

Rationalization of the chirality induction and inversion in a zinc trisporphyrinate by a chiral monoalcohol

Li Li,^a Chuanjiang Hu,^{*a} Bo Shi^b and Yong Wang^{*a}

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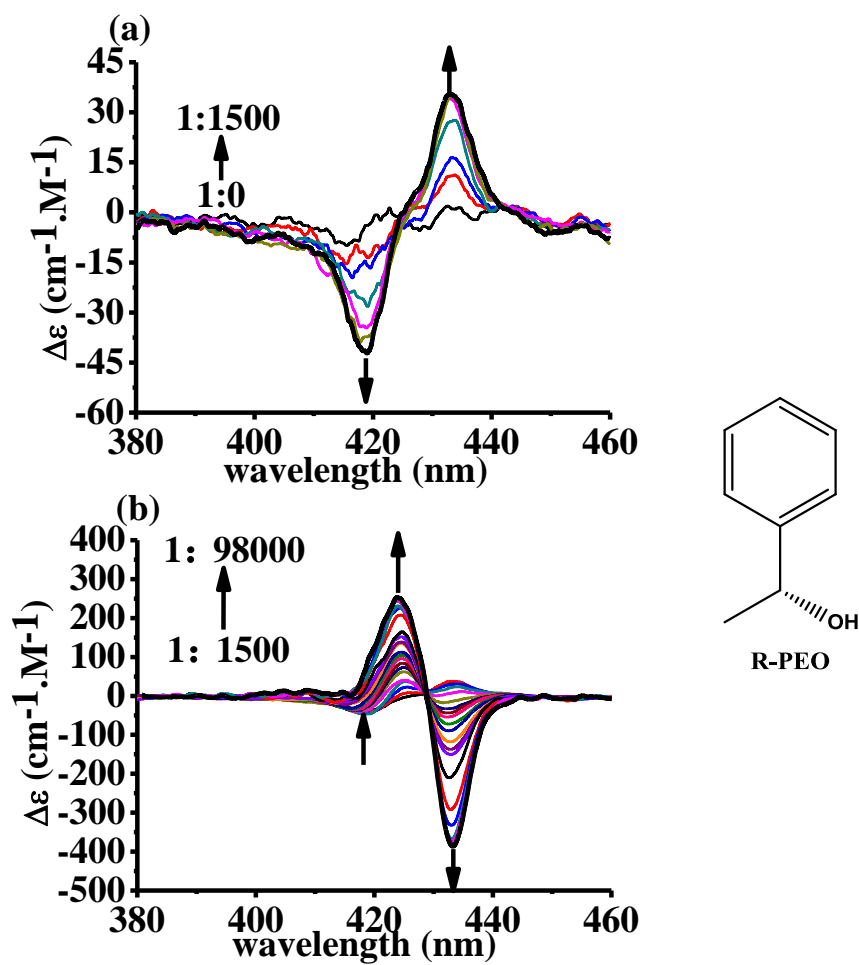


Figure S1. CD titration of [Zn₃-1] (1.08×10^{-6} M) by R-1-phenylethylalcohol in methylene chloride at 295 K. The host to guest ratio is a) from 1:0 to 1:1500; b) from 1:1500 to 1:98000.

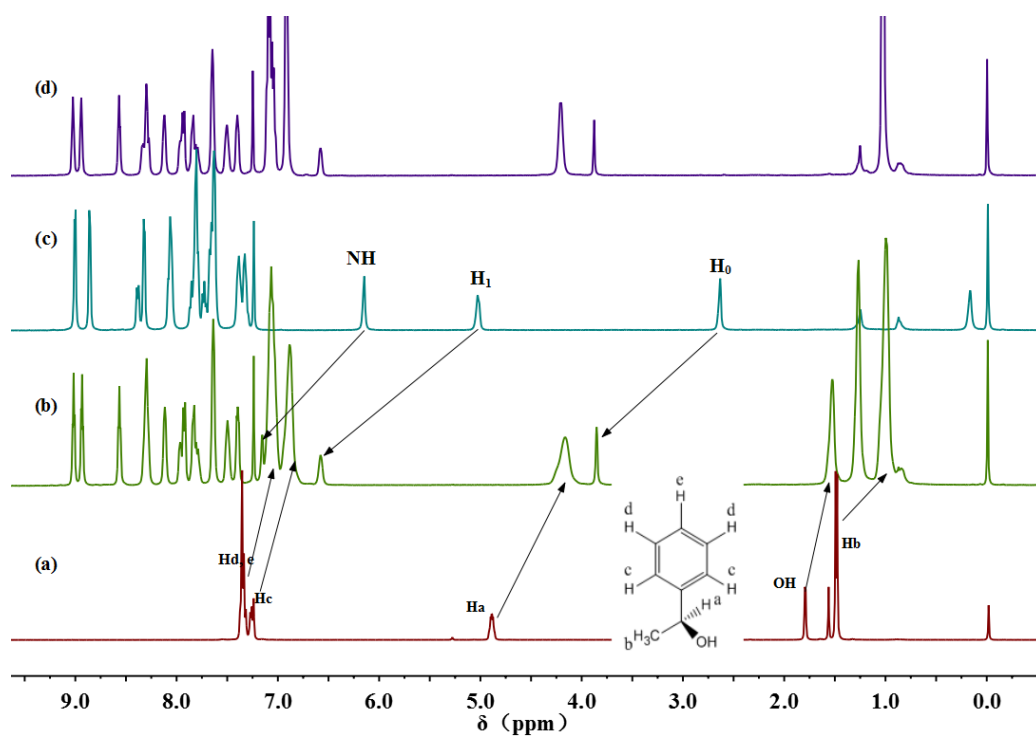


Figure S2. ^1H NMR spectra in CDCl_3 (at 295 K) of (a) S-PEO, (b) the mixture of [Zn₃-1] and S-PEO (12 eq.), (c) [Zn₃-1] (4.23×10^{-3} M), (d) Addition of D_2O into (b). Inset shows the proton numbering scheme of S-PEO. The arrows show the shift of the relevant protons.

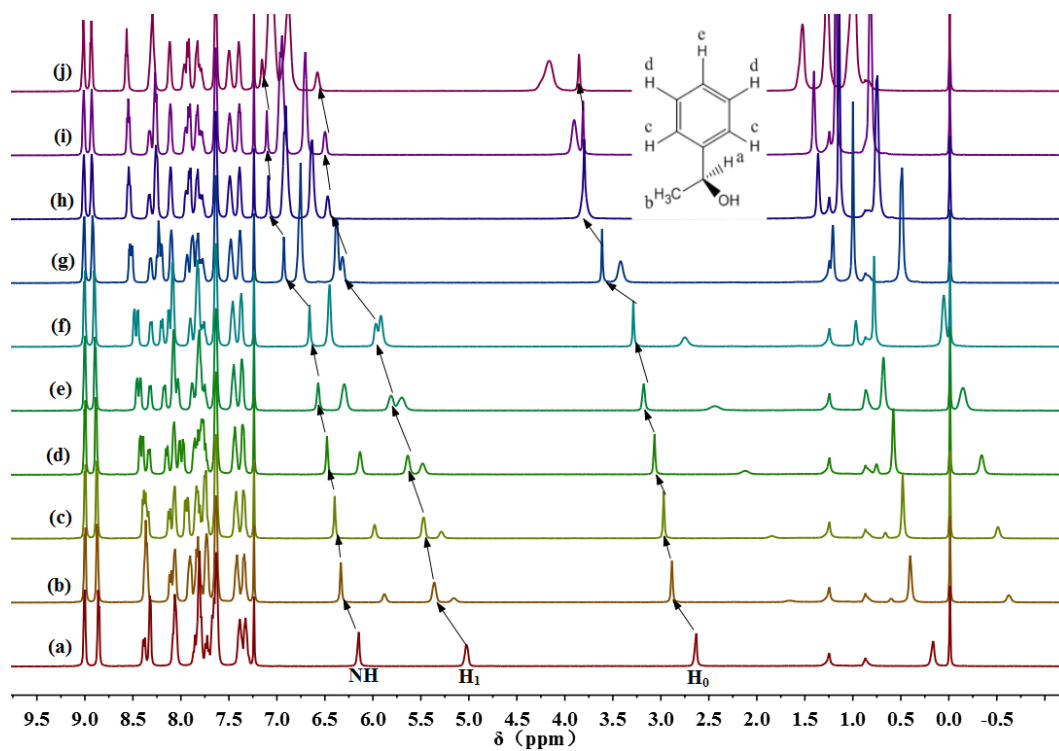


Figure S3. ^1H NMR spectral changes of of $[\text{Zn}_3\text{-1}]$ (4.23×10^{-3} M) upon addition of S-1-phenylethylalcohol in CDCl_3 at 295 K as the host-guest molar ratio: (a) 1:0, (b) 1:0.42, (c) 1:0.60, (d) 1:1.05, (e) 1:1.65, (f) 1:2.50, (g) 1:4.50, (h) 1:6.00, (i) 1:6.90, (j) 1:12.00. Insert shows the proton numbering scheme of S-1-phenylethylalcohol.

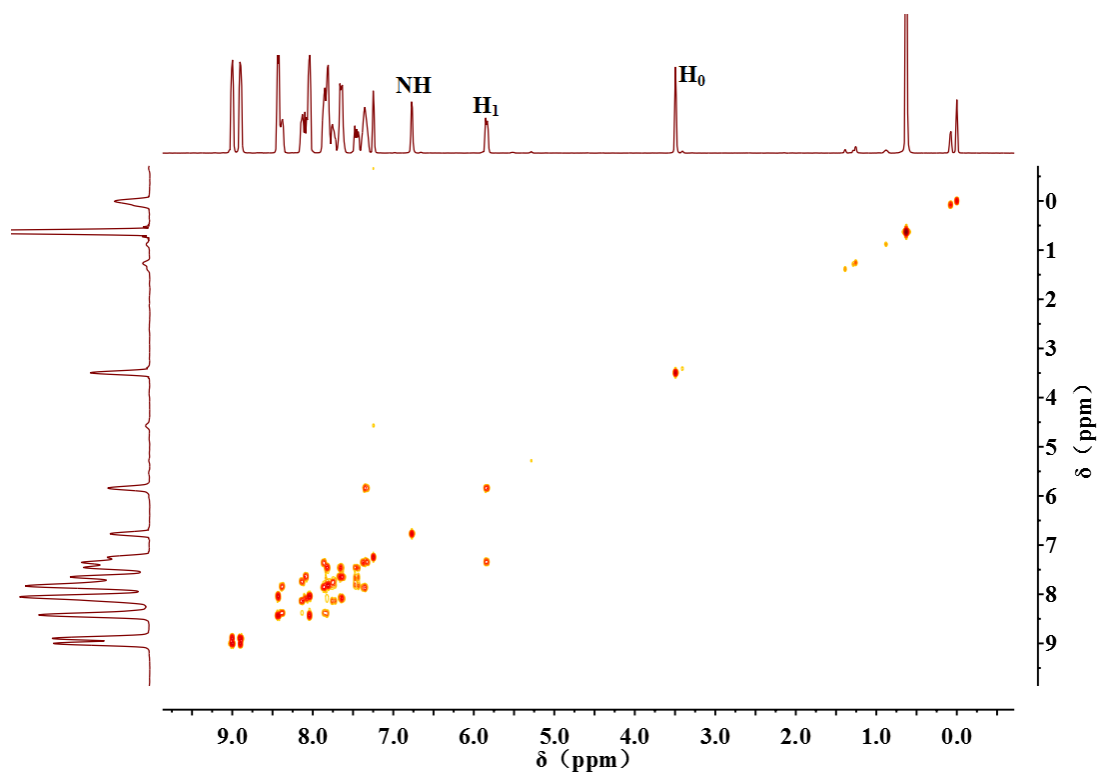


Figure S4. ^1H - ^1H gCOSY spectrum of $[\text{Zn}_3\text{-1}]$ (4.23×10^{-3} M) in CDCl_3 at 295 K. Inset shows the proton numbering scheme of $[\text{Zn}_3\text{-1}]$.

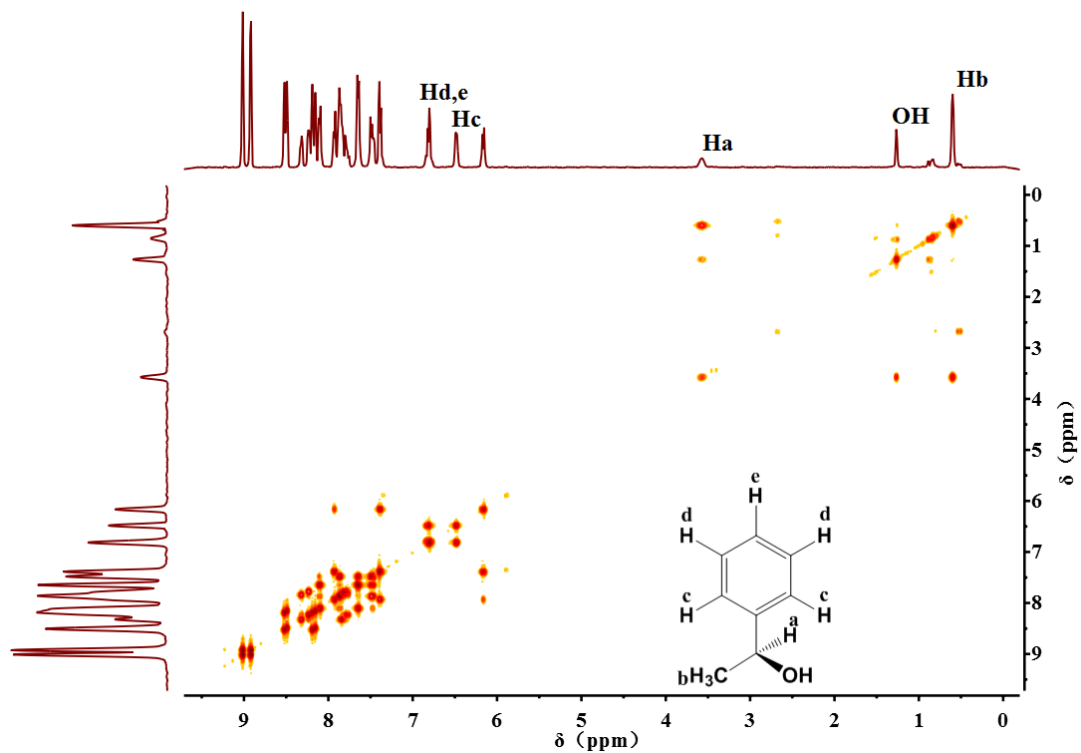


Figure S5. ^1H - ^1H gCOSY spectrum of the mixture of [Zn₃-1] (4.06×10^{-3} M) and S-PEO (6.0 eq.) in CDCl₃ at 295 K. Inset shows the proton numbering scheme of S-PEO.

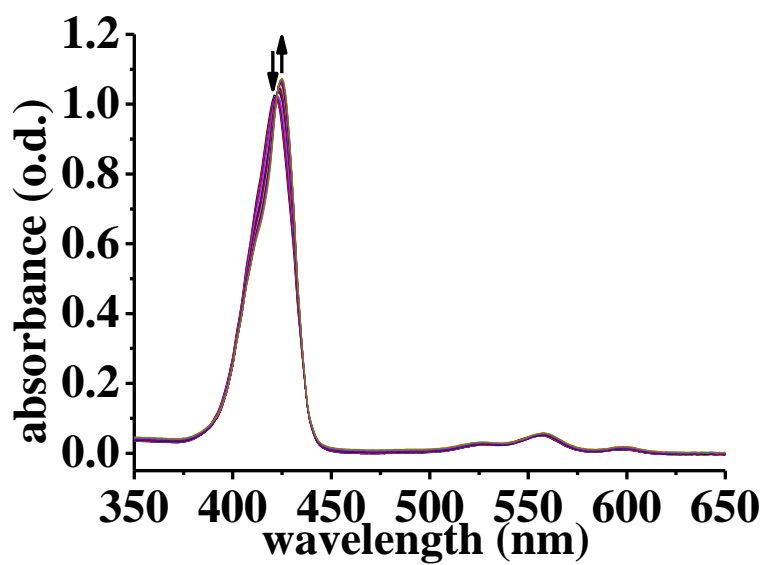


Figure S6. UV-vis spectral change of [Zn₂Ni-1] (1.17×10^{-6} M) upon addition of S-1-phenylethylalcohol as the host-guest molar ratio changes from 1:0 to 1: 18000.

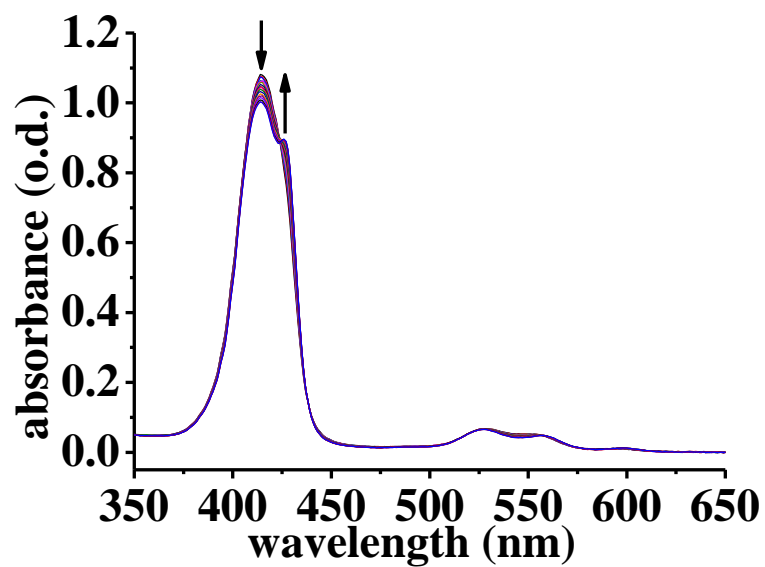


Figure S7. UV-vis spectral change of [ZnNi₂-1] (1.16×10^{-6} M) upon addition of S-1-phenylethylalcohol as the host-guest molar ratio changes from 1:0 to 1: 18000.

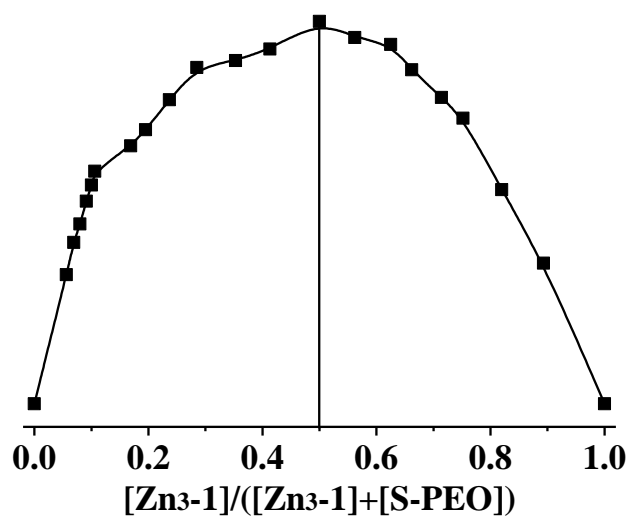


Figure S8. Job's plot for complexation of [Zn₃-1] and S-PEO by ¹H NMR spectroscopy.

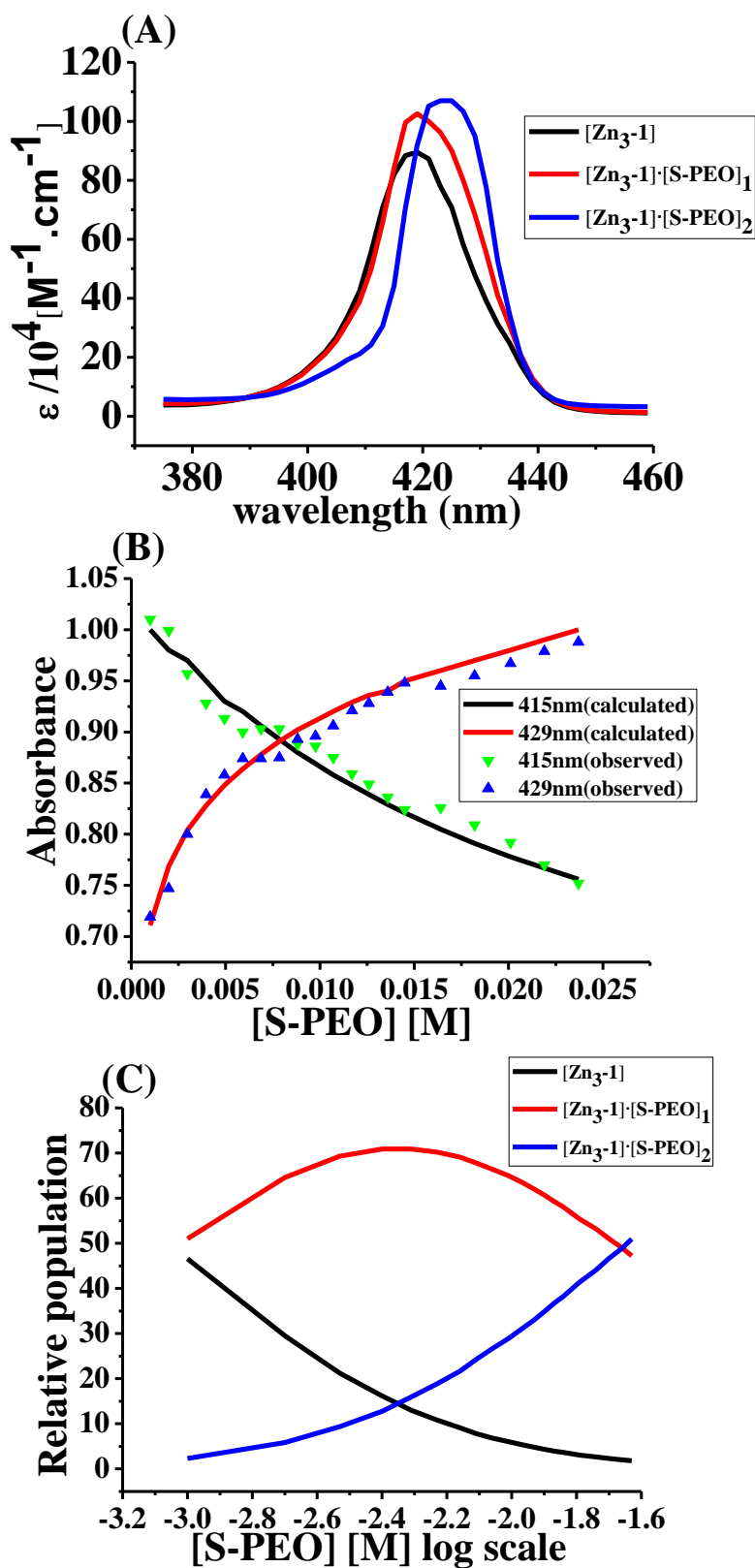


Figure S9. (A) Observed UV-visible spectrum of $[Zn_3-1]$ and calculated UV-visible spectra of $[Zn_3-1] \cdot (S-PEO)$, $[Zn_3-1] \cdot (S-PEO)_2$. (B) Fits of the absorbance data at selected wavelengths of 415 and 429 nm. (C) Species distribution plots of $[Zn_3-1] \cdot (S-PEO)$, $[Zn_3-1] \cdot (S-PEO)_2$.

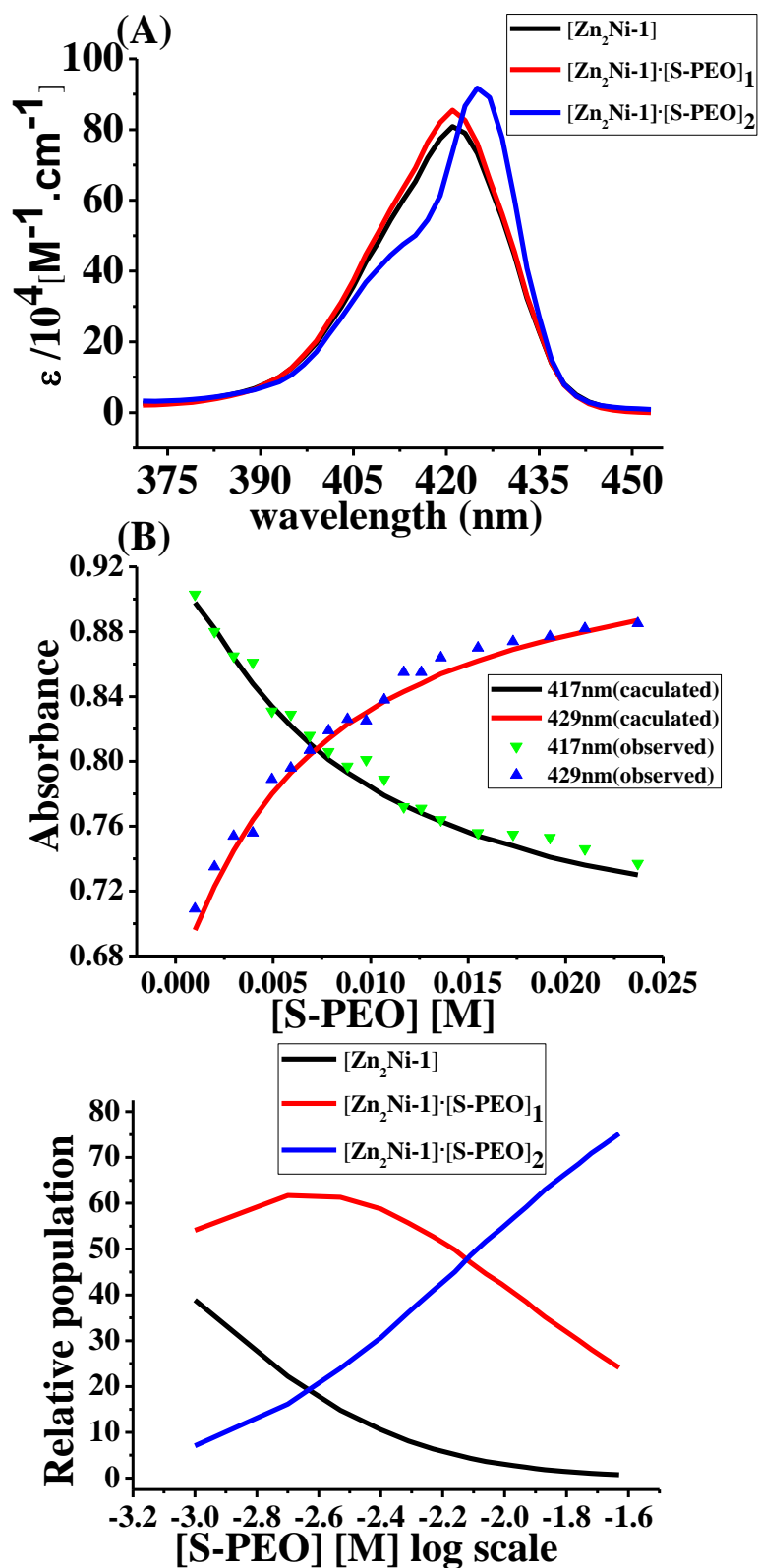


Figure S10. (A) Observed UV-visible spectrum of $[Zn_3-1]$ and calculated UV-visible spectra of $[Zn_2Ni-1] \cdot (S-PEO)$, $[Zn_2Ni-1] \cdot (S-PEO)_2$. (B) Fits of the absorbance data at selected wavelengths of 417 and 429 nm. (C) Species distribution plots of $[Zn_2Ni-1] \cdot (S-PEO)$, $[Zn_2Ni-1] \cdot (S-PEO)_2$.

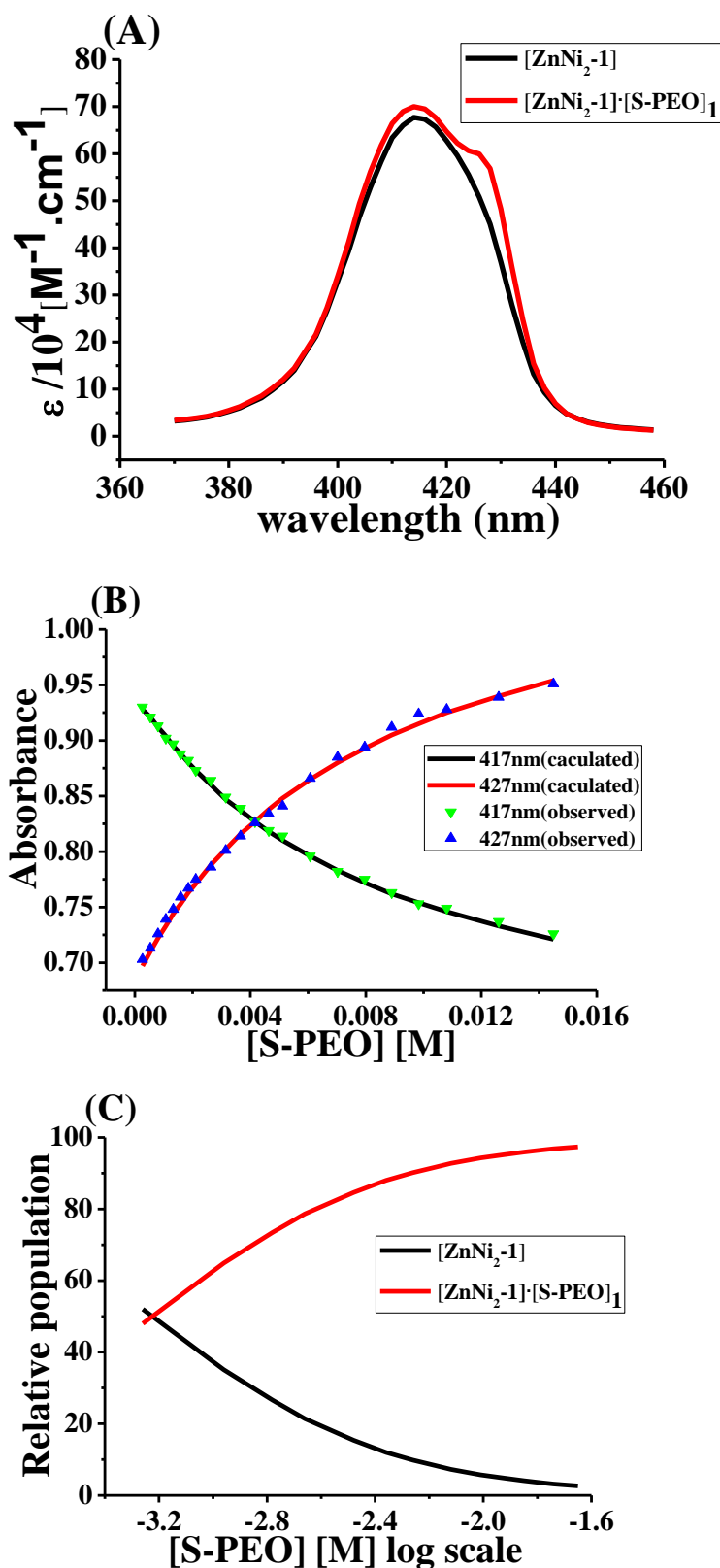


Figure S11. (A) Observed UV-visible spectrum of $[ZnNi_2-1]$ and calculated UV-visible spectra of $[ZnNi_2-1] \cdot (S-PEO)$. (B) Fits of the absorbance data at selected wavelengths of 417 and 427 nm. (C) Species distribution plots of $[ZnNi_2-1] \cdot (S-PEO)$.

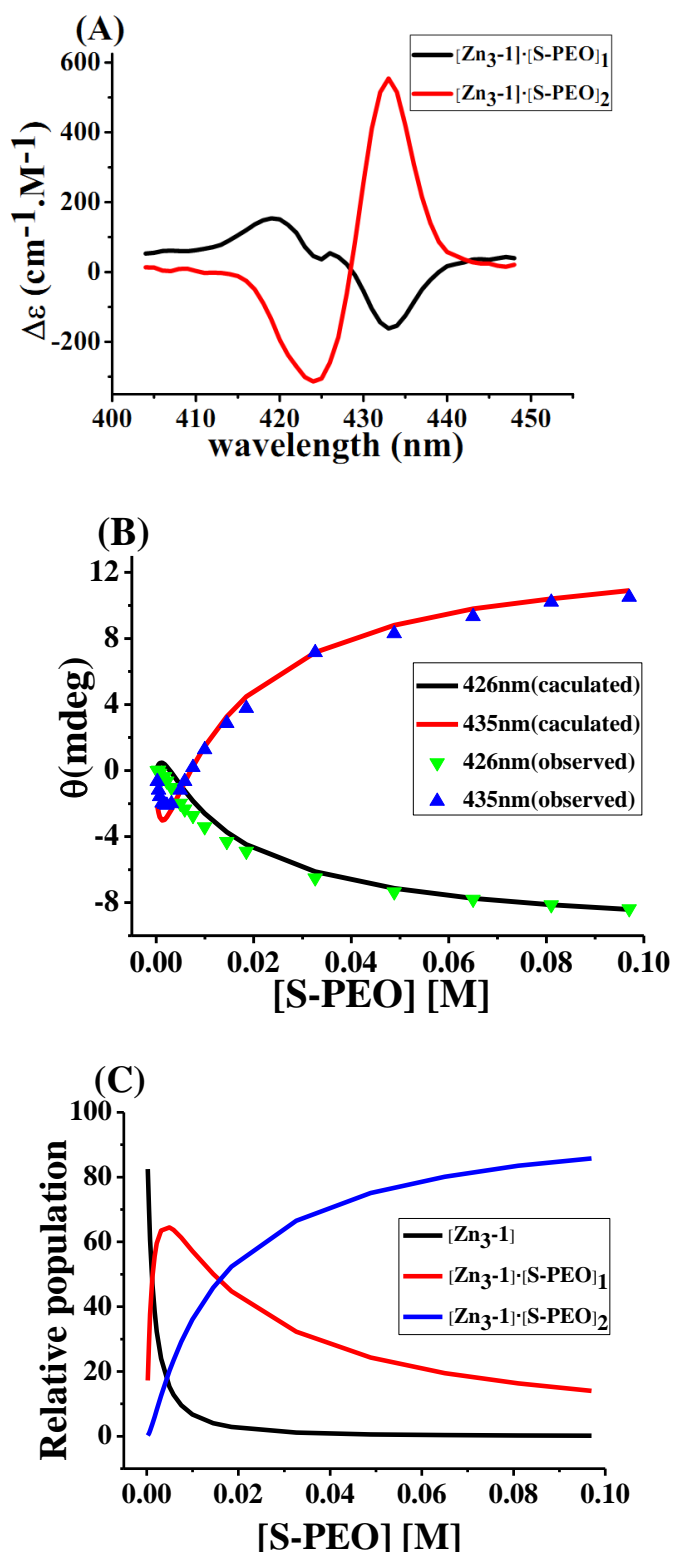


Figure S12. K_1 and K_2 are found to be $0.85 \pm (0.07) \times 10^3$ and $0.63 \pm (0.04) \times 10^2$. (A) Calculated CD spectra of $[Zn_3-1]\cdot(S-PEO)$ and $[Zn_3-1]\cdot(S-PEO)_2$. (B) Fits of the CD data at selected wavelengths of 426 and 435 nm. (C) Species distribution plots of $[Zn_3-1]$, $[Zn_3-1]\cdot(S-PEO)$, $[Zn_3-1]\cdot(S-PEO)_2$.

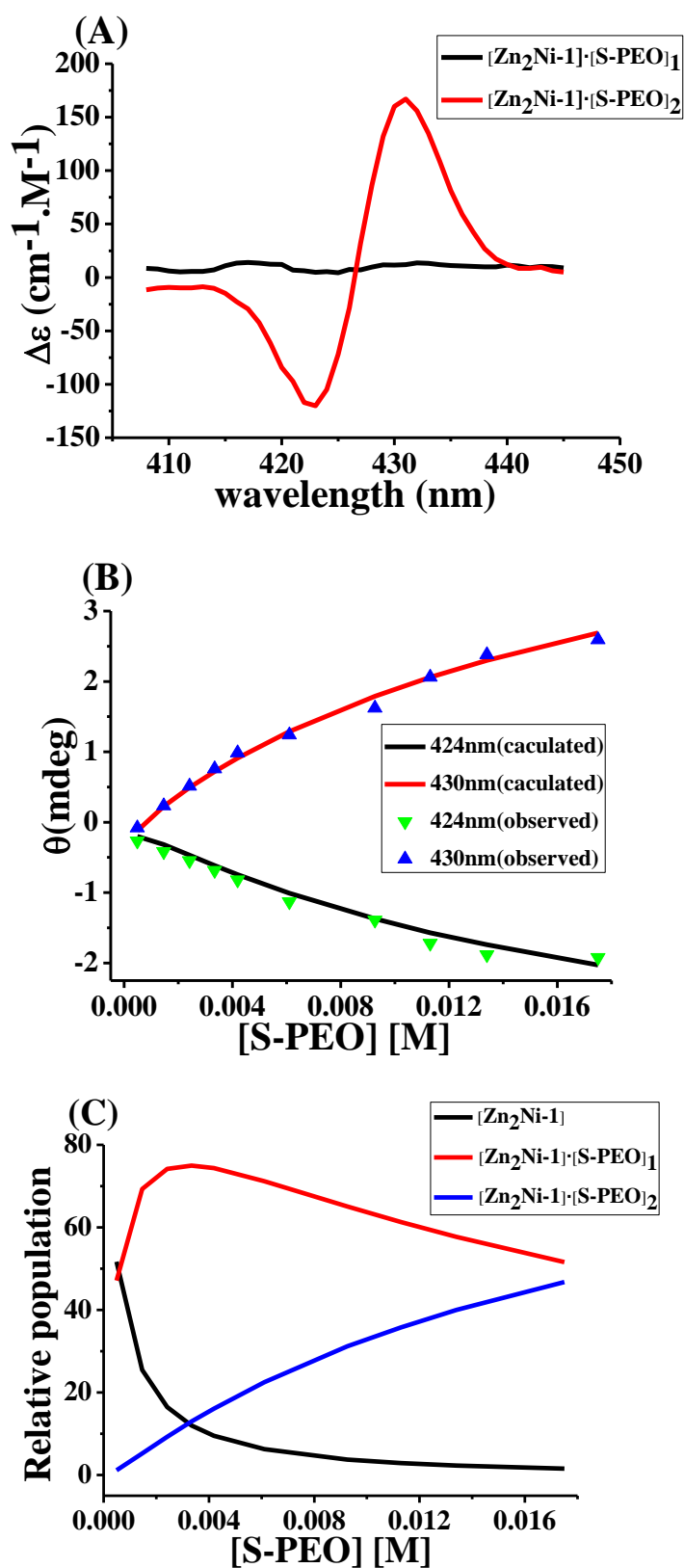


Figure S13. K_1 and K_2 are found to be $1.16 \pm (0.28) \times 10^3$ and $0.52 \pm (0.14) \times 10^2$. (A) Calculated CD spectra of $[\text{Zn}_2\text{Ni-1}]\cdot(\text{S-PEO})$, $[\text{Zn}_2\text{Ni-1}]\cdot(\text{S-PEO})_2$. (B) Fits of the CD data at selected wavelengths of 424 and 430 nm. (C) Species distribution plots of $[\text{Zn}_2\text{Ni-1}]$, $[\text{Zn}_2\text{Ni-1}]\cdot(\text{S-PEO})$ and $[\text{Zn}_2\text{Ni-1}]\cdot(\text{S-PEO})_2$.

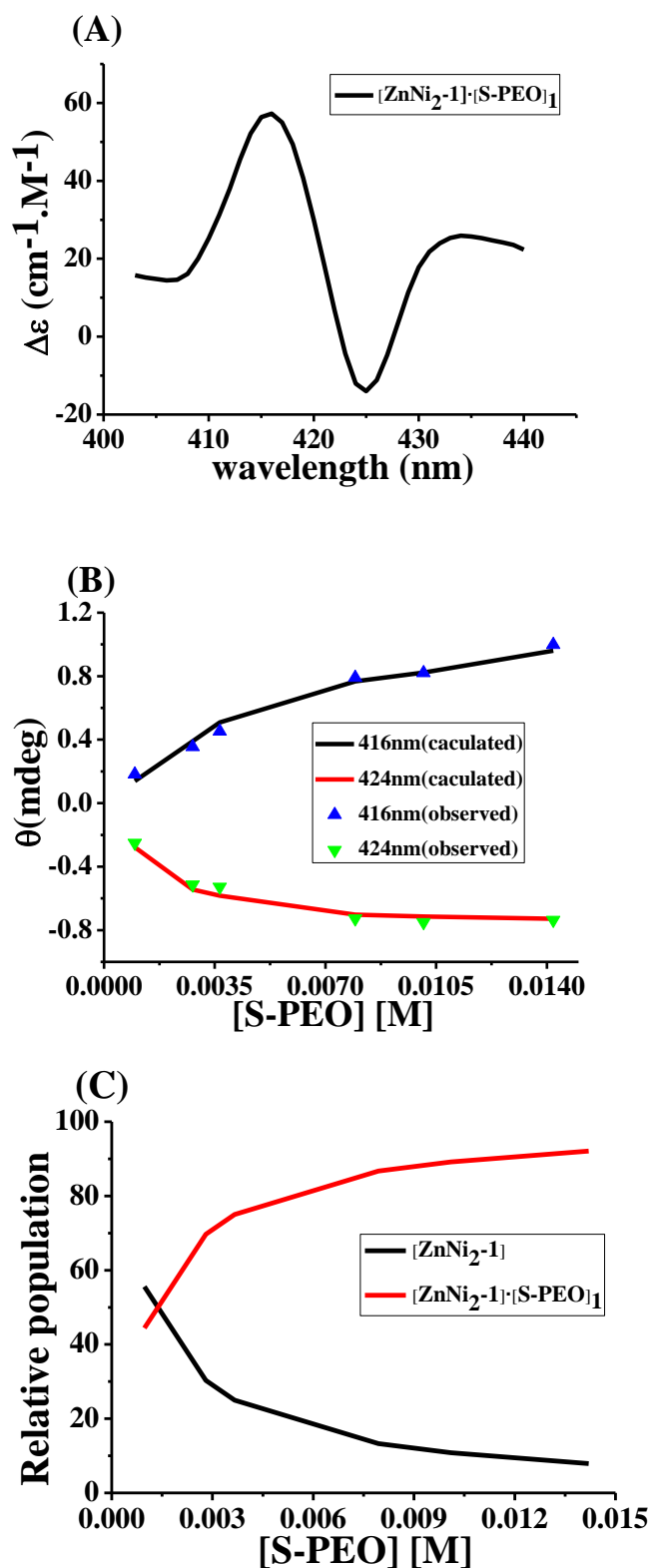


Figure S14. K_1 is found to be $0.82 \pm (0.10) \times 10^3$. (A) Calculated CD spectrum of $[\text{ZnNi}_2\text{-1}] \cdot (\text{S-PEO})$. (B) Fits of the CD data at selected wavelengths of 416 and 424 nm. (C) Species distribution plots of $[\text{ZnNi}_2\text{-1}]$ and $[\text{ZnNi}_2\text{-1}] \cdot (\text{S-PEO})$.

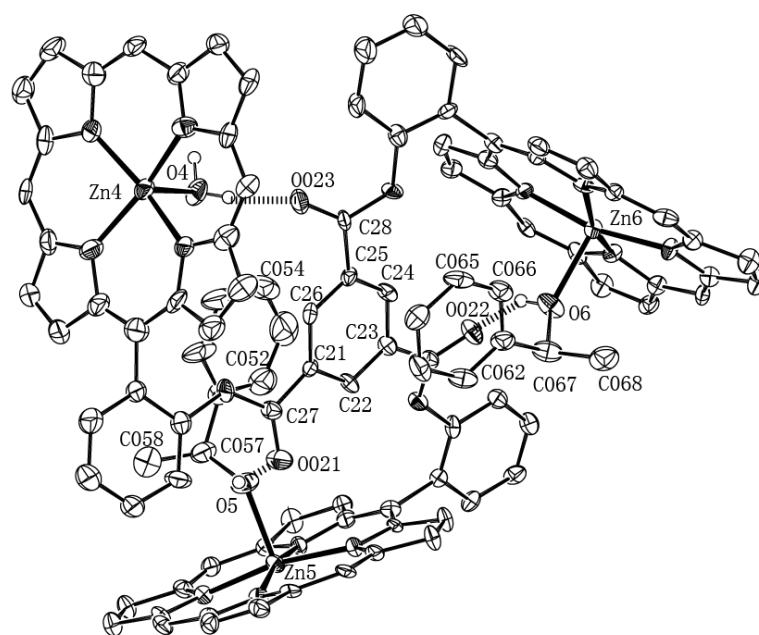


Figure S15. ORTEP view for $[Zn_3-1] \cdot (S-PEO)_2 \cdot H_2O$ (mol B) at 50% probability thermal ellipsoids. Hydrogen bonds are shown by dash lines. Some phenyl rings and some hydrogens have been omitted for clarity.

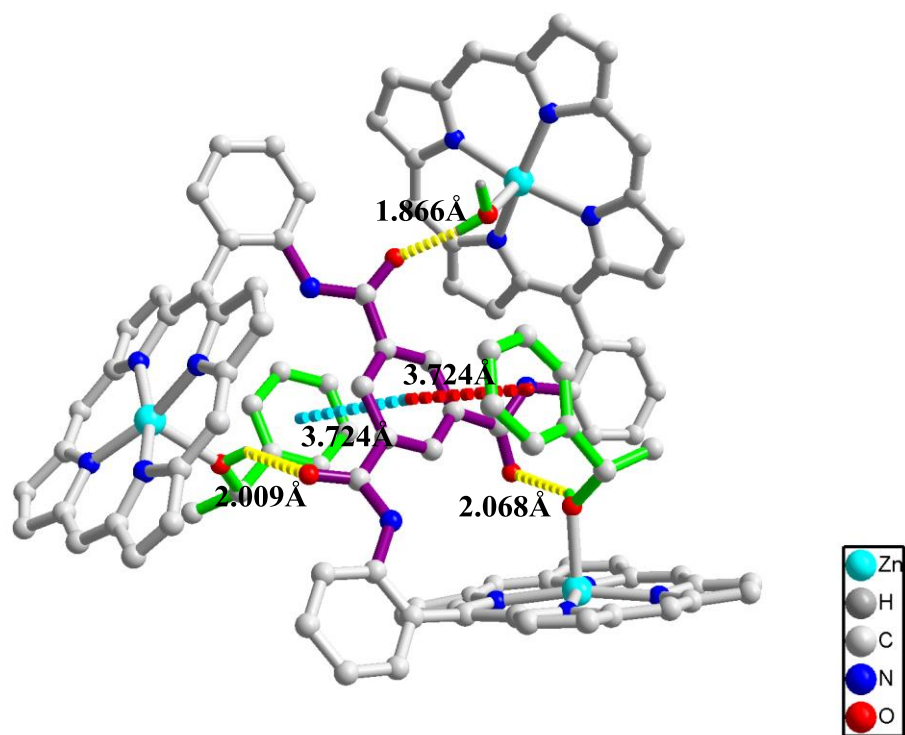


Figure S16. Another view showing hydrogen bonds and π - π interactions in $[\text{Zn}_3\text{-1}] \cdot (\text{S-PEO})_2 \cdot \text{H}_2\text{O}$ (mol B). All hydrogen and some phenyl rings have been omitted for clarity.

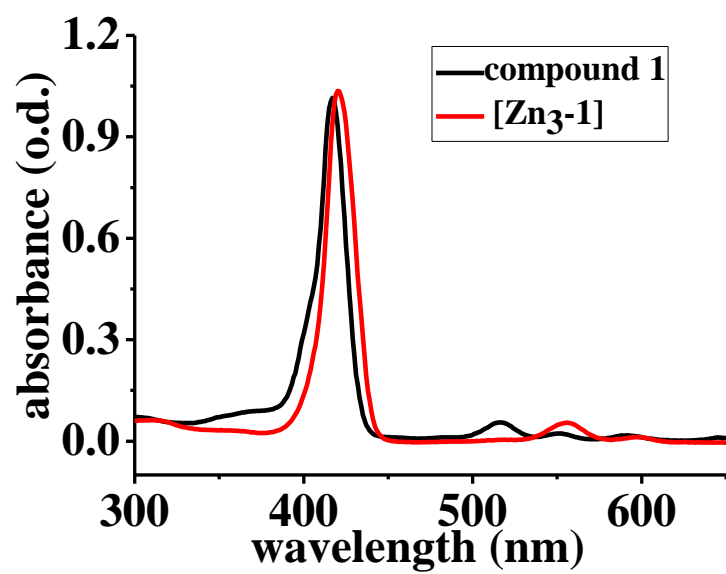


Figure S17. Comparison of **1** and [Zn₃-**1**] in UV-vis spectra .

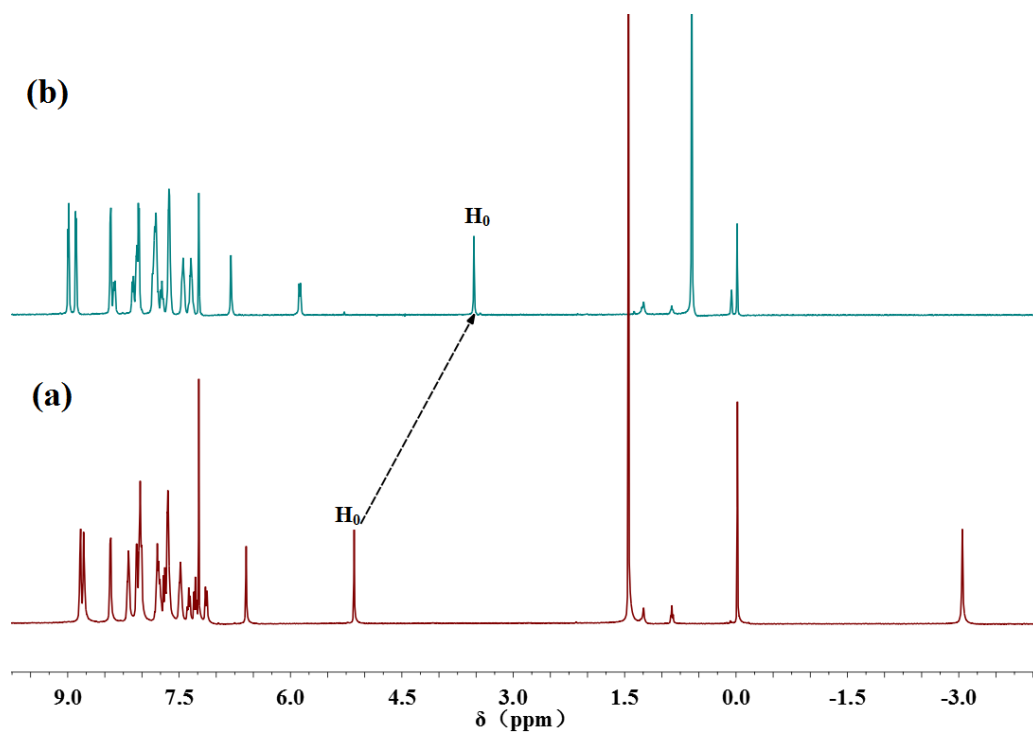


Figure S18. Comparison of ¹H NMR. (a) **1** and (b) [**Zn₃-1**] in CDCl₃.

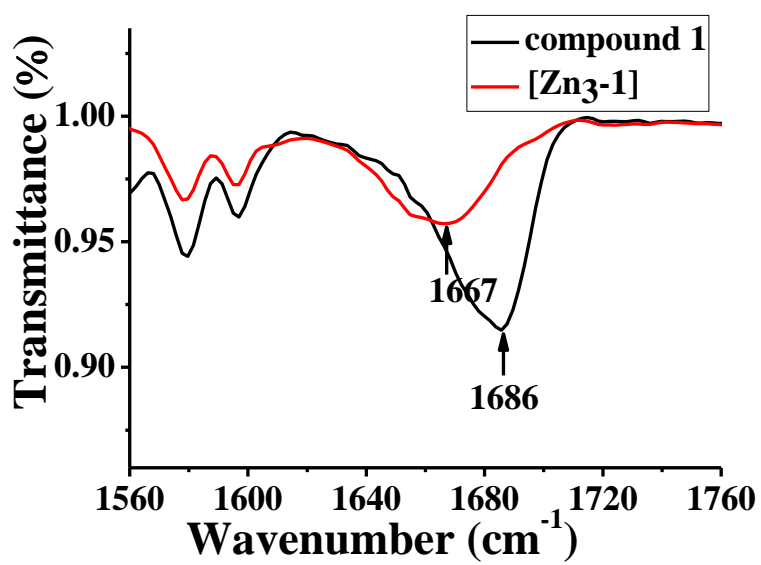


Figure S19. Comparison of **1** and [Zn₃-1] in IR.

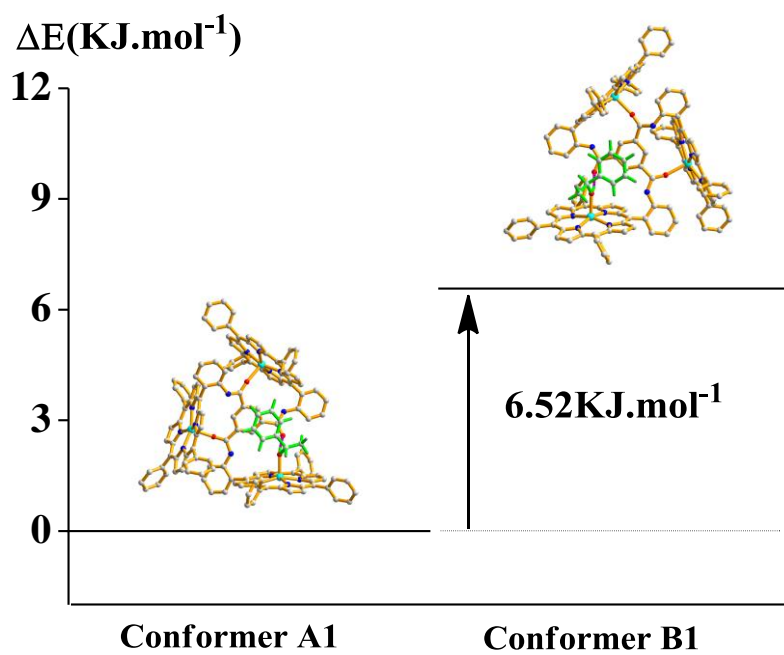


Figure S20. Relative energies of DFT-optimized conformer B1 and conformer A1 of $[Zn_3-1] \cdot (S-PEO)_1$.

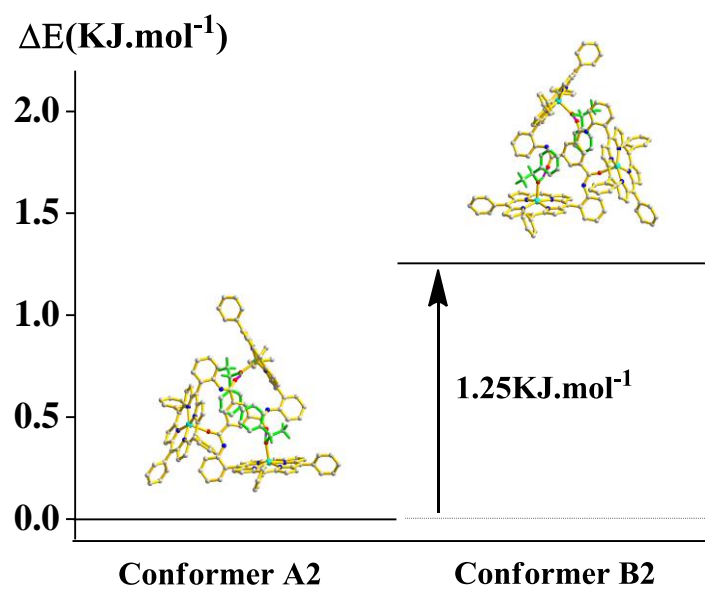


Figure S21. Relative energies of DFT-optimized conformer A2 and conformer B2 of $[\text{Zn}_3-1] \cdot (\text{S-PEO})_2$.

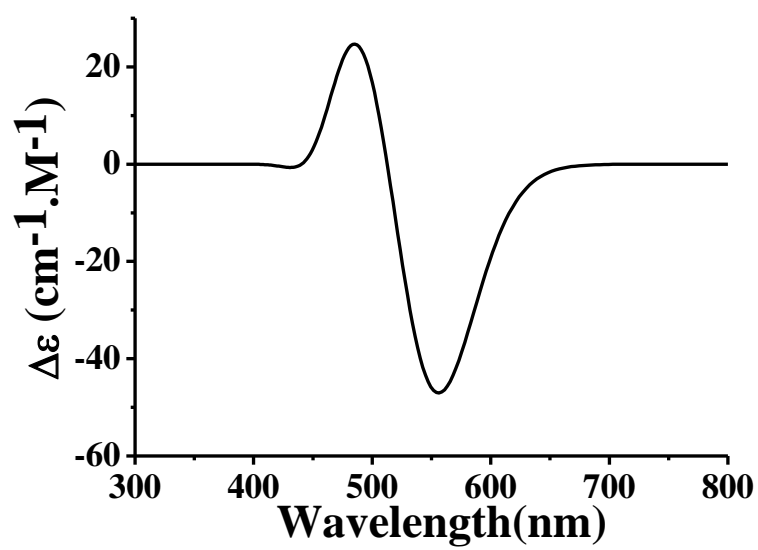


Figure S22. Calculated CD spectrum for the conformer A1.

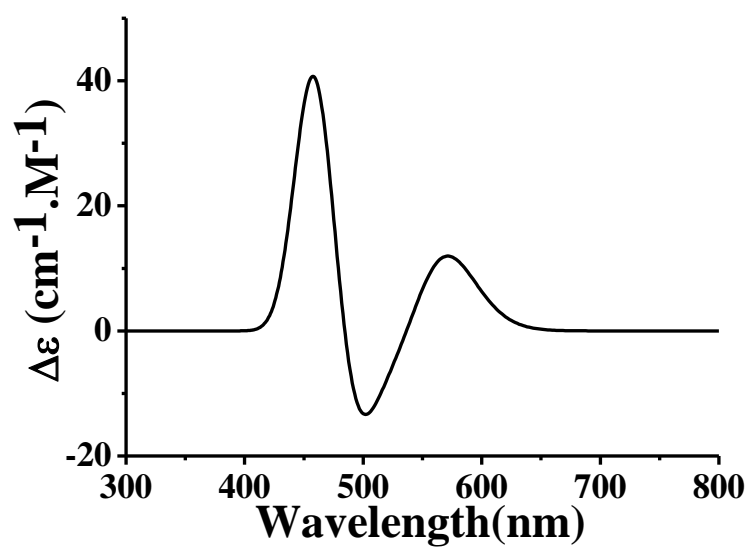


Figure S23. Calculated CD spectrum for the conformer A2.

Table S1. Calculated Binding Constants of the Complexes with 1-phenylethylalcohols at 295 K.

compound	Binding Constant $K_1^{a,b}$	Binding Constant $K_2^{a,b}$
[Zn ₃ -1]	1.10 (± 0.06) $\times 10^3$ [0.85 \pm (0.07) $\times 10^3$]	0.45 (± 0.05) $\times 10^2$ [0.63 \pm (0.04) $\times 10^2$]
[Zn ₂ Ni-1]	1.4 (± 0.2) $\times 10^3$ [1.16 \pm (0.28) $\times 10^3$]	1.3 (± 0.2) $\times 10^2$ [0.52 \pm (0.14) $\times 10^2$]
[ZnNi ₂ -1]	1.66 (± 0.20) $\times 10^3$ [0.82 \pm (0.10) $\times 10^3$]	

^aCalculated from UV-visible spectral measurement. ^bValues shown within the bracket are calculated from CD spectral measurement.

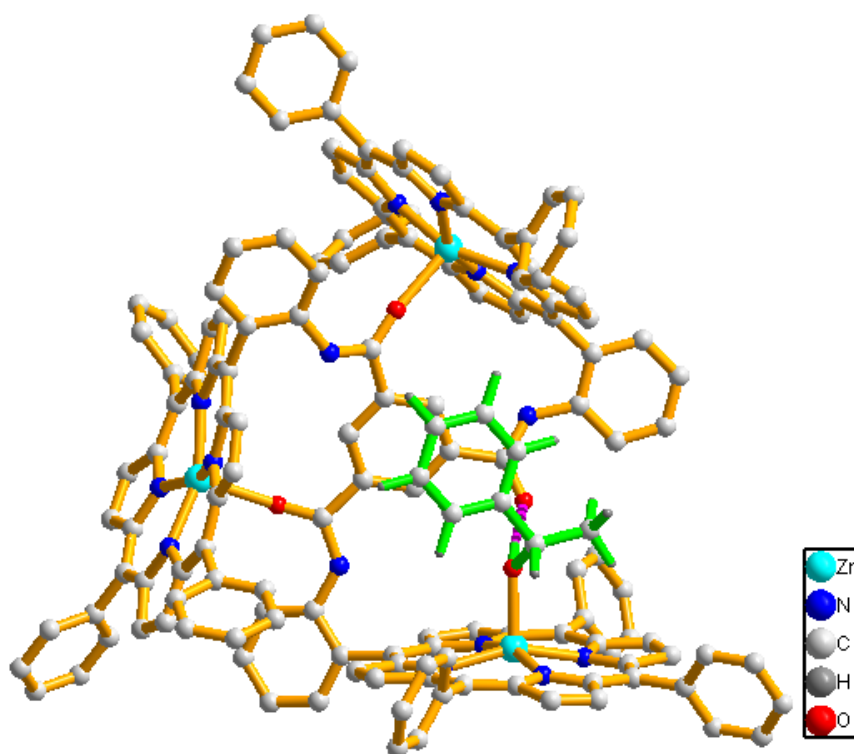
Table S2. Bond lengths (Å) and angles (°) for hydrogen bonds for
[Zn₃-1]·(S-PEO)₂·H₂O.

D-H...A	D-H	H..A	D...A	<(DHA)
O1-H1-O013	0.820	1.942	2.692	151.84
O2-H2-O011	0.820	1.911	2.722	169.24
O3-H3-O012	0.820	1.839	2.655	173.56
O4-H4-O023	0.820	1.866	2.681	172.68
O5-H5-O021	0.820	2.068	2.733	137.98
O6-H6-O022	0.820	2.009	2.700	141.62

Table S3. Selected bond distances (Å) for [Zn₃-1]·(S-PEO)₂·H₂O.

Zn(1)-N(14)	2.053(5)	Zn(3)-N(34)	2.058(4)	Zn(5)-N(52)	2.030(3)
Zn(1)-N(13)	2.057(5)	Zn(3)-N(32)	2.062(4)	Zn(5)-N(51)	2.054(4)
Zn(1)-N(12)	2.062(5)	Zn(3)-N(31)	2.062(4)	Zn(5)-N(54)	2.060(3)
Zn(1)-N(11)	2.065(5)	Zn(3)-O(33)	2.075(4)	Zn(5)-N(53)	2.088(4)
Zn(1)-O(1)	2.166(4)	Zn(3)-O(3)	2.116(3)	Zn(5)-O(5)	2.124(3)
Zn(2)-N(23)	2.043(4)	Zn(4)-N(41)	2.041(5)	Zn(6)-N(63)	2.017(4)
Zn(2)-N(24)	2.048(4)	Zn(4)-N(43)	2.040(5)	Zn(6)-N(61)	2.060(4)
Zn(2)-N(22)	2.056(4)	Zn(4)-N(44)	2.067(5)	Zn(6)-N(64)	2.063(4)
Zn(2)-N(21)	2.063(4)	Zn(4)-N(41)	2.084(4)	Zn(6)-N(62)	2.065(4)
Zn(2)-O(2)	2.199(4)	Zn(4)-O(4)	2.145(4)	Zn(6)-O(6)	2.180(3)

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 A1

$$\Delta E^{\theta} = -12196.26369020 \text{ hartree}$$

Cartesian coordinates for Geometry Optimized Conformer A1

Atoms	x	y	z
Zn	-1.94510700	4.79168600	-0.67341100
N	-3.77448100	3.83527000	-0.39899500
N	-2.49956100	6.12512200	0.80365500
N	-0.60071300	6.20496200	-1.37660900
N	-1.82311900	3.87115200	-2.53035500
C	-3.81983300	2.40840300	-2.42196800
C	-4.41851400	4.87011600	1.75203300
C	-0.86678500	7.94124500	0.37270900
C	0.23516900	4.97543200	-3.35653300

C	-4.30532100	2.82855300	-1.16956900
C	-4.54980100	3.90728400	0.73447600
C	-3.50172100	5.94060300	1.72378800
C	-1.93517900	7.34925800	1.07679600
C	-0.22412900	7.36346300	-0.74342800
C	0.29923800	6.00414100	-2.39681700
C	-0.80123500	4.02458100	-3.43603200
C	-2.65701400	2.90434200	-3.04149000
C	-5.43608200	2.23246900	-0.49243400
H	-6.03819400	1.42014200	-0.87413700
C	-5.57420300	2.88458900	0.69355400
H	-6.31129800	2.70204500	1.46183600
C	-3.57170600	7.08254300	2.60847600
H	-4.28823600	7.21260000	3.40632800
C	-2.61991200	7.96134600	2.19584500
H	-2.41541000	8.94344100	2.59519700
C	0.96801300	7.89663300	-1.36898700
H	1.49210500	8.78895700	-1.05983800
C	1.30050800	7.04792800	-2.37847300
H	2.14158200	7.12209000	-3.05224300
C	-0.99182000	3.11922400	-4.54860700
H	-0.34822800	3.04861100	-5.41350800
C	-2.14392000	2.43320000	-4.30988300
H	-2.61962300	1.69521700	-4.94127600
C	-4.52969000	1.25334500	-3.07528300
C	-5.61763000	1.43235200	-3.93357600

H	-5.93953900	2.44331200	-4.16686400
C	-6.29253600	0.33372000	-4.47203700
H	-7.13714200	0.49043700	-5.13710900
C	-5.88525600	-0.96144500	-4.14928900
H	-6.40971500	-1.82008400	-4.55667500
C	-4.79406900	-1.17104600	-3.30443400
H	-4.46785100	-2.17324500	-3.05607600
C	-4.12134400	-0.06668200	-2.77968700
C	-5.36013200	4.80797600	2.91503200
C	-4.87263200	4.55397400	4.20698700
H	-3.80788500	4.39052600	4.34790500
C	-5.73728400	4.50632700	5.30188300
H	-5.33892200	4.30921000	6.29388800
C	-7.10716700	4.71355100	5.12423300
H	-7.78081500	4.68066700	5.97640500
C	-7.60451900	4.97081700	3.84498500
H	-8.66758300	5.14252200	3.69770700
C	-6.73894700	5.01915000	2.75174200
H	-7.12790900	5.23388100	1.76046500
C	-0.38548200	9.28237200	0.83222600
C	-0.44348400	10.39169700	-0.02847800
H	-0.84957000	10.26380500	-1.02769700
C	-0.00021300	11.64710200	0.38790800
H	-0.06076800	12.49149300	-0.29377900
C	0.51186100	11.82134700	1.67499200
H	0.85817100	12.79909000	1.99890500

C	0.57288600	10.73042400	2.54348500
H	0.97041200	10.85330300	3.54759000
C	0.12643300	9.47556200	2.12690400
H	0.17406500	8.63194100	2.80971200
C	1.29994700	4.91666200	-4.40943900
C	1.40922300	5.91611600	-5.38943000
H	0.71031700	6.74781200	-5.37739400
C	2.39135000	5.84260400	-6.37825600
H	2.45614600	6.62417200	-7.13091600
C	3.28069300	4.76670600	-6.40662300
H	4.04447100	4.70789200	-7.17738100
C	3.18316600	3.76502100	-5.43891000
H	3.87053700	2.92309800	-5.45411200
C	2.20168300	3.84085900	-4.44906900
H	2.13918800	3.06639900	-3.68970500
Zn	-4.25144800	-3.93078900	0.19784100
N	-3.69547100	-3.92057400	2.20703800
N	-6.06928000	-3.12461100	0.76435800
N	-5.16374600	-4.63445300	-1.53116800
N	-2.72608000	-5.31315200	-0.13147900
C	-1.59203400	-5.23121000	2.06855000
C	-5.52241200	-2.50678700	3.10039000
C	-7.35898700	-3.50310900	-1.31600600
C	-3.27920200	-5.94574700	-2.46315000
C	-2.54951200	-4.45266600	2.74961100
C	-4.30401700	-3.20237500	3.20944900

C	-6.35020900	-2.51506000	1.96153500
C	-7.18891200	-2.98370700	-0.01887100
C	-6.39647900	-4.26257200	-2.01021400
C	-4.55050900	-5.34429900	-2.53556100
C	-2.45167600	-5.93889900	-1.32517700
C	-1.69472900	-5.62940200	0.72085800
C	-2.43597500	-4.06229700	4.13934900
H	-1.64223800	-4.36160300	4.81010700
C	-3.51213900	-3.27771300	4.41835500
H	-3.75798100	-2.80455200	5.35775600
C	-7.68690200	-1.96027600	1.92961300
H	-8.16870200	-1.44559900	2.74813200
C	-8.20913500	-2.25977500	0.71089500
H	-9.20011700	-2.03578800	0.34421300
C	-6.55931900	-4.74168000	-3.36670700
H	-7.43322900	-4.58967900	-3.98360400
C	-5.41534900	-5.40205700	-3.69431000
H	-5.17806400	-5.88829700	-4.62941800
C	-1.20036500	-6.66008100	-1.22453200
H	-0.75939500	-7.25739500	-2.00953800
C	-0.72801800	-6.46155400	0.03653600
H	0.17345400	-6.86448700	0.47549100
C	-0.31618000	-5.57306100	2.79240600
C	-0.06378100	-6.85392400	3.29107000
H	-0.83701000	-7.61100000	3.19602300
C	1.16048100	-7.16931000	3.88599000

H	1.33583600	-8.17230600	4.26443400
C	2.15412000	-6.19568000	3.98578600
H	3.11072700	-6.43496000	4.44162900
C	1.93011500	-4.90163400	3.51365400
H	2.69399700	-4.13847800	3.59077300
C	0.69882500	-4.59290300	2.92724500
C	-6.00055500	-1.73241300	4.29155600
C	-6.01597200	-0.32907500	4.26393900
H	-5.66791300	0.18821600	3.37373700
C	-6.46534700	0.40253200	5.36436700
H	-6.46531900	1.48863700	5.32392900
C	-6.90951900	-0.25958800	6.51061600
H	-7.26099600	0.30846400	7.36804600
C	-6.90248700	-1.65517900	6.54977900
H	-7.25317500	-2.17824900	7.43578800
C	-6.45219600	-2.38542400	5.44898200
H	-6.45690000	-3.47163200	5.47738100
C	-8.66718700	-3.24703800	-2.00093000
C	-9.03522500	-1.95084700	-2.39548500
H	-8.35137300	-1.12740400	-2.21257800
C	-10.25649400	-1.71742500	-3.02957200
H	-10.52148700	-0.70714500	-3.33088000
C	-11.13256400	-2.77519600	-3.27966700
H	-12.08387500	-2.59290200	-3.77248800
C	-10.77890700	-4.06878800	-2.89132400
H	-11.45637700	-4.89845600	-3.07600700

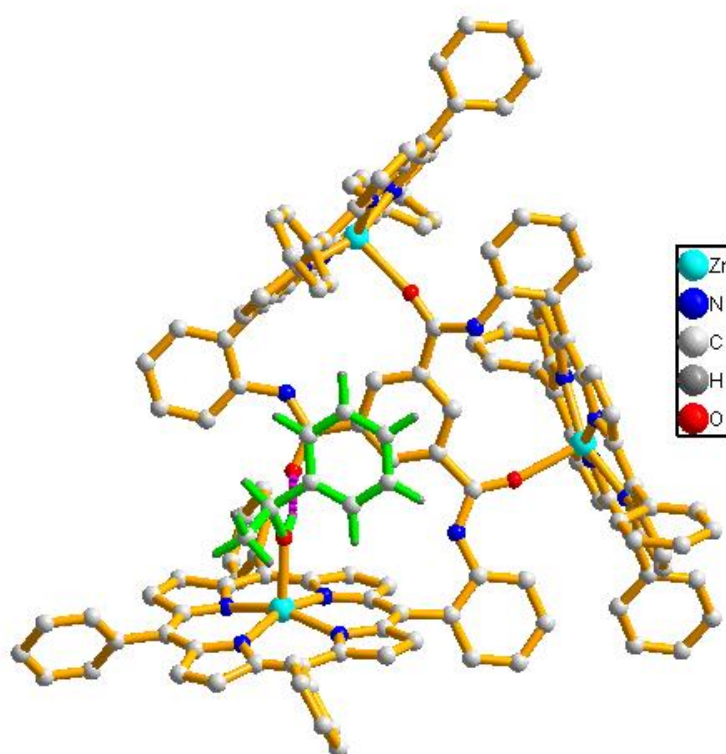
C	-9.55762900	-4.30191900	-2.25789300
H	-9.28892600	-5.30822500	-1.94881300
C	-2.79646300	-6.69828100	-3.66808700
C	-1.75416500	-6.19874800	-4.46373600
H	-1.29704000	-5.24691400	-4.20765500
C	-1.30600500	-6.90533100	-5.58110500
H	-0.49950900	-6.49938500	-6.18617900
C	-1.89275600	-8.12504300	-5.92208800
H	-1.54373300	-8.67553400	-6.79166900
C	-2.93029500	-8.63365600	-5.13837200
H	-3.39077300	-9.58469400	-5.39318300
C	-3.37779100	-7.92613500	-4.02201600
H	-4.18150400	-8.32641400	-3.41023900
Zn	5.96628200	-0.44380200	0.60529100
N	6.89434100	-1.77387700	1.91209400
N	7.24987500	-1.10722900	-0.88993100
N	5.69956300	1.30299000	-0.50464500
N	5.23485900	0.56568100	2.26208600
C	4.47186700	2.65108300	1.16724100
C	6.73372600	0.57928800	-2.63226000
C	8.29486300	-3.02027700	0.28991800
C	5.70195400	-1.14405700	3.99003900
C	4.96732600	2.39871000	-0.12623200
C	5.97265800	1.45962600	-1.84208700
C	7.36355500	-0.58880900	-2.15706600
C	8.08402400	-2.19866700	-0.83542800

C	7.71117500	-2.81959000	1.55806800
C	6.52740300	-1.98688200	3.21813700
C	5.14553100	0.06738300	3.53819600
C	4.61631400	1.79079000	2.27356200
C	4.76242300	3.27501100	-1.26116500
H	4.22069600	4.21018900	-1.24366200
C	5.37520000	2.68902300	-2.32466200
H	5.42861800	3.05988700	-3.33766000
C	8.29658900	-1.38032800	-2.92864600
H	8.58979400	-1.18105200	-3.94941400
C	8.74943100	-2.36813200	-2.10964800
H	9.48318200	-3.12796700	-2.33588900
C	7.85794400	-3.72710700	2.67706000
H	8.43598500	-4.63969300	2.67220900
C	7.11884500	-3.21749300	3.69897600
H	6.98269700	-3.63450000	4.68612000
C	4.44253400	1.01052900	4.38329900
H	4.25228600	0.88238500	5.43906300
C	4.12018100	2.07874900	3.60347100
H	3.61767600	2.98903400	3.90029000
C	3.75200500	3.95361900	1.38278300
C	4.47893200	5.11853600	1.64525300
H	5.56163700	5.05009200	1.69895900
C	3.83912600	6.34363800	1.83040900
H	4.42232700	7.23812500	2.02976600
C	2.44914400	6.41054300	1.75039800

H	1.94283300	7.36116200	1.87993100
C	1.69267100	5.26748900	1.49453500
H	0.61521200	5.32282000	1.42786800
C	2.34169900	4.04101600	1.31120100
C	6.91865200	0.92517600	-4.07936900
C	7.72476400	2.00578300	-4.46972900
H	8.22968000	2.59166500	-3.70676100
C	7.88562800	2.32623500	-5.81857700
H	8.51762900	3.16419300	-6.10114200
C	7.24133700	1.57204500	-6.80129300
H	7.36667500	1.82128900	-7.85170800
C	6.43818900	0.49290000	-6.42660800
H	5.93281300	-0.10034400	-7.18435000
C	6.28070200	0.17146500	-5.07721200
H	5.65274100	-0.66677500	-4.78743700
C	9.21415900	-4.19209200	0.12909900
C	8.87900500	-5.26375400	-0.71392300
H	7.93390500	-5.24057500	-1.24936900
C	9.73795400	-6.35341700	-0.86224200
H	9.45705800	-7.17522800	-1.51590400
C	10.95029400	-6.39093200	-0.17107400
H	11.62007300	-7.23884900	-0.28730800
C	11.29668800	-5.33171600	0.66988400
H	12.24072200	-5.34894100	1.20836900
C	10.43612700	-4.24356500	0.81900500
H	10.71138200	-3.41758000	1.46877200

C	5.39256100	-1.55844400	5.39524900
C	6.38740000	-1.59429000	6.38472900
H	7.40307000	-1.30819200	6.12587600
C	6.08115300	-1.98112900	7.69029100
H	6.86372100	-1.99716000	8.44453000
C	4.77484900	-2.33946800	8.02877100
H	4.53693400	-2.64094900	9.04547500
C	3.77596100	-2.30684400	7.05372000
H	2.75687400	-2.58746900	7.30731700
C	4.08177800	-1.91801400	5.74883100
H	3.30818700	-1.89703900	4.98595500
O	4.16404700	-1.51606000	0.09628300
H	3.52895000	-1.69723500	0.82932100
C	2.73530300	-2.40966200	-1.65859400
C	1.75113000	-3.40383400	-1.67326300
H	1.90331600	-4.33457800	-1.13572200
C	0.55866700	-3.22012100	-2.38109900
H	-0.19337300	-4.00447700	-2.36938800
C	0.33612100	-2.03719500	-3.08498300
H	-0.58906700	-1.89415000	-3.63726200
C	1.31173300	-1.03481100	-3.07612100
H	1.14561400	-0.10930100	-3.62213700
C	2.49796900	-1.22172400	-2.36979300
H	3.25501600	-0.44104200	-2.36359400
C	4.05618600	-2.55510100	-0.91049900
H	4.86749000	-2.31488900	-1.60417500

C	4.32679700	-3.92643500	-0.29753600
H	5.31587000	-3.92871500	0.16782700
H	4.30395200	-4.70719700	-1.06590100
H	3.58952700	-4.17510100	0.47284800
N	-2.97109100	-0.18386600	-1.95935400
N	0.37454900	-3.30461000	2.44674300
N	1.64913100	2.82700900	1.09104800
O	-3.32652500	-2.07108600	-0.70651100
O	2.37981000	-2.22589100	2.12988600
O	-0.49457700	3.45823900	0.55003500
C	-1.52615700	-0.58708400	-0.10248200
C	-1.15514200	0.75608600	0.03023100
H	-1.74573500	1.55849400	-0.39842200
C	-0.00692400	1.11504200	0.74424800
C	0.74397600	0.11588200	1.38070300
H	1.61567300	0.34960400	1.98499800
C	0.34933500	-1.22282600	1.29631300
C	-0.77628300	-1.56889100	0.54207400
H	-1.06846700	-2.60419300	0.40834400
C	-2.70040100	-1.02664700	-0.93340600
C	0.34999900	2.57980100	0.78683400
C	1.14945300	-2.28754200	1.99365100
H	-0.62183400	-3.17195500	2.32935500
H	2.26325500	2.02127600	1.10717600
H	-2.35557900	0.61566100	-2.03353500



Conformer B1

$$\Delta E^{\theta} = -12196.26120580 \text{ hartree}$$

Cartesian coordinates for Geometry Optimized Conformer B1

Atoms	x	y	z
Zn	2.16104600	4.91660600	-0.07679600
N	2.76996100	4.58730000	-2.03902700
N	1.27349700	6.67820400	-0.72859300
N	2.09334900	5.65857300	1.85172300
N	3.67595900	3.63242500	0.53328600
C	4.43291200	2.79067600	-1.67031800
C	3.49216700	3.95935300	2.98350400
C	0.68426900	7.65775100	1.47123300
C	1.39053000	6.30280200	-3.17508900

C	3.63972400	3.61988500	-2.48463400
C	2.25235400	5.19079600	-3.16066800
C	0.96642800	7.00261600	-2.02884500
C	0.67122300	7.62726500	0.06395100
C	1.34303800	6.72241300	2.29018800
C	2.60279600	5.05108600	2.97298900
C	4.01209900	3.33677800	1.83375300
C	4.45423000	2.82620000	-0.26248800
C	3.65089200	3.59468100	-3.93169300
H	4.25762400	2.93955700	-4.54115100
C	2.79712800	4.56849800	-4.34868300
H	2.57389200	4.86057200	-5.36456700
C	0.13736400	8.18780900	-2.05614700
H	-0.25646200	8.65596600	-2.94638400
C	-0.03573200	8.58002300	-0.76485000
H	-0.59213900	9.43245300	-0.40238700
C	1.36605600	6.77659800	3.73594100
H	0.86848200	7.51973800	4.34190200
C	2.13089900	5.73476000	4.15853700
H	2.36801400	5.46071000	5.17602700
C	5.03894000	2.31719600	1.85396600
H	5.50705500	1.92105300	2.74347800
C	5.31216200	2.00110000	0.55908100
H	6.03901700	1.29109900	0.19019400
C	5.26305600	1.73048000	-2.34020700
C	6.51875900	1.99942300	-2.89292700

H	6.90232400	3.01493200	-2.85171200
C	7.27692800	0.98086300	-3.47508800
H	8.25147400	1.20707300	-3.89882800
C	6.78446000	-0.32451000	-3.50846000
H	7.37049800	-1.12077700	-3.95596400
C	5.52865100	-0.61928300	-2.97579500
H	5.13123100	-1.62610700	-3.01379200
C	4.77680500	0.40566500	-2.40265600
C	3.95589000	3.45189100	4.31547300
C	3.55499100	2.18936100	4.77914900
H	2.89997200	1.58132400	4.16138800
C	3.97876800	1.71700100	6.02234300
H	3.65638500	0.73772900	6.36521400
C	4.81419700	2.49959000	6.82243700
H	5.13957900	2.13429700	7.79305200
C	5.22629500	3.75452400	6.36959900
H	5.88161000	4.36795400	6.98253800
C	4.80088700	4.22566900	5.12701500
H	5.12653000	5.20027000	4.77432200
C	-0.05495700	8.77398100	2.14796400
C	0.44441200	10.08520200	2.11698900
H	1.37933700	10.28387500	1.60016000
C	-0.24172900	11.12525900	2.74569000
H	0.16269100	12.13367900	2.71411100
C	-1.43951600	10.87131800	3.41661600
H	-1.97384200	11.68097500	3.90657500

C	-1.94637800	9.57114500	3.45467300
H	-2.87971100	9.36427900	3.97191900
C	-1.25967400	8.53097800	2.82612600
H	-1.66047800	7.52155300	2.84932600
C	0.92871700	6.80116700	-4.51131600
C	1.39886100	8.01797000	-5.02998000
H	2.11012400	8.60073100	-4.45122300
C	0.97058400	8.47592900	-6.27666900
H	1.34906300	9.41882200	-6.66291900
C	0.06537700	7.72406100	-7.02796200
H	-0.26797300	8.08062900	-7.99893800
C	-0.40802400	6.51106200	-6.52470800
H	-1.11543600	5.92023900	-7.10085000
C	0.02078800	6.05404200	-5.27772000
H	-0.35350300	5.11244900	-4.88536400
Zn	4.36329900	-3.85937800	-0.15394900
N	3.64421600	-4.18893600	1.77632800
N	6.19536700	-3.38705400	0.68352300
N	5.35057400	-4.30325800	-1.92555000
N	2.75600800	-4.99064200	-0.85141800
C	1.46309200	-5.24464500	1.24434600
C	5.52084500	-3.21190900	3.06183200
C	7.62533400	-3.51349600	-1.33684100
C	3.43658900	-5.19221500	-3.22408600
C	2.41576200	-4.69793200	2.12589600
C	4.23176700	-3.76056300	2.94345000

C	6.43583900	-3.08114900	2.00036300
C	7.39199500	-3.23839700	0.02396800
C	6.65403300	-3.99905400	-2.23568100
C	4.75984300	-4.73091600	-3.09096300
C	2.52357600	-5.32968400	-2.16393800
C	1.64080400	-5.37600500	-0.14681700
C	2.21985300	-4.57858700	3.55556100
H	1.34723700	-4.91689700	4.09709200
C	3.33767000	-3.98882900	4.05833000
H	3.54903500	-3.74351100	5.08887700
C	7.82309200	-2.70832500	2.17468900
H	8.28400100	-2.43953600	3.11401800
C	8.41641600	-2.81700100	0.95699900
H	9.45595700	-2.65462500	0.71374900
C	6.88595300	-4.22426400	-3.64710100
H	7.82182600	-4.06153800	-4.16167800
C	5.71319400	-4.66845100	-4.17648300
H	5.51056800	-4.93815000	-5.20295200
C	1.21293300	-5.93127100	-2.29145100
H	0.78579900	-6.30763700	-3.21006300
C	0.66622600	-5.95816600	-1.04480500
H	-0.29288000	-6.35992000	-0.74971200
C	0.11973300	-5.62165600	1.81064800
C	-0.85518100	-4.61605200	2.02202900
C	-2.13521000	-4.93551700	2.48627400
H	-2.86510600	-4.14982800	2.63229800

C	-2.44892800	-6.26951800	2.75025600
H	-3.44371800	-6.51699600	3.10990100
C	-1.49861500	-7.27357200	2.56543500
H	-1.74617100	-8.30913600	2.78067400
C	-0.22336000	-6.94505600	2.09843500
H	0.51953800	-7.72200600	1.94157600
C	5.98609000	-2.79771900	4.42594200
C	6.13965100	-1.44048400	4.74596400
H	5.89974800	-0.68873000	3.99898700
C	6.58711200	-1.05049000	6.00949100
H	6.69077300	0.00661100	6.23788300
C	6.88952600	-2.01358300	6.97391900
H	7.24008400	-1.71130900	7.95730800
C	6.74068400	-3.36776200	6.66802900
H	6.97846300	-4.12452300	7.41118700
C	6.29294800	-3.75620700	5.40465800
H	6.18706700	-4.81075500	5.16518400
C	9.01445700	-3.30575500	-1.85800800
C	9.78339200	-4.39587900	-2.29751100
H	9.35898000	-5.39492600	-2.25247400
C	11.08137200	-4.21040300	-2.77478400
H	11.66115600	-5.06873600	-3.10418600
C	11.63621300	-2.93013400	-2.82128100
H	12.64741700	-2.78513600	-3.19203400
C	10.88383900	-1.83788000	-2.38571000
H	11.30641000	-0.83688100	-2.41882900

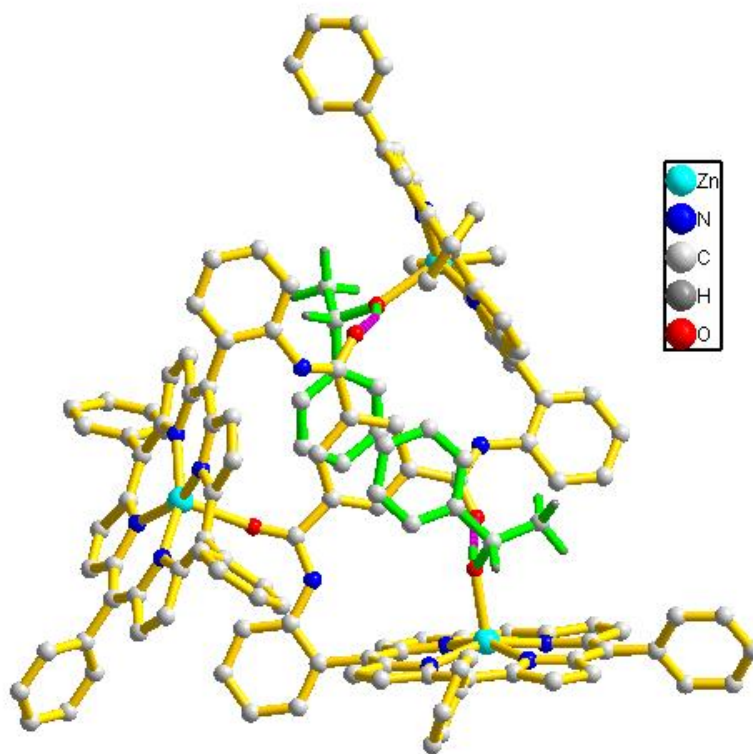
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C	2.98774000	-5.63232400	-4.58735000
C	2.14855600	-4.82278700	-5.36676900
H	1.83249800	-3.85744000	-4.98067600
C	1.72711100	-5.23809000	-6.63125300
H	1.07797300	-4.59575900	-7.22056800
C	2.13986300	-6.47170700	-7.13715500
H	1.81183100	-6.79627900	-8.12105100
C	2.97661800	-7.28629900	-6.37183600
H	3.30115500	-8.24950300	-6.75697900
C	3.39719800	-6.86952900	-5.10809000
H	4.04445200	-7.50683800	-4.51180800
Zn	-6.25793900	-0.72335300	0.36899600
N	-5.18233600	0.43820600	1.73037000
N	-6.78436800	-1.96374200	1.95684700
N	-7.85553400	-1.49620200	-0.69480600
N	-6.28851500	0.92563900	-0.90380800
C	-4.74043000	2.42645300	0.31640500
C	-5.22372200	-1.09915200	3.67349700
C	-8.46151500	-3.37511100	0.80526100
C	-7.83948000	0.05697000	-2.62725000
C	-4.63930500	1.68041100	1.50920600
C	-4.83945000	0.08244900	3.01251400
C	-6.12372100	-2.05231800	3.15705400
C	-7.58769600	-3.07361200	1.86930600

C	-8.60016900	-2.60359200	-0.36516600
C	-8.31680700	-1.06089500	-1.91243600
C	-6.88128700	0.96797500	-2.14395100
C	-5.49063900	2.03881100	-0.81329500
C	-3.93969500	2.12881200	2.69543500
H	-3.45036500	3.08604600	2.81054600
C	-4.05647300	1.13740900	3.62077600
H	-3.67890800	1.13129000	4.63301200
C	-6.50065500	-3.27393700	3.83625400
H	-6.11914700	-3.60212600	4.79222700
C	-7.40723200	-3.90407900	3.04120100
H	-7.90401700	-4.84570300	3.22434100
C	-9.58035700	-2.85794500	-1.39915300
H	-10.32042200	-3.64465800	-1.37963000
C	-9.40383500	-1.90681700	-2.35541200
H	-9.97156300	-1.77115600	-3.26446400
C	-6.40057200	2.12066300	-2.87706600
H	-6.68473900	2.38445000	-3.88537400
C	-5.54745100	2.78652800	-2.05258500
H	-5.00560700	3.69820300	-2.25965300
C	-4.09615000	3.78427300	0.27125500
C	-2.69513200	3.97548600	0.17942100
C	-2.15755000	5.26734800	0.10630400
H	-1.08997200	5.40031600	0.01763400
C	-3.00535600	6.37361700	0.13457500
H	-2.57145000	7.36615200	0.06917700

C	-4.38523400	6.20746800	0.23730100
H	-5.04533000	7.06984200	0.26359600
C	-4.91535100	4.92027100	0.30242500
H	-5.98876900	4.77503600	0.37960900
C	-4.64530600	-1.34709600	5.03237900
C	-3.27350900	-1.60562700	5.18326000
H	-2.64598100	-1.63941100	4.29729300
C	-2.72551400	-1.83207000	6.44650200
H	-1.66233000	-2.03659700	6.54364400
C	-3.53897300	-1.80134700	7.58082800
H	-3.11184800	-1.97604200	8.56482000
C	-4.90464700	-1.54497500	7.44372400
H	-5.54466700	-1.51421800	8.32176800
C	-5.45298700	-1.32081400	6.18025200
H	-6.51441500	-1.11361600	6.07615800
C	-9.31901100	-4.59633800	0.93461000
C	-9.14994800	-5.69014000	0.07046900
H	-8.38048100	-5.64561800	-0.69529900
C	-9.94894400	-6.82770700	0.19076400
H	-9.79807300	-7.66557900	-0.48506500
C	-10.93491600	-6.89183500	1.17703300
H	-11.55846800	-7.77702700	1.27039200
C	-11.11533500	-5.81083000	2.04198600
H	-11.88426900	-5.84861400	2.80930700
C	-10.31424000	-4.67470500	1.92222400
H	-10.46149000	-3.83208400	2.59186200

C	-8.42256100	0.30935600	-3.98428300
C	-8.17563900	-0.57453500	-5.04688400
H	-7.54752200	-1.44463800	-4.87695600
C	-8.71837400	-0.34331400	-6.31138900
H	-8.50987700	-1.03710700	-7.12175800
C	-9.52182000	0.77591400	-6.53636000
H	-9.94571500	0.95608800	-7.52071500
C	-9.77858500	1.66138400	-5.48793500
H	-10.40829600	2.53219000	-5.65117700
C	-9.23339900	1.43032300	-4.22436300
H	-9.44128600	2.11712400	-3.40869900
O	-4.45461600	-1.75345200	-0.31334700
H	-3.75408300	-1.68708500	0.37370800
C	-2.85509600	-2.08430100	-2.12628700
C	-1.71096100	-2.83892800	-2.40488000
H	-1.61612800	-3.84741400	-2.00732300
C	-0.67994600	-2.31077600	-3.18546300
H	0.20181700	-2.91425200	-3.38391900
C	-0.78258700	-1.01535800	-3.69331000
H	0.01809600	-0.60025300	-4.30025700
C	-1.92064300	-0.25234700	-3.41537000
H	-2.00805300	0.75800100	-3.80708900
C	-2.94996400	-0.78186900	-2.63728800
H	-3.83168100	-0.18473900	-2.42112800
C	-3.99308400	-2.68405100	-1.31575500
H	-3.62231600	-3.57730100	-0.79599000

C	-5.17690100	-3.07802000	-2.19334100
H	-5.96732400	-3.53801000	-1.59375300
H	-4.84768400	-3.79190300	-2.95559100
H	-5.59074100	-2.20043900	-2.69952400
N	3.45961700	0.20009200	-1.90946300
N	-0.44360900	-3.29594800	1.73138700
N	-1.88766500	2.81171700	0.15679400
O	3.59486800	-1.76880600	-0.73978300
O	-2.38753100	-2.10875900	1.48424200
O	0.26501700	3.60764600	0.04253900
C	1.67452300	-0.35732200	-0.40503800
C	0.90633800	-1.38503000	0.14142300
H	1.28589300	-2.39587800	0.04544500
C	-0.32326000	-1.11311800	0.75197700
C	-0.81354400	0.19665800	0.76603300
H	-1.76533000	0.37608100	1.25742700
C	-0.06426300	1.23614500	0.20129600
C	1.19196000	0.95577700	-0.34614700
H	1.77080200	1.80140300	-0.69923100
C	3.00102700	-0.71963000	-1.02258400
C	-0.53729400	2.66544700	0.13961500
C	-1.16028700	-2.20775200	1.35180100
H	0.56120200	-3.20954000	1.65435300
H	-2.42888800	1.95526600	0.15134000
H	2.87242400	1.01460500	-2.02606500



Conformer A2

$$\Delta E^{\theta} = -12582.37367400 \text{ hartree}$$

Cartesian coordinates for Geometry Optimized Conformer A2

Atoms	x	y	z
Zn	-1.18652200	5.53640100	0.07433600
N	0.88342000	5.61237900	0.17603300
N	-1.07711200	6.70300900	-1.63521300
N	-3.15122500	6.13445200	0.28717100
N	-1.19499000	5.04396800	2.09502800
C	1.23695200	4.81761700	2.49627200
C	1.34693100	6.48472100	-2.09597700
C	-3.43815600	7.44395000	-1.79710500

C	-3.64304200	5.01420700	2.44115500
C	1.68278200	5.21485600	1.22195900
C	1.72736700	5.92215400	-0.86344800
C	0.03831800	6.89038400	-2.41686500
C	-2.11064900	7.35595000	-2.26456700
C	-3.91214100	6.83603000	-0.61512900
C	-4.01042500	5.69001300	1.26406700
C	-2.31545800	4.77230800	2.84169200
C	-0.11339000	4.73110600	2.88342900
C	3.07328200	5.25884800	0.82288600
H	3.91403200	5.01318000	1.45587700
C	3.10037600	5.69200900	-0.46725000
H	3.96703300	5.87368400	-1.08642600
C	-0.30965800	7.65662000	-3.59299400
H	0.37390200	7.94283600	-4.37872600
C	-1.62736600	7.97160300	-3.48322100
H	-2.21607500	8.57393600	-4.15870400
C	-5.29972400	6.82343700	-0.19697500
H	-6.11726500	7.29280700	-0.72403500
C	-5.36079400	6.10596900	0.95640900
H	-6.23231400	5.89117800	1.55808700
C	-1.92987600	4.25161500	4.13506800
H	-2.61210400	3.96287300	4.92172800
C	-0.56689700	4.24744900	4.16981600
H	0.07515300	3.96256400	4.99263700
C	2.29071400	4.33347900	3.45445800

C	3.04983700	5.21346400	4.23145500
H	2.82132500	6.27480000	4.19329900
C	4.10342800	4.74662100	5.02077200
H	4.68694500	5.44594800	5.61288200
C	4.41164400	3.38595100	5.03448000
H	5.23888000	3.01820100	5.63481700
C	3.65631400	2.48119300	4.28755800
H	3.88712500	1.42346400	4.29656200
C	2.59561000	2.95529400	3.51234400
C	2.43415900	6.75660500	-3.09413300
C	3.02919100	5.70654100	-3.80953800
H	2.69087000	4.68764600	-3.64365200
C	4.04705000	5.95761700	-4.73129800
H	4.49247700	5.13051300	-5.27790700
C	4.48824500	7.26321800	-4.95228200
H	5.28056500	7.45880400	-5.66995600
C	3.90698700	8.31642400	-4.24354400
H	4.24820400	9.33594300	-4.40358800
C	2.88991100	8.06476600	-3.32193000
H	2.44489700	8.88512700	-2.76557700
C	-4.41104300	8.25029600	-2.60183700
C	-5.01721800	9.38966000	-2.04595900
H	-4.76499100	9.67952600	-1.02997200
C	-5.92343700	10.15230200	-2.78298900
H	-6.37558700	11.03238300	-2.33315000
C	-6.24309300	9.79282100	-4.09359500

H	-6.94933100	10.38652900	-4.66765600
C	-5.64626700	8.66634500	-4.66180300
H	-5.88767600	8.37586500	-5.68095200
C	-4.73853300	7.90504500	-3.92414600
H	-4.27621900	7.03139300	-4.37481500
C	-4.74184500	4.56158900	3.35744400
C	-5.05924000	5.27639600	4.52201200
H	-4.50522300	6.18128100	4.75692700
C	-6.07726600	4.83875500	5.37119300
H	-6.31168100	5.40674400	6.26783400
C	-6.79243500	3.67810300	5.07009400
H	-7.58262700	3.33562600	5.73287100
C	-6.48703900	2.95963300	3.91279700
H	-7.03315100	2.05166100	3.67134000
C	-5.47213800	3.40018900	3.06147900
H	-5.24027600	2.83863000	2.16015500
Zn	6.26579200	-2.06865900	0.53139000
N	5.88507900	-3.23459200	-1.15816700
N	8.16327700	-1.72115100	-0.22223000
N	6.98851700	-1.58457100	2.42434600
N	4.67817500	-3.04387000	1.47246300
C	3.72208300	-4.23275300	-0.48147600
C	7.87754100	-2.64480200	-2.50557400
C	9.18263700	-0.64468100	1.76556300
C	5.02453800	-2.23049600	3.78646700
C	4.72823600	-3.92688500	-1.41910600

C	6.60069200	-3.21166500	-2.33232700
C	8.60751600	-1.98773400	-1.49401000
C	9.19344300	-1.08436200	0.42741500
C	8.13619400	-0.87546300	2.68052500
C	6.26433300	-1.59061300	3.59044900
C	4.32176000	-2.93991800	2.79532500
C	3.74014400	-3.84905300	0.87553600
C	4.69480600	-4.32280200	-2.81165800
H	3.89648000	-4.87411500	-3.28766600
C	5.84991500	-3.87744200	-3.37651200
H	6.16885000	-3.99011100	-4.40246500
C	9.96848600	-1.52037400	-1.64627700
H	10.57179400	-1.63086500	-2.53555300
C	10.33019400	-0.96207600	-0.46013100
H	11.28549400	-0.53173100	-0.19717500
C	8.12288900	-0.39597000	4.04623200
H	8.89435600	0.20300200	4.50770000
C	6.96631500	-0.83859300	4.60886500
H	6.61702100	-0.67189800	5.61751700
C	3.12209900	-3.71244500	3.04124500
H	2.64337400	-3.83343300	4.00229700
C	2.76293700	-4.27555600	1.85522700
H	1.93563200	-4.94457600	1.66326900
C	2.58871900	-5.10627900	-0.94089800
C	2.81944400	-6.46759500	-1.17595600
H	3.82364500	-6.85119000	-1.02117800

C	1.79682500	-7.32320500	-1.58406700
H	2.00345100	-8.37629300	-1.75240600
C	0.51261900	-6.81368700	-1.76744100
H	-0.29957500	-7.46166600	-2.08462800
C	0.24743700	-5.46240200	-1.55161600
H	-0.74673500	-5.06884900	-1.70305900
C	1.27874700	-4.60658200	-1.13676200
C	8.52081500	-2.77075300	-3.85311700
C	8.75084600	-1.63605600	-4.64730100
H	8.44962900	-0.66031000	-4.27633800
C	9.35079700	-1.75017000	-5.90190400
H	9.51484300	-0.85970800	-6.50327500
C	9.73462100	-3.00245300	-6.38497200
H	10.20272900	-3.09196000	-7.36167800
C	9.51444900	-4.13894200	-5.60466300
H	9.81570700	-5.11761700	-5.96922700
C	8.91294200	-4.02384900	-4.35076800
H	8.75053000	-4.90906600	-3.74224100
C	10.38472300	0.10286400	2.25584000
C	10.69820600	1.37220100	1.74421800
H	10.05175800	1.81316100	0.99051900
C	11.81837500	2.06995200	2.19728800
H	12.04013300	3.05382600	1.79193100
C	12.64862600	1.50921300	3.16950600
H	13.52207800	2.05145200	3.52184300
C	12.35008900	0.24672300	3.68540800

H	12.99377800	-0.20106200	4.43816300
C	11.22843000	-0.44924400	3.23315100
H	11.00312100	-1.43488600	3.63056200
C	4.40798000	-2.15598300	5.14927400
C	3.21974700	-1.43496100	5.35162300
H	2.76570000	-0.92765300	4.50532400
C	2.63839600	-1.35514600	6.61821300
H	1.72424600	-0.78347000	6.75719400
C	3.23228200	-2.00063300	7.70467300
H	2.77959700	-1.94053600	8.69078600
C	4.41206200	-2.72274500	7.51596600
H	4.87905600	-3.23246800	8.35476400
C	4.99533700	-2.79859200	6.25003200
H	5.91063200	-3.36589600	6.10594100
O	5.06739100	-0.28278400	0.12679100
H	4.35012500	-0.18855100	0.79442200
C	3.91193200	0.78436700	-1.74604300
C	3.76057400	-0.36986800	-2.52814300
H	4.43492100	-1.20843400	-2.38384000
C	2.75176600	-0.44609700	-3.48867500
H	2.65122600	-1.34662700	-4.08925800
C	1.87760300	0.62788000	-3.67947900
H	1.08972100	0.56606700	-4.42569300
C	2.02023800	1.77883900	-2.90327600
H	1.33505800	2.61339300	-3.03004100
C	3.03319300	1.85501400	-1.94292700

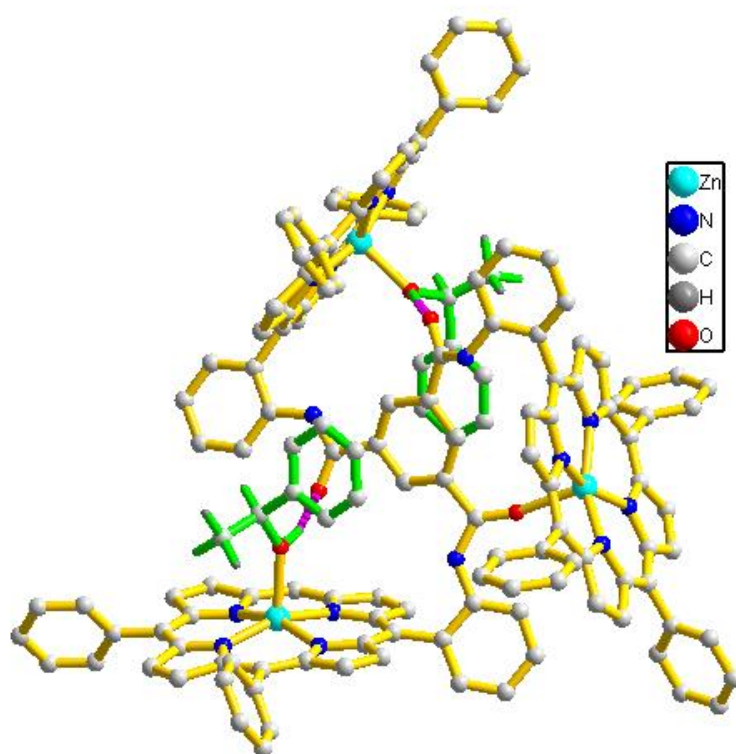
H	3.13428200	2.75413300	-1.33816400
C	5.03241500	0.88609900	-0.72215200
H	4.84033300	1.75313000	-0.07741000
C	6.40061900	1.05229300	-1.37605200
H	7.18122000	1.14428100	-0.61520300
H	6.40400500	1.95180600	-2.00068500
H	6.63464000	0.19238600	-2.01089000
Zn	-5.29084300	-3.23941700	-0.79569200
N	-4.84342400	-5.00232300	-1.81264000
N	-6.52196000	-4.34745200	0.46254000
N	-6.37033200	-1.54173500	-0.23437400
N	-4.60660800	-2.19152000	-2.45146400
C	-5.36475100	0.07877500	-1.81147400
C	-7.69810400	-2.49703200	1.62359500
C	-5.85605000	-6.63026800	-0.24331200
C	-3.56291800	-4.05091500	-3.70890300
C	-6.13951300	-0.26789000	-0.68683100
C	-7.19679800	-1.42776200	0.85659300
C	-7.40080500	-3.85696500	1.39864200
C	-6.57124400	-5.71791300	0.55846000
C	-5.04080700	-6.27580300	-1.33751300
C	-4.01102500	-5.11368700	-2.89894400
C	-3.87662000	-2.69532300	-3.49962400
C	-4.69128700	-0.83602500	-2.64618200
C	-6.82875600	0.68787400	0.15589500
H	-6.82232700	1.76064000	0.02400200

C	-7.48166400	-0.02970800	1.11063300
H	-8.10667400	0.34727900	1.90725400
C	-8.02953500	-4.95423400	2.10185900
H	-8.78420300	-4.85479600	2.86839500
C	-7.51760800	-6.10278800	1.58323800
H	-7.77595000	-7.11819500	1.84616900
C	-4.28553300	-7.21927300	-2.13476200
H	-4.24606700	-8.28656900	-1.97243000
C	-3.65046600	-6.50137800	-3.10068800
H	-2.99840900	-6.87201000	-3.87840400
C	-3.49551800	-1.61980900	-4.39158500
H	-2.94244900	-1.73758500	-5.31212500
C	-3.99568400	-0.46968100	-3.86312000
H	-3.93149400	0.52935800	-4.27148200
C	-5.30853300	1.53219200	-2.18668100
C	-6.41484500	2.12604500	-2.80368200
H	-7.28694200	1.50871400	-2.99857600
C	-6.40977200	3.47204800	-3.16476800
H	-7.28129100	3.91261900	-3.64050500
C	-5.27823700	4.24345700	-2.90779800
H	-5.26530900	5.29496900	-3.17222000
C	-4.15611800	3.68430900	-2.29847600
H	-3.28439700	4.28792600	-2.09412600
C	-4.16730200	2.33237300	-1.93418100
C	-8.63678300	-2.16976600	2.74429000
C	-9.90674600	-1.62961100	2.48437100

H	-10.20740600	-1.45751700	1.45467700
C	-10.78207300	-1.32545000	3.52765900
H	-11.76296100	-0.91372800	3.30445800
C	-10.40329200	-1.55532700	4.85166600
H	-11.08485700	-1.31892900	5.66450200
C	-9.14390800	-2.09262200	5.12448700
H	-8.83808100	-2.27193500	6.15201500
C	-8.27002600	-2.39800100	4.08020600
H	-7.28867400	-2.81092600	4.29694200
C	-6.00243300	-8.08782200	0.07074300
C	-5.51021600	-8.61929500	1.27339600
H	-5.01017600	-7.96046800	1.97795100
C	-5.64895400	-9.97665800	1.56590000
H	-5.25544500	-10.36906200	2.50006400
C	-6.28609400	-10.82804900	0.66141000
H	-6.39533400	-11.88505000	0.88916600
C	-6.78314400	-10.31243300	-0.53705500
H	-7.28667800	-10.96587500	-1.24481800
C	-6.64195800	-8.95553100	-0.82943400
H	-7.03694200	-8.55552400	-1.75903100
C	-2.69636800	-4.38614100	-4.88425100
C	-3.21267300	-5.08810400	-5.98488400
H	-4.25726800	-5.38690100	-5.97952600
C	-2.40380100	-5.39256900	-7.08055000
H	-2.82323800	-5.93155100	-7.92617700
C	-1.06333400	-5.00214800	-7.09378000

H	-0.43315400	-5.23979600	-7.94673600
C	-0.53746800	-4.30529900	-6.00434800
H	0.50680700	-4.00356800	-6.00297100
C	-1.34722600	-3.99897000	-4.90988200
H	-0.93681400	-3.46608900	-4.05720700
O	-3.57071100	-2.88126500	0.43337000
H	-2.70647900	-2.87629700	-0.04406600
C	-2.64999700	-2.23504300	2.58666600
C	-1.44163000	-2.46121900	3.25416800
H	-0.97993200	-3.44343700	3.23204800
C	-0.81234300	-1.43259700	3.96281000
H	0.12349700	-1.63328500	4.47840900
C	-1.38424100	-0.16219100	4.01027100
H	-0.89867200	0.64011900	4.56004400
C	-2.59284000	0.07628700	3.34785300
H	-3.04903700	1.06231900	3.38645300
C	-3.21793500	-0.95177100	2.64582900
H	-4.15807100	-0.76513200	2.13289500
C	-3.38596600	-3.31616500	1.80277000
H	-4.40957100	-3.37896400	2.18570300
C	-2.76672100	-4.71047900	1.83747300
H	-3.39668700	-5.39813700	1.26674200
H	-2.69106800	-5.08226000	2.86517100
H	-1.76685600	-4.71765200	1.38987100
N	1.75759400	2.09591300	2.75537000
N	1.07217000	-3.22183500	-0.90684200

N	-3.05813000	1.69149400	-1.32975000
O	3.20273100	0.48239400	2.02009500
O	-1.21086500	-3.04128600	-0.98873800
O	-1.59741900	3.39727600	-0.82513600
C	1.04095900	0.64550900	0.98099200
C	0.10491600	1.55578000	0.48068400
H	0.14067300	2.60797000	0.73982300
C	-0.89904300	1.14214700	-0.40069300
C	-0.93205300	-0.19655800	-0.80870200
H	-1.67036400	-0.56221700	-1.51571600
C	0.02736200	-1.10740200	-0.34497500
C	1.00926300	-0.68461800	0.55326200
H	1.73243800	-1.38007200	0.96770700
C	2.10789800	1.05584700	1.95405200
C	-1.87871900	2.18852800	-0.87193500
C	-0.09564900	-2.53995800	-0.77536400
H	1.92660300	-2.69209400	-0.77492100
H	-3.20465400	0.69805600	-1.19412800
H	0.82007500	2.45367900	2.62761400



Conformer B2

$$\Delta E^{\theta} = -12582.37319630 \text{ hartree}$$

Cartesian coordinates for Geometry Optimized Conformer B2

Atoms	x	y	z
Zn	0.50778900	5.71979600	-0.21345100
N	0.38654500	5.56030400	1.85599700
N	2.29747600	6.73825700	0.04645800
N	0.39063400	6.52534600	-2.11765000
N	-1.54969900	5.42281200	-0.28663600
C	-1.99397300	4.92457000	2.09887300
C	-1.92612900	5.86349100	-2.69650300
C	2.63081600	7.57485200	-2.26385000
C	2.71192200	6.19198700	2.42772100

C	-0.70181500	5.16528000	2.59815600
C	1.42866900	5.70351000	2.73990800
C	3.09079700	6.69561400	1.16942200
C	3.04096200	7.35074700	-0.93396200
C	1.39123700	7.17478600	-2.80006200
C	-0.65647900	6.38885100	-2.99832800
C	-2.33313000	5.44370600	-1.41641800
C	-2.37264700	5.04877300	0.74943200
C	-0.33041000	5.04148300	3.99082000
H	-1.00205500	4.77387300	4.79526100
C	0.98862000	5.36932700	4.07708500
H	1.60097400	5.41735200	4.96592700
C	4.38220300	7.27963000	0.88001000
H	5.20354600	7.35974500	1.57687300
C	4.34717200	7.69633500	-0.41369200
H	5.13546700	8.18025800	-0.97151000
C	0.96528700	7.44151600	-4.15794100
H	1.54687400	7.95820300	-4.90693600
C	-0.29084400	6.93856300	-4.28552600
H	-0.92416400	6.95694600	-5.16029300
C	-3.68684200	5.05562300	-1.08337800
H	-4.51165100	5.01002300	-1.77972800
C	-3.71161100	4.81125000	0.25571000
H	-4.55996400	4.52572000	0.86138000
C	-3.04276700	4.41365900	3.04824900
C	-3.96360400	5.26352300	3.66968200

H	-3.87745000	6.33475300	3.51114100
C	-4.99575300	4.74713900	4.45611700
H	-5.70737500	5.42143800	4.92433300
C	-5.11939500	3.36759500	4.62628900
H	-5.92977000	2.95947900	5.22338500
C	-4.19891300	2.49913600	4.03912800
H	-4.28368000	1.42722500	4.17149500
C	-3.16323600	3.02527500	3.26528900
C	-2.95195700	5.83816500	-3.79221200
C	-3.36319900	4.62890900	-4.37230100
H	-2.92471600	3.69524100	-4.03295400
C	-4.32589100	4.61355000	-5.38331800
H	-4.62743600	3.66611800	-5.82236100
C	-4.89468100	5.80693500	-5.83065200
H	-5.64402300	5.79466900	-6.61772100
C	-4.49548600	7.01696900	-5.25970800
H	-4.93594300	7.95156900	-5.59733500
C	-3.53328700	7.03178200	-4.24933700
H	-3.22931100	7.97404300	-3.80178700
C	3.57569800	8.30538300	-3.16936900
C	3.90557500	9.64819400	-2.92354700
H	3.46243900	10.15408400	-2.07035000
C	4.78179600	10.33535900	-3.76422700
H	5.01946400	11.37582500	-3.55843300
C	5.34555900	9.69324700	-4.86843800
H	6.02793900	10.22859200	-5.52315800

C	5.02539400	8.35929300	-5.12616800
H	5.46017600	7.84878700	-5.98155300
C	4.14768000	7.67276100	-4.28548900
H	3.90421300	6.63365100	-4.48829000
C	3.72455000	6.22219000	3.53229900
C	4.14569400	7.43623800	4.09734900
H	3.72534000	8.36696300	3.72655500
C	5.08547900	7.45577800	5.12878900
H	5.39592100	8.40573300	5.55612300
C	5.62038400	6.26104700	5.61431000
H	6.35260000	6.27626300	6.41718100
C	5.20814700	5.04662200	5.06292700
H	5.62151600	4.11154100	5.43186000
C	4.26755300	5.02844800	4.03221900
H	3.95259300	4.08266000	3.59948200
Zn	-5.89670500	-2.58009700	0.72449800
N	-5.44761700	-3.92397400	-0.81263400
N	-7.78877700	-2.37604500	-0.11082400
N	-6.67691700	-1.88823500	2.52463100
N	-4.29839600	-3.36371700	1.79762700
C	-3.20887500	-4.63198800	-0.03035300
C	-7.44831300	-3.60771200	-2.23679800
C	-8.87452200	-1.08854000	1.71062100
C	-4.74004200	-2.33427700	4.00284900
C	-4.22964700	-4.52741400	-0.99658100
C	-6.14638300	-4.08351000	-1.98412300

C	-8.21161400	-2.83914500	-1.33360400
C	-8.84772700	-1.69342700	0.43779500
C	-7.84807600	-1.18615200	2.67118400
C	-5.99073500	-1.75767200	3.70624100
C	-3.97805700	-3.10694200	3.10759300
C	-3.28665700	-4.13667200	1.28774500
C	-4.14529300	-5.06844200	-2.33776500
H	-3.29439500	-5.59036300	-2.75162700
C	-5.33220400	-4.79873700	-2.94657600
H	-5.62943700	-5.05203900	-3.95387200
C	-9.58718200	-2.44776400	-1.55603600
H	-10.17958000	-2.70833000	-2.42095000
C	-9.97797500	-1.73587000	-0.46507300
H	-10.94968000	-1.30575100	-0.27076200
C	-7.88863200	-0.56826500	3.97977500
H	-8.68764500	0.05514000	4.35369200
C	-6.74363400	-0.92636500	4.62157500
H	-6.43463100	-0.65569900	5.62102500
C	-2.73102100	-3.76324800	3.44317500
H	-2.26761400	-3.76338400	4.41945100
C	-2.29932000	-4.39350000	2.31601800
H	-1.41823400	-5.00881000	2.19585900
C	-1.95769900	-5.36281200	-0.42472600
C	-0.74894100	-4.67519200	-0.69635700
C	0.39686100	-5.38879500	-1.08122200
H	1.30912000	-4.85711300	-1.30591500

C	0.34854800	-6.77835000	-1.18392300
H	1.24766300	-7.30995000	-1.48279200
C	-0.83045900	-7.47043700	-0.91407600
H	-0.86705900	-8.55328400	-0.99242900
C	-1.96992600	-6.75763500	-0.54144600
H	-2.89715100	-7.28140900	-0.32776700
C	-8.07111400	-3.95281500	-3.55428300
C	-8.37790600	-2.95356100	-4.49205800
H	-8.15142100	-1.91762100	-4.25527900
C	-8.95793800	-3.27704200	-5.71918300
H	-9.18240100	-2.48867100	-6.43302900
C	-9.24391400	-4.60733400	-6.03156100
H	-9.69642200	-4.85970800	-6.98685900
C	-8.94515800	-5.61118100	-5.10839400
H	-9.16930500	-6.64929100	-5.33976700
C	-8.36401500	-5.28666100	-3.88213300
H	-8.14058100	-6.06906900	-3.16233800
C	-10.10522300	-0.31832100	2.08012200
C	-10.96208200	-0.76911800	3.09724900
H	-10.72626500	-1.69384000	3.61640100
C	-12.11034200	-0.05184200	3.43509500
H	-12.76372000	-0.42130600	4.22127700
C	-12.42320600	1.13072700	2.76218700
H	-13.31743000	1.68950800	3.02529900
C	-11.58106700	1.58957100	1.74774400
H	-11.81444400	2.51062200	1.21982100

C	-10.43414000	0.87045100	1.40937700
H	-9.77886200	1.23283900	0.62207000
C	-4.17512600	-2.10417500	5.37163200
C	-3.05680100	-1.27445800	5.55196900
H	-2.61479900	-0.79193100	4.68449300
C	-2.52534200	-1.05611600	6.82421900
H	-1.66330700	-0.40495200	6.94464800
C	-3.10256500	-1.66672600	7.93926900
H	-2.68868200	-1.49886100	8.92994600
C	-4.21583300	-2.49267400	7.77361400
H	-4.67026400	-2.97421100	8.63561300
C	-4.74804500	-2.70809600	6.50124000
H	-5.61172500	-3.35495000	6.37464200
O	-4.80575000	-0.93646200	-0.09432000
H	-4.27596300	-0.38770000	0.53348800
C	-3.88407200	-0.03318100	-2.15381000
C	-3.47558300	-1.12645400	-2.93298800
H	-4.07052900	-2.03651400	-2.92998100
C	-2.32094100	-1.05903000	-3.71213100
H	-2.02632700	-1.91473900	-4.31452800
C	-1.55105800	0.10656600	-3.72414400
H	-0.65076800	0.16199800	-4.33043500
C	-1.94793600	1.20046600	-2.95381000
H	-1.35341100	2.11048300	-2.95105800
C	-3.10838300	1.13253700	-2.17702800
H	-3.40250600	1.99981800	-1.59314200

C	-5.12976100	-0.18212500	-1.28934200
H	-5.83158400	-0.83295800	-1.81856200
C	-5.84368300	1.11520300	-0.91907300
H	-6.76165200	0.88046700	-0.37228000
H	-6.10559400	1.68517700	-1.81719700
H	-5.22291300	1.74931700	-0.27732600
Zn	5.59708900	-3.00729800	-0.62335000
N	4.75239700	-1.86905600	-2.15411700
N	5.26477400	-4.69617700	-1.79606200
N	6.98267900	-4.09621600	0.45982400
N	6.50679400	-1.26943500	0.07544500
C	5.38262100	0.39749500	-1.37075600
C	3.81197900	-3.69812700	-3.53585900
C	6.50005000	-6.35697700	-0.43704500
C	7.97128400	-2.26353400	1.80621600
C	4.75851600	-0.49996600	-2.26200600
C	4.03809500	-2.34399100	-3.22747900
C	4.37941200	-4.78545700	-2.84169300
C	5.59409300	-5.98339100	-1.45003700
C	7.16867000	-5.45748100	0.41650800
C	7.82836200	-3.61481800	1.42859800
C	7.33500700	-1.18127000	1.16939100
C	6.17176500	0.01697600	-0.26640300
C	4.03215800	-0.09712700	-3.44851100
H	3.91215700	0.92014900	-3.79441100
C	3.58268900	-1.23684300	-4.04127900

H	3.02371700	-1.32678000	-4.96141700
C	4.11880800	-6.17655900	-3.14685700
H	3.45103400	-6.53432200	-3.91714900
C	4.87035600	-6.91696400	-2.28674900
H	4.92997800	-7.99363800	-2.22100300
C	8.18353700	-5.84219100	1.37374100
H	8.55112000	-6.84658700	1.52556200
C	8.59004900	-4.70477300	1.99928400
H	9.35185200	-4.60470400	2.75867000
C	7.48789100	0.20611800	1.55667100
H	8.06832500	0.56216300	2.39535200
C	6.77578000	0.94704800	0.66504000
H	6.66840800	2.02206600	0.63582000
C	5.30441900	1.86630600	-1.68242700
C	4.13316000	2.63923800	-1.48788500
C	4.12519500	4.00518900	-1.79818500
H	3.22998800	4.58601600	-1.63560100
C	5.27714700	4.60765800	-2.30078100
H	5.25827700	5.66789100	-2.52948400
C	6.43906400	3.86472400	-2.49991000
H	7.33552000	4.33588200	-2.89288000
C	6.44218000	2.50645000	-2.18939900
H	7.33858500	1.91264300	-2.34170400
C	2.91843400	-4.00124500	-4.69926400
C	1.54822900	-3.69992300	-4.64193000
H	1.14488800	-3.25821700	-3.73551200

C	0.71218800	-3.97839700	-5.72401700
H	-0.34843200	-3.74795200	-5.65902800
C	1.23097100	-4.55829400	-6.88321000
H	0.57941500	-4.77352900	-7.72600800
C	2.59217500	-4.86088600	-6.95261000
H	3.00645400	-5.30788900	-7.85265000
C	3.42800200	-4.58591600	-5.86951100
H	4.48824600	-4.81585100	-5.92843800
C	6.78600000	-7.81728700	-0.26420900
C	6.39947000	-8.49191000	0.90497700
H	5.88114700	-7.94262000	1.68604300
C	6.66513100	-9.85199000	1.06775900
H	6.35237600	-10.35650700	1.97833600
C	7.32560900	-10.56303000	0.06420400
H	7.53397200	-11.62209700	0.19084900
C	7.71775400	-9.90443600	-1.10268000
H	8.23802200	-10.44789300	-1.88718000
C	7.44951400	-8.54476100	-1.26541200
H	7.76291100	-8.03335100	-2.17123100
C	8.89386500	-1.95803100	2.94658700
C	8.58485100	-2.37260500	4.25195200
H	7.66088500	-2.91576100	4.43024400
C	9.44267400	-2.08821200	5.31519100
H	9.18187500	-2.41347000	6.31904100
C	10.62838800	-1.38594600	5.09199300
H	11.29740400	-1.16528200	5.91953900

C	10.95004900	-0.97081900	3.79841600
H	11.87417300	-0.42937300	3.61319800
C	10.09044000	-1.25400700	2.73630500
H	10.34727600	-0.93669600	1.72953900
O	3.74134100	-2.97683500	0.53610500
H	2.99483000	-2.73730600	-0.05810300
C	2.59385700	-2.21163200	2.55209500
C	1.36284900	-2.33432100	3.20505600
H	0.80410800	-3.26517400	3.13155100
C	0.83845400	-1.27323600	3.94670600
H	-0.11656300	-1.39126700	4.45195600
C	1.53954700	-0.06982200	4.03316000
H	1.13416700	0.76031900	4.60622700
C	2.76605000	0.06422300	3.37615800
H	3.31787200	0.99894600	3.43831800
C	3.29157000	-0.99894400	2.64207000
H	4.24492200	-0.89199000	2.13256900
C	3.18387500	-3.39416000	1.79927900
H	2.38167500	-4.11483000	1.59030600
C	4.27616700	-4.09529100	2.60167300
H	4.65629700	-4.96511000	2.05864300
H	3.87114600	-4.42584400	3.56374500
H	5.11064800	-3.41413700	2.79447400
N	-2.17271300	2.19596500	2.66622100
N	-0.76234200	-3.26276700	-0.55875400
N	2.99516900	1.96577100	-0.98123700

O	-3.47021500	0.53386100	1.79479100
O	1.42694300	-2.72041400	-0.94035200
O	1.40549700	3.60944400	-0.71728100
C	-1.21885800	0.75410000	0.98548900
C	-1.07106500	-0.58516100	0.60703600
H	-1.78244000	-1.30837400	0.99294400
C	-0.00453800	-0.96823000	-0.20978100
C	0.91795000	-0.00337100	-0.63881300
H	1.71812700	-0.33761800	-1.29137000
C	0.78280600	1.33657400	-0.26326100
C	-0.30395700	1.70965700	0.53340100
H	-0.42321000	2.76253400	0.76369700
C	-2.39154300	1.13754900	1.84019100
C	1.74825800	2.41665600	-0.67990800
C	0.27889500	-2.39133200	-0.60251100
H	-1.68017200	-2.87697800	-0.36819500
H	3.16488000	0.98244600	-0.80619200
H	-1.25606100	2.62098400	2.61311000