0.74808600	-2.24149100
C	-2.80469100	-1.37347100	-3.47718200
H	-1.43055200	-1.78221900	-5.09061800
H	-3.95187400	-0.82095500	-1.74560200
H	-3.63040600	-1.91478700	-3.93064700
C	-2.10195600	0.65781300	-0.29860500
H	-1.38626500	1.49061000	-0.27238700
C	-1.77570200	-0.27522600	0.87349300
H	-1.85254800	0.25748000	1.82770900
H	-2.47667100	-1.11441700	0.89487700
H	-0.75992500	-0.66958100	0.77707700
N	-3.47827100	1.19724600	-0.10770000
H	-3.44529600	1.88791000	0.64271000
H	-3.75729000	1.71861400	-0.94018600



“inside-outside” **Conformer I•5S**
 $\Delta H^\circ = -8457.11073556$ hartree

Cartesian coordinates for Geometry Optimized “inside-outside” **Conformer I•5S**

Atoms	x	y	z
Zn	4.52919400	0.12387200	-0.05635200
N	4.49114000	-0.79388500	-1.94735500
N	4.21288700	-1.77818600	0.76923700
N	3.74088700	0.92988400	1.68958900
N	4.13698200	1.92708800	-1.00481400
C	4.55154200	-0.15390500	-3.16270300
C	4.63951600	-2.13601300	-2.20385400
C	4.40969400	-2.98317500	0.13859500
C	3.98179800	-2.05944800	2.09469500
C	3.60713300	0.28012400	2.89337000
C	3.56986200	2.27037900	1.94570000
C	3.84735500	3.12158500	-0.38898300
C	4.22080900	2.18795300	-2.35146200
C	4.75453600	-1.12571600	-4.21798900

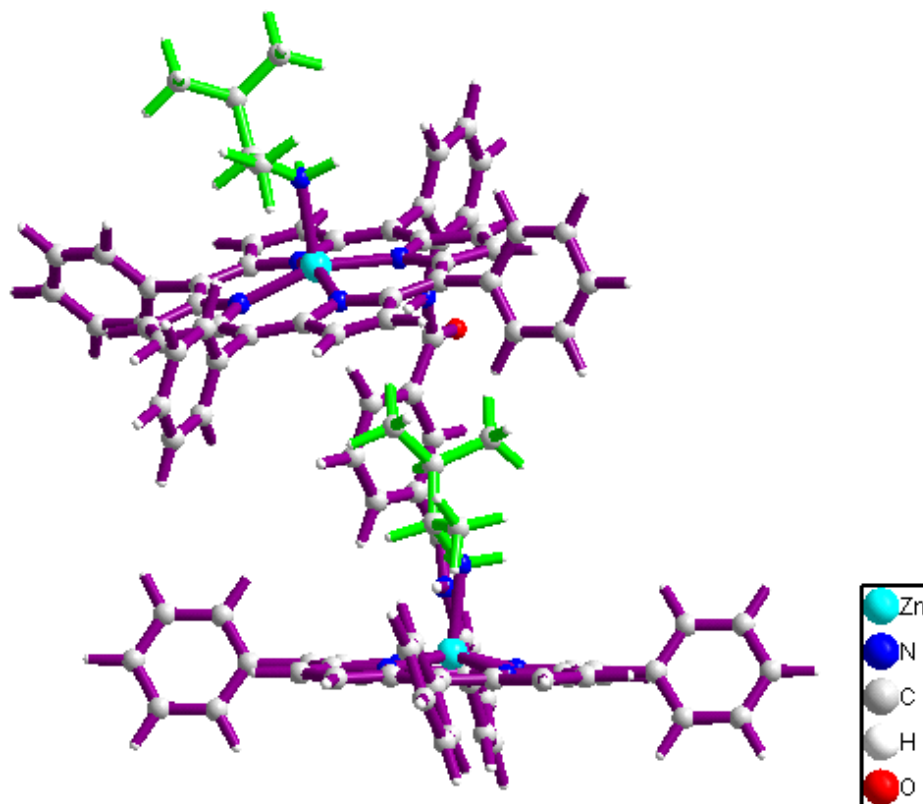
H	4.84575100	-0.89848700	-5.27011100
C	4.80022300	-2.34984000	-3.62712500
H	4.92730200	-3.31082900	-4.10430200
C	4.31530500	-4.06126900	1.10105500
H	4.43447500	-5.11222800	0.87763400
C	4.03412300	-3.49211000	2.30560200
H	3.87197900	-3.99342900	3.24873100
C	3.36607000	1.24479900	3.94517700
H	3.23893100	1.01163700	4.99215300
C	3.34491000	2.47290400	3.36089100
H	3.19738000	3.42878600	3.84176300
C	3.74776200	4.17037200	-1.38066300
H	3.50286800	5.20251300	-1.17627200
C	3.97720000	3.59417600	-2.59201100
H	3.95567700	4.06804600	-3.56260400
C	4.62513100	-3.16898600	-1.24351100
C	3.70558400	-1.11188600	3.10072200
C	3.61592100	3.30586500	0.98946700
C	4.44019500	1.23516600	-3.36796500
C	4.84843400	-4.57095800	-1.74201300
C	6.14058900	-4.98116500	-2.09030600
H	6.95553400	-4.27198300	-1.97224200
C	6.39553700	-6.26243700	-2.57742500
H	7.40833600	-6.55611000	-2.83819800
C	5.33477800	-7.15519900	-2.72522600
H	5.51228900	-8.15703800	-3.10713300
C	4.03481400	-6.78110500	-2.39140400
H	3.20741600	-7.46569800	-2.51220900
C	3.78188800	-5.49212700	-1.89460700
C	3.47362300	-1.62155700	4.49082300
C	4.51178000	-2.21256200	5.22828500
H	5.49943200	-2.29301100	4.78233400
C	4.29072800	-2.68683900	6.52200100
H	5.10925400	-3.13721700	7.07750700
C	3.02592400	-2.57800700	7.10286900
H	2.85416300	-2.94618100	8.11082200
C	1.98385200	-1.99238000	6.38131000
H	0.99353000	-1.90311400	6.82007700
C	2.20626900	-1.51992800	5.08744900
H	1.39004500	-1.07075200	4.52844600
C	3.38269800	4.70655400	1.46841700
C	4.41695000	5.65564200	1.42906200
H	5.39193400	5.36126800	1.05035800
C	4.20867700	6.96043300	1.87722000

H	5.02446100	7.67803100	1.84386400
C	2.95952900	7.34128300	2.37072800
H	2.79683800	8.35738600	2.72036300
C	1.92045200	6.40951000	2.41169600
H	0.94064200	6.69715100	2.78243200
C	2.13084600	5.10431400	1.96412400
H	1.31631100	4.38579600	1.99087400
C	4.52804300	1.74041800	-4.77639100
C	3.52098300	1.45119300	-5.71100700
H	2.66827400	0.85285600	-5.40180100
C	3.60232100	1.92673900	-7.02040900
H	2.81009700	1.69504800	-7.72750800
C	4.69340100	2.70080600	-7.41969500
H	4.75718000	3.07091500	-8.43940600
C	5.70147900	2.99673600	-6.50050400
H	6.55648400	3.59588100	-6.80286400
C	5.61824800	2.52136500	-5.19115300
H	6.40637400	2.75074300	-4.47910300
C	1.31233600	-5.77804300	-1.49879400
C	0.16149300	-5.07224500	-0.82788800
C	-1.13131800	-5.48537900	-1.16753100
H	-1.26571700	-6.27736600	-1.89572500
C	0.33212200	-4.09155100	0.16150500
H	1.32445000	-3.80238700	0.49638000
C	-0.78035100	-3.52809900	0.78615800
H	-0.64130200	-2.79829100	1.57909700
O	1.17548900	-6.89894700	-1.97577600
Zn	-4.51306500	0.75941600	0.31620600
N	-4.96295800	-0.95205600	1.41700500
N	-5.83249500	0.04883400	-1.16489100
N	-4.77552000	2.66719900	-0.49344800
N	-3.91530200	1.66284400	2.09000400
C	-4.56287400	-1.21763000	2.70460900
C	-5.65468600	-2.05787800	0.98302200
C	-6.32541400	-1.22759200	-1.27769300
C	-6.18167600	0.70682200	-2.31957200
C	-5.30336000	2.97117900	-1.72442500
C	-4.27475600	3.83871700	0.02042400
C	-3.47376100	2.95727100	2.21983600
C	-3.55494000	1.00509700	3.24166900
C	-5.02513500	-2.53274600	3.09798700
H	-4.88190600	-2.98170300	4.07013000
C	-5.70059700	-3.05083100	2.03539600
H	-6.20888500	-4.00293900	1.97357900

C	-6.98200900	-1.39060100	-2.55903000
H	-7.45569300	-2.29628800	-2.90876500
C	-6.90287600	-0.19257400	-3.19754300
H	-7.30664100	0.06765100	-4.16526700
C	-5.12269600	4.38133200	-1.99970800
H	-5.44239100	4.89036900	-2.89725100
C	-4.50174000	4.91990400	-0.91629800
H	-4.22925400	5.95334400	-0.75923200
C	-2.78309700	3.11262800	3.48201200
H	-2.31956900	4.02218600	3.83543900
C	-2.82823500	1.90628300	4.11059300
H	-2.40678400	1.64847400	5.07119400
C	-6.24535300	-2.22813000	-0.28798600
C	-5.93299100	2.06438300	-2.60173500
C	-3.64591900	3.98798500	1.27307100
C	-3.85220100	-0.33931300	3.54828000
C	-6.84499100	-3.56913900	-0.60794300
C	-8.23446000	-3.72800400	-0.66485400
H	-8.86092100	-2.86732300	-0.44777500
C	-8.81530200	-4.95382700	-0.98958800
H	-9.89658500	-5.05183800	-1.02459400
C	-7.99333900	-6.04534800	-1.26874300
H	-8.43004800	-7.00593900	-1.52886500
C	-6.60575400	-5.92519400	-1.21887600
H	-5.96147300	-6.76455900	-1.44088600
C	-6.02485300	-4.69348600	-0.88183500
C	-6.40676800	2.59041000	-3.92417600
C	-7.50441200	3.46182700	-4.00206400
H	-8.01510300	3.75245500	-3.08818200
C	-7.94574000	3.94679800	-5.23395700
H	-8.80007000	4.61761000	-5.27343900
C	-7.29811300	3.56722600	-6.41114100
H	-7.64224600	3.94410000	-7.37060000
C	-6.20703800	2.69886300	-6.34801900
H	-5.69522300	2.39856300	-7.25870000
C	-5.76620200	2.21552600	-5.11524000
H	-4.91435800	1.54230600	-5.06948600
C	-3.14310500	5.35243900	1.63471500
C	-3.73776100	6.08183300	2.67731800
H	-4.57061300	5.64402800	3.22026400
C	-3.28078300	7.35738800	3.01011500
H	-3.75963700	7.90741300	3.81609000
C	-2.21984100	7.92939900	2.30524800
H	-1.86732400	8.92532600	2.56042500

C	-1.61845500	7.21542800	1.26638000
H	-0.78975400	7.64909300	0.71303200
C	-2.07574000	5.93834500	0.93617900
H	-1.60298000	5.38502300	0.12949200
C	-3.41053900	-0.86887000	4.87758000
C	-2.47550900	-1.91379800	4.95658400
H	-2.07004300	-2.33225700	4.03943400
C	-2.06416900	-2.41833700	6.19122900
H	-1.34175500	-3.22975300	6.22680900
C	-2.58068700	-1.88488600	7.37388500
H	-2.26505200	-2.27925700	8.33614600
C	-3.51248500	-0.84684000	7.31117300
H	-3.92793000	-0.43123400	8.22552000
C	-3.92368400	-0.34521200	6.07585900
H	-4.65858600	0.45352500	6.03176500
C	-3.61049400	-5.41941500	-0.97018900
C	-2.25100500	-4.90336700	-0.56702300
C	-2.06777500	-3.92460500	0.42414600
H	-2.91693800	-3.51468000	0.96502400
O	-3.75606600	-6.54845300	-1.42464000
N	-4.63097800	-4.51599700	-0.78265300
N	2.49275000	-5.06700900	-1.51724800
H	-4.35859100	-3.58696000	-0.49381900
H	2.44865900	-4.10931700	-1.19615400
C	-0.11110300	-0.48269100	-2.39834400
C	-0.74818700	0.90109900	-2.19669600
H	0.71550600	-0.65033300	-1.69880900
H	-0.83331600	-1.29820300	-2.27059500
C	0.29574500	2.01544400	-2.36103300
H	-1.49855800	1.04189900	-2.99239900
C	-1.52686500	1.04702900	-0.86200700
H	-0.15102200	3.00686000	-2.21777200
H	1.12025500	1.90771200	-1.64818400
H	-1.90116700	2.07705300	-0.82141000
C	-0.69816700	0.78406400	0.39670300
N	-2.74314500	0.18290300	-0.82215900
H	-1.29448100	0.97517000	1.29331000
H	-0.34730100	-0.25463500	0.43378400
H	0.18311400	1.43100600	0.43120800
H	-3.16460800	0.14841800	-1.75215000
H	-2.47473600	-0.77851200	-0.60620200
H	0.29889800	-0.56875400	-3.41083900
H	0.73236500	1.99054600	-3.36565500
H	6.91812500	-0.58495700	-0.63862600

N	6.70165500	0.03626300	0.14291800
C	7.57450100	1.24145900	0.07869900
H	6.90545800	-0.49970100	0.98750700
C	9.03557300	0.89135500	-0.31277800
H	7.16215600	1.85597300	-0.73100700
C	7.42962300	2.01910500	1.38824100
C	9.77233500	0.04050800	0.73349200
C	9.84264100	2.15128000	-0.66206000
H	8.96114000	0.29175500	-1.23455900
H	6.38321300	2.28386600	1.56071300
H	7.77389900	1.43075500	2.24755100
H	8.01314700	2.94419800	1.36183800
H	9.94409400	0.60014200	1.66013200
H	9.22131300	-0.87272800	0.98890700
H	10.75163100	-0.26928800	0.35225300
H	9.32331700	2.76639500	-1.40673500
H	10.02239500	2.77360500	0.22221500
H	10.82050400	1.88079400	-1.07588900



“inside-outside” **Conformer II•5S**
 $\Delta H^\circ = -8457.10850551$ hartree

Cartesian coordinates for Geometry Optimized “inside-outside” **Conformer II•5S**

Atoms	x	y	z
Zn	-4.91837300	0.47914500	-0.59325500
N	-4.18210700	-0.27675400	-2.40459800
N	-5.02154900	-1.51510400	0.08461400
N	-4.92099400	1.06407200	1.39957800
N	-4.04694700	2.29642400	-1.07941200
C	-3.67776100	0.46017200	-3.44997400
C	-4.23663800	-1.58070300	-2.83452200
C	-5.04442700	-2.63360300	-0.71409100
C	-5.43158500	-1.91742000	1.33406400
C	-5.29309600	0.30054300	2.47998400
C	-4.73117600	2.34276100	1.86688200
C	-4.00569000	3.41036200	-0.27501900
C	-3.59866300	2.68726500	-2.31779100
C	-3.39245000	-0.41292700	-4.57061300
H	-2.96482600	-0.10166700	-5.51265500

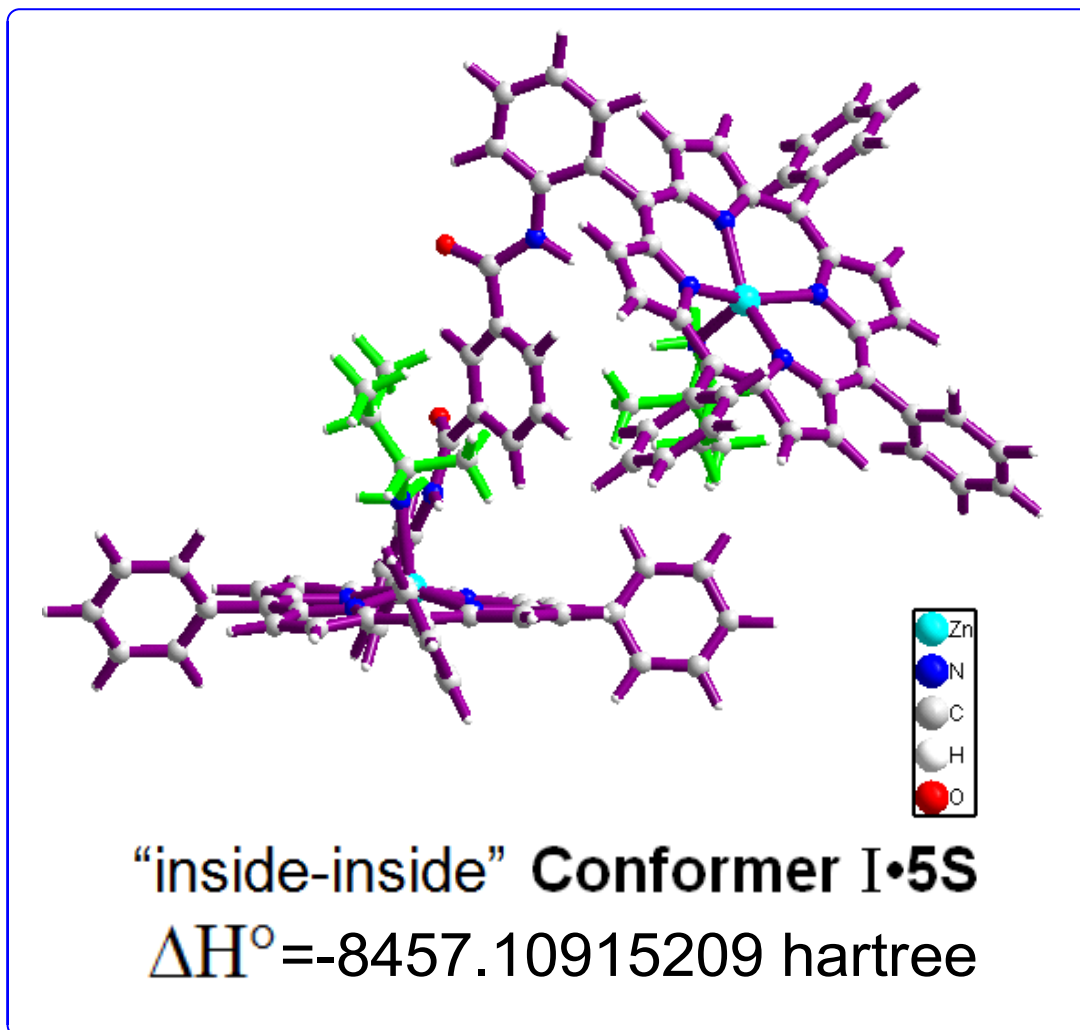
C	-3.74271600	-1.67211000	-4.19254100
H	-3.66041500	-2.58445800	-4.76606000
C	-5.49475100	-3.77672300	0.05215600
H	-5.61350200	-4.77981400	-0.33260300
C	-5.73505500	-3.33433600	1.31647700
H	-6.09063400	-3.91021500	2.15842200
C	-5.33961800	1.12669400	3.66768600
H	-5.58416200	0.78092300	4.66146800
C	-5.00333700	2.38899900	3.28728800
H	-4.93292900	3.26885500	3.91003100
C	-3.52871400	4.54480900	-1.03641500
H	-3.38751100	5.54329200	-0.64877200
C	-3.28944800	4.10162000	-2.30041300
H	-2.92512500	4.67369800	-3.14114800
C	-4.67659100	-2.68421900	-2.07583900
C	-5.56036600	-1.08483100	2.46374100
C	-4.32796100	3.45172400	1.09629600
C	-3.43013400	1.84696600	-3.43831200
C	-4.76726600	-4.01379900	-2.77242100
C	-5.83475200	-4.26697400	-3.64143100
H	-6.57206400	-3.48340000	-3.79450700
C	-5.96962000	-5.49060100	-4.29605100
H	-6.81020000	-5.66399400	-4.96192200
C	-5.01548900	-6.48421100	-4.08030400
H	-5.10427000	-7.44514900	-4.58005700
C	-3.93360800	-6.26372300	-3.23017400
H	-3.18691200	-7.02722700	-3.06592300
C	-3.79913300	-5.02936800	-2.57427800
C	-5.99820700	-1.72047200	3.74824800
C	-7.24028100	-1.40248900	4.32043300
H	-7.88731800	-0.68889900	3.81760200
C	-7.65154800	-1.99495200	5.51490100
H	-8.61930400	-1.73853600	5.93809700
C	-6.82628600	-2.91703300	6.16112400
H	-7.14577800	-3.37938100	7.09117100
C	-5.58762300	-3.24123700	5.60477000
H	-4.93595200	-3.95453200	6.10252900
C	-5.17793600	-2.64839400	4.40985700
H	-4.21072700	-2.89919200	3.98325600
C	-4.20009100	4.77318300	1.79479300
C	-5.11689200	5.80681900	1.54925400
H	-5.93076800	5.63833300	0.84917700
C	-4.99712500	7.03774100	2.19606800
H	-5.71971800	7.82441100	1.99486100

C	-3.95660200	7.25665600	3.10056300
H	-3.86262200	8.21484100	3.60453000
C	-3.03689300	6.23703600	3.35282100
H	-2.22033800	6.39923000	4.05155400
C	-3.15776800	5.00665100	2.70543000
H	-2.43674600	4.21733000	2.89930300
C	-2.92245700	2.46676200	-4.70566000
C	-1.60919100	2.95470200	-4.79840300
H	-0.95319900	2.87785500	-3.93566900
C	-1.13976100	3.52644600	-5.98161400
H	-0.11810300	3.89361100	-6.03370900
C	-1.97589100	3.62124000	-7.09557100
H	-1.61063700	4.06647200	-8.01709600
C	-3.28343700	3.13865300	-7.01830200
H	-3.94294200	3.20985000	-7.87933200
C	-3.75102400	2.56644300	-5.83452500
H	-4.77062300	2.19514500	-5.77726300
C	-1.69351600	-5.55661900	-1.30306900
C	-0.72070300	-4.92578500	-0.33834100
C	0.52929600	-5.54087600	-0.21815600
H	0.73687200	-6.43671200	-0.79215700
C	-1.00922800	-3.80387400	0.45471800
H	-1.99225500	-3.34038700	0.43803700
C	-0.04689100	-3.29805100	1.32900800
H	-0.28864800	-2.44923500	1.96250300
O	-1.54240000	-6.71216500	-1.68451000
Zn	5.02354100	0.50751300	0.53700100
N	4.82052400	-0.83980300	2.13312800
N	6.15228800	-0.96863500	-0.44164000
N	5.95130800	1.90992700	-0.69011900
N	4.58678200	2.03819000	1.86795600
C	4.22242400	-0.57426000	3.34056900
C	5.18496900	-2.16485700	2.15776100
C	6.29545500	-2.28527600	-0.07956300
C	6.74373100	-0.83416500	-1.67404300
C	6.53138100	1.64611400	-1.90718100
C	5.79750100	3.27247400	-0.61400900
C	4.65856500	3.38605400	1.61029900
C	3.99923800	1.90326200	3.10306100
C	4.18958800	-1.77724300	4.14673900
H	3.79619800	-1.84675300	5.15071500
C	4.79436800	-2.75761900	3.42043500
H	4.98966600	-3.77834300	3.71896600
C	6.98441000	-3.01101100	-1.12698800

H	7.23082600	-4.06253800	-1.10097000
C	7.26102400	-2.11487400	-2.11176500
H	7.78644700	-2.29428800	-3.03851900
C	6.72718000	2.88339100	-2.63344800
H	7.14658500	2.96866900	-3.62526500
C	6.28288900	3.88823200	-1.83133600
H	6.26993500	4.94685500	-2.04635900
C	4.09165800	4.12508200	2.71824100
H	4.03750200	5.20149300	2.79050800
C	3.66656000	3.20962800	3.63024800
H	3.19067000	3.39912900	4.58128000
C	5.85831700	-2.86049300	1.13151900
C	6.89599800	0.37140200	-2.38847300
C	5.21394500	3.97909700	0.45781300
C	3.78984400	0.68982500	3.78891400
C	6.20199400	-4.30660100	1.36365000
C	7.52587400	-4.65653000	1.65777800
H	8.26236400	-3.86172600	1.73530700
C	7.90643800	-5.98456500	1.84449400
H	8.94033600	-6.22848400	2.07157400
C	6.94633600	-6.98973700	1.73194500
H	7.22558800	-8.03120500	1.86782000
C	5.61889600	-6.67798200	1.44655800
H	4.87305500	-7.45374600	1.34618100
C	5.23729100	-5.33878200	1.26849800
C	7.53308900	0.29277100	-3.74269800
C	8.80650800	0.83665400	-3.97577500
H	9.33515500	1.31607800	-3.15665500
C	9.39812400	0.75689600	-5.23700100
H	10.38709600	1.17933700	-5.39502800
C	8.72748600	0.13131100	-6.28967200
H	9.18863100	0.06895800	-7.27175500
C	7.46187700	-0.41576700	-6.07162700
H	6.93058900	-0.90365000	-6.88473500
C	6.87179900	-0.33586300	-4.80963900
H	5.88533500	-0.76079600	-4.64485500
C	5.18568500	5.47475500	0.36446700
C	6.37691800	6.21662000	0.41008700
H	7.32207000	5.69251000	0.52087000
C	6.35631500	7.60925400	0.32453200
H	7.28959400	8.16483300	0.36708100
C	5.14301700	8.28688600	0.19133800
H	5.12658700	9.37152000	0.12500000
C	3.95099100	7.56180500	0.14419300

H	3.00134900	8.07953700	0.03590700
C	3.97283600	6.16915000	0.23013200
H	3.04323500	5.60833500	0.18724300
C	3.11895100	0.74893700	5.12857200
C	1.83032400	0.22192400	5.30569400
H	1.31836400	-0.22085200	4.45548500
C	1.20238500	0.26767000	6.55123300
H	0.20199100	-0.14168500	6.66591500
C	1.85478100	0.84019300	7.64447300
H	1.36715900	0.87542900	8.61505600
C	3.13862600	1.36486900	7.48355700
H	3.65761400	1.80598900	8.33061400
C	3.76471100	1.31879500	6.23735300
H	4.76719400	1.71973200	6.11691400
C	2.81845900	-5.76120600	0.71901800
C	1.50776600	-5.02181800	0.63386900
C	1.21301700	-3.89295400	1.41348100
H	1.93944700	-3.50644800	2.12456200
O	2.87722000	-6.97042000	0.52871400
N	3.90072200	-4.96529400	1.01833600
N	-2.71966600	-4.73736700	-1.71662800
H	3.74287400	-3.96661300	1.01577400
H	-2.69924900	-3.77974000	-1.39337100
H	3.47310800	-0.15937200	-1.49791800
N	3.18643100	-0.00246000	-0.53052100
C	1.93949900	0.81507000	-0.50150100
H	2.98742500	-0.93015300	-0.15241900
C	0.69810500	0.01596500	-0.98116000
H	1.77837300	1.06127500	0.55547700
C	2.19058600	2.11760700	-1.26265800
C	0.74062800	-0.36427200	-2.46982500
C	-0.60738000	0.75006400	-0.64037100
H	0.70103600	-0.92126100	-0.40211500
H	3.02530700	2.66526600	-0.81929100
H	2.43413700	1.92723500	-2.31487000
H	1.30676100	2.76198500	-1.23348000
H	0.66175400	0.51807300	-3.11555000
H	1.66096900	-0.89766800	-2.73890800
H	-0.09918200	-1.02190800	-2.71861700
H	-0.66003400	1.00257800	0.42569900
H	-0.71115500	1.68140600	-1.20833700
H	-1.47797400	0.13140200	-0.88182100
H	-7.22803800	-0.47483400	-1.12388500
N	-7.01229400	0.52035700	-1.20664800

C	-8.04666100	1.31815900	-0.49012100
H	-7.03891700	0.72759300	-2.20587400
C	-9.47170600	0.72986000	-0.67043100
H	-7.79619700	1.23316800	0.57431700
C	-7.89923600	2.78494400	-0.89870600
C	-9.98799900	0.78143500	-2.11692400
C	-10.47609500	1.37794600	0.29476100
H	-9.39191900	-0.33159400	-0.38513400
H	-6.88160300	3.13229300	-0.69978600
H	-8.10293500	2.92785900	-1.96702000
H	-8.59198300	3.41904900	-0.33761200
H	-10.15943500	1.81200700	-2.44859200
H	-9.29190900	0.31198300	-2.82261800
H	-10.94144900	0.24837000	-2.20068700
H	-10.11292400	1.35080300	1.32914500
H	-10.67040100	2.42490900	0.03409400
H	-11.43582900	0.85018600	0.26396100



Cartesian coordinates for Geometry Optimized “inside-inside” **Conformer I•5S**

Atoms	x	y	z
Zn	5.42951400	0.33893000	-0.75946600
N	4.05423500	0.29438100	-2.32609000
N	6.34378400	-1.34534800	-1.63264500
N	7.22402100	0.68598300	0.24803200
N	4.96061400	2.34328700	-0.48597700
C	3.11209500	1.25353100	-2.61138600
C	3.84885400	-0.73631000	-3.21115200
C	5.75086100	-2.20583200	-2.52395800
C	7.47214000	-1.97818200	-1.16821500
C	8.28571100	-0.17679000	0.36424300
C	7.53937400	1.80053500	0.98703300
C	5.52951200	3.18314500	0.44108600
C	3.83377900	2.97602300	-0.95291000
C	2.29056300	0.81635700	-3.72075700
H	1.49549900	1.39185800	-4.17303600

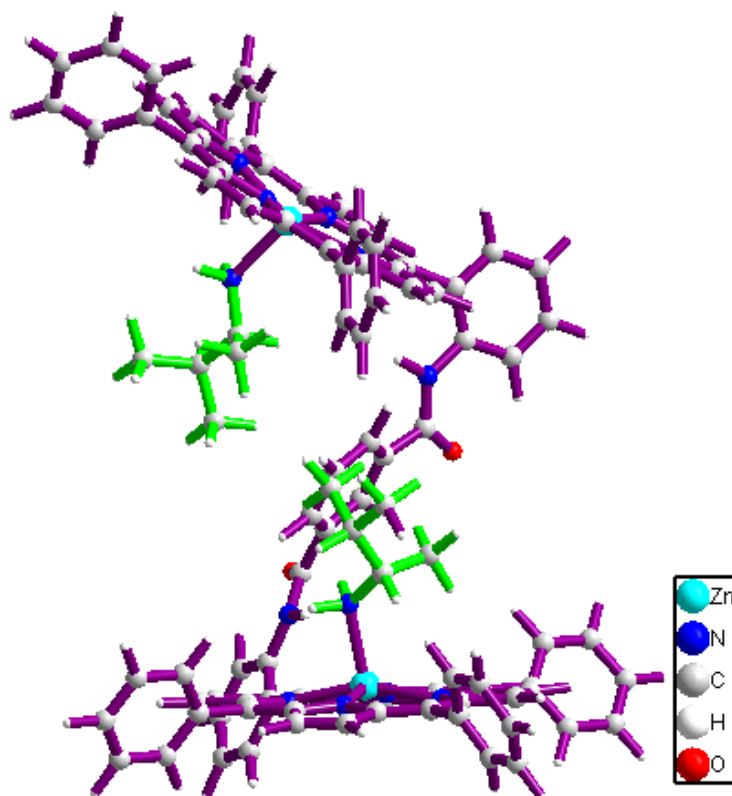
C	2.74388900	-0.41441500	-4.08988200
H	2.39067700	-1.03602800	-4.90114600
C	6.51049300	-3.43695900	-2.59902100
H	6.26070700	-4.29100100	-3.21158100
C	7.57437100	-3.29561500	-1.76367700
H	8.35410900	-4.01570400	-1.56280400
C	9.31307700	0.42034500	1.19189600
H	10.26996200	-0.02601600	1.42019600
C	8.85229300	1.64069100	1.57662400
H	9.36200000	2.37882400	2.17862500
C	4.70828300	4.36473200	0.59701700
H	4.90875700	5.18236400	1.27391900
C	3.66248400	4.23849300	-0.26627800
H	2.85054400	4.93299300	-0.42669100
C	4.58789600	-1.93788900	-3.27491200
C	8.39752800	-1.44237100	-0.24971300
C	6.73872800	2.95203200	1.12943000
C	2.96927200	2.49137900	-1.95530400
C	4.10495600	-3.01708400	-4.20415300
C	4.80227200	-3.30744100	-5.38233300
H	5.67526400	-2.70840000	-5.62588300
C	4.40139800	-4.33980000	-6.23071800
H	4.95912100	-4.54433500	-7.14012700
C	3.28494800	-5.10551200	-5.89539700
H	2.96583500	-5.91863700	-6.54193600
C	2.56266200	-4.84198800	-4.73279600
H	1.70194000	-5.43757000	-4.46036900
C	2.96124300	-3.79483100	-3.88980000
C	9.60351000	-2.26606100	0.08345800
C	10.56744300	-2.56078700	-0.89438700
H	10.43372600	-2.17629600	-1.90156000
C	11.69115600	-3.32679800	-0.58258700
H	12.42829800	-3.53891800	-1.35263100
C	11.87191200	-3.81400200	0.71321200
H	12.74664200	-4.41149000	0.95572500
C	10.92237100	-3.52773000	1.69565800
H	11.05229000	-3.90526100	2.70659300
C	9.80017500	-2.75972300	1.38319600
H	9.06128000	-2.54223400	2.14961000
C	7.22992600	4.02306000	2.05430300
C	7.61641500	5.28038200	1.56221000
H	7.56183700	5.46986300	0.49393000
C	8.07841200	6.27501200	2.42480700
H	8.37850000	7.23911000	2.02251400

C	8.16215000	6.03178100	3.79703200
H	8.52181100	6.80644700	4.46897000
C	7.78271200	4.78601700	4.30003000
H	7.84159400	4.58749700	5.36707000
C	7.32259100	3.79154400	3.43615600
H	7.02514500	2.82433100	3.83204900
C	1.83703200	3.37951200	-2.37793100
C	0.50874000	3.06411400	-2.05342900
H	0.30170800	2.15933200	-1.48784300
C	-0.54177400	3.90166300	-2.43254600
H	-1.56154600	3.65211400	-2.15178700
C	-0.27936500	5.06750700	-3.15413700
H	-1.09558300	5.72086100	-3.45061200
C	1.03661400	5.39095700	-3.49016400
H	1.24894200	6.29475600	-4.05541700
C	2.08537400	4.55620300	-3.10250600
H	3.10870600	4.80993400	-3.36482400
C	1.15950500	-4.04923800	-2.13862100
C	0.57712100	-3.24799500	-1.00021200
C	-0.02984100	-3.93407200	0.05695000
H	-0.03794300	-5.01881000	0.05918800
C	0.57873100	-1.84304600	-1.00296300
H	1.00305600	-1.29191600	-1.83838900
C	-0.00849800	-1.14123400	0.05036200
H	-0.00001600	-0.05452700	0.04806000
O	0.67649600	-5.12182100	-2.48233200
Zn	-5.43221800	0.36944900	0.75952700
N	-4.08691700	0.34848500	2.35088500
N	-6.33966400	-1.32433600	1.61695700
N	-7.21880700	0.70249000	-0.26773500
N	-4.97116800	2.37394600	0.47524500
C	-3.15037800	1.31294700	2.63751000
C	-3.89279100	-0.67045100	3.25200700
C	-5.79293000	-2.14642700	2.57133500
C	-7.47849500	-1.94864500	1.16703900
C	-8.24936000	-0.18935600	-0.43513400
C	-7.49476000	1.77921200	-1.07552000
C	-5.52826700	3.19959700	-0.47133400
C	-3.86117500	3.02225500	0.96061800
C	-2.34121600	0.88930800	3.76091000
H	-1.55280200	1.47124700	4.21654500
C	-2.79816500	-0.33720500	4.13949500
H	-2.45473900	-0.94798500	4.96306600
C	-6.60078700	-3.34106000	2.71276400

H	-6.39966200	-4.15629600	3.39228000
C	-7.64935200	-3.21161600	1.85672700
H	-8.47026200	-3.89841900	1.70997500
C	-9.20548100	0.34005300	-1.38564500
H	-10.11247900	-0.15386200	-1.70246300
C	-8.74539600	1.56000300	-1.77237700
H	-9.21096900	2.25426500	-2.45676700
C	-4.72242800	4.39361900	-0.61212000
H	-4.92193300	5.20671100	-1.29484500
C	-3.69363100	4.28530900	0.27359200
H	-2.89522800	4.99183900	0.44861700
C	-4.63881800	-1.86696000	3.33157700
C	-8.37449700	-1.43876400	0.20704200
C	-6.70531700	2.93945300	-1.20293800
C	-3.00565700	2.54735500	1.97505900
C	-4.16947200	-2.92822700	4.28843900
C	-4.86824300	-3.18558800	5.47317500
H	-5.73463900	-2.57236900	5.70476600
C	-4.47752800	-4.20460300	6.34245600
H	-5.03666200	-4.38430900	7.25622900
C	-3.36961700	-4.98908100	6.02243400
H	-3.05902200	-5.79220800	6.68540100
C	-2.64447600	-4.75635400	4.85503000
H	-1.78911000	-5.36530300	4.59533100
C	-3.03257600	-3.72249600	3.99119300
C	-9.56501700	-2.28192600	-0.14225500
C	-10.85367900	-1.91641600	0.27729200
H	-10.98212700	-1.01278600	0.86674600
C	-11.96036500	-2.70190400	-0.04807400
H	-12.94962900	-2.40387700	0.28943700
C	-11.79796800	-3.86828000	-0.79796100
H	-12.65967800	-4.48019900	-1.05086100
C	-10.52146400	-4.24432300	-1.21949500
H	-10.38472400	-5.14950500	-1.80543200
C	-9.41571600	-3.45753200	-0.89388900
H	-8.42401300	-3.75177700	-1.22698000
C	-7.16507600	3.98599300	-2.17270800
C	-7.64383000	5.22583500	-1.72009000
H	-7.68478900	5.41917300	-0.65178400
C	-8.07275900	6.19937200	-2.62316700
H	-8.44484400	7.15085500	-2.25218000
C	-8.03020400	5.95125700	-3.99638600
H	-8.36403100	6.70939900	-4.69977500
C	-7.55731000	4.72237500	-4.46010100

H	-7.51759200	4.52058100	-5.52741500
C	-7.12961600	3.74931000	-3.55590600
H	-6.75787300	2.79560500	-3.92069600
C	-1.87775400	3.43931400	2.40136500
C	-0.54752300	3.12185900	2.08675700
H	-0.33753500	2.21453300	1.52641000
C	0.50104300	3.96026700	2.46903700
H	1.52247600	3.70783000	2.19661900
C	0.23453600	5.12965300	3.18342600
H	1.04905800	5.78390400	3.48259900
C	-1.08348600	5.45536700	3.50921600
H	-1.29891400	6.36187500	4.06892700
C	-2.13030400	4.61927800	3.11890800
H	-3.15513000	4.87458700	3.37382800
C	-1.22462800	-4.01917800	2.25226400
C	-0.62710200	-3.23396300	1.11027500
C	-0.60706000	-1.82914700	1.10649600
H	-1.02488900	-1.26792200	1.93842900
O	-0.75365300	-5.09207900	2.61101100
N	-2.31606300	-3.40619700	2.82002300
N	2.25176600	-3.45240700	-2.72183800
H	-2.66014200	-2.58338900	2.34443500
H	2.60734200	-2.62691100	-2.25959900
C	-3.01527400	-2.40280000	-3.07922200
C	-4.25051300	-1.49766600	-3.20555400
H	-2.09584500	-1.87309100	-3.35317300
H	-2.88490400	-2.79535500	-2.06395400
C	-4.40987400	-0.98342300	-4.64452400
H	-5.13790200	-2.11362400	-2.98658100
C	-4.29005000	-0.33392200	-2.17904600
H	-5.29308300	-0.34111800	-4.74592700
H	-3.53455600	-0.40803900	-4.96800500
H	-5.20335500	0.23877300	-2.37902500
C	-3.09888700	0.62358300	-2.24509300
N	-4.42814800	-0.82315200	-0.77710800
H	-3.23249400	1.44101300	-1.53065100
H	-2.15903300	0.11037100	-2.00784400
H	-2.99995200	1.05903200	-3.24363700
H	-5.04500600	-1.63728300	-0.75946000
H	-3.52361400	-1.15499100	-0.43883700
H	-3.10484400	-3.26589900	-3.74767000
H	-4.52492900	-1.82107800	-5.34139600
H	5.06719500	-1.66888800	0.77266900
N	4.45128800	-0.85392000	0.79184500

C	4.33185600	-0.35593100	2.19255500
H	3.54210500	-1.18751900	0.46824700
C	4.29732400	-1.51446100	3.22525500
H	5.25089000	0.21255200	2.37831300
C	3.14669200	0.60845800	2.26777000
C	3.05731000	-2.41515300	3.11496000
C	4.47233000	-0.99404800	4.66022200
H	5.17972700	-2.13566200	3.00073000
H	3.27734700	1.42385000	1.55058800
H	2.20165000	0.09993700	2.04122700
H	3.06040100	1.04638100	3.26642900
H	2.14216100	-1.88031900	3.39322500
H	2.91721100	-2.81336400	2.10322000
H	3.14929000	-3.27454400	3.78781700
H	5.35744000	-0.35256700	4.74994500
H	3.60148500	-0.41545600	4.98987000
H	4.59258200	-1.82881600	5.35969200



“inside-inside” Conformer II•5S

$\Delta H^\circ = -8457.10486736$ hartree

Cartesian coordinates for Geometry Optimized “inside-inside” **Conformer II•5S**

Atoms	x	y	z
Zn	6.40964800	-0.01693100	0.47436100
N	6.16110000	0.42651300	2.51384800
N	5.92286500	-1.98376900	0.91220800
N	7.34197700	-0.68195400	-1.25453400
N	7.53074000	1.74917500	0.32140700
C	6.32075700	1.66219300	3.09605200
C	5.52343700	-0.36343400	3.43717200
C	5.42819700	-2.47325900	2.09687300
C	5.99013300	-3.04734900	0.04450600
C	7.11577800	-1.89240300	-1.86473200
C	8.02343500	0.09558300	-2.16061500
C	8.28018900	2.15051000	-0.75749400
C	7.59479300	2.76301800	1.24490900
C	5.72138600	1.66071200	4.41519800

H	5.68335600	2.50500300	5.08810500
C	5.23756000	0.40702600	4.62937600
H	4.73428600	0.03378700	5.50985600
C	5.18342100	-3.89521900	1.97525700
H	4.82096000	-4.53680600	2.76590900
C	5.52519600	-4.24845500	0.70756000
H	5.49610200	-5.23433400	0.26710300
C	7.63545100	-1.86237200	-3.21496100
H	7.57354500	-2.67074000	-3.92867000
C	8.19942200	-0.63703200	-3.39582000
H	8.68338900	-0.25960400	-4.28474900
C	8.85273000	3.45449100	-0.49679500
H	9.51388300	3.99218000	-1.16077200
C	8.42544600	3.83500500	0.73763000
H	8.67299400	4.74130200	1.27096500
C	5.19763900	-1.72642900	3.27139200
C	6.49020800	-3.01034200	-1.27200600
C	8.48778000	1.40876300	-1.93880400
C	6.98862700	2.76205100	2.52018400
C	4.64683100	-2.45544300	4.46480900
C	5.49062300	-2.72630300	5.55012900
H	6.52361000	-2.39544800	5.49221700
C	5.03701400	-3.41179700	6.67564700
H	5.71491800	-3.61519700	7.49969100
C	3.71002300	-3.83772600	6.72460000
H	3.33943600	-4.37659200	7.59251600
C	2.84076600	-3.57957900	5.66704600
H	1.81393600	-3.91499600	5.69733700
C	3.30080700	-2.88885100	4.53503700
C	6.38271400	-4.26433300	-2.08383600
C	7.52956100	-4.96832900	-2.48580900
H	8.50809100	-4.59597700	-2.19586000
C	7.42256800	-6.14009400	-3.23565400
H	8.32223100	-6.67376000	-3.53103500
C	6.16636800	-6.62997100	-3.59818500
H	6.08296700	-7.54295500	-4.18170000
C	5.01788200	-5.94153800	-3.20341300
H	4.03523000	-6.31407500	-3.48045400
C	5.12584500	-4.77068300	-2.45225800
H	4.22958900	-4.23665200	-2.14910500
C	9.27725900	2.05970200	-3.03302900
C	10.53456200	1.55998800	-3.40942300
H	10.93566500	0.69340100	-2.89152500
C	11.27129900	2.16882500	-4.42602600

H	12.24496600	1.76947200	-4.69777700
C	10.76449400	3.28927600	-5.08698800
H	11.33818600	3.76319300	-5.87898100
C	9.51622500	3.79730500	-4.72297800
H	9.11112900	4.66699200	-5.23392700
C	8.78145300	3.18850600	-3.70498400
H	7.80872800	3.58499100	-3.42667000
C	7.10234900	4.01423500	3.33497000
C	6.46557700	5.19638000	2.92416900
H	5.88157800	5.19173800	2.00772300
C	6.56950900	6.36637800	3.67725000
H	6.06442300	7.26905700	3.34321100
C	7.31626900	6.37677900	4.85664200
H	7.39901900	7.28753700	5.44371100
C	7.95850000	5.21001300	5.27546700
H	8.54871600	5.21019900	6.18816800
C	7.85252600	4.04042400	4.52193100
H	8.36132200	3.13702300	4.84603400
C	1.22841900	-3.12455100	3.13836100
C	0.60088600	-2.57610900	1.88339500
C	-0.17315700	-3.44856300	1.11363500
H	-0.26005100	-4.48871300	1.40706200
C	0.71649900	-1.23331800	1.49342300
H	1.28829500	-0.53687700	2.10209100
C	0.05925800	-0.77731400	0.34978000
H	0.14544400	0.26432200	0.05339500
O	0.66592100	-3.99281800	3.79521100
Zn	-6.43176900	0.53351100	-0.63006200
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N	-7.02629200	-1.46516500	-0.73436100
N	-8.32610300	0.96171600	0.18881900
N	-6.29139200	2.54249200	-1.14948300
C	-4.18873700	1.03276800	-2.70543400
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C	-6.33980900	-2.49194300	-1.33403900
C	-8.06984200	-2.03921400	-0.04764900
C	-9.20823900	0.05306200	0.71851200
C	-8.81418300	2.20819200	0.49278500
C	-7.02819300	3.57003100	-0.60969600
C	-5.24806600	3.12143500	-1.83012300
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H	-2.57935900	0.82460300	-4.26815900
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H	-3.12952300	-1.79427800	-4.07828100

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H	-6.61403100	-4.72880700	-1.32505400
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H	-8.72842700	-4.17677400	0.22617300
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C	-10.05636300	2.08165000	1.22753100
H	-10.66666600	2.90330800	1.57321900
C	-6.40709400	4.83729200	-0.93234600
H	-6.76398500	5.80766000	-0.61947200
C	-5.30859300	4.56051600	-1.68555700
H	-4.60057100	5.26308800	-2.10033700
C	-5.22742700	-2.35135200	-2.18990200
C	-9.08537400	-1.35019500	0.64543600
C	-8.21060900	3.43449600	0.14696300
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C	-4.70899600	-3.60295800	-2.84236900
C	-5.48614500	-4.22420300	-3.82975400
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C	-5.08342400	-5.40974200	-4.44113300
H	-5.70679500	-5.86947200	-5.20270100
C	-3.87740600	-5.99616800	-4.05863300
H	-3.54954100	-6.92482200	-4.51807200
C	-3.07509100	-5.40194900	-3.08776400
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C	-10.13430800	-2.17643200	1.32880600
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H	-11.69387600	-1.68230400	-0.07153800
C	-12.41619600	-3.01172900	1.46379500
H	-13.42348000	-3.05066000	1.05729900
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C	-8.88817400	4.69123000	0.60380400
C	-9.48603100	5.56142000	-0.32180400
H	-9.45731500	5.31008400	-1.37832200
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H	-4.70865700	4.13129900	-4.65116900
C	-1.56703900	-4.02253100	-0.86091400
C	-0.83097300	-2.99859500	-0.03523800
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H	-1.19739500	-1.29109300	-1.31878100
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N	-2.66865900	-3.54078200	-1.53054000
N	2.44866800	-2.57047600	3.45476400
H	-2.98183700	-2.61113900	-1.28318000
H	2.88934300	-2.01746600	2.73038300
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N	-5.61846900	0.45524400	1.39569700
C	-4.23463400	0.05605800	1.76900100
H	-6.28535900	-0.20211200	1.80374800
C	-4.12402000	-0.35981600	3.26105500
H	-4.01585400	-0.83805100	1.17140700
C	-3.27588300	1.16729300	1.33754800
C	-4.37294800	0.79375500	4.24587800
C	-2.78911200	-1.05787100	3.56029200
H	-4.91914100	-1.10641400	3.41941100
H	-3.37441800	1.35658200	0.26464600
H	-3.48443800	2.10598500	1.86474000
H	-2.23852100	0.88789300	1.54186000
H	-3.57591000	1.54478200	4.19774100
H	-5.32699600	1.30258500	4.06120100
H	-4.40295600	0.41555300	5.27363700
H	-2.60453600	-1.89112300	2.87300800
H	-1.94320300	-0.36540500	3.48061600
H	-2.78541500	-1.46225100	4.57841800
H	4.64301500	1.79639900	0.52783700

N	4.55515400	0.99384300	-0.09760800
C	4.36183100	1.46270300	-1.49824500
H	3.73135400	0.47909100	0.21557800
C	3.48017600	2.73770400	-1.57586500
H	5.35982000	1.74653100	-1.85189600
C	3.87181500	0.28434600	-2.34215000
C	2.03102600	2.52190400	-1.11355900
C	3.52334500	3.37035900	-2.97507700
H	3.94283300	3.45964900	-0.88386300
H	4.58144400	-0.54545000	-2.28154200
H	2.89416300	-0.07896400	-2.00105300
H	3.77694900	0.56702900	-3.39455700
H	1.48786000	1.85415300	-1.79304000
H	1.98315600	2.09147500	-0.10574400
H	1.49110800	3.47495500	-1.08419100
H	4.55518800	3.52194700	-3.31398500
H	3.01519700	2.74553300	-3.71881300
H	3.02755600	4.34795300	-2.97194400