

Supporting Information

Stoichiometrically controlled chirality inversion in zinc bisporphyrinate – monoamine complexes

Tingting Hu,^a Chuanjiang Hu,^{ a, b} Yong Wang,^{* a} David James Young,^c
Jian-Ping Lang^{* a}*

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1. CD titration spectra

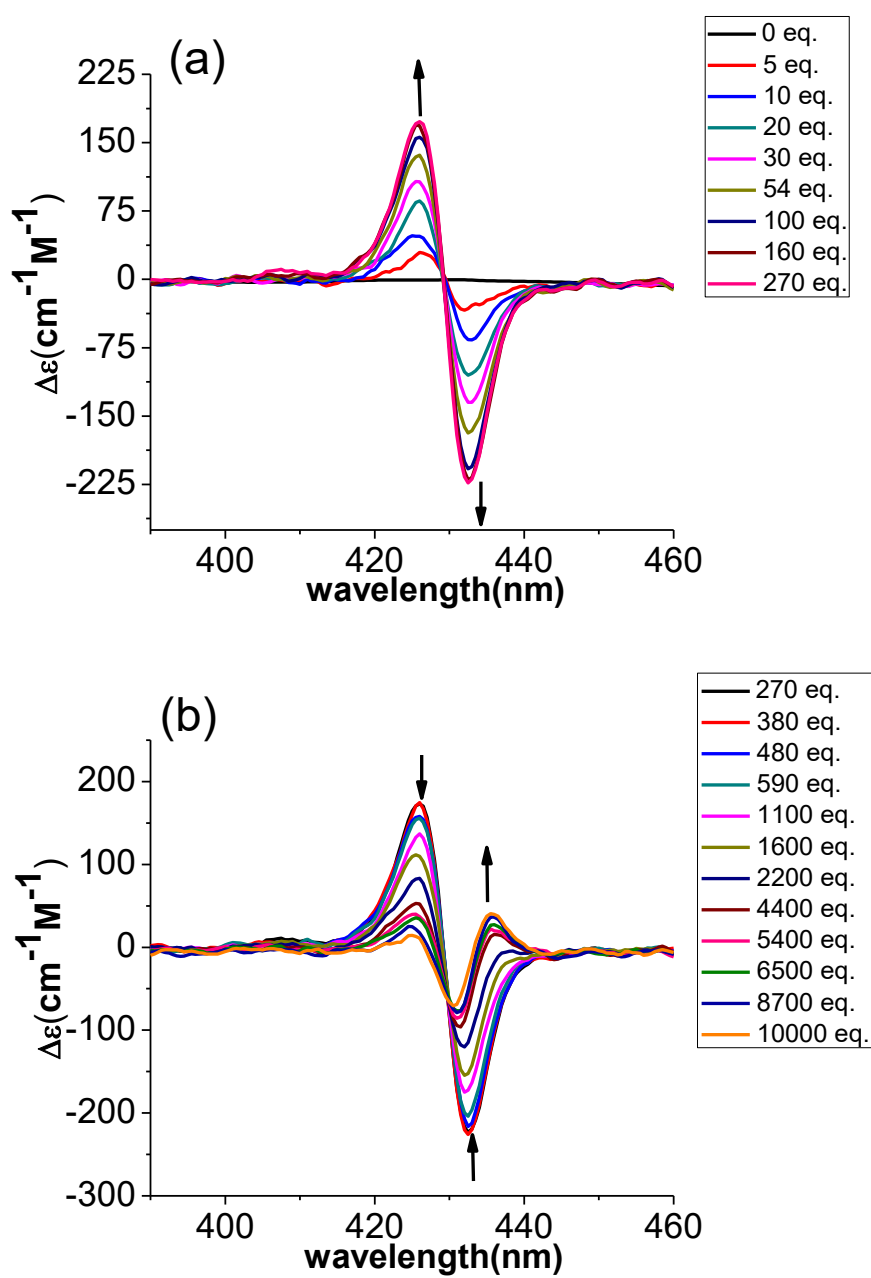


Figure S1. Circular dichroism spectra of [Zn₂-NABis] (1.78×10⁻⁶ M) with 1S in methylene chloride at 25°C. The host to guest ratio is (a) from 1:0 to 1:270; (b) from 1:270 to 1:10000.

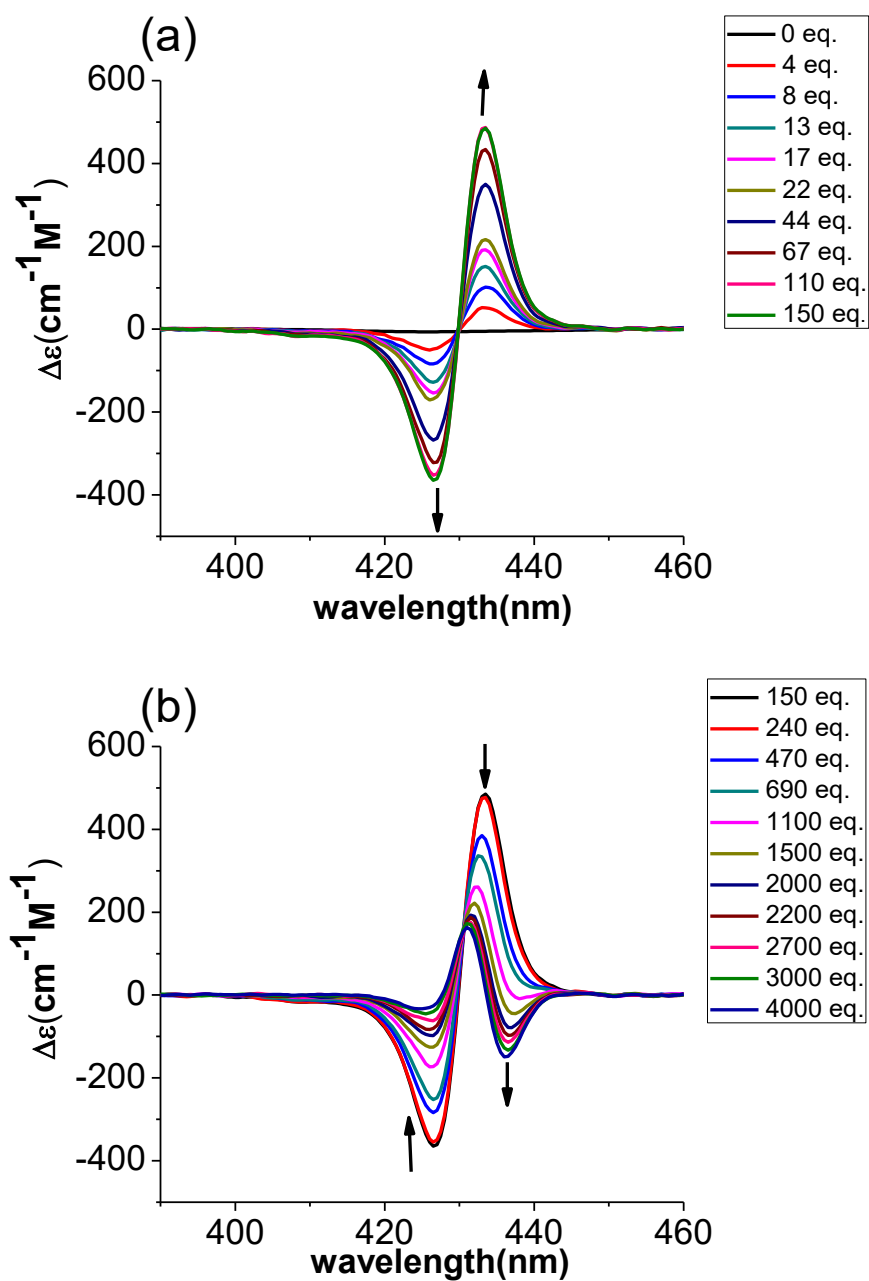


Figure S2. Circular dichroism spectra of $[\text{Zn}_2\text{-NABis}]$ ($1.78 \times 10^{-6} \text{ M}$) with **1R** in **toluene** at 25°C . The host to guest ratio is (a) from 1:0 to 1:150; (b) from 1:150 to 1:4000.

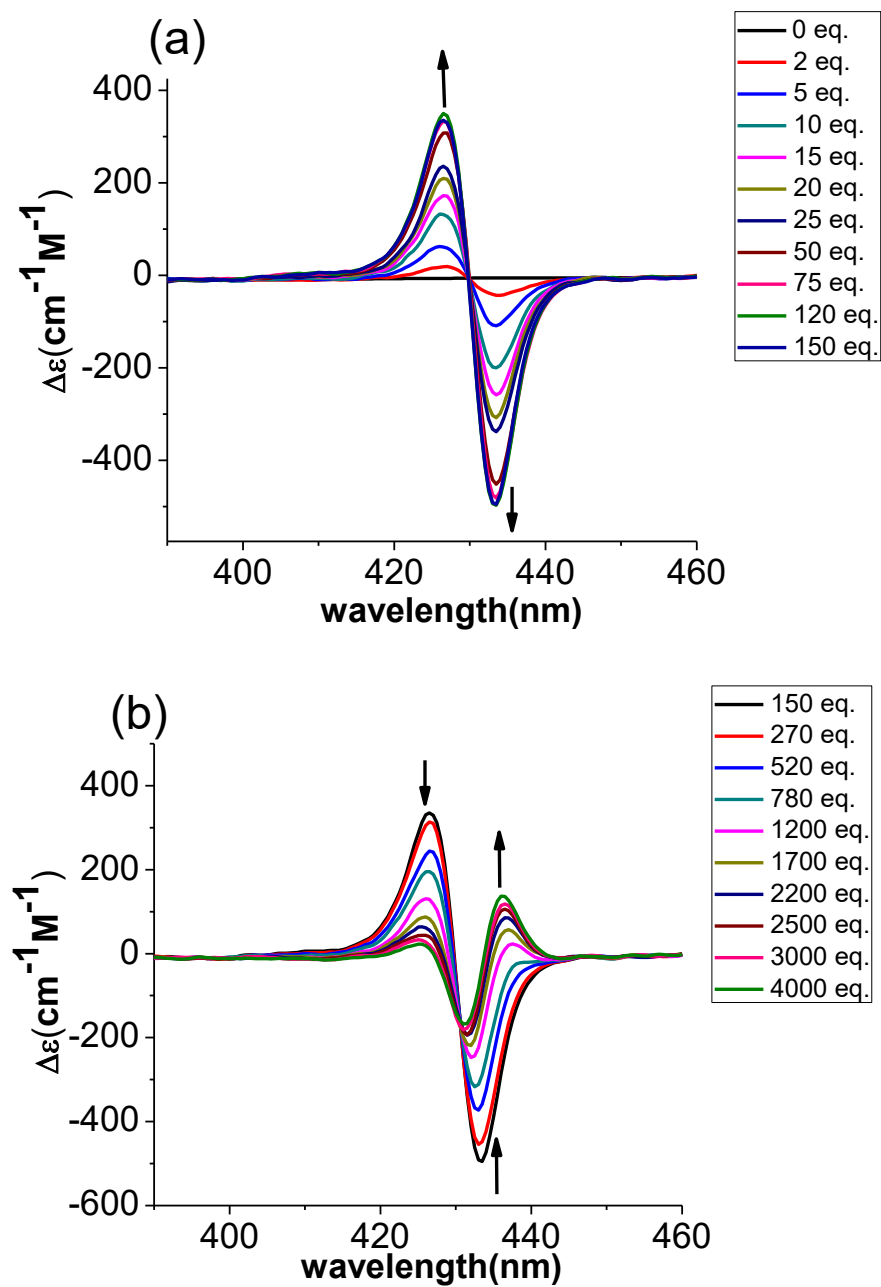


Figure S3. Circular dichroism spectra of $[\text{Zn}_2\text{-NABis}]$ ($1.78 \times 10^{-6} \text{ M}$) with **1S** in **toluene** at 25°C . The host to guest ratio is (a) from 1:0 to 1:150; (b) from 1:150 to 1:4000.

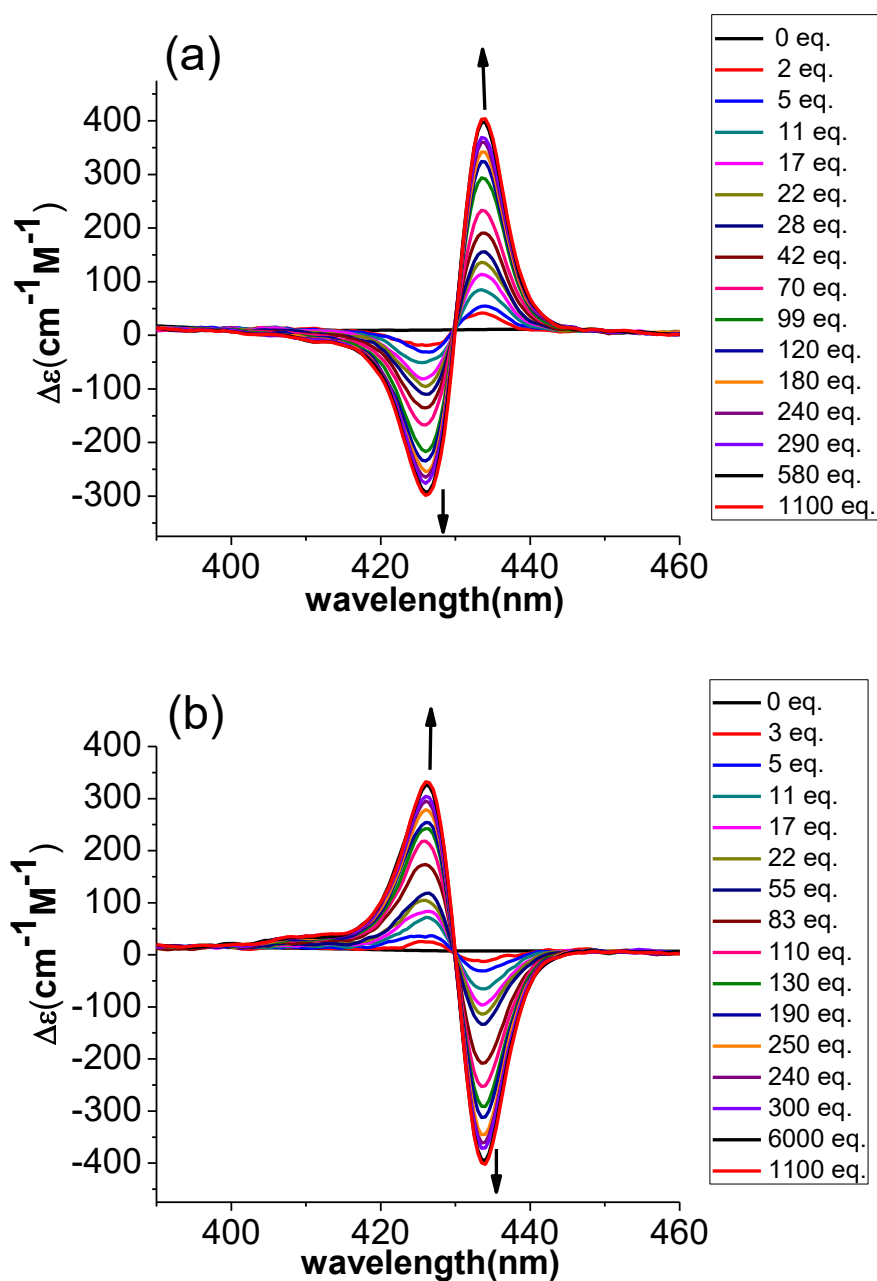


Figure S4. Circular dichroism spectra of $[\text{Zn}_2\text{-NABis}]$ ($1.78 \times 10^{-6} \text{ M}$) in upon addition of (a) 2R, (b) 2S from 1: 0 to 1:1100 equivalents in methylene chloride at 25°C .

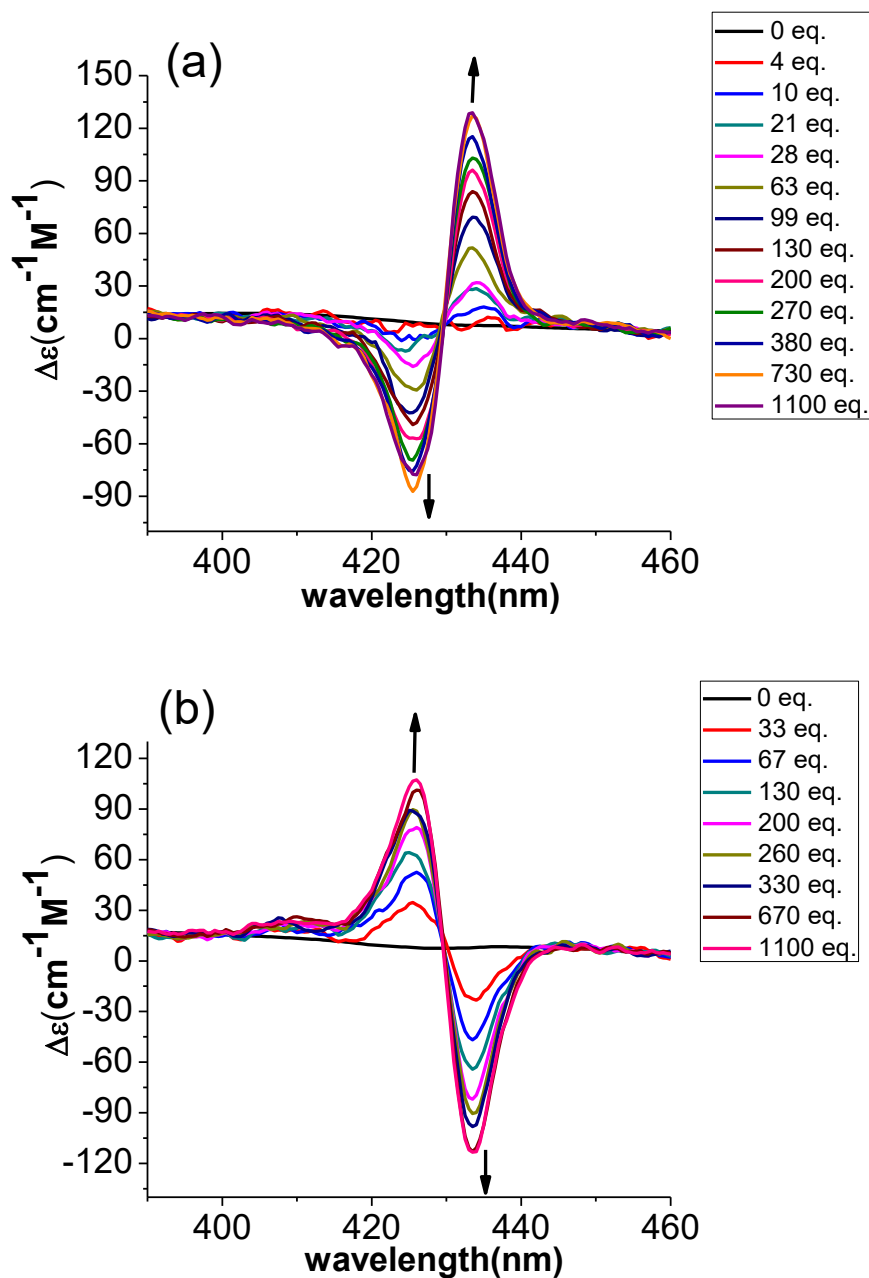


Figure S5. Circular dichroism spectra of $[\text{Zn}_2\text{-NABis}]$ ($1.78 \times 10^{-6} \text{ M}$) in upon addition of (a) 3R, (b) 3S from 1: 0 to 1:1100 equivalents in methylene chloride at 25°C .

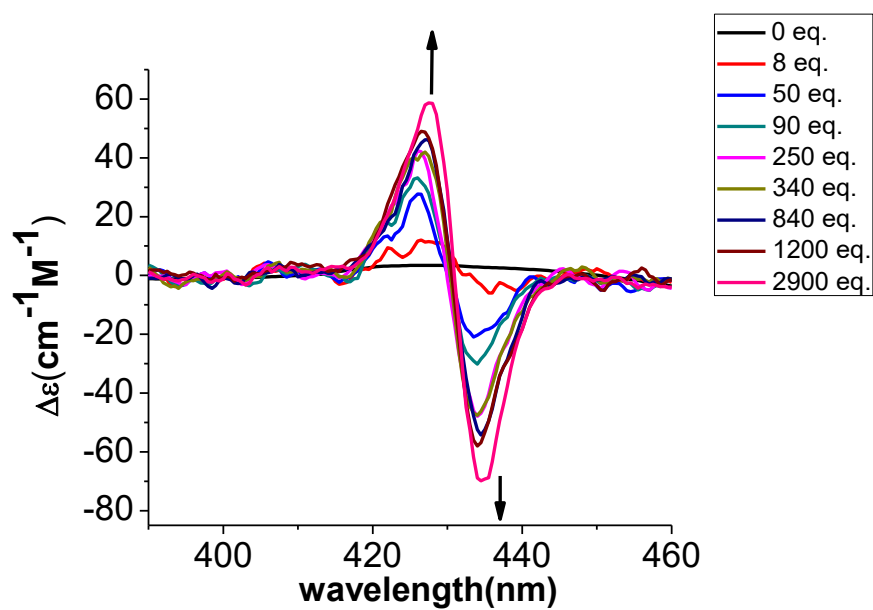


Figure S6. Circular dichroism spectra of $[\text{Zn}_2\text{-NABis}]$ ($1.78 \times 10^{-6} \text{ M}$) in upon addition of 4R from 1: 0 to 1:2900 equivalents in methylene chloride at 25°C .

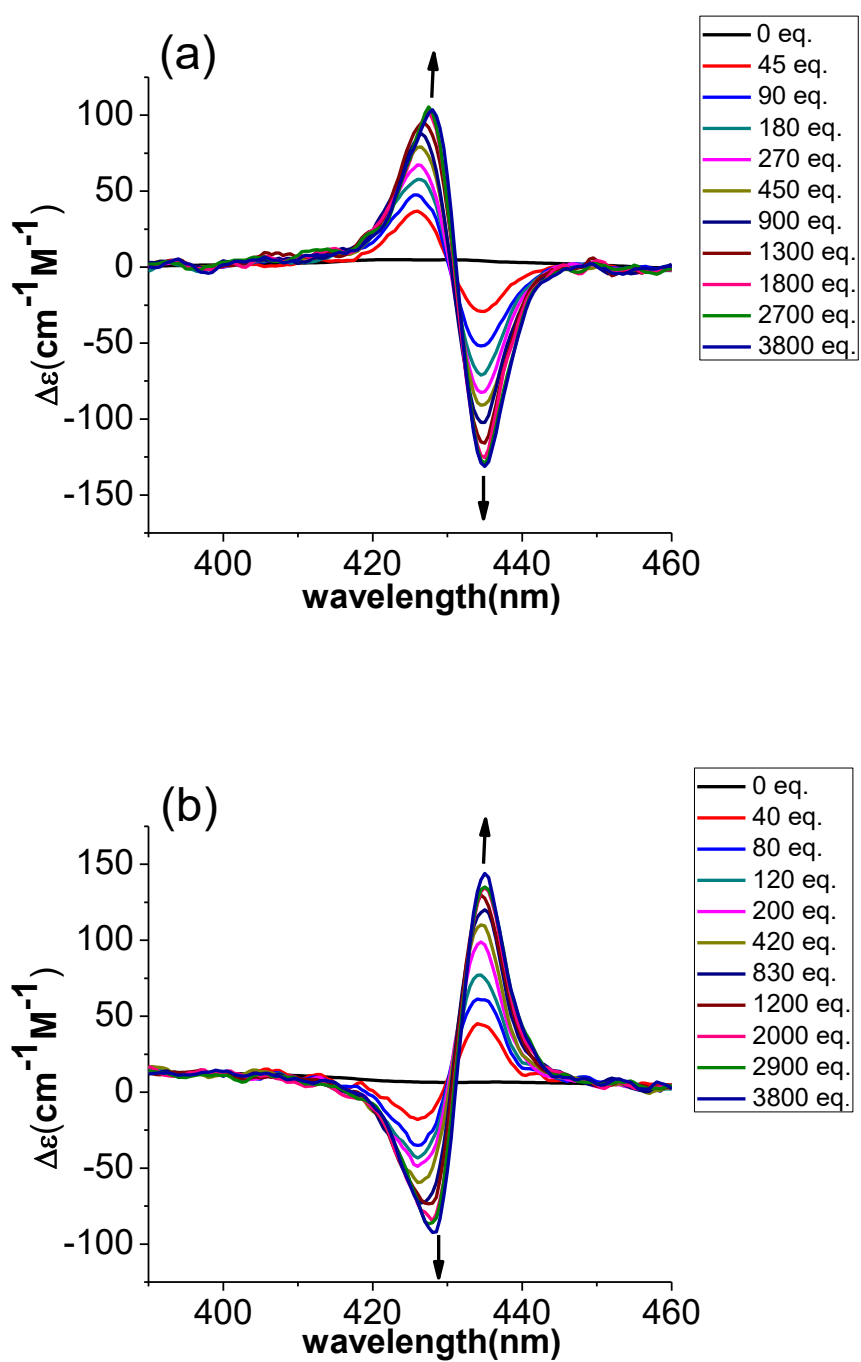


Figure S7. Circular dichroism spectra of $[\text{Zn}_2\text{-NABis}]$ ($1.78 \times 10^{-6} \text{ M}$) in upon addition of (a) 5R, (b) 5S from 1: 0 to 1:3800 equivalents in methylene chloride at 25°C .

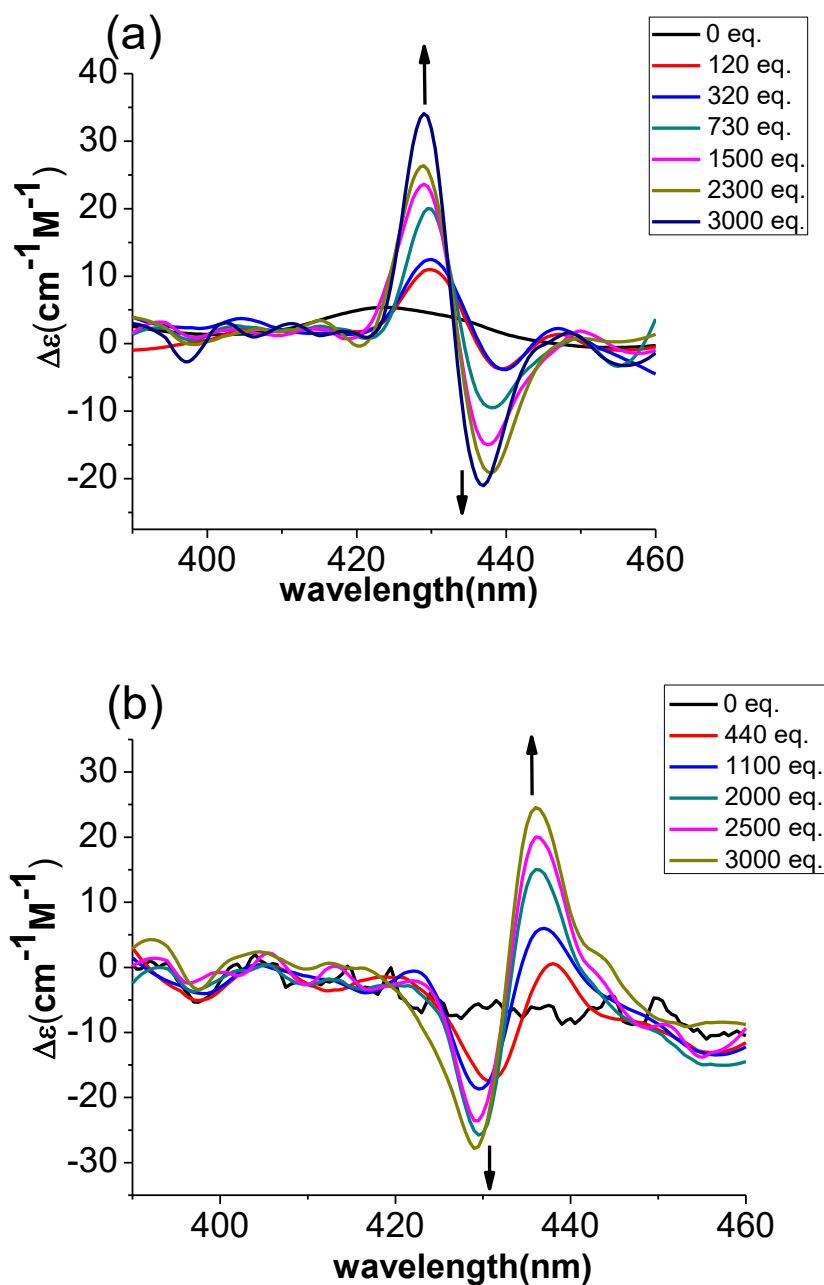


Figure S8. Circular dichroism spectra of $[\text{Zn}_2\text{-NABis}]$ ($1.78 \times 10^{-6} \text{ M}$) in upon addition of (a) 6R, (b) 6S from 1: 0 to 1:3000 equivalents in methylene chloride at 25°C .

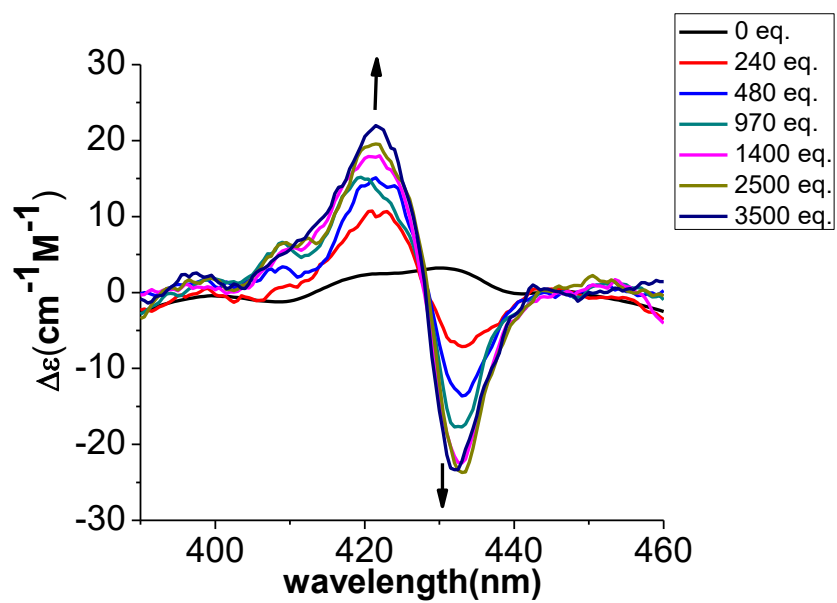


Figure S9. Circular dichroism spectra of [ZnNi-NABis] (2.26×10^{-6} M) in upon addition of 1S from 1: 0 to 1:3500 equivalents in methylene chloride at 25°C.

2. Plots of CD intensity as the function of the equivalents of the guests

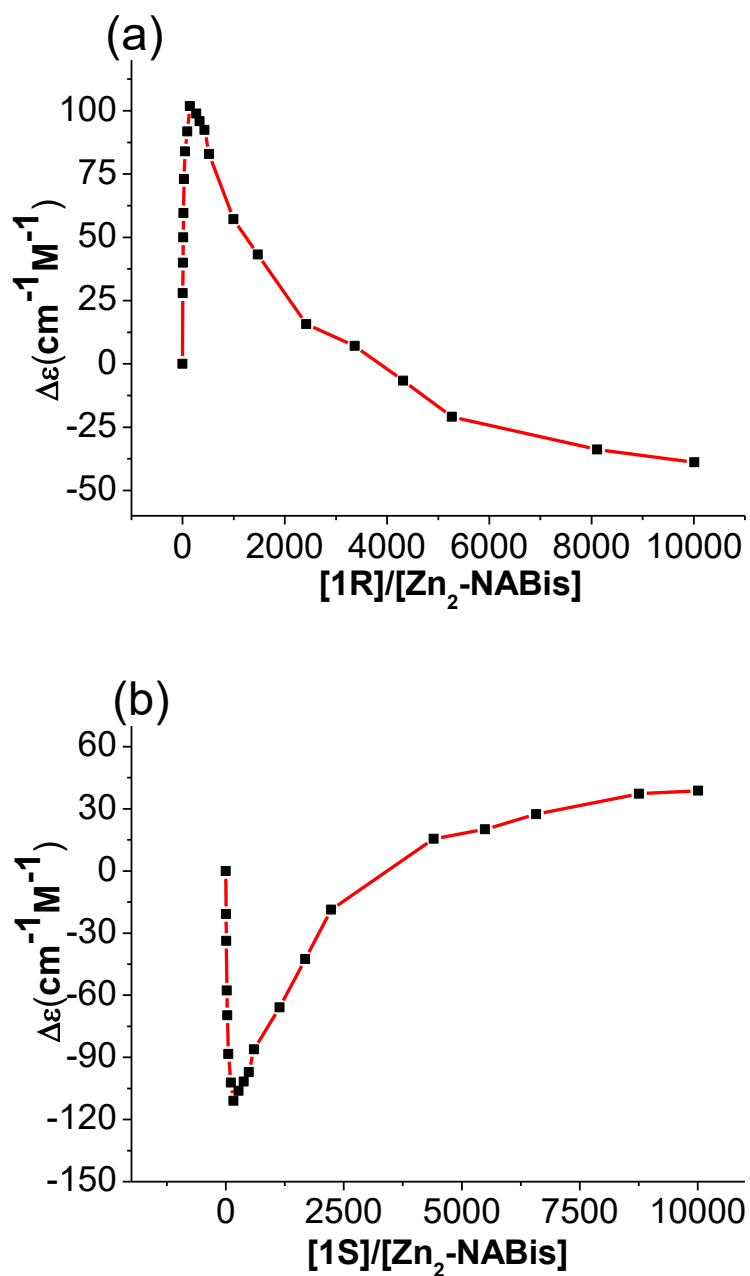


Figure S10. Plots of CD intensity at 436 nm as the function of the equivalents of (a) 1R (b) 1S in methylene chloride at 25°C.

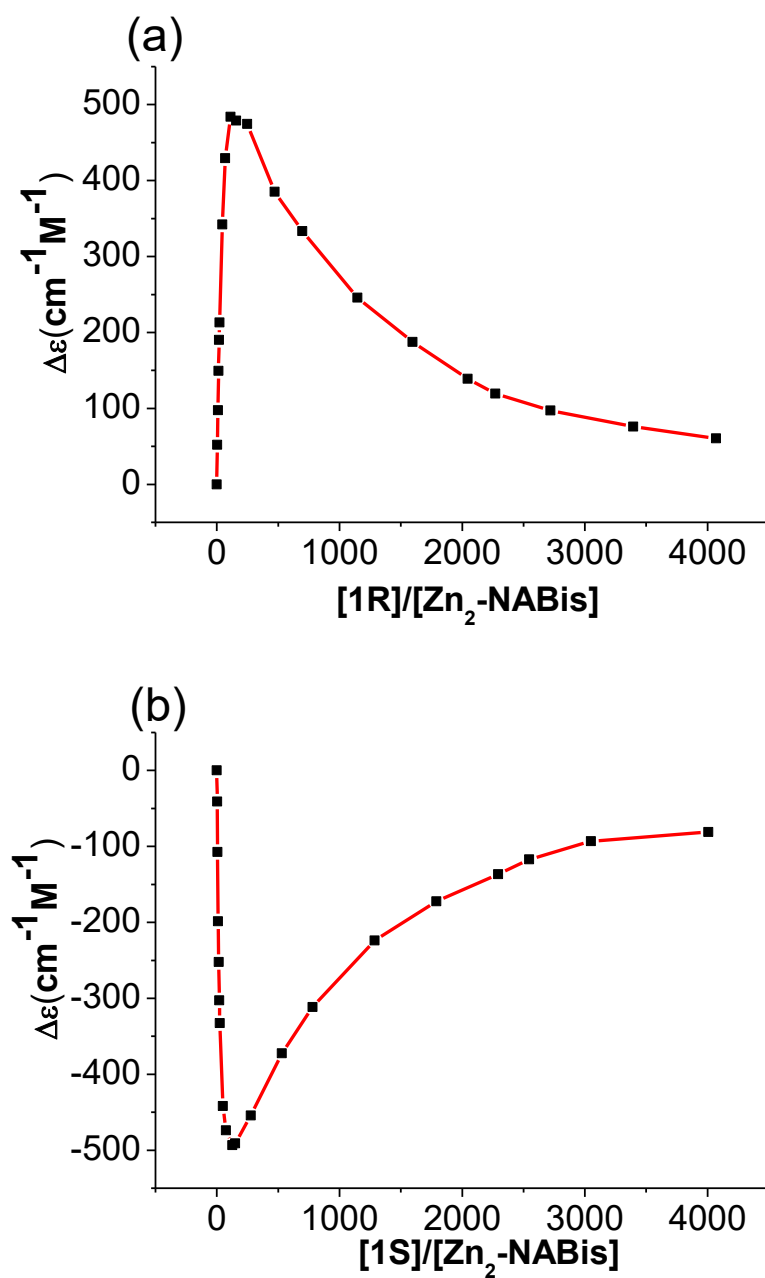


Figure S11. Plots of CD intensity at 433 nm as the function of the equivalents of (a) 1R (b) 1S in toluene at 25°C.

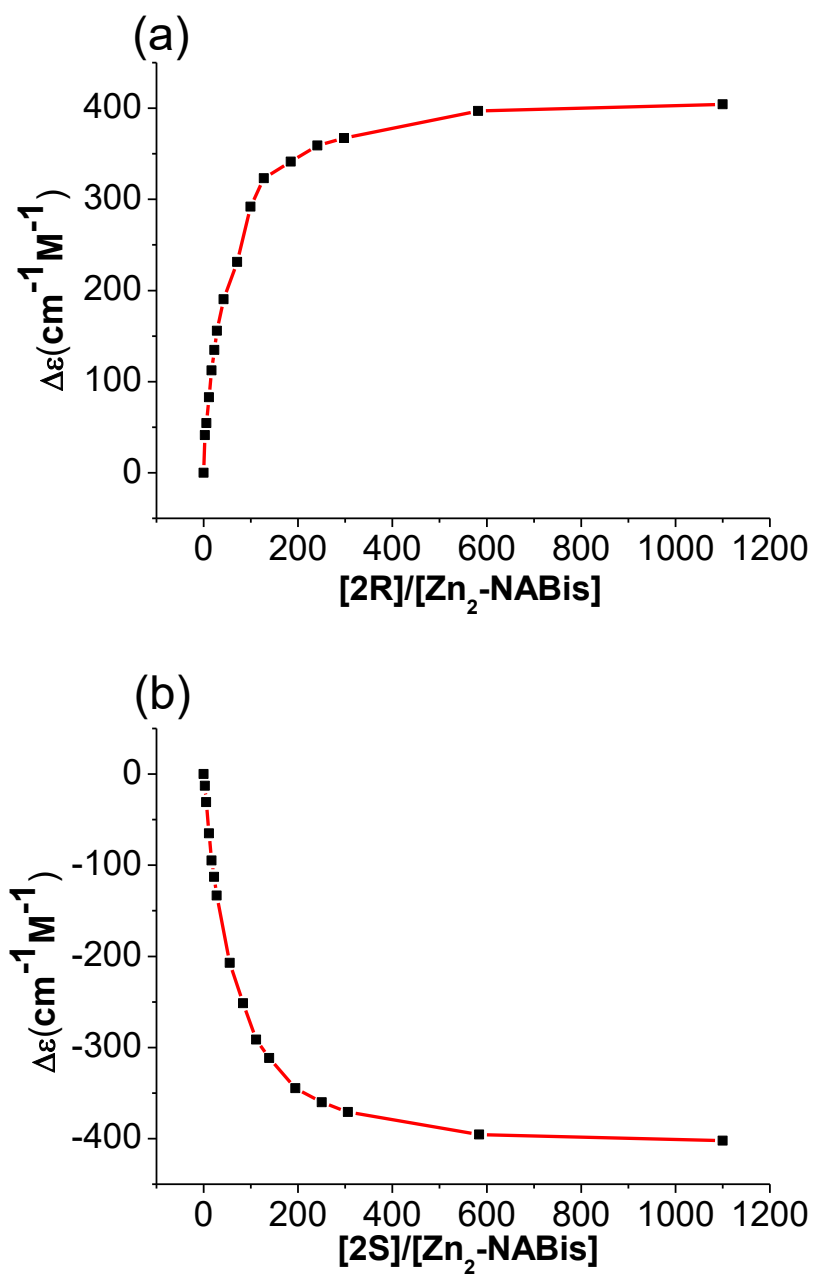


Figure S12. Plots of CD intensity at 434 nm as the function of the equivalents of (a) 2R (b) 2S in methylene chloride at 25°C.

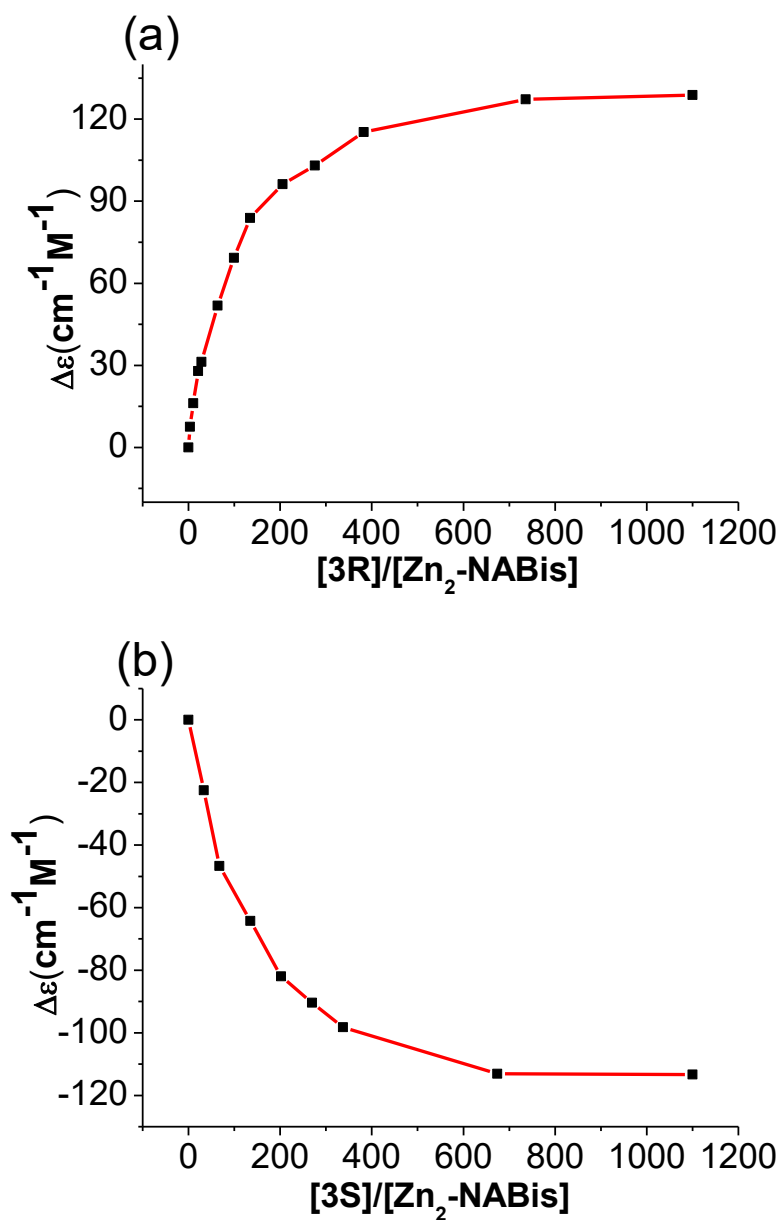


Figure S13. Plots of CD intensity at 433.5 nm as the function of the equivalents of (a) 3R (b) 3S in methylene chloride at 25°C.

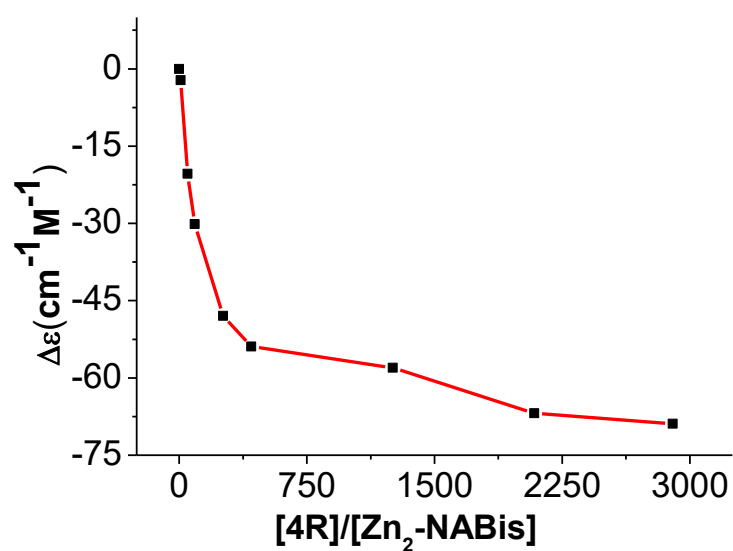


Figure S14. Plots of CD intensity at 434 nm as the function of the equivalents of 4R in methylene chloride at 25°C.

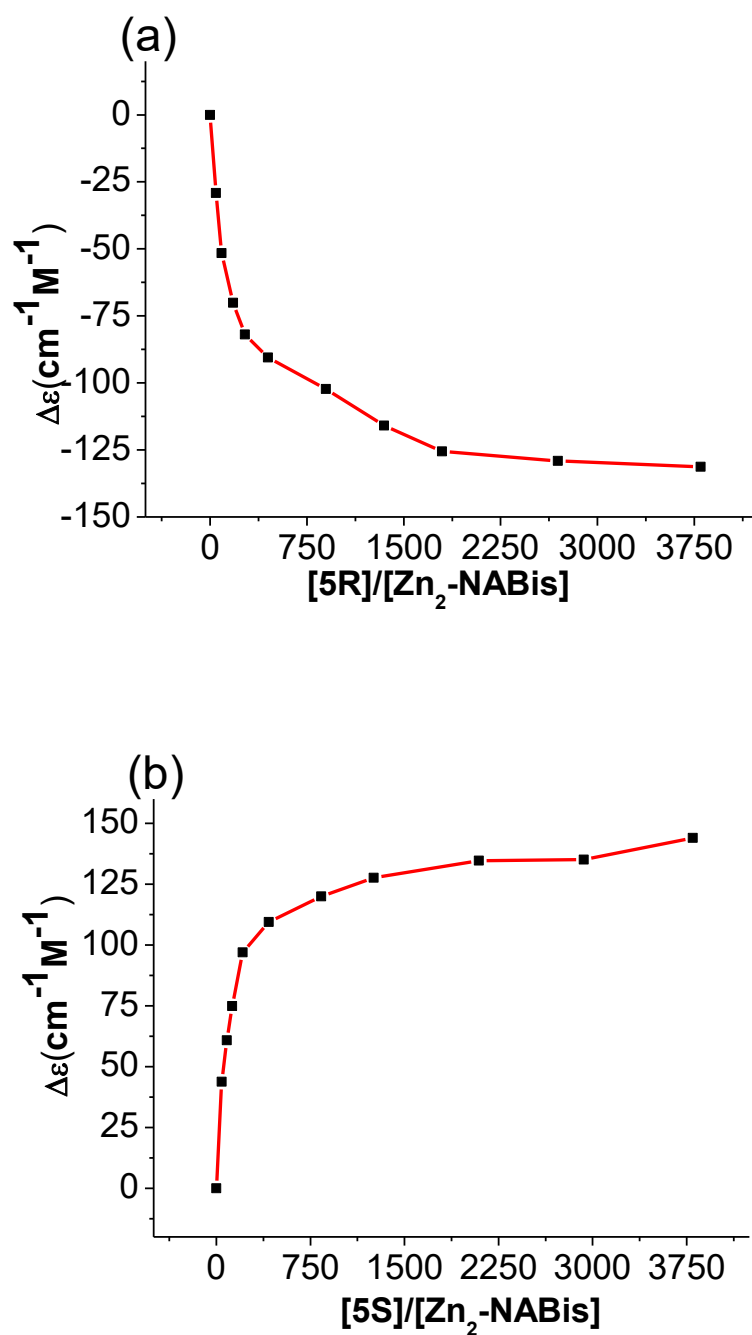


Figure S15. Plots of CD intensity at 435 nm as the function of the equivalents of (a) 5R (b) 5S in methylene chloride at 25°C.

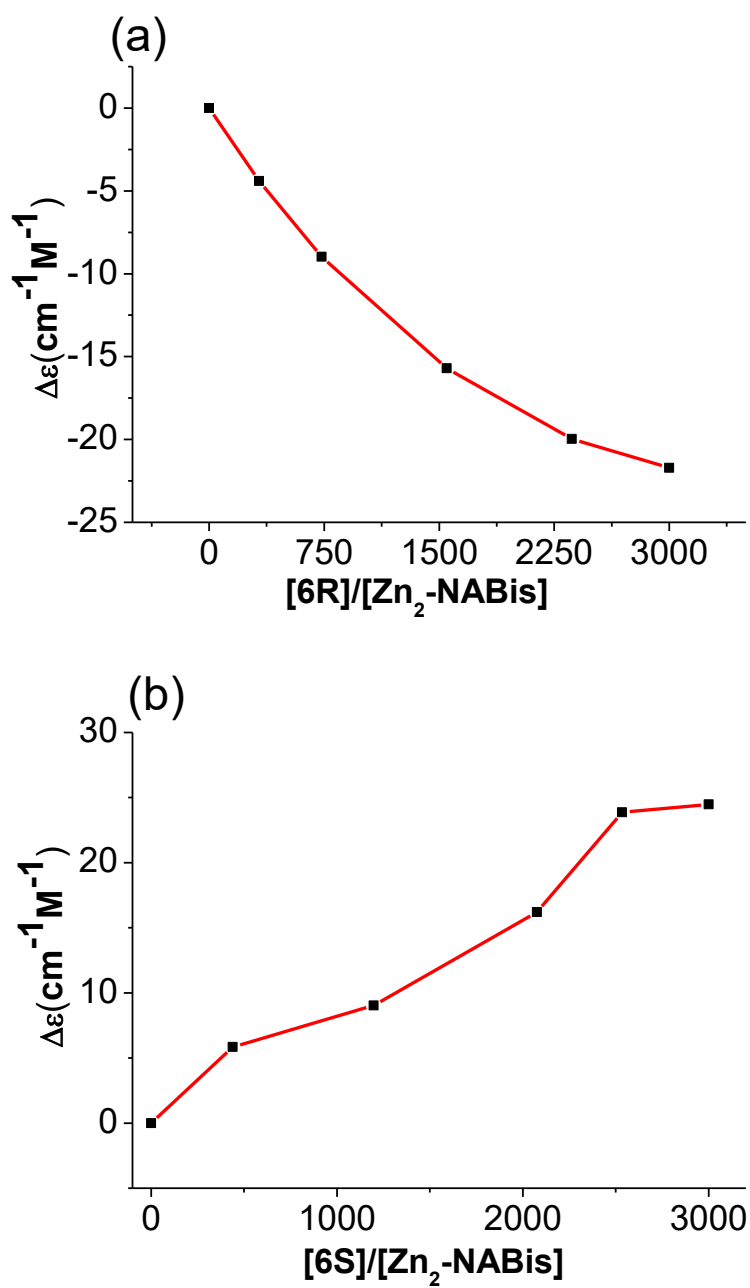


Figure S16. Plots of CD intensity at 437 nm as the function of the equivalents of (a) 6R (b) 6S in methylene chloride at 25°C.

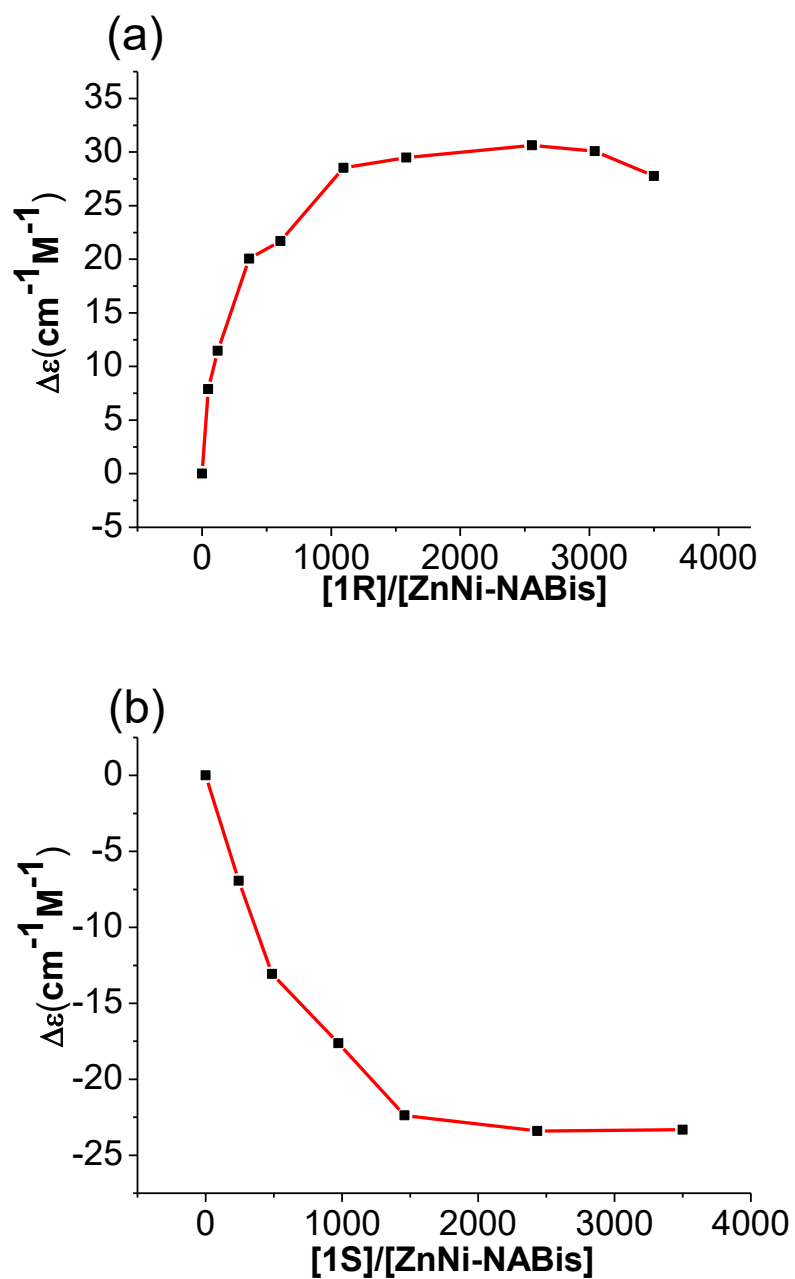


Figure S17. Plots of CD intensity at 432.5 nm as the function of the equivalents of (a) 1R (b) 1S in methylene chloride at 25°C.

3. UV-vis spectra of free base bisporphyrin NABis and [Zn₂-NABis]

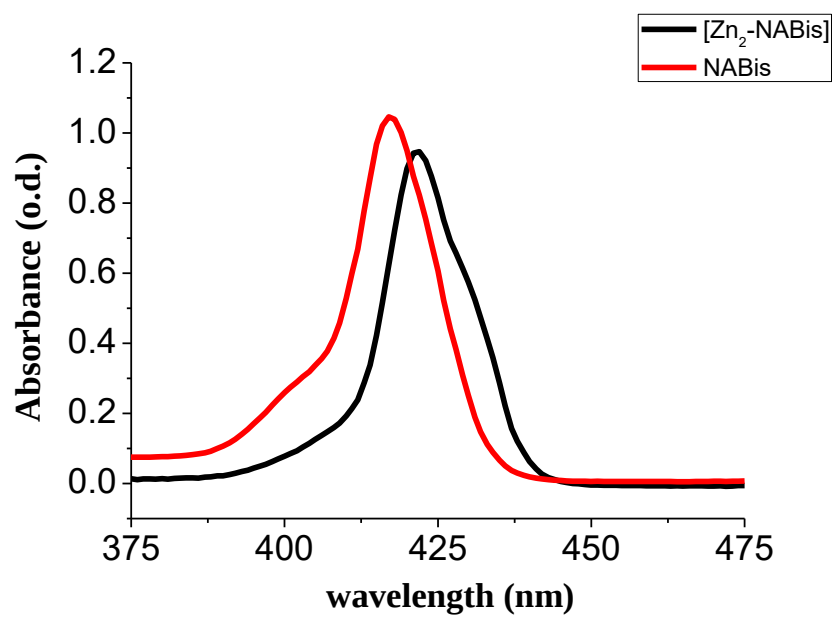


Figure S18. UV-vis spectra of free base bisporphyrin NABis and [Zn₂-NABis].

4. UV-vis titration spectra

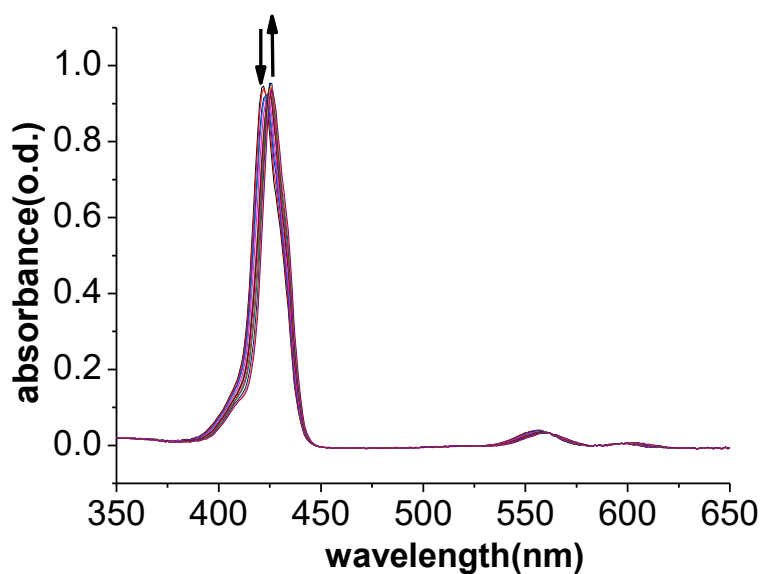


Figure S19. UV-vis spectra of [Zn₂-NABis] (1.78×10^{-6} M) with 1R from 1: 0 to 1:600 equivalents in methylene chloride at 25°C.

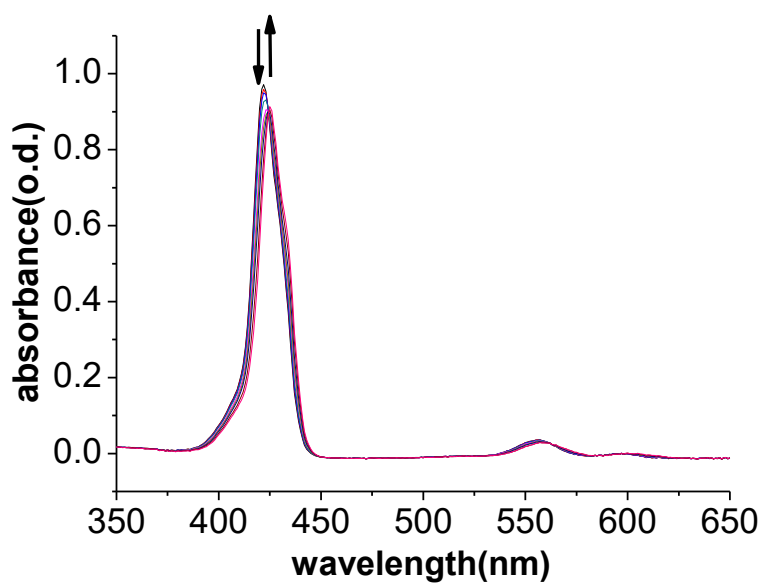


Figure S20. UV-vis spectra of [Zn₂-NABis] (1.78×10^{-6} M) with 2R from 1: 0 to 1:600 equivalents in methylene chloride at 25°C.

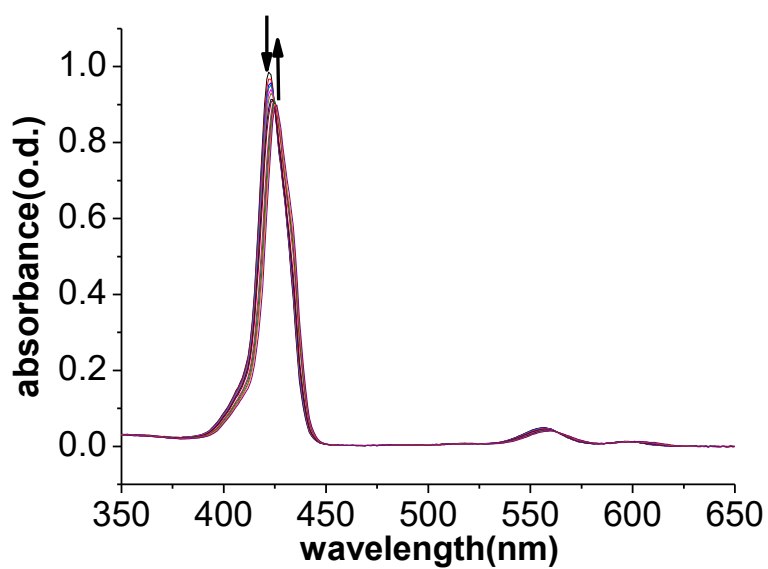


Figure S21. UV-vis spectra of [Zn₂-NABis] (1.78×10^{-6} M) with 3R from 1: 0 to 1:600 equivalents in methylene chloride at 25°C.

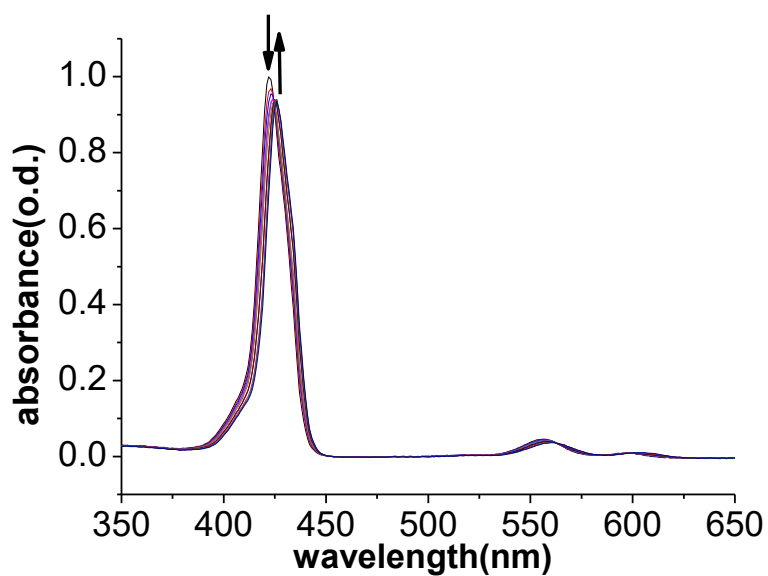


Figure S22. UV-vis spectra of [Zn₂-NABis] (1.78×10^{-6} M) with 4R from 1: 0 to 1:600 equivalents in methylene chloride at 25°C.

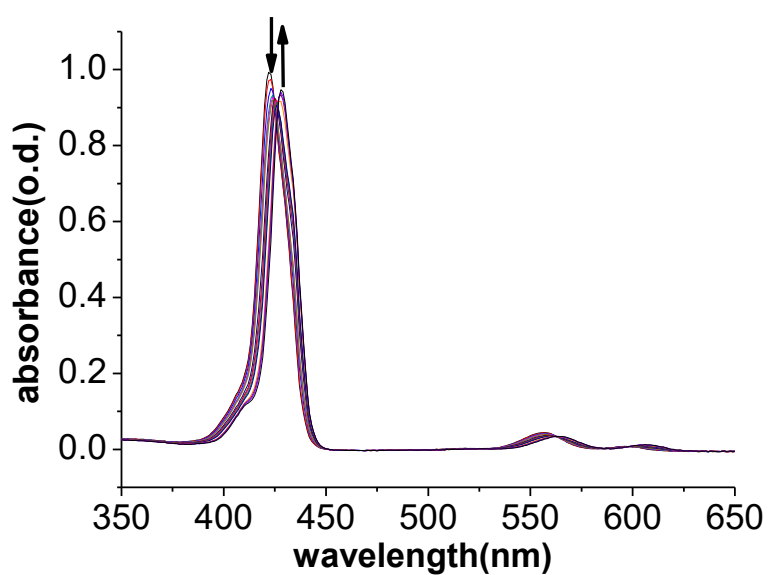


Figure S23. UV-vis spectra of [Zn₂-NABis] (1.78×10^{-6} M) with 5R from 1: 0 to 1:600 equivalents in methylene chloride at 25°C.

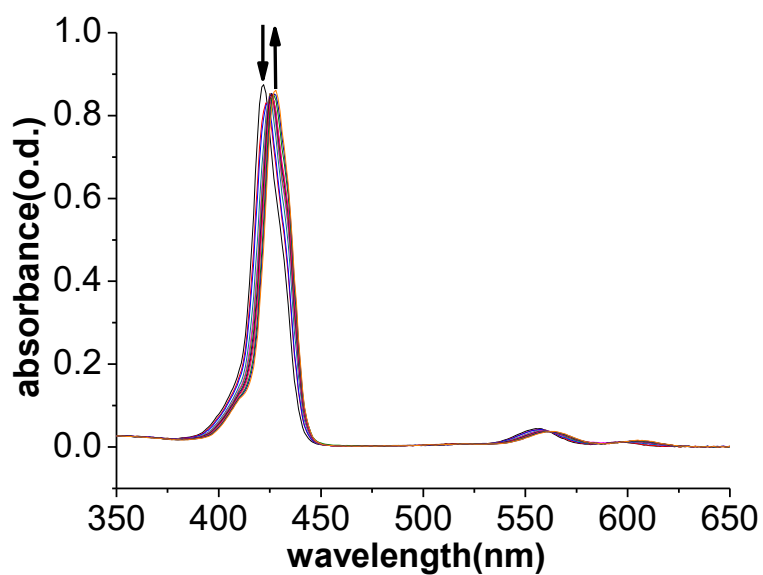


Figure S24. UV-vis spectra of [Zn₂-NABis] (1.78×10^{-6} M) with 6R from 1: 0 to 1:600 equivalents in methylene chloride at 25°C.

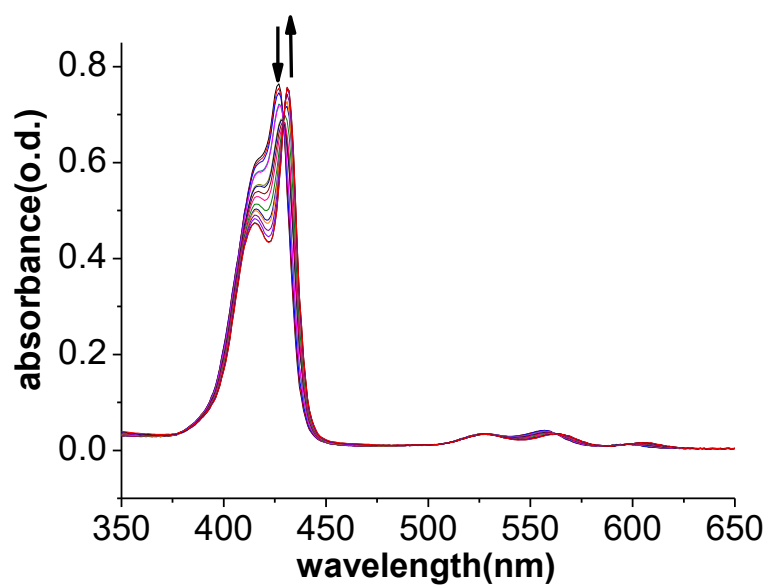


Figure S25. UV-vis spectra of [ZnNi-NABis] (2.26×10^{-6} M) with 1R from 1: 0 to 1:3000 equivalents in methylene chloride at 25°C.

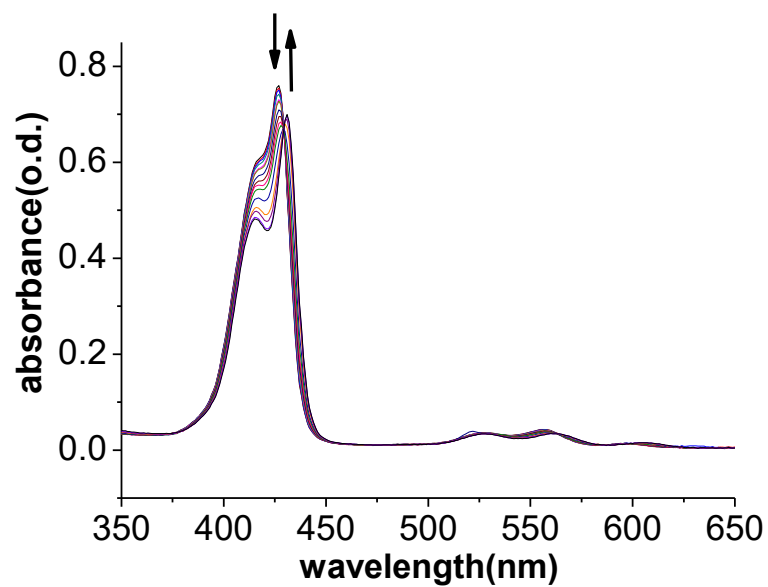


Figure S26. UV-vis spectra of [ZnNi-NABis] (2.26×10^{-6} M) with 2R from 1: 0 to 1:3000 equivalents in methylene chloride at 25°C.

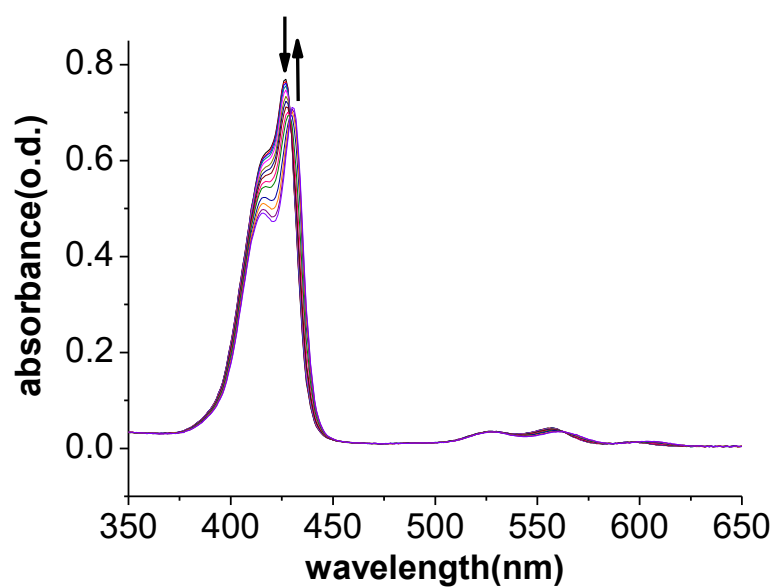


Figure S27. UV-vis spectra of [ZnNi-NABis] (2.26×10^{-6} M) with 3R from 1: 0 to 1:3000 equivalents in methylene chloride at 25°C.

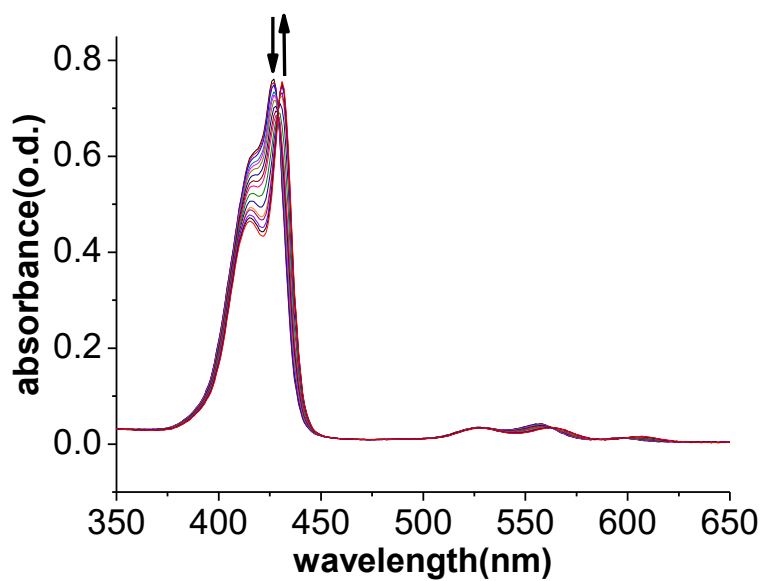


Figure S28. UV-vis spectra of [ZnNi-NABis] (2.26×10^{-6} M) with 4R from 1: 0 to 1:3000 equivalents in methylene chloride at 25°C.

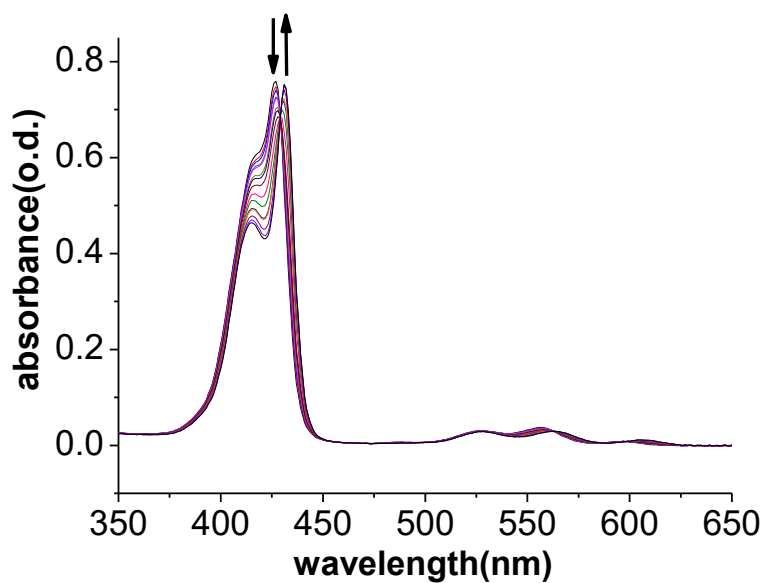


Figure S29. UV-vis spectra of [ZnNi-NABis] (2.26×10^{-6} M) with 5R from 1: 0 to 1:3000 equivalents in methylene chloride at 25°C.

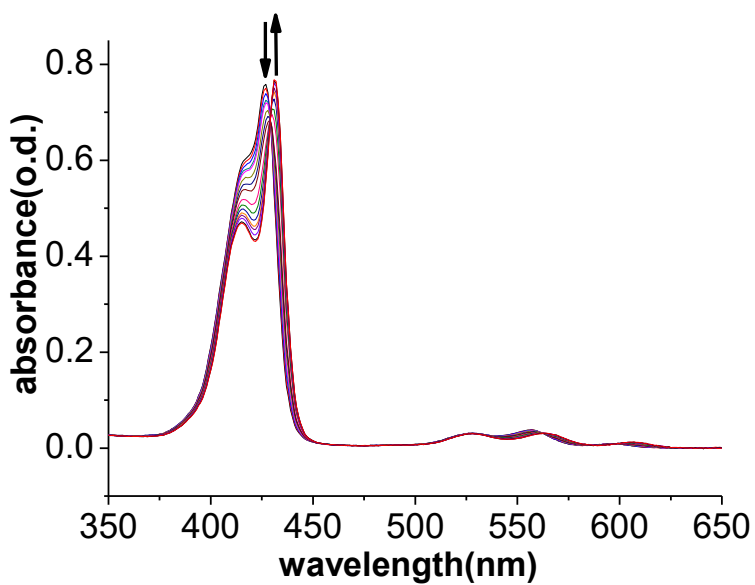


Figure S30. UV-vis spectra of [ZnNi-NABis] (2.26×10^{-6} M) with 6R from 1: 0 to 1:3000 equivalents in methylene chloride at 25°C.

5. NMR spectra of new compounds

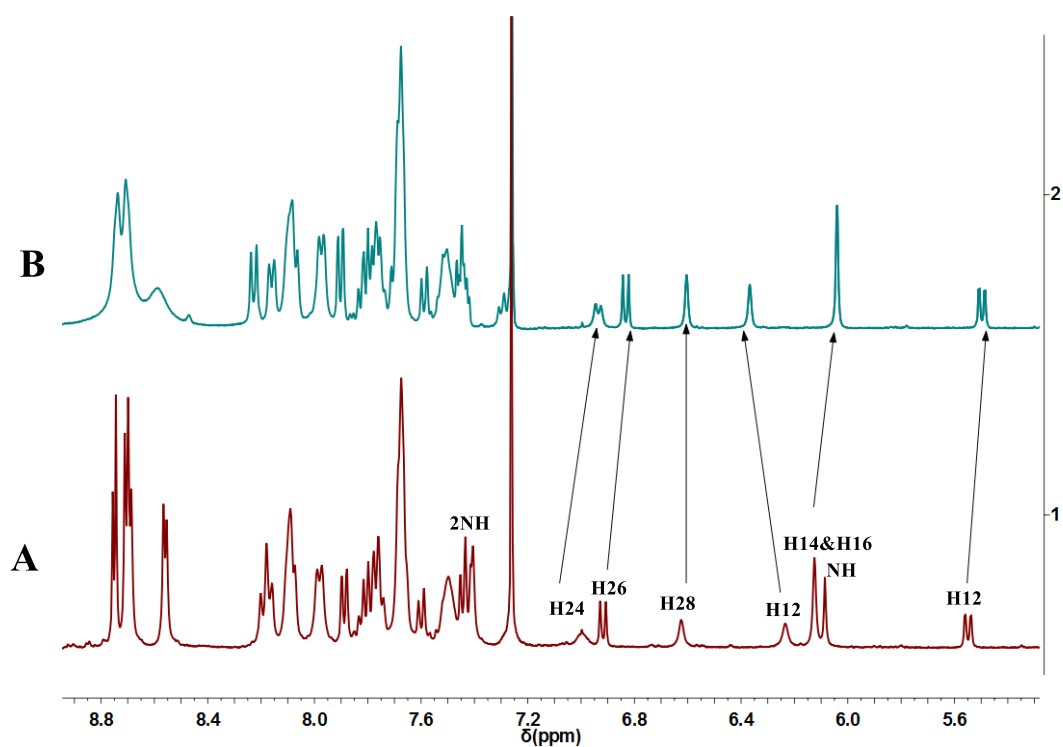


Figure S31. ^1H NMR for NABis (7.1×10^{-3} M) A) before and B) after addition of D_2O .

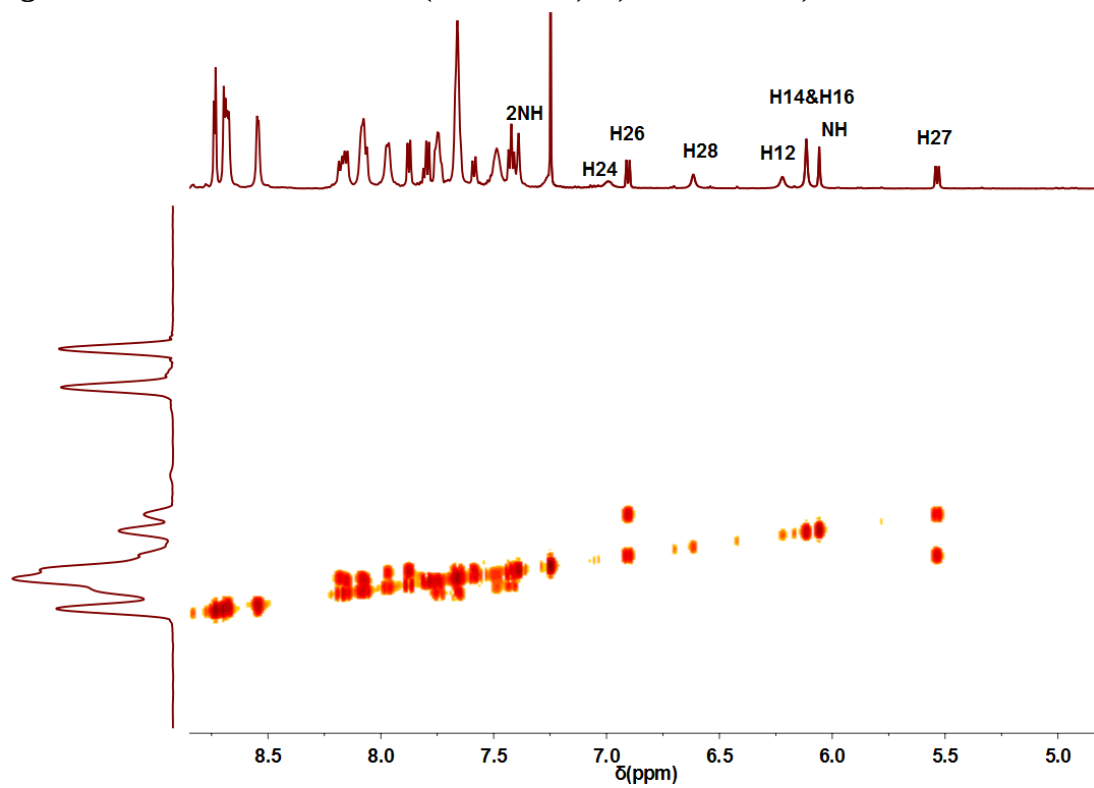


Figure S32. ^1H - ^1H COSY NMR spectrum for NABis.

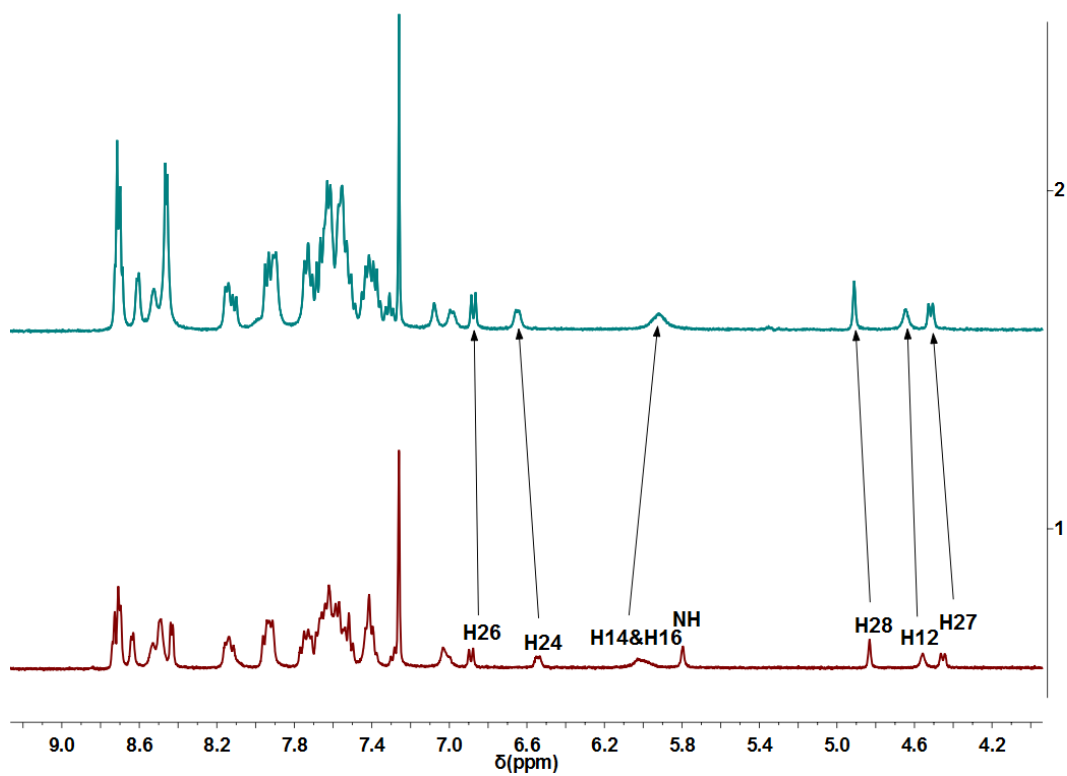


Figure S33. ^1H NMR for $[\text{ZnNi-NABis}]$ (4.2×10^{-3} M) A) before and B) after addition of D_2O .

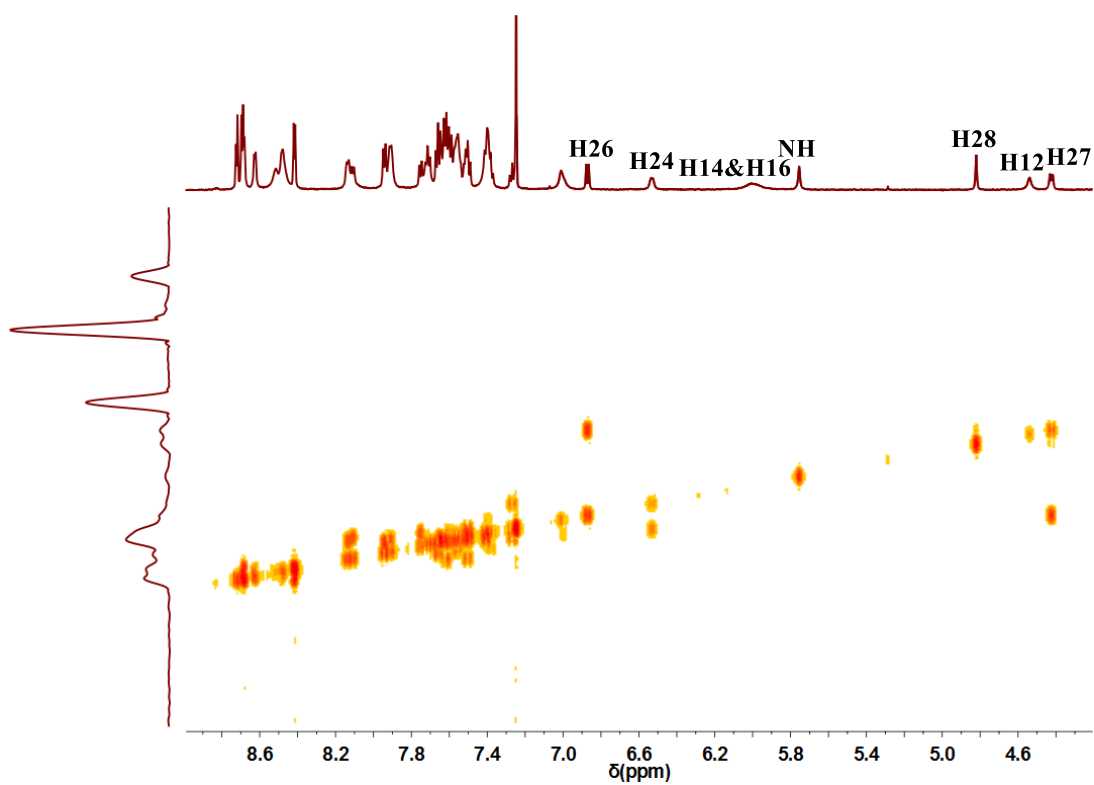


Figure S34. ^1H - ^1H COSY NMR spectrum for $[\text{ZnNi-NABis}]$.

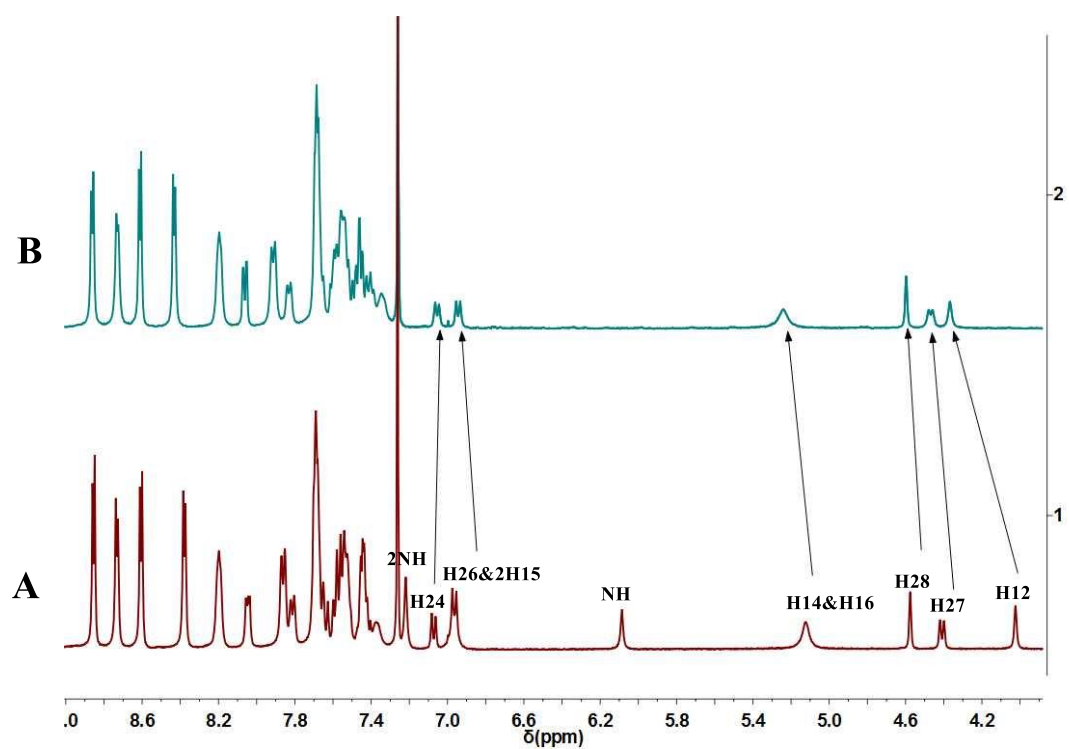


Figure S35. ^1H NMR for $[\text{Zn}_2\text{-NABis}]$ (5.3×10^{-3} M) A) before and B) after addition of D_2O .

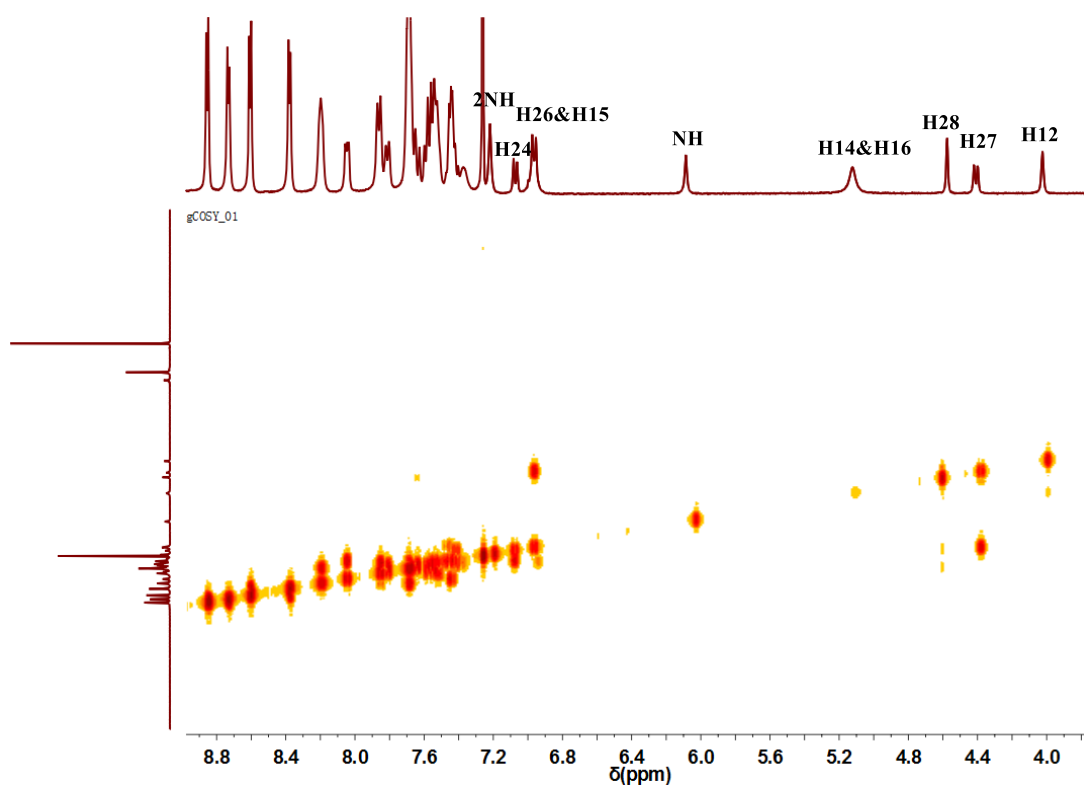


Figure S36. ^1H - ^1H COSY NMR spectrum for $[\text{Zn}_2\text{-NABis}]$.

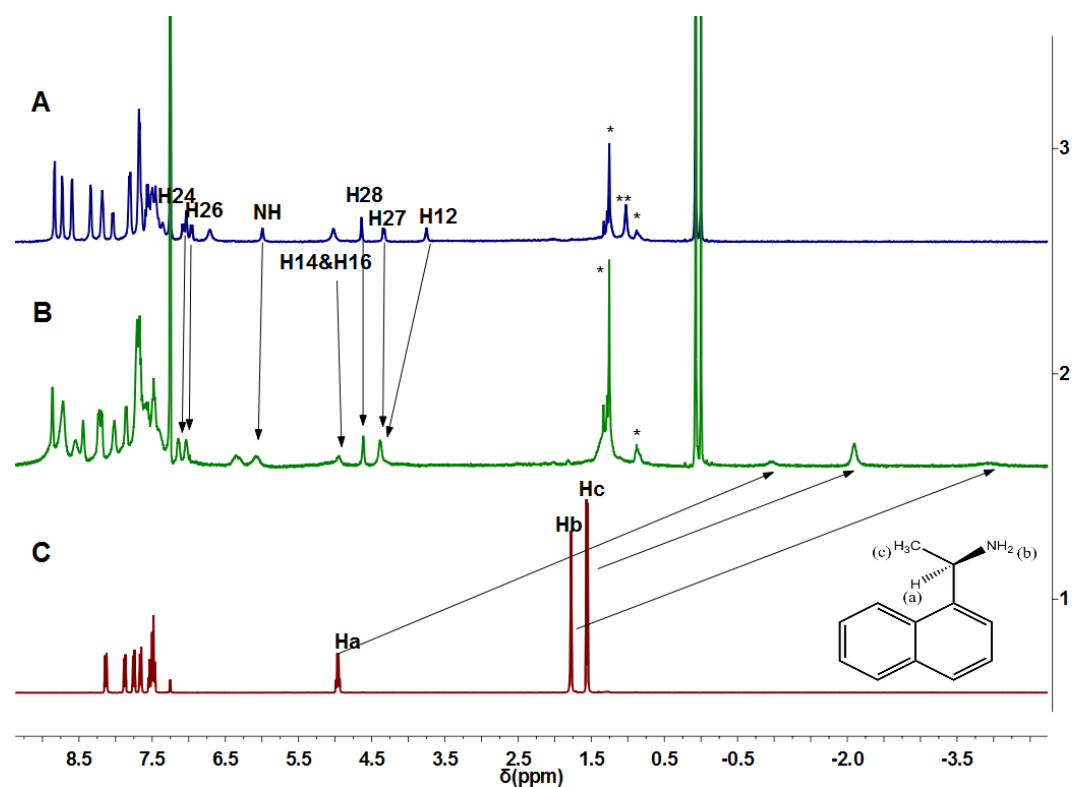


Figure S37. ^1H NMR spectra in CDCl_3 (at 298 K) of (A) $[\text{Zn}_2\text{-NABis}]$ (6.67×10^{-3} M), (B) the mixture of $[\text{Zn}_2\text{-NABis}]$ (6.67×10^{-3} M) and 1R (0.6 eq.), (C) 1R. Inset shows the proton numbering scheme of 1R. *: impurity from petroleum ether; **: Impurity from water.

6. Relative energies of DFT -optimized conformer A·1R and conformer B·1R

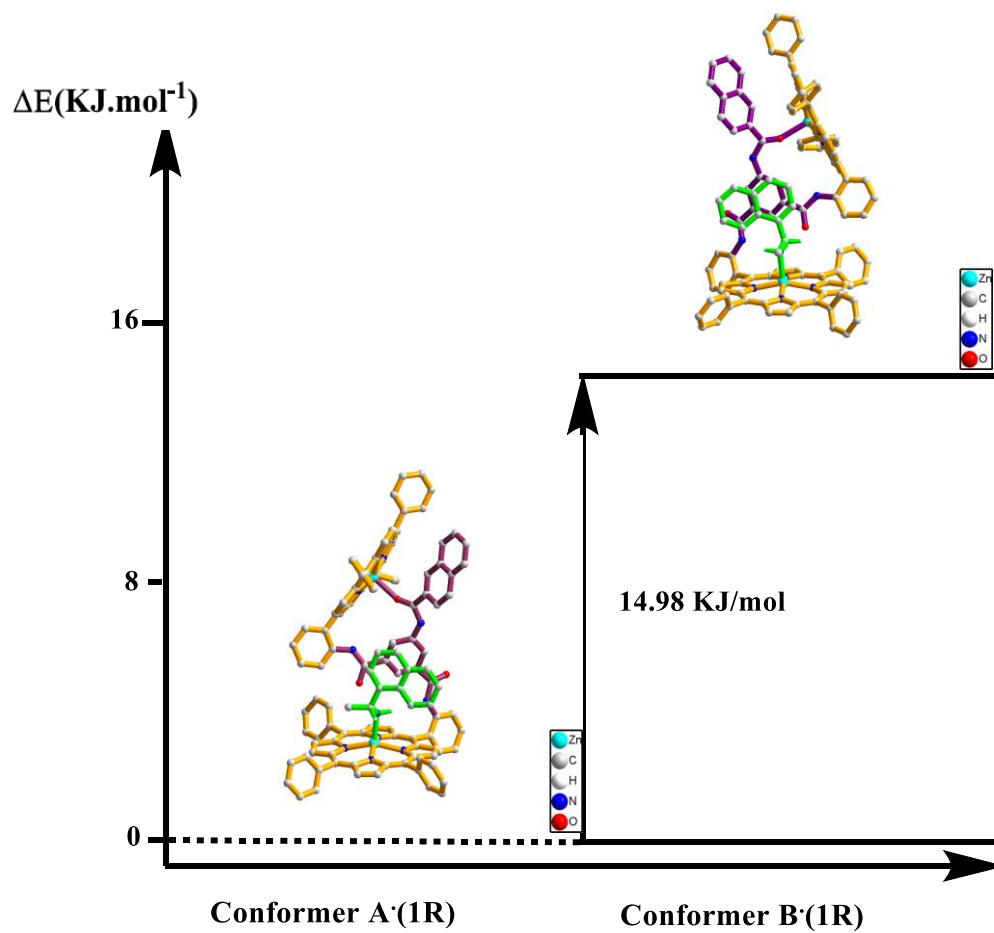


Figure S38. Relative energies of DFT-optimized conformer A·1R and conformer B·1R.

7. Relative energies of DFT-optimized conformer A·(1R)₂ and conformer B·(1R)₂

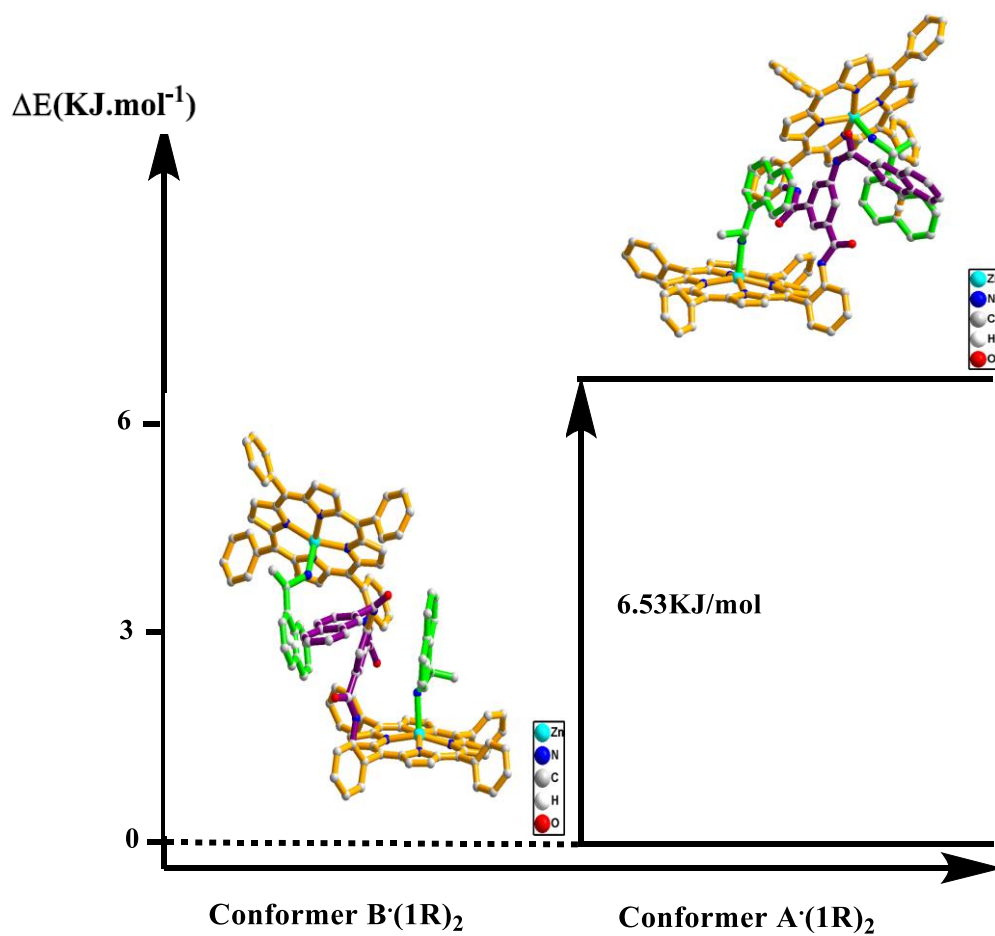


Figure S39. Relative energies of DFT-optimized conformer A·(1R)₂ and conformer B·(1R)₂.

8. Relative energies of DFT-optimized conformer A·2R and conformer B·2R

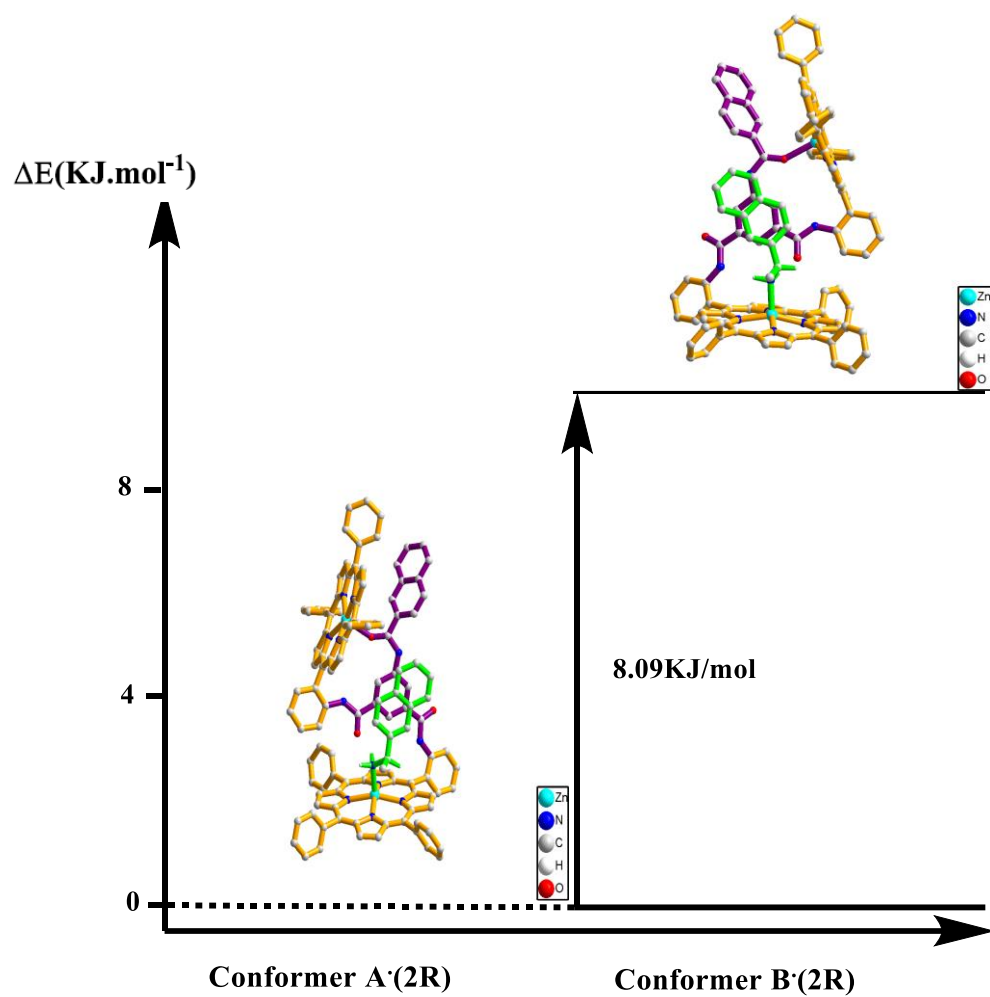


Figure S40. Relative energies of DFT-optimized conformer A·2R and conformer B·2R

9. Relative energies of DFT-optimized conformer A·(2R)₂ and conformer B·(2R)₂

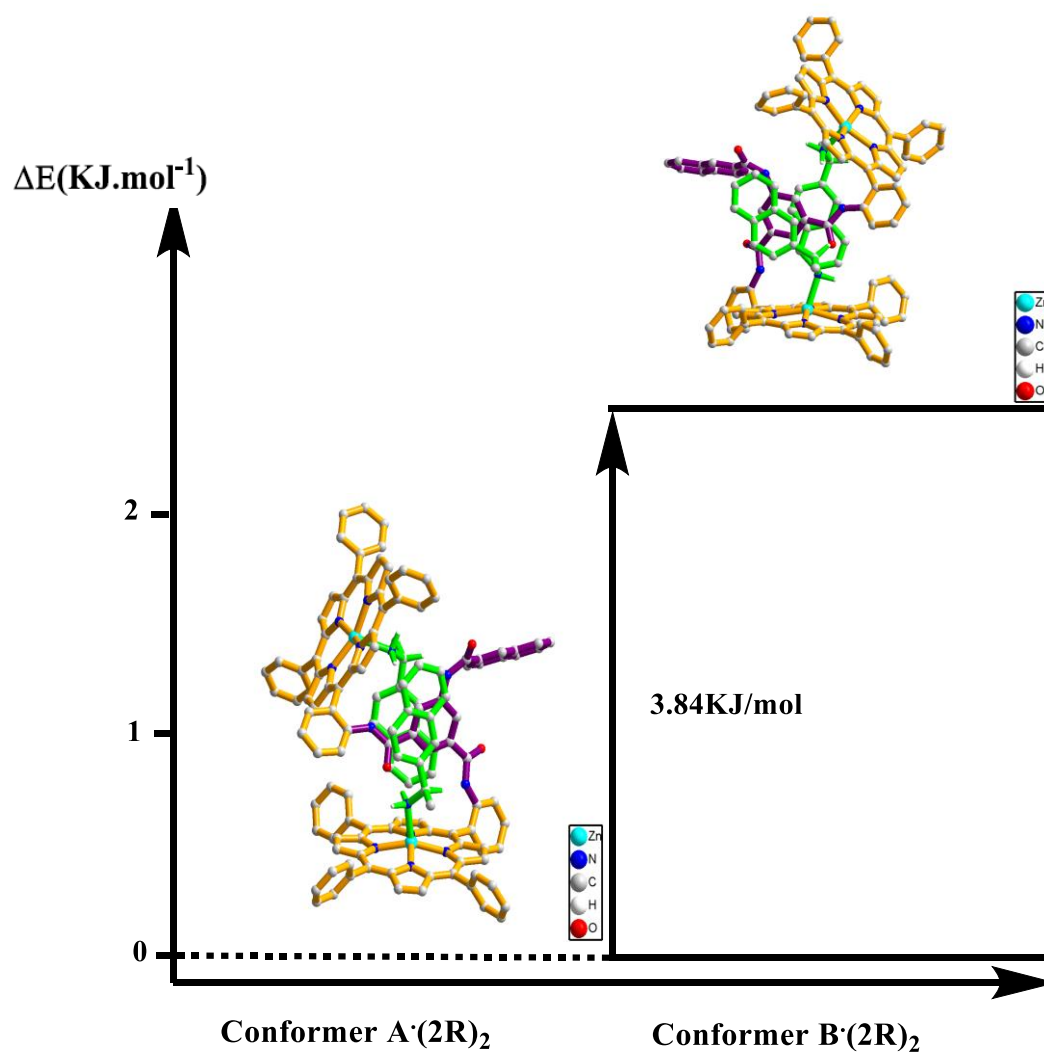
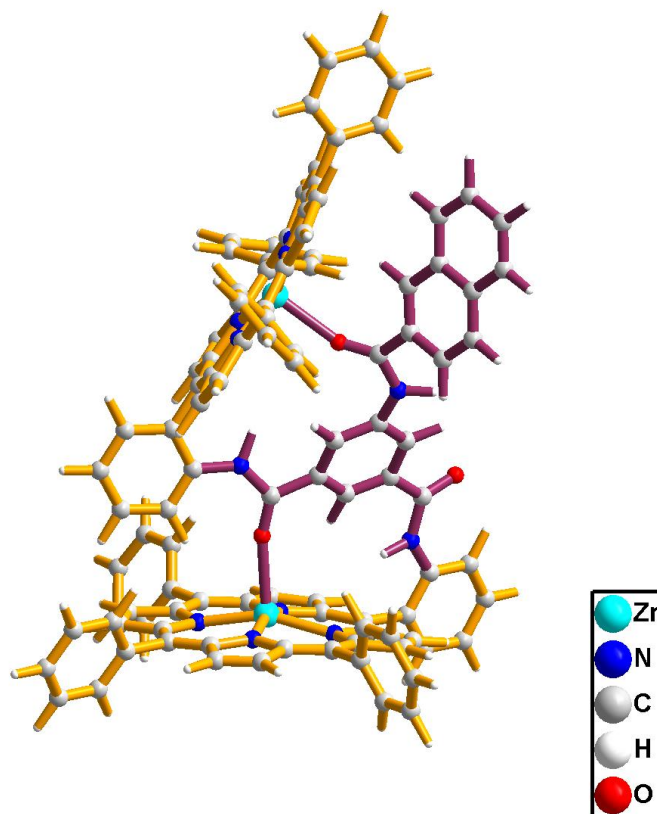


Figure S41. Relative energies of DFT-optimized conformer A·(2R)₂ and conformer B·(2R)₂

10. Cartesian coordinates for Geometry Optimized Conformers for all the calculated structures.



Conformer A

$\Delta E = -8504.24671789$ a.u.

Atoms	x	y	z
Zn	5.25838500	-0.34627500	0.36387600
Zn	-4.30496700	0.34938600	-1.30990500
N	5.85816000	1.60626300	0.73997600
C	5.64084300	1.65506100	3.20683100
C	5.39077600	0.28235700	3.40418500
C	5.15800200	-0.31805200	4.69990900
H	5.18747700	0.20691300	5.64448700
N	3.15850300	2.45214100	4.06658300
H	3.46868200	1.76002400	3.39996400
O	1.21010200	3.31152200	4.96036800
C	-0.94070900	0.65184400	2.42518300
N	5.29478600	-0.67356300	2.42002700
C	4.85419200	-3.10986300	2.43351900

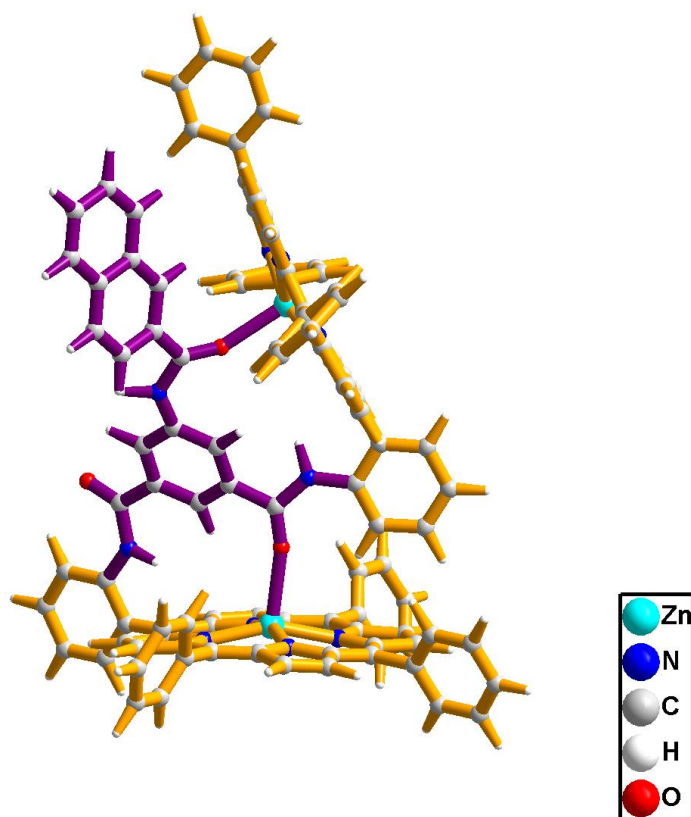
C	5.01023300	-1.85917500	3.05749300
C	4.91126500	-1.63794100	4.48480000
H	4.69214300	-2.39641400	5.22192700
N	0.95414700	-0.11387800	-1.28416400
H	-0.01465900	0.14231900	-1.13815000
O	3.00095800	-0.02385800	-0.23529300
C	-0.24875400	1.47139100	3.32260500
H	-0.72402700	1.84248900	4.22643000
N	5.30929900	-2.39684300	0.10386500
C	5.89392500	-2.49712100	-2.30225000
C	5.03652700	-3.34673400	1.05691000
C	5.06922500	-4.66481500	0.46112000
H	4.91338200	-5.59367400	0.99028900
C	1.08330600	1.81060200	3.08543600
N	6.02077400	-0.13634900	-1.55636200
C	6.32146600	2.32302700	-1.58534300
C	5.52615800	-3.07458500	-1.07240100
C	5.38093900	-4.49746000	-0.85163300
H	5.52676200	-5.26417300	-1.59834200
C	1.70658400	1.36357500	1.91480200
H	2.72142500	1.64683600	1.65933400
C	6.11192000	-1.12080800	-2.51185200
C	6.42862000	-0.52984800	-3.79429600
H	6.55641100	-1.07234700	-4.71986500
C	1.02013400	0.55507000	1.00853300
C	6.27907400	1.05314200	-2.19457200
C	6.52051000	0.81392800	-3.59985300
H	6.73400300	1.57423200	-4.33676400
C	-0.30775000	0.18634100	1.26695700
H	-0.84564700	-0.48909000	0.61251600
C	6.15049300	2.55761900	-0.20976200
C	6.33528400	3.84513700	0.42601400
H	6.59238200	4.76199200	-0.08430600
C	1.80492700	2.62341000	4.13717200
C	5.86512200	2.25428700	1.95257400
C	6.15303100	3.65905500	1.76067500
H	6.22820700	4.39362600	2.54971400
C	1.76697000	0.10195800	-0.21950400
N	-2.81024200	1.50416800	-2.17596600
C	-1.29418100	-0.30817000	-2.93173800
C	-3.83722500	-2.62346000	-1.98312600
C	-2.81792900	-3.54298500	-2.44429600
H	-2.91645200	-4.61832100	-2.47935200
N	-3.38447300	-1.33137000	-2.09629200

C	-5.12060400	-3.00819300	-1.55696600
C	-2.12008800	-1.40612900	-2.62546000
C	-1.75533300	-2.79106800	-2.83815900
H	-0.81728100	-3.13381600	-3.25072000
N	-6.07200500	-0.74179300	-1.22486800
C	-7.68940900	1.08520400	-0.77608800
C	-1.63975800	1.04310100	-2.72631400
C	-0.76841600	2.15736700	-3.03809600
H	0.20596800	2.07988000	-3.49979200
N	-5.44811000	2.07805700	-1.15108100
C	-3.69022900	3.75635500	-1.65434200
C	-2.70033100	2.87310300	-2.11933800
C	-1.41607900	3.28595700	-2.64453400
H	-1.06606000	4.30540200	-2.71315700
C	-4.98401100	3.36738600	-1.25624800
C	-6.06663000	4.30016400	-1.03755100
H	-5.98262600	5.37605800	-1.08533500
C	-6.79704000	2.16974100	-0.89707400
C	-7.18946400	3.56150600	-0.83343200
H	-8.19587300	3.92366000	-0.68499600
C	-7.32568100	-0.27140200	-0.91142800
C	-8.22523400	-1.38501200	-0.69703700
H	-9.26707700	-1.30710900	-0.42345600
C	-6.15995000	-2.11446600	-1.23277200
C	-7.50193000	-2.52189900	-0.88311200
H	-7.84377200	-3.54274100	-0.79508500
C	5.51722100	2.56591200	4.40087400
C	6.62309900	3.04460300	5.10560600
H	7.61593600	2.73075500	4.79528800
C	6.46536400	3.91462900	6.18815700
H	7.33797900	4.27691600	6.72417000
C	5.18521700	4.31412600	6.57307500
H	5.05622400	4.99189400	7.41275800
C	4.05738200	3.85173400	5.89399100
H	3.05768200	4.15103500	6.18232800
C	4.22383000	2.97877000	4.81341200
C	4.51642400	-4.28873200	3.29523300
C	3.26266500	-4.91098700	3.18925400
H	2.53825000	-4.52213400	2.47882200
C	2.94048300	-6.01119500	3.98498600
H	1.96283000	-6.47690600	3.89005200
C	3.86834300	-6.51071100	4.90069400
H	3.61861000	-7.36796800	5.52029400
C	5.12071700	-5.90404900	5.01295800

H	5.85278000	-6.29053800	5.71737400
C	5.44182400	-4.80382500	4.21674300
H	6.42067200	-4.33975500	4.29968900
C	6.08072600	-3.41577900	-3.47138800
C	4.99168000	-4.10658800	-4.02706100
H	4.00132300	-3.95952100	-3.60600500
C	5.16850100	-4.96267200	-5.11523800
H	4.31160400	-5.48418300	-5.53393100
C	6.43801100	-5.14544800	-5.66634400
H	6.57604800	-5.81263300	-6.51305500
C	7.52955300	-4.46608300	-5.12193400
H	8.52302200	-4.60617100	-5.54012600
C	7.35218800	-3.60933600	-4.03491400
H	8.20471800	-3.08791900	-3.60871200
C	6.61068200	3.50732300	-2.45764800
C	7.87943400	3.68962600	-3.03000200
H	8.65975500	2.96038800	-2.83052000
C	8.14613300	4.79496900	-3.83896000
H	9.13626000	4.92074700	-4.26946100
C	7.14805900	5.73856000	-4.08935800
H	7.35521800	6.59950000	-4.71943400
C	5.88276000	5.57024100	-3.52409400
H	5.09866600	6.29833400	-3.71528900
C	5.61716900	4.46478500	-2.71471300
H	4.63031800	4.33357500	-2.27952500
C	0.08200200	-0.59704900	-3.46389000
C	0.27990900	-0.97162600	-4.79571600
H	-0.58577200	-1.04337000	-5.44807300
C	1.55767200	-1.24393600	-5.28739000
H	1.69012400	-1.52870300	-6.32730900
C	2.65876300	-1.14163700	-4.43784600
H	3.65897100	-1.34416700	-4.80727200
C	2.49716600	-0.77355700	-3.10181000
H	3.35014900	-0.69087800	-2.44321900
C	1.21389600	-0.50160500	-2.61645600
C	-5.41524700	-4.47714200	-1.49367700
C	-4.84444700	-5.27816300	-0.49281800
H	-4.19230900	-4.81877100	0.24497200
C	-5.11106800	-6.64690100	-0.43425700
H	-4.66257500	-7.24995200	0.35106800
C	-5.95270800	-7.23893100	-1.37761200
H	-6.16013900	-8.30478800	-1.33284000
C	-6.52499200	-6.45348300	-2.37995900
H	-7.17694300	-6.90647400	-3.12241100

C	-6.25807400	-5.08494600	-2.43725700
H	-6.69853400	-4.47697300	-3.22264500
C	-9.13118000	1.39785100	-0.51676800
C	-10.12001900	1.03428100	-1.44665100
H	-9.82387500	0.52923300	-2.36146200
C	-11.46469800	1.32392900	-1.21458100
H	-12.21068800	1.03796700	-1.95150600
C	-11.85113900	1.98533600	-0.04714400
H	-12.89865300	2.21143500	0.13301800
C	-10.88082700	2.35812200	0.88427900
H	-11.16880700	2.87508000	1.79601700
C	-9.53543400	2.06933000	0.65007400
H	-8.78551100	2.36648600	1.37792100
C	-3.37844400	5.22215900	-1.63677900
C	-3.21509900	5.94686200	-2.82799900
H	-3.32026300	5.43319300	-3.77961400
C	-2.93265800	7.31322300	-2.79924900
H	-2.81433700	7.85790000	-3.73240800
C	-2.80924700	7.97945000	-1.57852000
H	-2.58849900	9.04330800	-1.55619700
C	-2.97286000	7.27088700	-0.38687400
H	-2.87611900	7.78002100	0.56850000
C	-3.25666000	5.90493400	-0.41654100
H	-3.37963300	5.35465400	0.51219400
C	-3.32288300	-0.07340200	2.00223700
O	-3.34512300	0.16364500	0.78811500
N	-2.23667000	0.21889600	2.79225700
H	-2.41125500	0.19573700	3.78804400
C	-4.44656000	-0.69847600	2.76687900
C	-5.75813700	-0.41601400	2.43414300
C	-6.83297500	-0.95810000	3.18632700
C	-6.54840100	-1.82901500	4.28908600
C	-5.19316000	-2.13061200	4.58661100
C	-4.17051200	-1.57884700	3.85516100
H	-8.40675100	-0.00166000	2.04842000
H	-5.97267600	0.24219900	1.59822600
C	-8.18868100	-0.65427800	2.88659400
C	-7.62575900	-2.36332400	5.04336700
H	-4.97302800	-2.81379200	5.40316800
H	-3.14371600	-1.85223800	4.08082000
C	-8.92795800	-2.04667900	4.72749700
C	-9.21110000	-1.18429400	3.63996700
H	-7.40448300	-3.02547800	5.87688100
H	-9.74521500	-2.45908300	5.31292400

H	-10.24237700	-0.94227800	3.39890200
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Conformer B

$\Delta E = -8504.24671719 \text{ a.u.}$

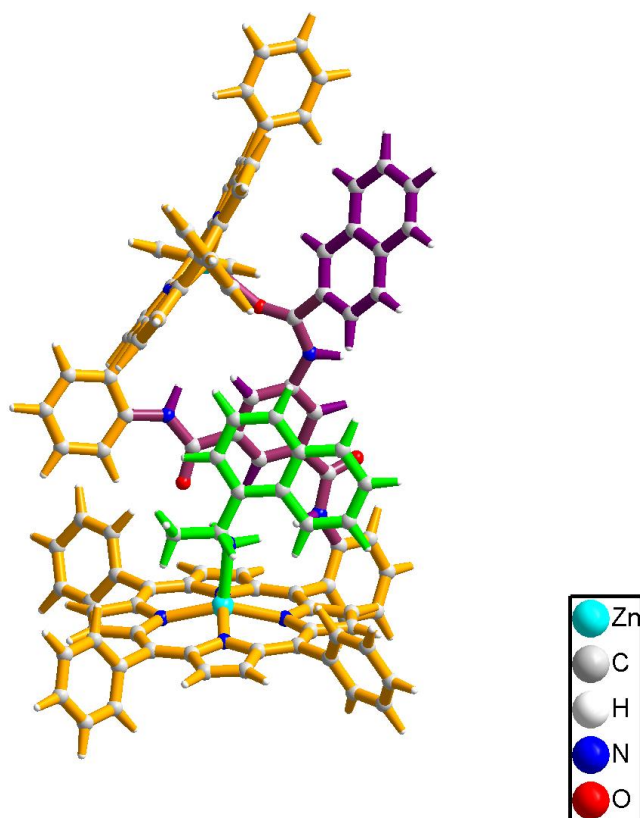
Atoms	x	y	z
Zn	-5.25838300	-0.34596700	0.36405500
Zn	4.30496400	0.34840000	-1.31001600
N	-5.85774500	1.60693600	0.73903900
C	-5.64059700	1.65704300	3.20588500
C	-5.39079900	0.28439900	3.40401700
C	-5.15822800	-0.31534300	4.70009300
H	-5.18769700	0.21015000	5.64437900
N	-3.15817100	2.45448600	4.06502700
H	-3.46841400	1.76200000	3.39882200
O	-1.20970400	3.31434600	4.95819400
C	0.94099000	0.65312200	2.42461700
N	-5.29490600	-0.67208800	2.42039500
C	-4.85476400	-3.10844900	2.43526000
C	-5.01059800	-1.85739000	3.05853700
C	-4.91168800	-1.63538800	4.48572900

H	-4.69275600	-2.39350400	5.22328300
N	-0.95401300	-0.11548500	-1.28401100
H	0.01480900	0.14077200	-1.13819000
O	-3.00083600	-0.02433500	-0.23525500
C	0.24906400	1.47328600	3.32149900
H	0.72437100	1.84502800	4.22504000
N	-5.30981100	-2.39665600	0.10522500
C	-5.89448900	-2.49814900	-2.30082500
C	-5.03717800	-3.34605900	1.05878500
C	-5.07015200	-4.66447100	0.46374400
H	-4.91446800	-5.59306000	0.99343600
C	-1.08302000	1.81228500	3.08417300
N	-6.02071000	-0.13690000	-1.55630200
C	-6.32081700	2.32252300	-1.58669300
C	-5.52683800	-3.07501700	-1.07065700
C	-5.38190900	-4.49779800	-0.84908500
H	-5.52793000	-5.26491000	-1.59534400
C	-1.70635300	1.36441300	1.91388700
H	-2.72121300	1.64747300	1.65827400
C	-6.11208700	-1.12189300	-2.51122700
C	-6.42857700	-0.53158800	-3.79402200
H	-6.55645600	-1.07458000	-4.71929000
C	-1.01993900	0.55527300	1.00815600
C	-6.27868600	1.05228200	-2.19520700
C	-6.52012400	0.81232300	-3.60035700
H	-6.73338700	1.57226100	-4.33771200
C	0.30797300	0.18675900	1.26677200
H	0.84584800	-0.48914100	0.61280200
C	-6.14986600	2.55783000	-0.21123400
C	-6.33448500	3.84571900	0.42383500
H	-6.59138500	4.76233900	-0.08700900
C	-1.80458600	2.62576500	4.13543200
C	-5.86468600	2.25562200	1.95128700
C	-6.15233900	3.66033200	1.75861000
H	-6.22744900	4.39533100	2.54725600
C	-1.76682300	0.10128500	-0.21952900
N	2.80994800	1.50251900	-2.17651300
C	1.29424200	-0.31042900	-2.93154100
C	3.83781100	-2.62480800	-1.98213700
C	2.81868400	-3.54473600	-2.44288700
H	2.91743200	-4.62006400	-2.47752000
N	3.38478300	-1.33286100	-2.09579100
C	5.12129600	-3.00910000	-1.55589800
C	2.12039400	-1.40809700	-2.62487200

C	1.75591500	-2.79320100	-2.83700500
H	0.81791900	-3.13630900	-3.24938500
N	6.07222500	-0.74236100	-1.22474300
C	7.68924400	1.08515900	-0.77668700
C	1.63954700	1.04099000	-2.72664800
C	0.76794800	2.15494600	-3.03882100
H	-0.20643400	2.07706300	-3.50045700
N	5.44769900	2.07738800	-1.15189200
C	3.68944600	3.75510800	-1.65575400
C	2.69974300	2.87145600	-2.12040900
C	1.41537800	3.28382700	-2.64571000
H	1.06512800	4.30316700	-2.71470500
C	4.98331800	3.36657800	-1.25752100
C	6.06573400	4.29966800	-1.03916500
H	5.98148800	5.37552700	-1.08732100
C	6.79662300	2.16945200	-0.89798200
C	7.18874600	3.56132700	-0.83485700
H	8.19508400	3.92375300	-0.68660100
C	7.32581600	-0.27157800	-0.91154000
C	8.22561800	-1.38490900	-0.69676700
H	9.26746400	-1.30667500	-0.42329100
C	6.16046600	-2.11501900	-1.23211700
C	7.50255200	-2.52202500	-0.88237200
H	7.84462800	-3.54275400	-0.79396500
C	-5.51685900	2.56851200	4.39944500
C	-6.62266800	3.04762700	5.10399600
H	-7.61554000	2.73367000	4.79390500
C	-6.46481800	3.91820000	6.18609200
H	-7.33737800	4.28080100	6.72198100
C	-5.18462300	4.31783300	6.57071500
H	-5.05553500	4.99603100	7.41003800
C	-4.05685800	3.85504300	5.89178700
H	-3.05712500	4.15445900	6.17989000
C	-4.22342100	2.98153400	4.81166800
C	-4.51717100	-4.28689400	3.29762300
C	-3.26346700	-4.90932600	3.19203400
H	-2.53898400	-4.52092400	2.48142300
C	-2.94142600	-6.00913700	3.98837200
H	-1.96381400	-6.47499400	3.89373000
C	-3.86937400	-6.50806800	4.90430800
H	-3.61975300	-7.36501600	5.52438200
C	-5.12169300	-5.90122200	5.01619200
H	-5.85382400	-6.28726100	5.72078700
C	-5.44266100	-4.80139700	4.21936800

H	-6.42146400	-4.33718000	4.30202500
C	-6.08162200	-3.41742800	-3.46942100
C	-4.99281700	-4.10884900	-4.02480700
H	-4.00238100	-3.96180000	-3.60393100
C	-5.16996600	-4.96550400	-5.11247800
H	-4.31324400	-5.48748200	-5.53094800
C	-6.43957300	-5.14824900	-5.66336800
H	-6.57786600	-5.81587600	-6.50969100
C	-7.53088100	-4.46827800	-5.11924600
H	-8.52442400	-4.60833200	-5.53726900
C	-7.35318600	-3.61095700	-4.03273400
H	-8.20554000	-3.08907000	-3.60675600
C	-6.60974400	3.50639100	-2.45966700
C	-7.87842500	3.68863300	-3.03219100
H	-8.65890400	2.95966200	-2.83234200
C	-8.14486000	4.79357900	-3.84178300
H	-9.13494100	4.91931700	-4.27240600
C	-7.14658300	5.73682400	-4.09265600
H	-7.35352500	6.59745300	-4.72322400
C	-5.88134700	5.56856500	-3.52722700
H	-5.09710100	6.29639700	-3.71878900
C	-5.61602300	4.46351200	-2.71721100
H	-4.62922400	4.33234800	-2.28188800
C	-0.08191300	-0.59981700	-3.46348000
C	-0.27981400	-0.97522800	-4.79507000
H	0.58585200	-1.04720500	-5.44742400
C	-1.55754900	-1.24808600	-5.28651500
H	-1.68999900	-1.53350600	-6.32625500
C	-2.65861500	-1.14549900	-4.43697100
H	-3.65879900	-1.34847300	-4.80622100
C	-2.49702300	-0.77657300	-3.10117000
H	-3.34998700	-0.69366800	-2.44258800
C	-1.21378400	-0.50405700	-2.61605200
C	5.41625200	-4.47795800	-1.49204200
C	4.84561000	-5.27871200	-0.49087600
H	4.19337200	-4.81917300	0.24673300
C	5.11251700	-6.64737200	-0.43177900
H	4.66414400	-7.25021000	0.35378000
C	5.95428500	-7.23959300	-1.37489700
H	6.16193800	-8.30539000	-1.32971000
C	6.52641100	-6.45441600	-2.37754800
H	7.17845700	-6.90756100	-3.11982000
C	6.25921200	-5.08595600	-2.43538000
H	6.69954500	-4.47820200	-3.22100400

C	9.13096300	1.39821500	-0.51757100
C	10.11982200	1.03456700	-1.44740300
H	9.82373000	0.52915300	-2.36202800
C	11.46444900	1.32459800	-1.21551500
H	12.21045800	1.03856900	-1.95239400
C	11.85081400	1.98647500	-0.04831700
H	12.89829000	2.21287600	0.13169900
C	10.88047900	2.35934100	0.88304900
H	11.16840100	2.87666500	1.79459800
C	9.53513700	2.07016200	0.64902900
H	8.78519600	2.36737600	1.37683300
C	3.37733800	5.22084900	-1.63873300
C	3.21383100	5.94507500	-2.83022300
H	3.31909700	5.43107500	-3.78164800
C	2.93110200	7.31138300	-2.80197900
H	2.81265600	7.85569000	-3.73534000
C	2.80755700	7.97804100	-1.58149800
H	2.58658000	9.04186100	-1.55957400
C	2.97134100	7.26996200	-0.38959100
H	2.87450500	7.77942900	0.56559600
C	3.25543100	5.90405600	-0.41875100
H	3.37853400	5.35415500	0.51018900
C	3.32311400	-0.07257100	2.00210900
O	3.34524700	0.16329900	0.78775300
N	2.23699000	0.22050100	2.79194800
H	2.41163300	0.19817700	3.78774200
C	4.44683200	-0.69701600	2.76721500
C	5.75839700	-0.41495200	2.43410900
C	6.83326200	-0.95643200	3.18669100
C	6.54872400	-1.82632700	4.29026800
C	5.19349000	-2.12757600	4.58816600
C	4.17081800	-1.57640000	3.85630000
H	8.40701300	-0.00112700	2.04779000
H	5.97291600	0.24249500	1.59758100
C	8.18896400	-0.65297300	2.88657300
C	7.62611100	-2.36000700	5.04495200
H	4.97337100	-2.81001300	5.40535100
H	3.14402600	-1.84954900	4.08228300
C	8.92830500	-2.04372900	4.72869100
C	9.21141100	-1.18235800	3.64035300
H	7.40486200	-3.02138600	5.87909100
H	9.74558100	-2.45564500	5.31443800
H	10.24268500	-0.94061900	3.39898100



Conformer A•1R

$\Delta E = -9024.13880691$ a.u.

Atoms	x	y	z
Zn	5.94272300	0.21325000	0.24994200
C	2.25373900	-2.16272200	-0.94801100
C	1.15540300	-1.85184600	-1.72683000
H	1.25047300	-1.12841800	-2.52945700
C	-0.10831000	-2.45592800	-1.52025600
H	-0.93954100	-2.18217800	-2.16489800
C	-0.27317800	-3.38326800	-0.52050500
H	-1.23834300	-3.85846100	-0.35710600
C	2.10136800	-3.13205500	0.10505600
C	0.81832500	-3.74417100	0.31406500
C	0.66398500	-4.70362300	1.35053500
H	-0.31159500	-5.16659500	1.48569000
C	1.71811800	-5.05066200	2.16429900
H	1.58414700	-5.78471700	2.95425200
C	2.98287400	-4.45162300	1.96620500
H	3.81869000	-4.72311600	2.60447700

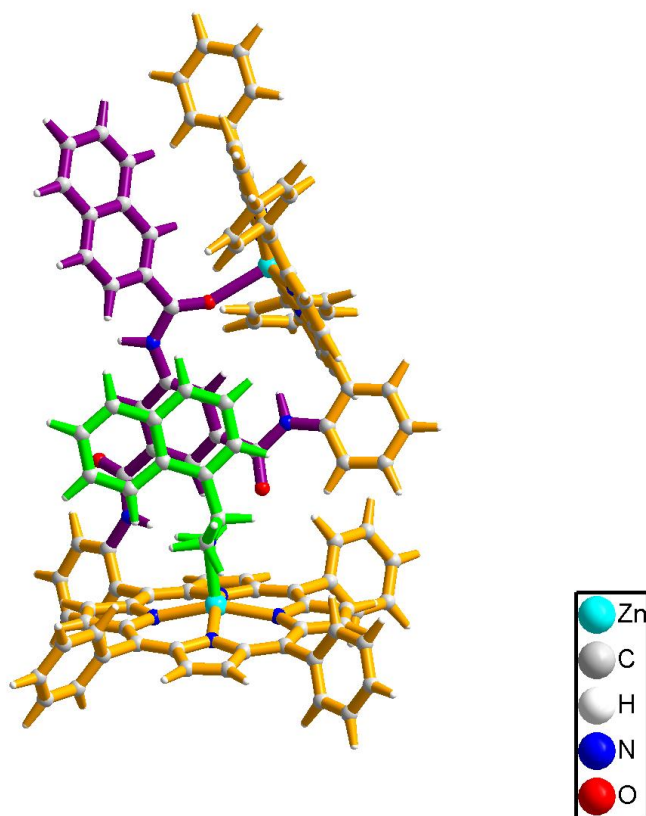
C	3.16883000	-3.52361800	0.96360400
H	4.15699400	-3.09374300	0.83746800
C	3.61052800	-1.49382100	-1.17620900
H	4.38780100	-2.25925000	-1.08553400
C	3.77571900	-0.84030800	-2.54893600
H	3.55949200	-1.55864800	-3.34587600
H	4.80314300	-0.49016200	-2.66637100
H	3.11271900	0.02316200	-2.66794300
Zn	-5.37293900	0.73917000	-1.01287600
N	5.45272300	1.94568800	1.31844700
C	5.26773700	1.00769200	3.60544400
C	5.75025700	-0.28925800	3.33389300
C	5.83989400	-1.34945400	4.31649500
H	5.54540100	-1.26848300	5.35307000
N	2.54045800	1.17501300	4.41840700
H	2.92913400	1.06657800	3.49067000
O	0.57773100	0.98423300	5.60959300
C	-1.49157800	-0.12141300	2.13539300
N	6.20428400	-0.73853100	2.11861900
C	7.16964500	-2.87556900	1.32356200
C	6.60066100	-2.04061800	2.30600600
C	6.35915700	-2.43404800	3.68001100
H	6.57005300	-3.40677600	4.10050800
N	-0.26085000	1.91212300	-1.37573100
H	-1.21795000	1.82035300	-1.05996900
O	1.90901000	1.79448000	-0.62946300
C	-0.75409700	0.12626800	3.29519000
H	-1.09700800	-0.22605100	4.26371700
N	7.18041000	-1.25954500	-0.55768400
C	7.66797100	-0.21348500	-2.75115900
C	7.46208400	-2.48239600	0.00069900
C	8.17509600	-3.30452500	-0.95427200
H	8.52989200	-4.30890200	-0.77353200
C	0.45646900	0.82116000	3.23543400
N	6.47869200	1.44216000	-1.34356900
C	5.43886900	3.55112500	-0.56766900
C	7.70796300	-1.27611000	-1.82666900
C	8.32304000	-2.56117800	-2.08397100
H	8.81212500	-2.84809300	-3.00353100
C	0.90902500	1.30997100	2.00600800
H	1.82146700	1.89207700	1.92101000
C	7.08961900	1.04896500	-2.50875400
C	7.06333600	2.13524800	-3.46572100
H	7.48981900	2.10643900	-4.45795700

C	0.15350200	1.09619700	0.84704900
C	6.06806200	2.73835500	-1.53205800
C	6.41431600	3.17166700	-2.86972400
H	6.20584300	4.14632900	-3.28638000
C	-1.04318400	0.37088000	0.90561700
H	-1.60300800	0.13217300	0.01046100
C	5.20514100	3.17877400	0.76988700
C	4.73247500	4.08657300	1.79555400
H	4.48502500	5.12719100	1.64320400
C	1.18625700	1.01033200	4.54347100
C	5.15811000	2.04409400	2.65512800
C	4.71088100	3.38802100	2.96297800
H	4.44396700	3.74888000	3.94657300
C	0.69655400	1.62908500	-0.45114200
N	-4.38461800	2.56406200	-1.15549400
C	-2.65080800	1.95281800	-2.82103200
C	-4.33752100	-1.16887900	-3.20227400
C	-3.23432000	-1.36512300	-4.11958400
H	-3.08050900	-2.24036900	-4.73421200
N	-4.23818500	0.06776600	-2.61308300
C	-5.38721400	-2.08657800	-3.01444000
C	-3.11710900	0.66234100	-3.13635800
C	-2.47830600	-0.23352300	-4.07727300
H	-1.58688400	-0.01118000	-4.64632300
N	-6.78305700	-0.70918700	-1.49704400
C	-8.68566000	0.05381600	-0.09910700
C	-3.26253300	2.82864500	-1.90247600
C	-2.75424000	4.14575500	-1.57965800
H	-1.89346500	4.61356700	-2.03668000
N	-6.84885700	1.71027300	0.08125700
C	-5.66286400	3.84364900	0.53149900
C	-4.59402100	3.66861900	-0.36518500
C	-3.56524900	4.65589400	-0.61511300
H	-3.48562100	5.61510500	-0.12517400
C	-6.73300300	2.94099600	0.68210500
C	-7.95201000	3.26034100	1.39078200
H	-8.13780200	4.17709600	1.93110000
C	-8.11508400	1.25527800	0.36804700
C	-8.81250600	2.22933200	1.18091200
H	-9.83538400	2.14903000	1.51729000
C	-8.03456500	-0.86510200	-0.94980500
C	-8.58274000	-2.14620300	-1.34212500
H	-9.54400000	-2.53664100	-1.04236700
C	-6.53494500	-1.84266700	-2.23570000

C	-7.65112900	-2.75445900	-2.12443900
H	-7.71288000	-3.72882700	-2.58640600
C	4.87190700	1.31398400	5.02389400
C	5.85812300	1.52905000	5.99313200
H	6.89922600	1.48475200	5.68618800
C	5.52859100	1.79336700	7.32245000
H	6.31314500	1.95799100	8.05556900
C	4.18601400	1.84309000	7.69601400
H	3.91255400	2.04558300	8.72816100
C	3.17704600	1.63668300	6.75690900
H	2.13468100	1.66307000	7.04165200
C	3.51368000	1.37517900	5.42041400
C	7.54422700	-4.27067600	1.72740700
C	6.84349800	-5.37825900	1.22396200
H	6.01502900	-5.21660800	0.53969600
C	7.19321900	-6.67691100	1.59818800
H	6.63489400	-7.52025800	1.19990400
C	8.25308600	-6.89185900	2.48084800
H	8.52665300	-7.90270400	2.77155300
C	8.96069600	-5.79948900	2.98614400
H	9.79167300	-5.95657000	3.66904700
C	8.60946300	-4.50166600	2.61238900
H	9.16691500	-3.65400900	3.00105800
C	8.30264700	-0.43693500	-4.09200900
C	7.51727400	-0.57106700	-5.24741900
H	6.43537100	-0.51783600	-5.16165300
C	8.10875400	-0.77613300	-6.49477100
H	7.48257800	-0.88120700	-7.37709500
C	9.49805900	-0.85093700	-6.60868000
H	9.95945000	-1.01070700	-7.57964000
C	10.29102000	-0.71845400	-5.46732200
H	11.37387400	-0.77052200	-5.54646800
C	9.69835500	-0.51301700	-4.22064900
H	10.31790900	-0.40394600	-3.33479400
C	5.00478400	4.92490600	-0.98097700
C	5.93743700	5.93623600	-1.25819400
H	6.99809200	5.71979500	-1.16469100
C	5.51478900	7.21035800	-1.64053400
H	6.25146300	7.98265400	-1.84677500
C	4.15227800	7.49431800	-1.75137100
H	3.82348600	8.48645500	-2.04950700
C	3.21510700	6.49705400	-1.47465300
H	2.15232000	6.70868100	-1.56028600
C	3.63710100	5.22336100	-1.09048100

H	2.91011600	4.44399600	-0.87859700
C	-1.36101800	2.39762500	-3.45256600
C	-1.31224200	2.83573300	-4.77871500
H	-2.23757800	2.87195700	-5.34668800
C	-0.10683800	3.21713200	-5.37147400
H	-0.09206100	3.55571800	-6.40347100
C	1.07175800	3.16168200	-4.62857100
H	2.01580500	3.45820400	-5.07716800
C	1.05913600	2.73387200	-3.30064900
H	1.96999900	2.69539800	-2.71928600
C	-0.15389100	2.35280600	-2.71137100
C	-5.29702500	-3.39562500	-3.74010900
C	-4.36236100	-4.36642900	-3.34831700
H	-3.71071600	-4.16327300	-2.50283100
C	-4.26939700	-5.58383100	-4.02425400
H	-3.54109200	-6.32408700	-3.70327800
C	-5.10987200	-5.85127300	-5.10619900
H	-5.03737000	-6.79863600	-5.63369200
C	-6.04258100	-4.89317600	-5.50791300
H	-6.69709600	-5.08986000	-6.35308800
C	-6.13452400	-3.67622900	-4.83107300
H	-6.85555200	-2.92890600	-5.15048600
C	-10.09289400	-0.25344300	0.31143700
C	-11.10659000	-0.37896700	-0.65373700
H	-10.85702300	-0.24228600	-1.70186900
C	-12.42080300	-0.66232200	-0.28173700
H	-13.18865100	-0.74854200	-1.04612800
C	-12.75183900	-0.82575500	1.06485600
H	-13.77581200	-1.04610400	1.35424500
C	-11.75799900	-0.69903800	2.03663300
H	-12.00326100	-0.82213700	3.08835000
C	-10.44373300	-0.41338300	1.66316100
H	-9.67654800	-0.31093600	2.42569000
C	-5.71073400	5.10647000	1.33699700
C	-5.94352700	6.35028600	0.72909700
H	-6.09642700	6.39477800	-0.34564700
C	-5.99123800	7.51890400	1.49031800
H	-6.17712500	8.47201100	1.00201100
C	-5.80792500	7.46419000	2.87335700
H	-5.84429700	8.37440700	3.46594800
C	-5.57963900	6.23301600	3.49042700
H	-5.43356700	6.18055100	4.56616200
C	-5.53348100	5.06471600	2.72875400
H	-5.35173000	4.10799900	3.21058500

N	3.91606700	-0.47293600	-0.12293100
H	3.30888600	0.34300400	-0.26680600
H	3.65091600	-0.85000100	0.78779800
C	-3.73880300	-1.06944300	1.46089300
O	-4.03058200	-0.22832600	0.60042400
N	-2.61491500	-0.97278300	2.24330400
H	-2.59366400	-1.59717400	3.03841800
C	-4.54844800	-2.29161100	1.76380300
C	-5.92922300	-2.24646000	1.72835400
C	-6.70355400	-3.38812600	2.06358500
C	-6.03838600	-4.60810600	2.41647200
C	-4.61892800	-4.63565800	2.41274000
C	-3.89207800	-3.51195000	2.10485100
H	-8.63044500	-2.43768000	1.79781200
H	-6.43287500	-1.32323900	1.45914300
C	-8.12433300	-3.35721300	2.07058900
C	-6.81634800	-5.74633900	2.75502800
H	-4.11046400	-5.56577100	2.65452100
H	-2.80705900	-3.56461200	2.08059200
C	-8.19158100	-5.68177400	2.75290700
C	-8.85069400	-4.47617400	2.40838300
H	-6.30686200	-6.66993800	3.01881500
H	-8.77761200	-6.55817500	3.01595600
H	-9.93635300	-4.43674800	2.40866600



Conformer B•1R

$\Delta E = -9024.13309980$ a.u.

Atoms	x	y	z
Zn	-6.03515800	0.24427300	0.19811300
C	-2.23314500	-2.19892700	-0.99647700
C	-1.27034500	-1.89253100	-1.94099200
H	-1.53053900	-1.22548600	-2.75937300
C	0.04434100	-2.41039400	-1.88129000
H	0.76646700	-2.13702800	-2.64565200
C	0.40070300	-3.24666300	-0.85202900
H	1.40757600	-3.65383800	-0.79067000
C	-1.87991400	-3.07319100	0.09180800
C	-0.53998000	-3.59417400	0.15381000
C	-0.17132600	-4.45649100	1.22176400
H	0.84176400	-4.85410500	1.23481700
C	-1.06688900	-4.79759200	2.20846100
H	-0.76997700	-5.45769100	3.01891500
C	-2.38460200	-4.29004500	2.15802400
H	-3.09857900	-4.55795900	2.93171000

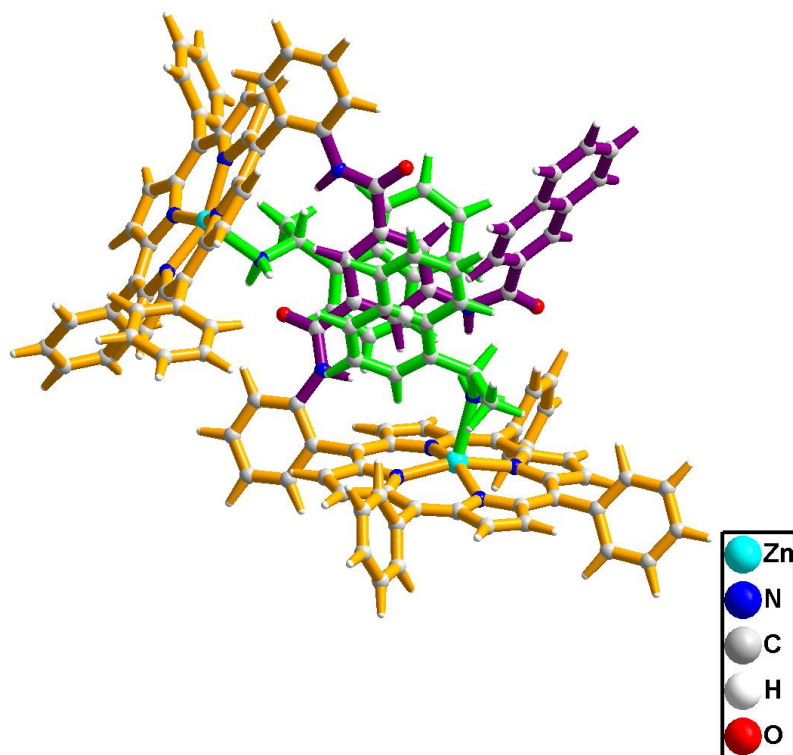
C	-2.77767200	-3.46102500	1.12979400
H	-3.80585100	-3.11938100	1.11997100
C	-3.63306400	-1.61173600	-1.19770600
Zn	5.37417200	0.73274700	-0.99539100
N	-5.27695400	1.86487000	1.30340100
C	-5.24499000	0.86345800	3.57344100
C	-5.90090300	-0.34725300	3.26842300
C	-6.12607300	-1.41859000	4.21666300
H	-5.79478300	-1.42411900	5.24522200
N	-2.51063600	0.80161500	4.42465500
H	-2.89367800	0.72478100	3.49179400
O	-0.55259600	0.58439500	5.61973900
C	1.55677200	-0.40014400	2.13670300
N	-6.44189500	-0.68018300	2.05100400
C	-7.79141600	-2.58598400	1.23067700
C	-7.04321300	-1.90546200	2.21144100
C	-6.82483500	-2.38511500	3.56147200
H	-7.17148900	-3.32951300	3.95542900
N	0.22132400	1.55375600	-1.38481800
H	1.18496900	1.48579500	-1.08420500
O	-1.92993200	1.42013300	-0.58872600
C	0.81248800	-0.18499200	3.29878600
H	1.16959300	-0.52711700	4.26584800
N	-7.52822400	-0.95375000	-0.61855300
C	-7.71923800	0.13223600	-2.83880300
C	-8.03854900	-2.10542600	-0.07217300
C	-8.89353300	-2.76665000	-1.03498600
H	-9.44153300	-3.68129600	-0.86137900
C	-0.42185100	0.46727400	3.24354000
N	-6.29533500	1.55103700	-1.39435100
C	-5.01123300	3.49112600	-0.54900300
C	-8.02027600	-0.87410200	-1.90006100
C	-8.87589900	-2.01107500	-2.16613600
H	-9.39793900	-2.19875300	-3.09314900
C	-0.89194300	0.94405600	2.01662000
H	-1.81896100	1.50235600	1.93348600
C	-6.90898700	1.25704900	-2.58643000
C	-6.65632500	2.31560900	-3.54098800
H	-7.03122500	2.34780200	-4.55381200
C	-0.13761000	0.75267400	0.85381600
C	-5.68628900	2.77073900	-1.55435700
C	-5.88932700	3.24431500	-2.90780700
H	-5.51262000	4.17408700	-3.30872500
C	1.08473500	0.07188200	0.90778700

H	1.64928000	-0.14888100	0.01132100
C	-4.87562700	3.07291800	0.78884600
C	-4.33185600	3.90067000	1.84625400
H	-3.96553800	4.90964500	1.72431100
C	-1.15699600	0.63061700	4.55159200
C	-5.00235000	1.90126400	2.64854800
C	-4.41455800	3.17913100	2.99677100
H	-4.13167400	3.48700500	3.99381300
C	-0.71282600	1.26638400	-0.43764400
N	4.25646400	2.48279700	-1.10067300
C	2.60251900	1.80049400	-2.81940900
C	4.53347300	-1.16616700	-3.27391500
C	3.46770400	-1.41151100	-4.22276300
H	3.39444900	-2.27268800	-4.87127200
N	4.32752600	0.03680400	-2.64349700
C	5.64527100	-2.00840200	-3.09428900
C	3.17395800	0.56242200	-3.16989800
C	2.62550000	-0.34392600	-4.15688500
H	1.73179000	-0.16799000	-4.73851300
N	6.89752500	-0.59133500	-1.49078700
C	8.70323700	0.25397700	-0.01423400
C	3.13296000	2.68969900	-1.86363400
C	2.52605800	3.95735900	-1.51437100
H	1.64330000	4.37577700	-1.97729700
N	6.74812200	1.76800600	0.16899100
C	5.40103900	3.79395000	0.65704900
C	4.36995000	3.57435200	-0.27323100
C	3.27979300	4.49455400	-0.51865100
H	3.12410900	5.43104000	-0.00363900
C	6.52725200	2.96320200	0.81051100
C	7.69770700	3.33758000	1.57217100
H	7.80078400	4.24234500	2.15329600
C	8.03361800	1.39087900	0.48129500
C	8.63439100	2.37695500	1.35465500
H	9.64858700	2.35289300	1.72453800
C	8.14578600	-0.67349000	-0.91999100
C	8.80144600	-1.88955500	-1.35253400
H	9.78532800	-2.21454200	-1.04798800
C	6.75438400	-1.70868500	-2.28015000
C	7.93636200	-2.53463300	-2.18057600
H	8.08392500	-3.47972900	-2.68227300
C	-4.83750900	1.08421700	5.00437100
C	-5.81892800	1.33154600	5.97202400
H	-6.85608800	1.37295600	5.65190000

C	-5.49121800	1.52309300	7.31385700
H	-6.27286100	1.71587300	8.04319500
C	-4.15383900	1.46493200	7.70389100
H	-3.88067700	1.60949300	8.74582600
C	-3.14942000	1.22228700	6.76894700
H	-2.11164900	1.16650500	7.06574100
C	-3.48347500	1.03528700	5.41905100
C	-8.40731700	-3.89854000	1.61163000
C	-7.97042800	-5.09628000	1.02355500
H	-7.17232700	-5.06422200	0.28675900
C	-8.54368400	-6.31870800	1.37647200
H	-8.18747100	-7.23457400	0.91178300
C	-9.56730400	-6.36620300	2.32454300
H	-10.01476200	-7.31772200	2.59939000
C	-10.01382500	-5.18273500	2.91539600
H	-10.81495200	-5.20807400	3.64963100
C	-9.43921300	-3.96120500	2.56187300
H	-9.79435200	-3.04113400	3.01743600
C	-8.32924300	0.01326400	-4.20378500
C	-7.54007900	-0.30739200	-5.31897100
H	-6.47537300	-0.47688200	-5.18286100
C	-8.10737200	-0.41492700	-6.58969700
H	-7.47947800	-0.66789200	-7.44024800
C	-9.47577800	-0.20354900	-6.76750100
H	-9.91811800	-0.28743600	-7.75666300
C	-10.27205800	0.11708800	-5.66647900
H	-11.33768200	0.28844400	-5.79539600
C	-9.70329300	0.22518800	-4.39664000
H	-10.32373600	0.48185900	-3.54242600
C	-4.42477100	4.82123100	-0.91392600
C	-5.24594600	5.91875300	-1.21632200
H	-6.32523800	5.79831300	-1.18240900
C	-4.69042800	7.15570200	-1.54653000
H	-5.34230700	7.99577800	-1.77231400
C	-3.30379700	7.31571600	-1.58030300
H	-2.87094800	8.27896100	-1.83746800
C	-2.47703300	6.23132800	-1.28085700
H	-1.39638300	6.34612700	-1.30860700
C	-3.03208400	4.99463200	-0.94873700
H	-2.39212600	4.14631300	-0.72434800
C	1.28533400	2.15998500	-3.44849800
C	1.20522100	2.61819200	-4.76632600
H	2.12592000	2.73763300	-5.33054100
C	-0.02481600	2.91740200	-5.35582800

H	-0.06326200	3.27449300	-6.38096700
C	-1.19710400	2.75671500	-4.61818600
H	-2.16075200	2.98790200	-5.06356400
C	-1.15438800	2.30630000	-3.29852000
H	-2.06084000	2.18882900	-2.72072700
C	0.08335600	2.01063100	-2.71139900
C	5.66796900	-3.29361800	-3.86635600
C	4.81329500	-4.35027100	-3.51699200
H	4.14238800	-4.22982900	-2.67070800
C	4.82383700	-5.54649500	-4.23580200
H	4.15656900	-6.35454400	-3.94726200
C	5.68999800	-5.70601800	-5.31884900
H	5.69835500	-6.63678800	-5.87975300
C	6.54416000	-4.66177700	-5.67820000
H	7.21789700	-4.77480100	-6.52361400
C	6.53287700	-3.46624300	-4.95832200
H	7.19320500	-2.65240400	-5.24488000
C	10.11621200	0.03176800	0.43051900
C	11.16832400	0.03868600	-0.50099000
H	10.94435400	0.21404100	-1.54921300
C	12.48761400	-0.16253400	-0.09467700
H	13.28531800	-0.14651400	-0.83272700
C	12.78473400	-0.37463600	1.25304300
H	13.81261600	-0.53075700	1.56914700
C	11.75176100	-0.37965500	2.19166700
H	11.97035300	-0.54203700	3.24392100
C	10.43230500	-0.17606200	1.78416200
H	9.63408600	-0.17625400	2.52127500
C	5.33830900	5.02981800	1.50263800
C	5.50866300	6.30527400	0.94159800
H	5.69368500	6.39476200	-0.12528100
C	5.45368700	7.44903500	1.73929500
H	5.59235800	8.42765000	1.28706500
C	5.22806300	7.33731600	3.11260500
H	5.18428900	8.22805700	3.73359700
C	5.06062800	6.07435900	3.68321000
H	4.88178200	5.97725600	4.75085600
C	5.11711700	4.93103600	2.88508100
H	4.98199800	3.94948900	3.33102000
N	-4.07310300	-0.69998400	-0.09792100
H	-3.42452800	0.09602900	-0.08881600
H	-3.95358700	-1.16044000	0.80351300
C	3.84277200	-1.24240100	1.45292100
O	4.08666500	-0.39560200	0.58328300

N	2.71903000	-1.19794600	2.24101300
H	2.73449200	-1.81395400	3.04263900
C	4.71718800	-2.41841900	1.75955400
C	6.09277500	-2.30699800	1.68453400
C	6.93159000	-3.40247000	2.01876700
C	6.33745400	-4.64671300	2.41164100
C	4.92147300	-4.74344400	2.44858400
C	4.13201600	-3.66288300	2.14073300
H	8.80137700	-2.36320700	1.68539500
H	6.54205600	-1.36600100	1.38311900
C	8.34891300	-3.30172400	1.98614700
C	7.17946500	-5.73908000	2.74770900
H	4.46607800	-5.69236900	2.72107900
H	3.05077700	-3.77037700	2.14795500
C	8.54931500	-5.60741500	2.70593500
C	9.13840100	-4.37741900	2.32304700
H	6.72355900	-6.68138200	3.04164800
H	9.18484100	-6.44904900	2.96757200
H	10.22040700	-4.28452400	2.29388700
C	-4.68463600	-2.68255400	-1.52327700
H	-4.31782600	-3.31567200	-2.33827100
H	-4.90611100	-3.33319600	-0.67292900
H	-5.61741200	-2.21194100	-1.83885500
H	-3.56775400	-0.95984900	-2.07435700



Conformer A·(1R)₂

$\Delta E = -9544.00736729$ a.u.

Atoms	x	y	z
Zn	-5.56918100	-1.43635300	1.03971400
N	-3.87242100	-1.47125800	2.27029300
N	-4.82986200	-3.13209700	0.10416100
N	-7.46915800	-1.96012800	0.39323600
N	-6.48650000	-0.22922500	2.50273300
C	-2.55719600	-3.21673400	1.08571900
C	-6.82493900	-3.70017900	-1.25247000
C	-8.80846500	-0.28413500	1.64058800
C	-4.54805300	0.19620200	3.98412100
C	-3.63934000	-0.69643300	3.38476800
C	-2.74566900	-2.23693800	2.08485500
C	-3.55084200	-3.63157800	0.17621600
C	-5.47570000	-3.84529600	-0.87802500
C	-7.74198500	-2.81744800	-0.64516200
C	-8.63223500	-1.27415300	0.65210500
C	-7.80334000	0.16311500	2.52254300

C	-5.88147000	0.38322100	3.57448800
C	-2.31360700	-0.96564800	3.89856300
H	-1.88026100	-0.50706300	4.77542400
C	-1.76604400	-1.92476200	3.10228700
H	-0.80098900	-2.40037600	3.20464700
C	-3.37832100	-4.67818600	-0.80928400
H	-2.47269500	-5.24527900	-0.96873800
C	-4.56927500	-4.81611500	-1.45224600
H	-4.82027300	-5.52154800	-2.23085600
C	-9.11830400	-2.65795600	-1.06354700
H	-9.59484700	-3.19768800	-1.86872500
C	-9.66719400	-1.70447300	-0.26384800
H	-10.67606900	-1.31993400	-0.29459900
C	-8.03037000	1.06408500	3.63357700
H	-8.98059500	1.50531800	3.89672900
C	-6.84241200	1.20066000	4.28201900
H	-6.63400300	1.77993200	5.16991800
C	-1.23607700	-3.93441400	1.04912100
C	-1.16763200	-5.27101600	1.46391200
H	-2.07969600	-5.74747300	1.81160800
C	0.03038700	-5.98384000	1.44617900
H	0.05291200	-7.01809600	1.77742700
C	1.19148200	-5.35400900	1.00108100
H	2.13530500	-5.89141200	0.97283000
C	1.16267700	-4.02577200	0.58086400
H	2.06057400	-3.54111100	0.22629200
C	-0.04274100	-3.30806800	0.60884000
C	-7.32544700	-4.55898200	-2.37444500
C	-6.87584200	-4.35281500	-3.68826700
H	-6.16322600	-3.55653800	-3.88552100
C	-7.33856600	-5.15183200	-4.73460500
H	-6.98229900	-4.97370000	-5.74589400
C	-8.25845400	-6.17196800	-4.48509000
H	-8.61856900	-6.79467900	-5.29967300
C	-8.71245900	-6.38781100	-3.18260000
H	-9.42447500	-7.18309700	-2.97784400
C	-8.25013200	-5.58799800	-2.13670700
H	-8.59954000	-5.76234900	-1.12279900
C	-10.17161200	0.31934800	1.78841700
C	-11.26207900	-0.45525700	2.21587000
H	-11.10698200	-1.50525000	2.44747400
C	-12.52972300	0.11086700	2.35547400
H	-13.35949000	-0.50464300	2.69305400
C	-12.73097800	1.46263700	2.07000900

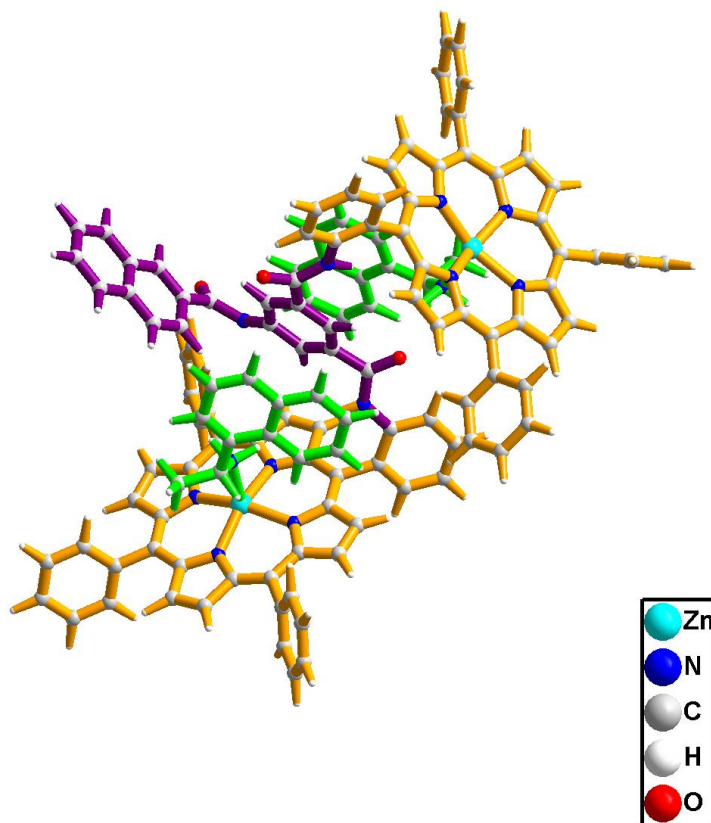
H	-13.71836600	1.90330600	2.17856500
C	-11.65526500	2.24488600	1.64614200
H	-11.80192300	3.29759400	1.41898500
C	-10.38773500	1.67808000	1.50833400
H	-9.55370000	2.28986300	1.17546000
C	-4.08172200	0.95048300	5.19686800
C	-3.98262000	0.30478300	6.43927800
H	-4.25336500	-0.74497900	6.51506100
C	-3.54679500	0.99690500	7.57011200
H	-3.47952200	0.48130600	8.52463900
C	-3.20265500	2.34690200	7.47592100
H	-2.86312000	2.88672500	8.35601400
C	-3.30009100	2.99868600	6.24535600
H	-3.03768400	4.05013900	6.16089800
C	-3.73821600	2.30865400	5.11190600
H	-3.80584800	2.83118700	4.16137700
Zn	6.28152200	-0.65371700	-0.45533900
N	7.09253500	1.22885700	-0.86053700
N	7.97444300	-1.04297800	0.70933200
N	6.05758700	-2.73302700	-0.65337400
N	5.17300200	-0.45643800	-2.21966600
C	8.99187300	1.21792000	0.73134700
C	7.60058300	-3.45723100	1.14093700
C	4.39275400	-2.79325500	-2.48593900
C	5.50916200	1.96995100	-2.61433900
C	6.51198100	2.19354000	-1.64831300
C	8.10234100	1.84712900	-0.16287000
C	8.93435000	-0.14251100	1.10109600
C	8.29136500	-2.23926600	1.30573400
C	6.55591400	-3.67059200	0.21746200
C	5.12576500	-3.37355700	-1.43049500
C	4.45462600	-1.43727400	-2.85869900
C	4.95073700	0.70761500	-2.91131800
C	7.13602700	3.47532200	-1.39352000
H	6.86248900	4.40965700	-1.86192700
C	8.12311300	3.25962100	-0.48220000
C	9.90144100	-0.79833200	1.95616600
H	10.78179500	-0.33429800	2.37645600
C	9.49877100	-2.09043100	2.09063100
H	9.98963200	-2.88124000	2.63912000
C	5.87841700	-4.93443800	0.01642700
H	6.05694800	-5.83910500	0.57935300
C	5.00164300	-4.75356100	-1.00945600
H	4.33231900	-5.48310700	-1.44230300

C	3.76842400	-0.87326900	-4.00315400
H	3.16015800	-1.42779000	-4.70292900
C	4.06876200	0.45369300	-4.03202300
H	3.75533500	1.18936400	-4.75965900
C	10.08449300	2.05351900	1.32481300
C	11.09672300	2.59244400	0.51398800
H	11.08343200	2.38906100	-0.55307100
C	12.11570900	3.37109500	1.06371100
H	12.89248500	3.77400600	0.41888300
C	12.14193000	3.62694600	2.43591900
H	12.93530600	4.23378600	2.86421200
C	11.14254700	3.09731500	3.25421000
H	11.15137000	3.29409200	4.32321300
C	10.12491700	2.31754900	2.70345400
H	9.34637000	1.91126600	3.34307600
C	8.04947600	-4.61958200	1.97194000
C	8.63989300	-5.74904600	1.38176400
H	8.77578900	-5.77210400	0.30424800
C	9.06151300	-6.82636500	2.16184500
H	9.52183600	-7.68805300	1.68527300
C	8.90054100	-6.79559700	3.54836600
H	9.22877600	-7.63471800	4.15602800
C	8.31777400	-5.67833500	4.14909500
H	8.18649000	-5.64504100	5.22763600
C	7.89842600	-4.60089000	3.36794200
H	7.44324700	-3.73389900	3.83888100
C	3.49117500	-3.68960800	-3.27832000
C	4.02058400	-4.70737800	-4.08776700
H	5.09822400	-4.83563700	-4.13907800
C	3.18145100	-5.54115400	-4.82802100
H	3.61102700	-6.31967900	-5.45327700
C	1.79660700	-5.37333200	-4.77016700
H	1.14246700	-6.02354300	-5.34517300
C	1.25779600	-4.36613700	-3.96744300
H	0.17994700	-4.23518800	-3.90908400
C	2.09716000	-3.53090600	-3.22901200
H	1.68091700	-2.75656700	-2.59241800
C	5.07492500	3.14424500	-3.44598400
C	3.79182800	3.73195200	-3.30796600
C	3.44198600	4.84881900	-4.08340300
H	2.46671600	5.29469200	-3.94986900
C	4.35128100	5.37027100	-5.00140200
H	4.06371300	6.23387100	-5.59539000
C	5.61233500	4.79726000	-5.15998300

H	6.31875200	5.20157700	-5.87944700
C	5.96066800	3.69467800	-4.38125300
H	6.93957500	3.23695300	-4.49099300
N	-2.06379800	2.69786700	1.15893100
H	-2.17338900	2.19363700	2.03415400
H	3.26662300	2.32236900	-1.92620500
O	2.06585300	-1.38454300	-0.18817700
O	1.07415300	4.54603100	-2.44576500
C	-0.97161200	2.25168200	0.37461600
C	-0.63370400	0.89488600	0.49222500
H	-1.19582200	0.27495500	1.18590100
C	0.44982400	0.36732000	-0.21202200
C	1.20741500	1.19670700	-1.04774800
H	2.01389800	0.74662100	-1.61721900
C	0.88403600	2.55125000	-1.15914600
C	-0.19808300	3.07853600	-0.44290900
H	-0.40356200	4.13562200	-0.54168600
C	0.88000100	-1.06379900	-0.06293800
C	1.61898400	3.51627600	-2.05908600
N	-0.12440200	-1.95321400	0.20857100
N	2.89994800	3.14524000	-2.38524000
H	-1.06447300	-1.57901000	0.20883200
C	-2.75446000	3.90441600	1.22293300
O	-3.29337600	4.21192700	2.28430800
H	8.80215600	3.98706000	-0.06168100
C	4.53565600	0.95552600	1.70326000
H	4.59504600	1.69322800	0.89881400
C	5.71028400	1.19177600	2.66384200
H	5.69765700	0.44609400	3.46845400
H	6.66444400	1.12582700	2.13823000
H	5.62958600	2.17974700	3.12695300
N	4.70074700	-0.35850800	1.02966200
H	4.85853500	-1.08885700	1.72468300
H	3.83446300	-0.61685300	0.54278900
C	3.21085100	1.13368100	2.44672200
C	2.62421300	2.43858500	2.58828400
C	2.60372500	0.05833900	3.06549800
C	1.41927700	2.58069900	3.35946900
C	1.42648500	0.20415200	3.83480900
C	0.84406700	1.44007800	3.97973600
H	0.98997900	-0.66891600	4.31150400
H	-0.06079700	1.56516900	4.57023400
C	-5.28757600	0.87246200	-1.55344800
H	-5.22953700	1.96961600	-1.57747400

C	-6.69549900	0.45760400	-2.00528300
H	-6.90512500	0.84164100	-3.00750700
H	-6.78607000	-0.63068200	-2.02922600
H	-7.45745000	0.85024300	-1.32229200
N	-5.08109300	0.44055700	-0.13677900
H	-4.13494300	0.70015200	0.15022000
H	-5.69699100	1.00893100	0.44738100
C	-4.20481200	0.33134400	-2.47879100
C	-3.94560600	0.97142800	-3.74081500
C	-3.48317000	-0.79588400	-2.13911300
C	-2.93753900	0.42146700	-4.60460700
C	-2.49056200	-1.33215300	-2.99357300
H	-3.69371400	-1.30283100	-1.20528600
C	-2.21976000	-0.73513100	-4.19938400
H	-1.95386900	-2.22459400	-2.68447900
H	-1.45855600	-1.13880200	-4.86251300
H	3.03004500	-0.93538600	2.96089100
C	0.81908300	3.86226600	3.49158000
C	1.37704600	4.97186600	2.89979000
H	0.90751400	5.94574700	3.00769000
C	2.56832200	4.84271000	2.14933700
H	3.00949000	5.71971200	1.68376600
C	3.17361500	3.61387000	1.99940900
H	4.08870300	3.55472000	1.42038100
H	-0.09814200	3.94792200	4.06992500
C	-2.67587500	1.03978200	-5.85662500
C	-3.37488400	2.15284800	-6.26210700
H	-3.16589100	2.61269600	-7.22392600
C	-4.36930700	2.69936700	-5.41904200
H	-4.92545500	3.57647100	-5.73959200
C	-4.64355700	2.12739700	-4.19468100
H	-1.90677500	0.61008600	-6.49404900
H	-5.41132900	2.57359300	-3.57251700
C	-3.69540200	9.23447600	-1.75046400
C	-3.49016100	8.39901700	-0.67635000
C	-3.31244600	7.00168800	-0.86849600
C	-3.35281000	6.47118000	-2.19924500
C	-3.56430800	7.36070200	-3.28528600
C	-3.73100000	8.71008200	-3.06660300
H	-3.09042500	6.49833100	1.23045000
H	-3.82930300	10.30124400	-1.59400100
H	-3.46026600	8.79567800	0.33549600
C	-3.10109900	6.11454900	0.21477500
C	-3.18566900	5.07201100	-2.38299000

H	-3.58880600	6.95801200	-4.29488000
H	-3.89007400	9.38126600	-3.90623700
C	-2.96879800	4.23594700	-1.31392800
C	-2.91183400	4.75973200	0.00853700
H	-3.23092200	4.66233200	-3.38799000
H	-2.83973100	3.17233900	-1.48400000



Conformer B·(1R)₂

$\Delta E = -9544.00985317$ a.u.

Atoms	x	y	z
Zn	6.32398400	-0.67439400	0.44772700
N	7.99060700	-0.46617200	-0.76770900
N	6.72457100	1.20906800	1.22493200
N	5.22131600	-1.07628300	2.18033400
N	6.53328400	-2.76972700	0.22908200
C	8.38198600	1.96384900	-0.45060000
C	5.22410500	1.18372600	3.19711200
C	4.78881500	-3.49231100	1.83007000
C	8.25231700	-2.80647500	-1.55240600

C	8.59184200	-1.43831700	-1.53137800
C	8.63657100	0.71221400	-1.04988800
C	7.49629500	2.17547200	0.62224900
C	6.08459500	1.81650000	2.27802900
C	4.84670800	-0.17364700	3.14410100
C	4.62532700	-2.26942700	2.50801400
C	5.70008300	-3.71510700	0.77774000
C	7.27375500	-3.40953000	-0.73434800
C	9.66292700	-0.85272300	-2.30975000
H	10.32479600	-1.39414500	-2.96974400
C	9.68532500	0.47578000	-2.01864700
H	10.36741300	1.22382800	-2.39587100
C	7.29444600	3.44509200	1.28831400
H	7.76266500	4.37853500	1.01172500
C	6.43280000	3.22066600	2.31828400
H	6.06831500	3.93379400	3.04403900
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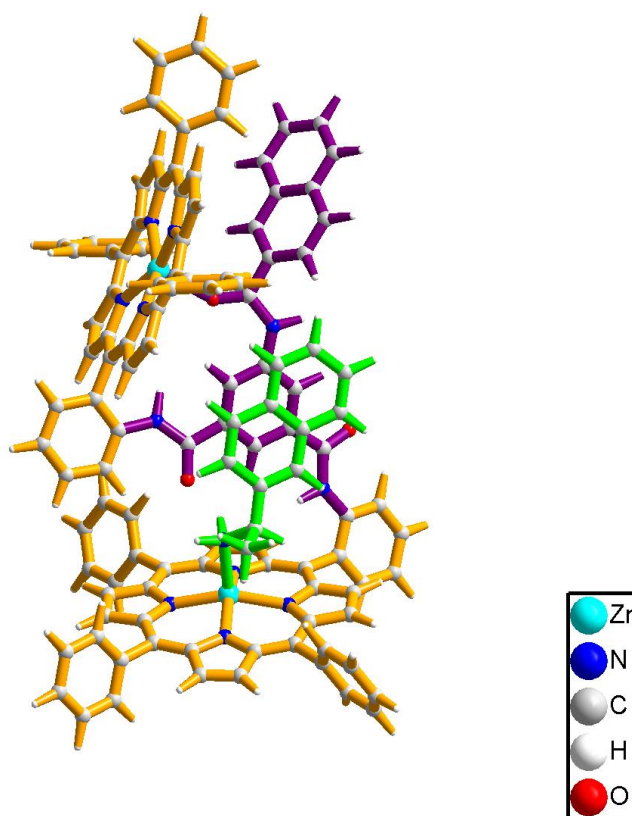
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Conformer A•2R

$\Delta E = -9024.14422108 \text{ a.u.}$

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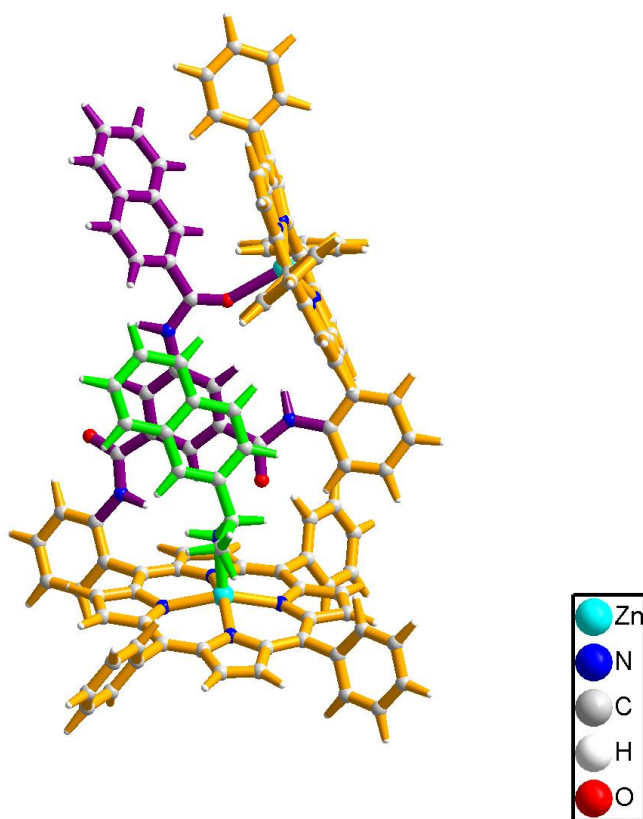
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H	0.47186300	5.49292200	-4.33454500
C	-0.87152500	4.18560500	-3.26998800
H	-1.74315500	4.46659000	-3.85452000
C	-1.02553800	3.23572200	-2.25652700
C	-4.29154800	-2.46490000	-4.70789800
C	-4.14097200	-3.80589900	-4.31995600
H	-4.25306100	-4.06902400	-3.27150400
C	-3.85007100	-4.79599700	-5.25951900
H	-3.73025700	-5.82672600	-4.93623500
C	-3.70997300	-4.46360600	-6.60795600
H	-3.48413500	-5.23375900	-7.34055400
C	-3.86496700	-3.13537800	-7.00933600
H	-3.76728100	-2.86779000	-8.05825400
C	-4.15339100	-2.14611100	-6.06854100
H	-4.28384100	-1.11562800	-6.38676900
C	-9.96408300	-0.74792100	-0.99354500
C	-11.00150000	0.06196100	-1.48401800
H	-10.76179400	1.04059700	-1.89045700
C	-12.32469800	-0.38026400	-1.46516900

H	-13.11165200	0.26007300	-1.85518100
C	-12.63571600	-1.64217300	-0.95512100
H	-13.66610200	-1.98759900	-0.94091500
C	-11.61391100	-2.45745500	-0.46558600
H	-11.84489900	-3.43992400	-0.06205300
C	-10.29045900	-2.01481900	-0.48490000
H	-9.50101900	-2.65089300	-0.09640400
C	-6.41568300	4.46278000	2.07141400
C	-6.63625200	5.80517600	1.72465700
H	-6.57829800	6.09841200	0.68012600
C	-6.93618500	6.75568900	2.70136300
H	-7.10759800	7.78920100	2.41174100
C	-7.02229700	6.38063900	4.04339500
H	-7.25541900	7.12073200	4.80423300
C	-6.80777400	5.04850300	4.40156500
H	-6.86880200	4.74728500	5.44415200
C	-6.50830300	4.09879800	3.42383100
H	-6.33583300	3.06395100	3.70690100
C	0.49020200	-1.28444200	3.07844100
C	-0.82239300	-1.73740100	2.93644300
H	-1.19190800	-2.45747900	3.66098500
C	-1.63717100	-1.26631200	1.90301900
C	-1.13798800	-0.32825900	0.99356600
H	-1.76935300	-0.01696100	0.17260200
C	0.17025500	0.14875200	1.15005000
C	0.98035200	-0.32674100	2.18643000
H	1.97163800	0.10302200	2.28349500
C	1.26467300	-1.84454400	4.24787200
C	0.78498500	1.15716800	0.21841400
C	-4.06845300	-1.32049900	1.21665600
N	2.62363800	-1.67864600	4.18386800
H	2.99633200	-1.26277000	3.34072800
N	-0.10745200	1.92783600	-0.46429300
H	-1.08553500	1.78321800	-0.25001800
N	-2.94445100	-1.79783600	1.83266100
H	-3.10794600	-2.57087900	2.46464600
O	0.67400000	-2.40872100	5.16614200
O	2.01077700	1.26918100	0.11346200
O	-4.07045900	-0.30029900	0.51060100
C	2.74603400	-2.29906400	-1.02145800
C	0.52770200	-2.09442000	-2.00952500
C	1.82954900	-1.66535800	-1.90707400
H	-0.16317400	-1.59407900	-2.68349200
H	2.16228100	-0.82084900	-2.50543700

C	4.20112700	-1.85898400	-0.95433500
H	4.67188700	-2.38847100	-0.11950500
N	4.37566000	-0.40294000	-0.67905400
H	4.35100200	0.11949300	-1.55543400
H	3.58525200	-0.03269900	-0.14083300
C	4.95407600	-2.22703800	-2.23980200
H	6.00008600	-1.91581100	-2.17752900
H	4.91647300	-3.30867400	-2.40195500
H	4.49689900	-1.74417100	-3.11282000
C	-0.79631900	-5.37280400	0.32986900
C	-1.69273500	-4.74070500	-0.56713800
C	-1.27593800	-3.67074500	-1.32961400
C	0.05766200	-3.19126300	-1.23618400
C	0.96643300	-3.83272000	-0.33439100
C	0.50212400	-4.92667800	0.44419300
H	-1.13474100	-6.21785000	0.92393300
H	-2.71021000	-5.11283800	-0.66224600
H	-1.95864900	-3.18583000	-2.02333700
H	1.19260800	-5.41219400	1.12991700
C	2.30265800	-3.35499400	-0.25187600
H	2.98922500	-3.84809700	0.43436700
C	-5.23805700	-3.54927500	1.54943000
C	-6.33121800	-4.27950100	1.94914800
C	-7.51771600	-3.63608600	2.39401100
C	-7.57069500	-2.20334700	2.38400200
C	-6.44200400	-1.47341300	1.92921000
C	-5.28775700	-2.12545400	1.54106900
H	-8.60708700	-5.44891000	2.85897600
H	-4.34107900	-4.05618600	1.20274300
H	-6.29709300	-5.36606400	1.93465500
C	-8.64724500	-4.36232800	2.85617300
C	-8.74557000	-1.55326900	2.85058000
H	-6.47994700	-0.38849700	1.91831900
C	-9.81913100	-2.28666800	3.30242200
C	-9.77053000	-3.70261300	3.30323500
H	-8.78311400	-0.46778500	2.83202300
H	-10.71332800	-1.78079500	3.65504000
H	-10.62647100	-4.26831700	3.66106300



Conformer B•2R

$\Delta E = -9024.14114081 \text{ a.u.}$

Atoms	x	y	z
Zn	-6.14458200	-0.23906700	-0.36444600
N	-6.69203800	1.27814400	-1.72510800
N	-5.32264100	-1.25893600	-2.01346000
N	-6.24772300	-2.06582000	0.61644600
N	-7.66356300	0.44738500	0.87794300
C	-5.39327900	0.55483500	-3.70619600
C	-4.93524700	-3.46440500	-0.95010400
C	-7.64060500	-1.38489200	2.54659800
C	-8.16727700	2.60247400	-0.24167700
C	-7.40027100	2.41157300	-1.40801000
C	-6.14094600	1.49411800	-2.96460900
C	-5.07551100	-0.74777700	-3.26391300
C	-4.86029200	-2.55185300	-2.02008200
C	-5.68802000	-4.17811900	1.35608900
H	-5.25691700	-5.16875000	1.35652000
C	-6.79648100	-2.27751300	1.85671600

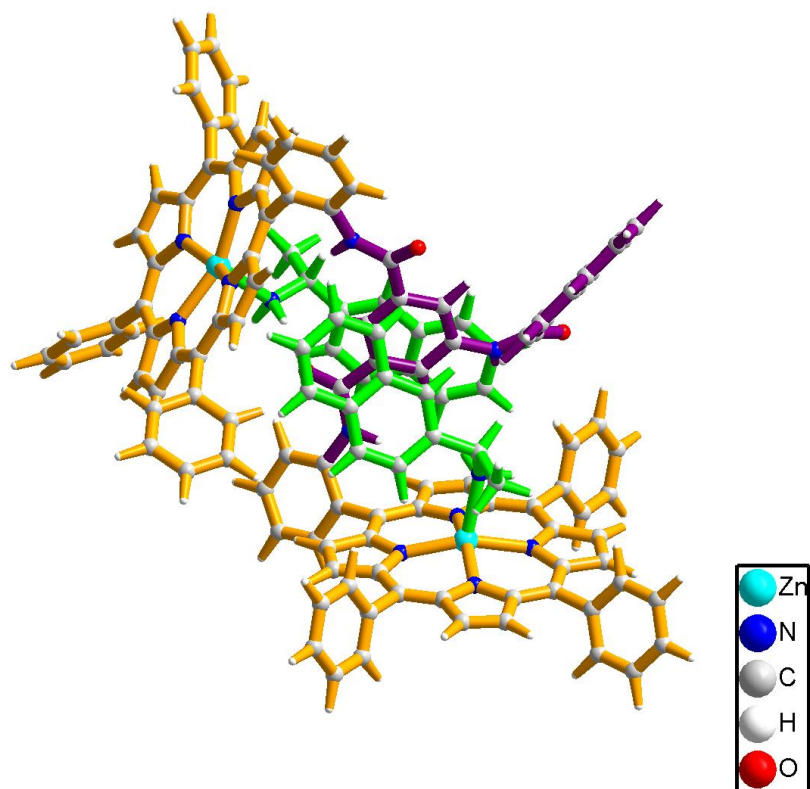
C	-8.06406800	-0.13331800	2.05817600
C	-8.30184200	1.66107000	0.79961900
C	-7.25192700	3.39333200	-2.46329300
H	-7.68740600	4.38206500	-2.46627200
C	-6.47405700	2.82673700	-3.42498000
H	-6.15836200	3.26415800	-4.36119400
C	-4.44162700	-1.75472500	-4.09094000
H	-4.16757100	-1.63044400	-5.12935500
C	-4.30987400	-2.86940500	-3.32200900
H	-3.90346500	-3.82735000	-3.61237700
C	-5.58467100	-3.21834600	0.27620900
C	-6.44386500	-3.59963500	2.32876800
H	-6.75214500	-4.03103200	3.27020600
C	-8.98709400	0.74450100	2.74550700
H	-9.45947200	0.53735500	3.69468100
C	-9.14448100	1.84565200	1.96198700
H	-9.77696900	2.70167800	2.14690400
C	-3.63104300	1.20307700	-5.44628600
C	-4.98120800	0.94573500	-5.09823800
C	-5.95859100	1.07766100	-6.09300800
H	-6.99138800	0.87335300	-5.82611100
C	-5.63368000	1.45679000	-7.39455900
H	-6.41278600	1.54801500	-8.14604400
C	-4.30186000	1.71493500	-7.71565700
H	-4.02964800	2.01491900	-8.72414600
C	-3.30124900	1.59241200	-6.75379200
H	-2.26831200	1.79843100	-6.99488400
C	-4.30375800	-4.80901900	-1.14785100
C	-2.90843900	-4.93511100	-1.23665600
H	-2.29413200	-4.04463400	-1.14334800
C	-2.31604700	-6.18430700	-1.42689700
H	-1.23352500	-6.26292100	-1.48678500
C	-3.10826600	-7.32873600	-1.53453900
H	-2.64674800	-8.30135300	-1.68388600
C	-4.49740200	-7.21616600	-1.44984600
H	-5.12289500	-8.10077300	-1.53840500
C	-5.08955200	-5.96719000	-1.25812000
H	-6.17106400	-5.88068000	-1.20084900
C	-8.15321900	-1.81947700	3.88751700
C	-9.49354700	-2.19900000	4.05926000
H	-10.16291400	-2.17890700	3.20364000
C	-9.96660800	-2.60597500	5.30762700
H	-11.00722400	-2.89954400	5.41930700
C	-9.10674200	-2.64194500	6.40694800

H	-9.47484800	-2.95910800	7.37908800
C	-7.77072600	-2.26921800	6.24904800
H	-7.09393900	-2.29173500	7.09940600
C	-7.29914600	-1.86177000	5.00026800
H	-6.25971500	-1.56820300	4.88084700
C	-8.91291500	3.89594400	-0.10703700
C	-9.98515200	4.19983000	-0.96103800
H	-10.27613700	3.47923700	-1.72016400
C	-10.67879000	5.40446600	-0.83823300
H	-11.50905000	5.61800100	-1.50651700
C	-10.31266100	6.32892900	0.14180900
H	-10.85256000	7.26726200	0.23768800
C	-9.24944200	6.03922500	0.99885900
H	-8.95489500	6.75356300	1.76345000
C	-8.55738700	4.83375200	0.87556500
H	-7.72858800	4.61294000	1.54263000
Zn	5.20716100	-0.72753700	1.11274800
N	4.38824000	-2.59578600	0.69030000
N	3.80493300	-0.52732400	2.63680300
N	6.35161200	0.71241400	2.08096300
N	6.93325000	-1.35800500	0.14401100
C	2.38093800	-2.49204500	2.13630700
C	4.69462200	1.50019000	3.74823200
C	8.50613500	0.40639000	0.89481100
C	6.03623700	-3.38241500	-0.97742100
C	3.17835100	-3.07109800	1.13188100
C	4.81502200	-3.46500700	-0.28423000
C	2.69980800	-1.31621900	2.84255800
C	3.73269500	0.49161400	3.55717700
C	5.92150000	1.57495900	3.06138400
C	7.64423400	1.07535500	1.78423600
C	8.15714200	-0.73065000	0.14046000
C	7.02925800	-2.41203700	-0.73414400
C	2.82406200	-4.27346100	0.40658900
H	1.92831200	-4.85789000	0.56548700
C	3.82940600	-4.50932800	-0.47809900
H	3.90622600	-5.31925000	-1.18874300
C	1.89936000	-0.77436700	3.91961500
H	0.98669400	-1.21104400	4.29933700
C	2.54125100	0.34000800	4.36578200
H	2.25288800	0.98829000	5.18062800
C	6.95745000	2.54074800	3.35589700
H	6.88128800	3.33920100	4.07940000
C	8.02828500	2.21965700	2.58252000

H	8.99455200	2.70160700	2.56168100
C	9.04739200	-1.40282000	-0.78080200
H	10.07353900	-1.12472300	-0.97288200
C	8.34982100	-2.43877600	-1.32380900
H	8.70211300	-3.17252800	-2.03428600
C	-0.09078400	-2.81816300	1.70212800
C	-1.33833700	-3.36019100	2.03925500
H	-2.21239300	-3.09185200	1.46240600
C	-1.43461200	-4.23912700	3.11792900
H	-2.40625600	-4.65493700	3.36982700
C	-0.30522600	-4.58722800	3.85814200
H	-0.38454400	-5.27764200	4.69303700
C	0.93322800	-4.03612700	3.52291200
H	1.81913000	-4.28723100	4.09953300
C	1.06272200	-3.14286400	2.45597100
C	4.43474500	2.51088700	4.82716400
C	3.46562500	3.51232900	4.66590000
H	2.90044900	3.56504000	3.73987100
C	3.22395400	4.44414400	5.67681500
H	2.47116400	5.21413100	5.52931700
C	3.94682600	4.38934300	6.86935400
H	3.75841400	5.11411300	7.65689900
C	4.91224300	3.39596700	7.04457800
H	5.47660600	3.34084600	7.97186500
C	5.15276500	2.46547400	6.03310700
H	5.89956600	1.68919900	6.17473200
C	9.91394000	0.91095300	0.78374000
C	10.98112200	0.14870200	1.28638800
H	10.77260700	-0.80985500	1.75344900
C	12.29427500	0.61262600	1.20231200
H	13.10493600	0.00921900	1.60253400
C	12.56502900	1.84960800	0.61410500
H	13.58745600	2.21247600	0.54947400
C	11.51332900	2.61725800	0.11114500
H	11.71281600	3.57950200	-0.35327100
C	10.19989400	2.15235600	0.19495300
H	9.38729600	2.75121100	-0.20469700
C	6.33019900	-4.42700500	-2.01122700
C	6.55858600	-5.76288900	-1.64491400
H	6.52493000	-6.03680200	-0.59410100
C	6.83572100	-6.73142000	-2.61061300
H	7.01369600	-7.75949400	-2.30601100
C	6.89094300	-6.38127800	-3.96097500
H	7.10627600	-7.13546500	-4.71316400

C	6.66852100	-5.05586800	-4.33868500
H	6.70551800	-4.77399400	-5.38778500
C	6.39185400	-4.08819600	-3.37199900
H	6.21334500	-3.05862600	-3.67008700
C	-0.53432400	0.84568300	-3.26137400
C	0.75637200	1.36376700	-3.14391800
H	1.11712400	2.01161000	-3.93784400
C	1.56234000	1.04380000	-2.04733300
C	1.07643600	0.19311500	-1.04912900
H	1.69766200	-0.00269600	-0.18584000
C	-0.20971500	-0.34801100	-1.17656000
C	-1.01131200	-0.02396600	-2.27628700
H	-1.98199900	-0.50328100	-2.34784300
C	-1.30063900	1.24107200	-4.50202800
C	-0.80554000	-1.27112300	-0.14872900
C	3.97781100	1.26500300	-1.33178900
N	-2.65503400	1.04345100	-4.43799500
H	-3.02946200	0.71564900	-3.55778400
N	0.10296800	-1.94440300	0.60952800
H	1.07706000	-1.80288500	0.37529000
N	2.84595500	1.63246100	-2.00896800
H	2.99468600	2.33991000	-2.71699000
O	-0.70935300	1.71300200	-5.47021000
O	-2.02949100	-1.40382100	-0.03805100
O	4.00787500	0.32808800	-0.52038900
C	-2.43840500	1.97264500	1.35163800
C	-0.07335800	2.02619200	1.94475600
C	-1.31899900	1.44964800	2.05242100
H	0.76789000	1.60653300	2.49057600
H	-1.45327400	0.57155700	2.67972400
C	-3.80344900	1.29896300	1.47389300
H	-3.70892100	0.46511500	2.17734100
C	-4.87473100	2.25918000	2.00005200
H	-5.80708800	1.72563200	2.19460300
H	-4.53423900	2.73048100	2.92782400
H	-5.08437200	3.05501600	1.27582600
N	-4.23390200	0.68265100	0.18382300
H	-4.17983500	1.39463800	-0.54686000
H	-3.53720900	-0.02916200	-0.06600500
C	1.55577900	4.90804600	0.19532100
C	0.44447500	5.45434600	-0.49524900
C	-0.79660400	4.86898000	-0.38636300
C	-0.99110600	3.71574600	0.42281500
C	0.13074600	3.16819500	1.12631500

C	1.40220100	3.78780900	0.98214200
H	2.52939500	5.38467900	0.11095100
H	0.57624900	6.33957100	-1.11172200
H	-1.64928800	5.28460700	-0.91836600
H	2.25444400	3.35911600	1.50442400
C	-2.25813300	3.09133800	0.55914800
H	-3.09886700	3.52415500	0.01904400
C	9.55486400	3.68943300	-3.69215300
C	8.41694100	4.33907800	-3.26820600
C	7.32382600	3.60809100	-2.73194400
C	7.42973400	2.18244700	-2.62130900
C	8.61800500	1.54267000	-3.06785900
C	9.65478300	2.27958500	-3.59388400
H	6.04749700	5.32194600	-2.37505900
H	10.38242800	4.25808200	-4.10743700
H	8.33657300	5.42057300	-3.34678000
C	6.12193200	4.23915200	-2.31173800
C	6.33763800	1.44724600	-2.09078000
H	8.69474300	0.46296700	-2.97622400
H	10.55932500	1.78143400	-3.93080000
C	5.06261900	3.50098600	-1.84157100
H	6.41640000	0.36810900	-2.00250700
H	4.15105300	3.99817200	-1.51976900
C	5.16648700	2.08438000	-1.73008000



Conformer A•(2R)₂

$\Delta E = -9544.01858308$ a.u.

Atoms	x	y	z
Zn	-5.68684800	-1.34505500	0.82430200
N	-4.27262100	-0.97106700	2.32943200
N	-4.61854600	-3.04962500	0.33946400
N	-7.34653900	-2.17673600	-0.08806100
N	-6.99928100	-0.08410300	1.88669600
C	-2.61455700	-2.72623200	1.76089700
C	-6.21722300	-4.03610100	-1.27560000
C	-9.08905700	-0.57390700	0.65205800
C	-5.40335400	0.89716100	3.50633200
C	-4.31810200	0.03249400	3.26799500
C	-3.07326800	-1.61780400	2.50392700
C	-3.34966500	-3.37810000	0.74933800
C	-4.97232700	-3.96625300	-0.62185700
C	-7.31862500	-3.19993800	-1.00525100
C	-8.61388100	-1.64607500	-0.12942200
C	-8.32487400	0.13437100	1.60162600

C	-6.66123700	0.80369300	2.88073600
C	-3.09846300	0.03112000	4.04728500
H	-2.87400500	0.70572400	4.86076300
C	-2.33487100	-0.99812100	3.58559800
H	-1.37271900	-1.32377100	3.95604500
C	-2.87759800	-4.52738500	0.00391300
H	-1.91359500	-4.99993900	0.12542800
C	-3.88139900	-4.89218200	-0.83956900
H	-3.89637200	-5.72311900	-1.53013200
C	-8.60301600	-3.30254500	-1.66391600
H	-8.85455400	-4.01475800	-2.43640600
C	-9.40312800	-2.34518400	-1.12173700
H	-10.43105600	-2.12608200	-1.37120100
C	-8.83895900	1.19545700	2.44324500
H	-9.85725800	1.55622900	2.44340200
C	-7.80707500	1.61922100	3.22219200
H	-7.81914500	2.39556300	3.97367400
C	-1.27146800	-3.30491300	2.10774300
C	-1.20715100	-4.54066200	2.76493400
H	-2.13999700	-5.02845400	3.03246100
C	0.01108300	-5.14612000	3.06854400
H	0.03052100	-6.10623400	3.57615600
C	1.19719700	-4.50889900	2.70708600
H	2.15722700	-4.97022600	2.92179100
C	1.17157800	-3.27451900	2.06185900
H	2.08907900	-2.78592500	1.76921300
C	-0.05639100	-2.66244700	1.76767800
C	-6.39506500	-5.10512400	-2.31392300
C	-5.80573900	-4.98038800	-3.58124600
H	-5.22623600	-4.09074500	-3.81337600
C	-5.96937400	-5.97630500	-4.54555200
H	-5.50938600	-5.85982500	-5.52342900
C	-6.72476900	-7.11431600	-4.25759100
H	-6.85198600	-7.89008100	-5.00793200
C	-7.31711400	-7.24940000	-3.00057500
H	-7.90533700	-8.13299800	-2.76687500
C	-7.15399100	-6.25260600	-2.03744300
H	-7.61196900	-6.36132000	-1.05812700
C	-10.52277600	-0.17169400	0.47907100
C	-11.55969700	-1.02112600	0.89655300
H	-11.31074300	-1.97539100	1.35233300
C	-12.89540700	-0.64902200	0.74018200
H	-13.68331500	-1.31894000	1.07447100
C	-13.21892300	0.58004100	0.16244200

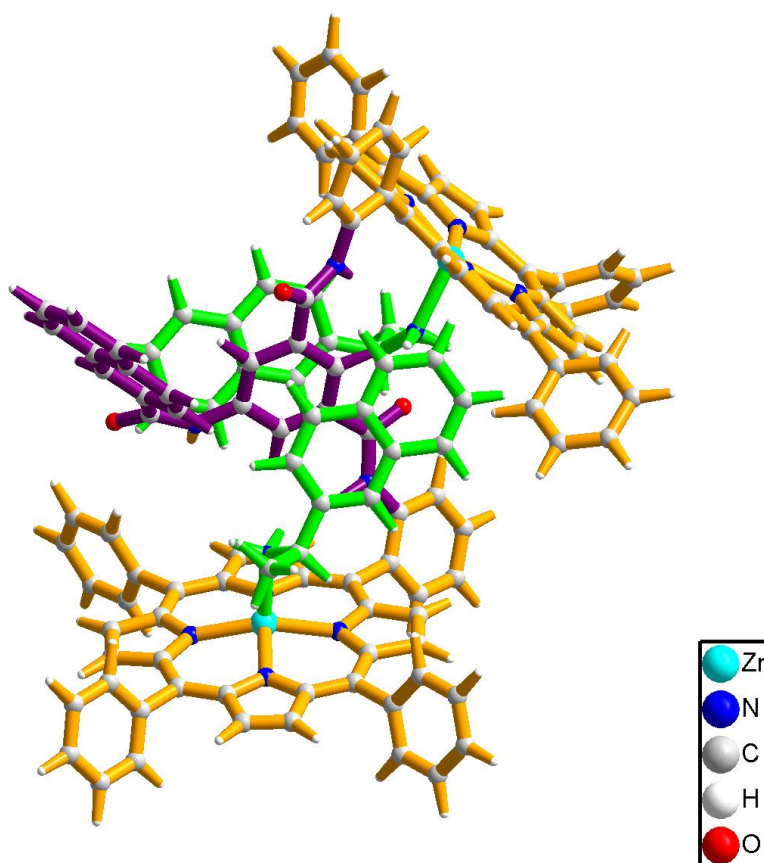
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C	-12.19763200	1.43441700	-0.25678000
H	-12.43929500	2.39185800	-0.71096900
C	-10.86214500	1.06162300	-0.09888200
H	-10.07041800	1.72798200	-0.43056600
C	-5.20564500	1.98276600	4.52433600
C	-5.69940700	1.85979400	5.83155100
H	-6.23931300	0.95993700	6.11392100
C	-5.49581500	2.87742900	6.76574400
H	-5.88233300	2.76555100	7.77555800
C	-4.79838800	4.03339300	6.40673000
H	-4.64480000	4.82546100	7.13507100
C	-4.30468400	4.16880800	5.10738800
H	-3.76699700	5.06146500	4.80119200
C	-4.50755600	3.14822900	4.17718400
H	-4.12698000	3.26198600	3.16667800
Zn	6.23183600	-0.57930600	-0.47354900
N	6.91684300	1.20075600	-1.31244600
N	8.07908400	-0.75154600	0.48865100
N	6.02806000	-2.66663100	-0.24565500
N	4.88188100	-0.71808500	-2.06221100
C	8.98511900	1.50813700	0.01456200
C	7.86756000	-3.06533100	1.36142200
C	4.06878000	-3.03575800	-1.71241000
C	5.15307800	1.55869000	-3.01303000
C	6.24477200	1.97700000	-2.22463500
C	7.97570100	1.95261100	-0.86134600
C	9.03910300	0.22380200	0.59784300
C	8.52955500	-1.82927000	1.21299700
C	6.68856700	-3.43555500	0.68060200
C	4.98080700	-3.42277400	-0.70909200
C	4.06841900	-1.78542300	-2.35904700
C	4.56414100	0.27694900	-2.95258600
C	6.86246300	3.28418800	-2.30552100
H	6.52601300	4.09796300	-2.93175600
C	7.92977200	3.26988100	-1.46209800
C	10.14331200	-0.26229900	1.39756200
H	11.04859000	0.28595800	1.61421900
C	9.82711800	-1.52872700	1.78025800
H	10.42708800	-2.21054900	2.36520100
C	6.00656200	-4.70323400	0.84051200
H	6.29686100	-5.49130300	1.52018300
C	4.95275600	-4.69628300	-0.02147800
H	4.22185700	-5.47648200	-0.17747800

C	3.21455900	-1.45240200	-3.48041500
H	2.48924100	-2.11106900	-3.93464600
C	3.52305300	-0.18014000	-3.84946100
H	3.10088400	0.39209200	-4.66295700
C	10.10686800	2.45360100	0.32101900
C	11.00874400	2.84732000	-0.68082300
H	10.88701200	2.45334300	-1.68587100
C	12.05670900	3.72366700	-0.39653200
H	12.74680700	4.01130500	-1.18555200
C	12.22265200	4.22416800	0.89614500
H	13.03853000	4.90702700	1.11790900
C	11.33446300	3.84024100	1.90239100
H	11.45320400	4.22658800	2.91146800
C	10.28779700	2.96250500	1.61698900
H	9.59647300	2.66901800	2.40207600
C	8.48637300	-4.07298200	2.28043700
C	8.99276100	-5.28622300	1.78589700
H	8.93717100	-5.48621600	0.71964800
C	9.57290300	-6.22238200	2.64246600
H	9.96436600	-7.15206100	2.23753100
C	9.65751800	-5.96419700	4.01194100
H	10.10925800	-6.69329100	4.67936800
C	9.16001500	-4.76187800	4.51768400
H	9.21910800	-4.55195900	5.58260700
C	8.58176600	-3.82577200	3.65955900
H	8.19392900	-2.89201300	4.05748300
C	3.03717300	-4.03453300	-2.14075100
C	3.40576600	-5.21486800	-2.80604000
H	4.45621000	-5.40116000	-3.01204300
C	2.43991500	-6.13669600	-3.21229800
H	2.74451600	-7.04178800	-3.73167000
C	1.08806600	-5.89552500	-2.95869200
H	0.33654000	-6.61473000	-3.27421200
C	0.70853300	-4.72675300	-2.29535200
H	-0.34026300	-4.53286400	-2.08368500
C	1.67508600	-3.80491200	-1.89051700
H	1.38546500	-2.90258600	-1.36255500
C	4.64945300	2.51204200	-4.06210400
C	3.38908800	3.15284800	-3.96502100
C	2.96461500	4.03647800	-4.96973500
H	2.00594900	4.52480700	-4.86650400
C	3.78260000	4.27882800	-6.07177800
H	3.44066000	4.96504000	-6.84209600
C	5.02469200	3.65605000	-6.18626000

H	5.66144300	3.84384900	-7.04610800
C	5.44440100	2.78333200	-5.18306500
H	6.40766900	2.28745200	-5.25970500
N	-1.61710300	3.55731300	1.46634100
H	-1.49494100	3.29560500	2.44171200
H	3.03442500	2.22607000	-2.17976500
O	2.01990500	-1.00333000	0.46558800
O	0.68327200	4.10478100	-3.17047700
C	-0.77198700	2.83981400	0.58641300
C	-0.47200300	1.51522900	0.95053300
H	-0.92009800	1.10407500	1.85198600
C	0.44163600	0.76400100	0.20856700
C	1.05622000	1.32390800	-0.91698000
H	1.73796200	0.70912200	-1.49584500
C	0.74215600	2.63031000	-1.29794700
C	-0.16662000	3.38875700	-0.54883200
H	-0.36843300	4.40497200	-0.86270600
C	0.85668300	-0.62051900	0.61908700
C	1.32657600	3.27651600	-2.52904400
N	-0.13720000	-1.39142300	1.15213000
N	2.59800600	2.86414000	-2.83299700
H	-1.07459600	-1.01352100	1.09791700
C	-2.21026000	4.81302100	1.39167300
O	-2.41173600	5.42868300	2.43733300
H	8.62684900	4.07189400	-1.26728900
C	4.79436600	1.10430700	1.95469800
H	4.67310900	1.90633300	1.21785100
C	6.12188200	1.32412000	2.68999300
H	6.30478400	0.52357400	3.41754500
H	6.95555300	1.34424500	1.98515600
H	6.09498600	2.27174500	3.23698400
N	4.84824800	-0.16186900	1.17502700
H	5.05411900	-0.93930900	1.80435800
H	3.91666000	-0.36342400	0.79366500
C	3.61761100	1.17469900	2.92206900
C	3.38483600	0.13581800	3.86714800
C	2.35573700	0.21527100	4.77557500
H	2.19153800	-0.59098500	5.48669700
C	-5.01856200	0.86230900	-1.77426800
H	-4.86954800	1.95116000	-1.81336800
C	-6.41405000	0.56076800	-2.33128200
H	-6.50255800	0.95092200	-3.35028400
H	-6.60966900	-0.51453400	-2.35198500
H	-7.18850300	1.03201700	-1.71493300

N	-4.94804800	0.42625200	-0.34366700
H	-3.98820400	0.53144200	-0.01224100
H	-5.50312900	1.07743500	0.21496000
C	-3.90328900	0.23280000	-2.58910700
C	-3.80932400	-1.17968200	-2.73235600
C	-2.81894400	-1.74514800	-3.50121400
H	-4.52506900	-1.81633500	-2.22391700
H	-2.75559100	-2.82703800	-3.59301900
H	4.02853100	-0.74064900	3.87274200
C	-0.18998700	3.60775200	4.77930000
C	0.85269700	3.52579600	3.88047600
C	-0.41020000	2.56355900	5.71312300
H	-0.84984400	4.47049000	4.76411300
H	1.02589900	4.32959400	3.16880200
H	-1.23361600	2.64224900	6.41760100
C	0.41467600	1.45988700	5.72638900
H	0.25137200	0.65909100	6.44413600
C	2.78680200	2.27564800	2.93619700
H	2.94496100	3.08096700	2.22104200
C	-0.98057400	1.29803300	-4.68870900
C	-0.00757500	0.73278300	-5.48330500
C	0.05650400	-0.67337300	-5.64753500
C	-0.84591100	-1.49176800	-5.00429600
H	-1.01235400	2.37468000	-4.54176700
H	0.71861000	1.36801500	-5.98348600
H	0.82693900	-1.10521400	-6.28076700
H	-0.78903100	-2.57188700	-5.11680400
C	-2.97135000	1.02982300	-3.22268100
H	-3.01732800	2.11226000	-3.11818700
C	1.71687900	2.39747900	3.86348700
C	1.49126100	1.34318800	4.80565400
C	-1.93834900	0.48111000	-4.02967100
C	-1.86482400	-0.94078700	-4.18228600
C	-3.82716200	9.28725600	-2.55110700
C	-3.33725100	8.73581800	-1.38930900
C	-3.25877000	7.32512400	-1.23358500
C	-3.70025100	6.48132000	-2.30471900
C	-4.19988300	7.08177100	-3.48975000
C	-4.26113400	8.45232800	-3.61051700
H	-2.45406100	7.35230500	0.78191500
H	-3.88244200	10.36662200	-2.66134700
H	-3.00271100	9.37141900	-0.57323400
C	-2.76496200	6.72611100	-0.04897400
C	-3.62528900	5.07164300	-2.13708300

H	-4.53157700	6.44121000	-4.30322200
H	-4.64372900	8.90056400	-4.52336000
C	-3.12364700	4.51822800	-0.98387300
C	-2.67673600	5.35205100	0.07916600
H	-3.97558900	4.43165500	-2.94328900
H	-3.07384600	3.43992900	-0.87665500



Conformer B•(2R)₂

$\Delta E = -9544.01712011$ a.u.

Atoms	x	y	z
Zn	6.32578400	-0.58433900	0.32035300
N	8.00385000	-0.37560400	-0.88548900
N	6.67585400	1.33822200	1.02776500
N	5.23754300	-0.95257400	2.06372900
N	6.60766900	-2.68270200	0.19059800
C	8.31225400	2.07788000	-0.67374700
C	5.20096200	1.33509000	3.01779900
C	4.85893000	-3.38920700	1.79268500

C	8.35020200	-2.73770400	-1.56690400
C	8.64623400	-1.35971200	-1.59928200
C	8.61242200	0.81024100	-1.21569400
C	7.41966200	2.30399900	0.39047000
C	6.03168500	1.96167000	2.06753500
C	4.85098000	-0.03071000	3.00413000
C	4.66625000	-2.14740900	2.42812700
C	5.78793100	-3.62807100	0.75870800
C	7.37674000	-3.33675800	-0.73977000
C	9.70488300	-0.77312800	-2.39363400
H	10.39225500	-1.32054500	-3.02181600
C	9.67759000	0.56737300	-2.16453400
H	10.33690200	1.32122900	-2.56976200
C	7.18910300	3.58963900	1.01646800
H	7.63151700	4.52533800	0.70677400
C	4.01315500	-0.66536800	4.00024700
H	3.59469000	-0.17570300	4.86806300
C	3.88560000	-1.96932900	3.63503100
H	3.34423800	-2.75015500	4.14862600
C	6.02582000	-4.91628000	0.14294100
H	5.50619100	-5.83232300	0.38411400
C	7.01438100	-4.73846200	-0.77621900
H	7.44966900	-5.48245900	-1.42748800
C	9.04407900	3.25802200	-1.23813600
C	10.02203300	3.93181000	-0.48943600
H	10.25293900	3.58453500	0.51380400
C	10.70133100	5.02782500	-1.02315400
H	11.45860100	5.53298000	-0.42912400
C	10.41490400	5.46994100	-2.31611500
H	10.94379600	6.32351900	-2.73179000
C	9.44621600	4.80741200	-3.07215800
H	9.21417500	5.14554900	-4.07878400
C	8.76858600	3.71066300	-2.53804400
H	8.01130900	3.20065400	-3.12710400
C	4.72661600	2.16630100	4.17874000
C	5.62830800	2.48810200	5.20046700
H	6.64939200	2.12706100	5.11660800
C	5.24079300	3.24332500	6.30674800
H	5.96010000	3.47513200	7.08706900
C	3.92370500	3.69142600	6.39801000
H	3.60436700	4.28239100	7.25239500
C	2.99993900	3.39510600	5.39758700
H	1.98047100	3.74918900	5.45526500
C	3.39452100	2.63308000	4.28662500

C	4.02783600	-4.53848400	2.27400700
C	2.63997000	-4.53884000	2.05747500
H	2.18741600	-3.70671900	1.52472900
C	1.85113700	-5.59890900	2.50704800
H	0.77984800	-5.58621900	2.32277100
C	2.43385300	-6.67321000	3.18249900
H	1.81886000	-7.49821600	3.53264800
C	3.81239200	-6.68242200	3.40445500
H	4.27419600	-7.51174700	3.93415400
C	4.60257300	-5.62411900	2.95337500
H	5.67369100	-5.62857500	3.13569400
C	9.13508100	-3.63834600	-2.47087200
C	10.00189700	-4.60759200	-1.94028700
H	10.10510200	-4.69020500	-0.86202000
C	10.73249100	-5.45041500	-2.77857300
H	11.40219300	-6.18980600	-2.34699200
C	10.60921000	-5.34114800	-4.16493500
H	11.17763300	-5.99773100	-4.81829200
C	9.75160300	-4.38180100	-4.70636600
H	9.64571400	-4.29109500	-5.78438900
C	9.02260100	-3.53856700	-3.86706400
H	8.35246700	-2.79669800	-4.29268000
Zn	-5.86402800	-1.18320300	-1.20896800
N	-6.88897400	0.35144900	-2.16501800
N	-7.69313900	-1.93467000	-0.57374000
N	-5.04244900	-3.07972400	-0.86366300
N	-4.27023700	-0.84318000	-2.53940900
C	-9.12208700	0.00931800	-1.14834400
C	-6.92587100	-4.08461800	0.39553900
C	-2.84785800	-2.79949300	-1.97985800
C	-5.08702600	1.23369500	-3.61875700
C	-7.38176000	2.25144200	-3.38099000
C	-8.19280500	0.71677700	-1.93793000
C	-8.87330000	-1.23084200	-0.52530900
C	-7.88655100	-3.07908500	0.16125900
C	-5.60457800	-4.06982500	-0.09346200
C	-3.49710500	-4.75977200	-0.51690600
C	-3.12383800	-1.59070100	-2.65558700
C	-4.13146900	0.22512100	-3.39291500
C	-6.37371100	1.26735400	-3.05010100
C	-8.50595300	1.91138800	-2.69532900
H	-9.46818900	2.40175100	-2.71963000
C	-9.83660300	-1.94909200	0.28274700
C	-9.22873400	-3.09122100	0.70328400

H	-9.64464400	-3.86724700	1.32920600
C	-4.63919000	-5.12754300	0.12420200
H	-4.82014900	-6.03610100	0.68001700
C	-3.76247100	-3.48498200	-1.15248900
C	-2.22812100	-0.97031800	-3.61027600
H	-1.27069900	-1.36725200	-3.91851500
C	-2.84829000	0.15677200	-4.05947000
H	-2.49187500	0.85932800	-4.79940000
C	-10.48660400	0.60758700	-0.98941600
C	-11.61449700	-0.00455600	-1.55912000
H	-11.48869900	-0.92209400	-2.12710200
C	-12.88321600	0.55748700	-1.41229600
H	-13.74290900	0.07106600	-1.86584600
C	-13.04771700	1.74230700	-0.69238100
H	-14.03581900	2.17994000	-0.57795700
C	-11.93446400	2.36224700	-0.12216000
H	-12.05228900	3.28367600	0.44216700
C	-10.66592300	1.80022100	-0.27090900
H	-9.80213900	2.28380100	0.17703500
C	-7.34777300	-5.26654500	1.21643200
C	-6.83534200	-5.46941100	2.50730700
C	-7.22872500	-6.57084000	3.26875100
H	-6.82372000	-6.70715400	4.26815300
C	-8.14278000	-7.49038800	2.75149800
H	-8.44955100	-8.34844200	3.34360900
C	-8.66071200	-7.30047300	1.46899700
H	-9.36994700	-8.01321600	1.05626400
C	-8.26681700	-6.19846200	0.70892700
H	-8.66678100	-6.05616500	-0.29116400
C	-1.51488500	-3.45202400	-2.21932800
C	-1.45082300	-4.62632500	-2.98091000
H	-2.37369100	-5.01513600	-3.40133000
C	-0.24699600	-5.29380900	-3.20109700
H	-0.22878700	-6.20263700	-3.79562300
C	0.92544900	-4.78300900	-2.64693600
H	1.87215500	-5.29440300	-2.79810800
C	0.90237800	-3.61191300	-1.89216400
H	1.80725900	-3.22044300	-1.45118300
C	-0.30922700	-2.93515400	-1.68175800
C	-4.71861300	2.33467500	-4.57164400
C	-4.76627800	2.12972100	-5.95925000
H	-5.08549000	1.16437400	-6.34303400
C	-4.41279100	3.15130800	-6.84242800
H	-4.45842600	2.97605800	-7.91422700

C	-4.00389500	4.39345300	-6.35184700
H	-3.72764700	5.18789200	-7.04021500
C	-3.95359500	4.60847600	-4.97321000
H	-3.63475200	5.56633800	-4.57174800
C	-4.31077600	3.58691500	-4.09026500
H	-4.26345800	3.77116100	-3.02185100
N	2.50818900	2.31059800	3.23741700
H	2.93936300	1.81519900	2.46615700
N	-1.81540900	3.24494200	-0.80945700
N	-0.37996100	-1.72080800	-0.96123100
H	-1.30140700	-1.30324200	-0.94655000
O	0.51154700	3.25796500	3.90278300
O	1.74429200	-1.47868600	-0.11852100
C	0.21823900	0.32578700	0.19861200
C	0.85459100	0.79148700	1.35478800
C	0.56049000	2.06810000	1.83604300
C	-0.34341200	2.89499700	1.16085600
H	-0.52616100	3.88821300	1.54947500
C	-0.96605600	2.44682700	-0.00824900
C	-0.68868800	1.14932700	-0.47556100
H	-1.14968600	0.82059800	-1.40417300
C	0.60596400	-1.03708100	-0.30416600
C	1.17696100	2.60531400	3.10042800
H	-2.56806300	-5.30790300	-0.57440200
H	-7.24725200	3.07532800	-4.06702500
H	-10.84097600	-1.61799100	0.50273400
H	-6.12860700	-4.75238300	2.91648800
C	-2.40301400	4.49078100	-0.62088500
O	-2.65220600	5.17562600	-1.61160700
H	1.54362400	0.13485500	1.87591500
H	-1.71697500	3.06681200	-1.80540200
C	4.22214100	-0.30907600	-2.41296800
N	4.56621100	-0.81079900	-1.04834500
H	3.71932300	-0.76050800	-0.47298300
H	4.74254500	-1.81317200	-1.13924100
C	3.59852500	1.07327800	-2.35798300
C	4.23233900	2.14054600	-1.66407600
C	3.67251400	3.39729900	-1.64255400
H	5.16515600	1.95760300	-1.14121800
H	4.16617200	4.19977800	-1.09939000
C	-5.16610200	-0.85178400	1.88322800
N	-4.98753200	-0.20998800	0.53911000
H	-5.25243600	0.77509300	0.58464600
H	-3.99691000	-0.21666500	0.29418300

C	-3.94537000	-0.66338800	2.76926600
C	-3.56464700	0.63110100	3.22312400
C	-2.42783200	0.81858600	3.97361900
H	-4.18591100	1.48618200	2.96886300
H	-2.12526400	1.81633500	4.28159900
C	-0.43424800	-0.12858400	5.12269900
C	-1.17518500	-2.70109300	4.27056900
C	-0.04284200	-2.52009600	5.03331900
C	0.32988200	-1.22291700	5.46400900
H	-0.14594600	0.87140800	5.43646500
H	-1.46121100	-3.69568800	3.93614800
H	0.57194200	-3.37451800	5.30285500
H	1.22518300	-1.09465900	6.06603300
C	-3.15911900	-1.74457500	3.11189900
H	-3.42636600	-2.74038100	2.76167500
C	1.84051900	4.95378000	-2.30840400
C	0.65328400	5.17613200	-2.96936100
C	0.02354200	4.12443400	-3.68202500
C	0.59160800	2.86918000	-3.70968500
H	2.32680900	5.75936200	-1.76281400
H	0.18527000	6.15566600	-2.94341700
H	-0.91311900	4.31384700	-4.19875300
H	0.11348100	2.06021000	-4.25844300
C	2.41344600	1.31943900	-3.02109300
H	1.91510800	0.51221600	-3.55565500
C	1.81260100	2.60545600	-3.02929700
C	2.45219700	3.67078400	-2.31795900
C	-1.60972300	-0.28495000	4.34084000
C	-1.98912300	-1.59561400	3.90571200
C	-2.81047600	4.94966600	0.74240600
C	-2.89248000	6.31413400	0.95250600
C	-3.33449600	6.84383100	2.18940600
C	-3.72859600	5.93976900	3.22940100
C	-3.65998900	4.54235100	2.97902900
C	-3.21071800	4.05704100	1.77442600
H	-3.10855000	8.92488600	1.63528700
H	-2.61811100	6.98683800	0.14559800
C	-3.40663400	8.24333100	2.42814000
C	-4.17558700	6.47114400	4.46747600
H	-3.96936000	3.85652000	3.76414100
H	-3.16072700	2.98740500	1.60597200
C	-4.23207200	7.83241000	4.66817500
C	-3.84535300	8.72705100	3.63951100
H	-4.47086700	5.78460700	5.25718500

H	-4.57453100	8.22738100	5.62074700
H	-3.89619200	9.79835400	3.81286700
C	6.34396300	3.37493100	2.06156200
H	5.96644300	4.10084700	2.76772800
C	5.46085200	-0.34864000	-3.31605500
H	6.23049300	0.34119400	-2.95995700
H	5.89374200	-1.35563900	-3.33702600
H	5.18668100	-0.06989500	-4.33883000
H	3.46679900	-0.98064300	-2.84615000
H	-5.27243800	-1.92210000	1.68629800
C	-6.46622500	-0.34517100	2.51455800
H	-7.31471100	-0.52332300	1.84774700
H	-6.65287200	-0.86541600	3.45871100
H	-6.41508500	0.72919700	2.73145900