

Supporting Information

Chirality Transfer from Chiral Monoamines to an *m*-Phthalic Diamide-Linked Zinc Bisporphyrinate with a Benzylamide Substituent

Qingyun Hu,[†] Congcong Zhuo,[†] Yong Wang,^{*,†} Chuanjiang Hu,^{*,†,‡} Jianping Lang^{*,†}

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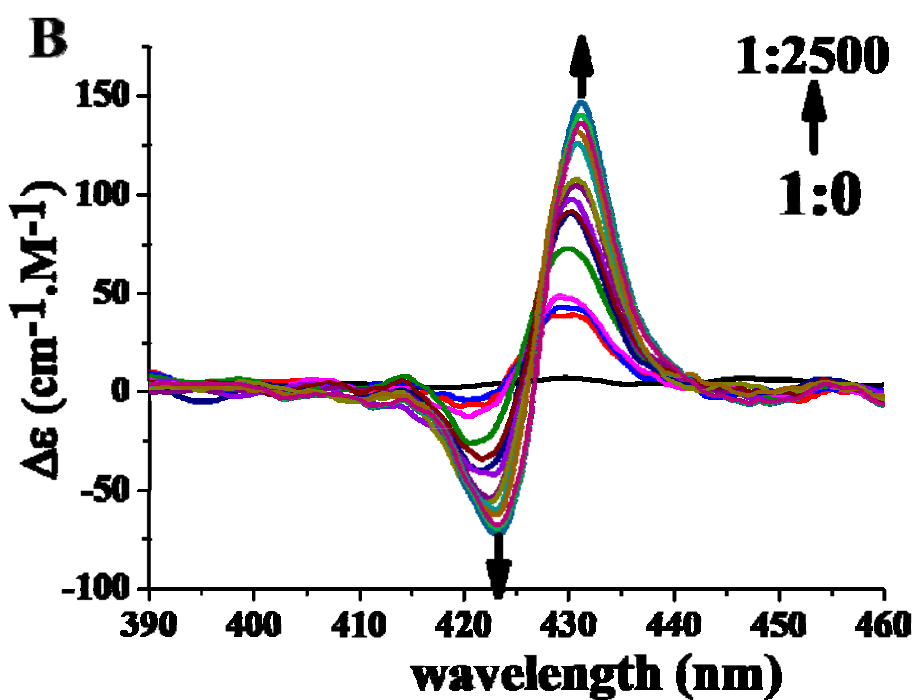
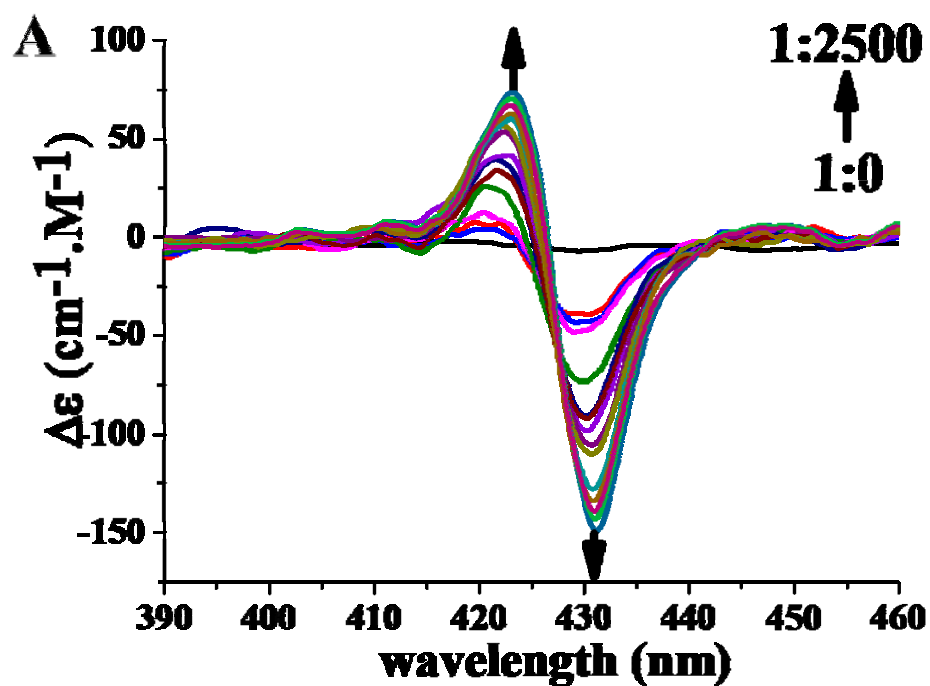


Figure S1. Circular dichroism spectra of a solution of $[\text{Zn}_2\text{-III}]$ (1.75×10^{-6} M) and from 1: 0 to 1:2500 equivalents of (A) 1R, (B) 1S in methylene chloride at 25°C.

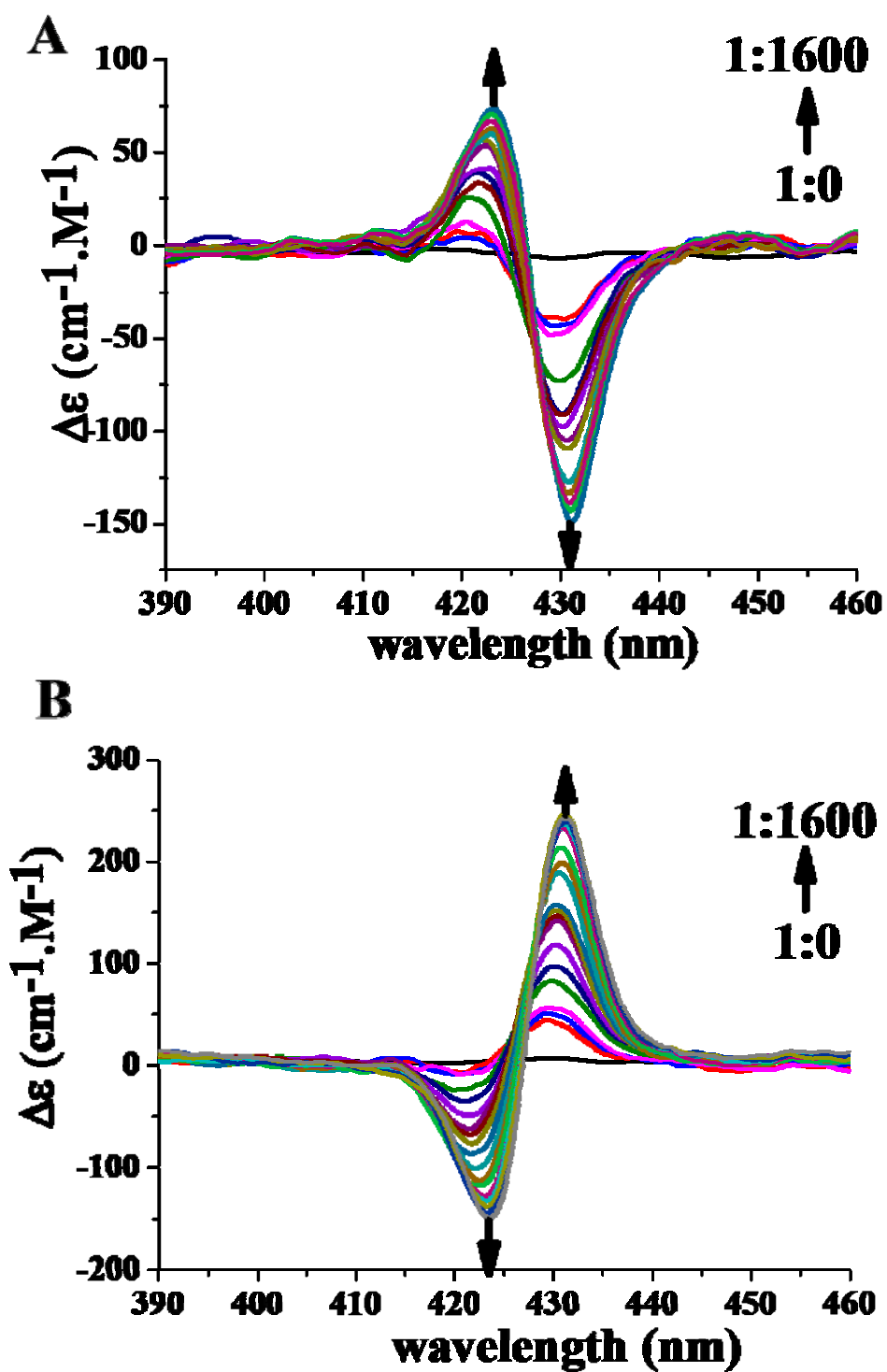


Figure S2. Circular dichroism spectra of a solution of $[\text{Zn}_2\text{-III}]$ (1.75×10^{-6} M) and from 1: 0 to 1:1600 equivalents of (A) 2R, (B) 2S in methylene chloride at 25°C.

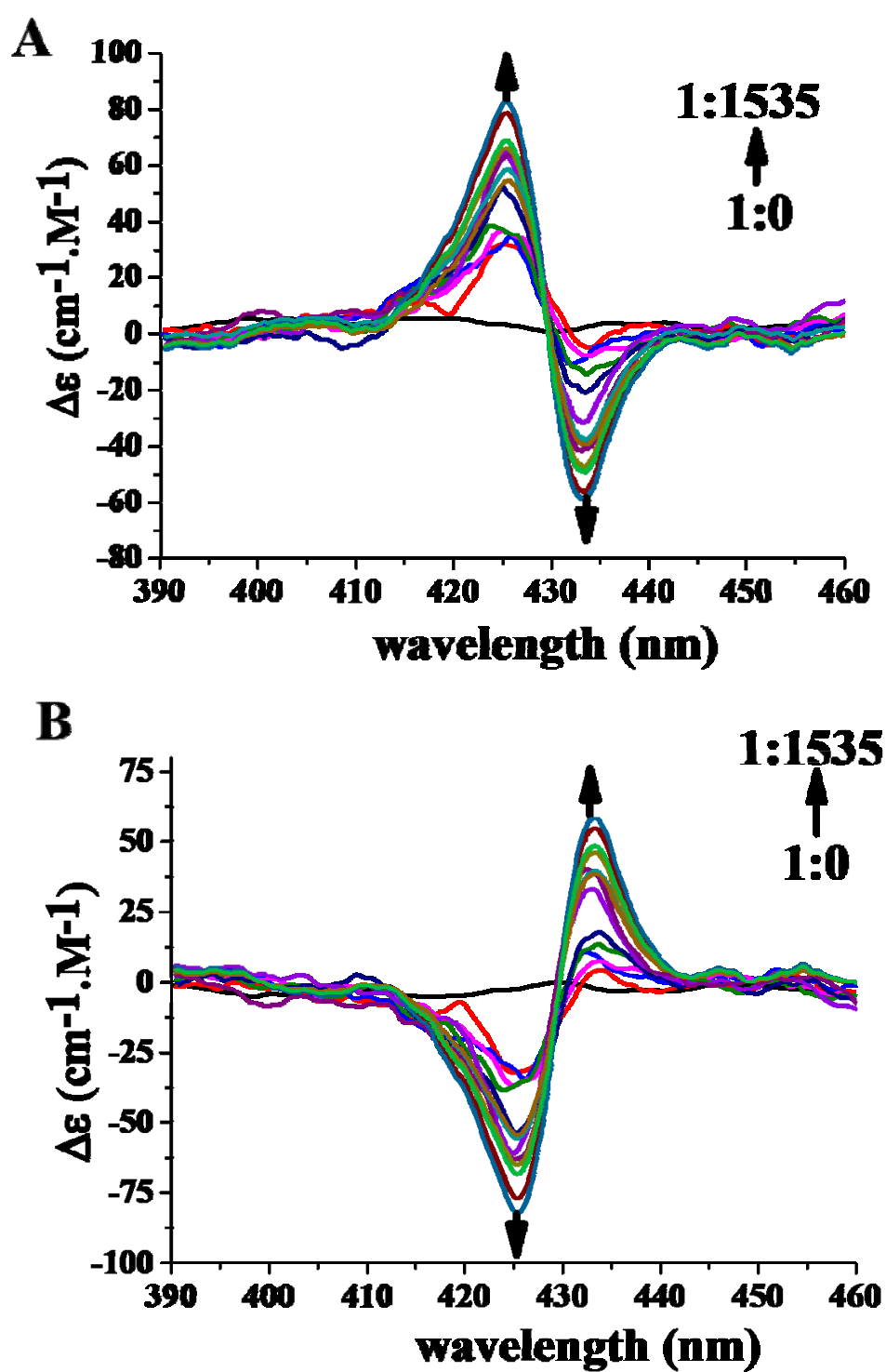


Figure S3. Circular dichroism spectra of a solution of $[\text{Zn}_2\text{-III}]$ (1.75×10^{-6} M) and from 1: 0 to 1:1535 equivalents of (A) 3R, (B) 3S in methylene chloride at 25°C.

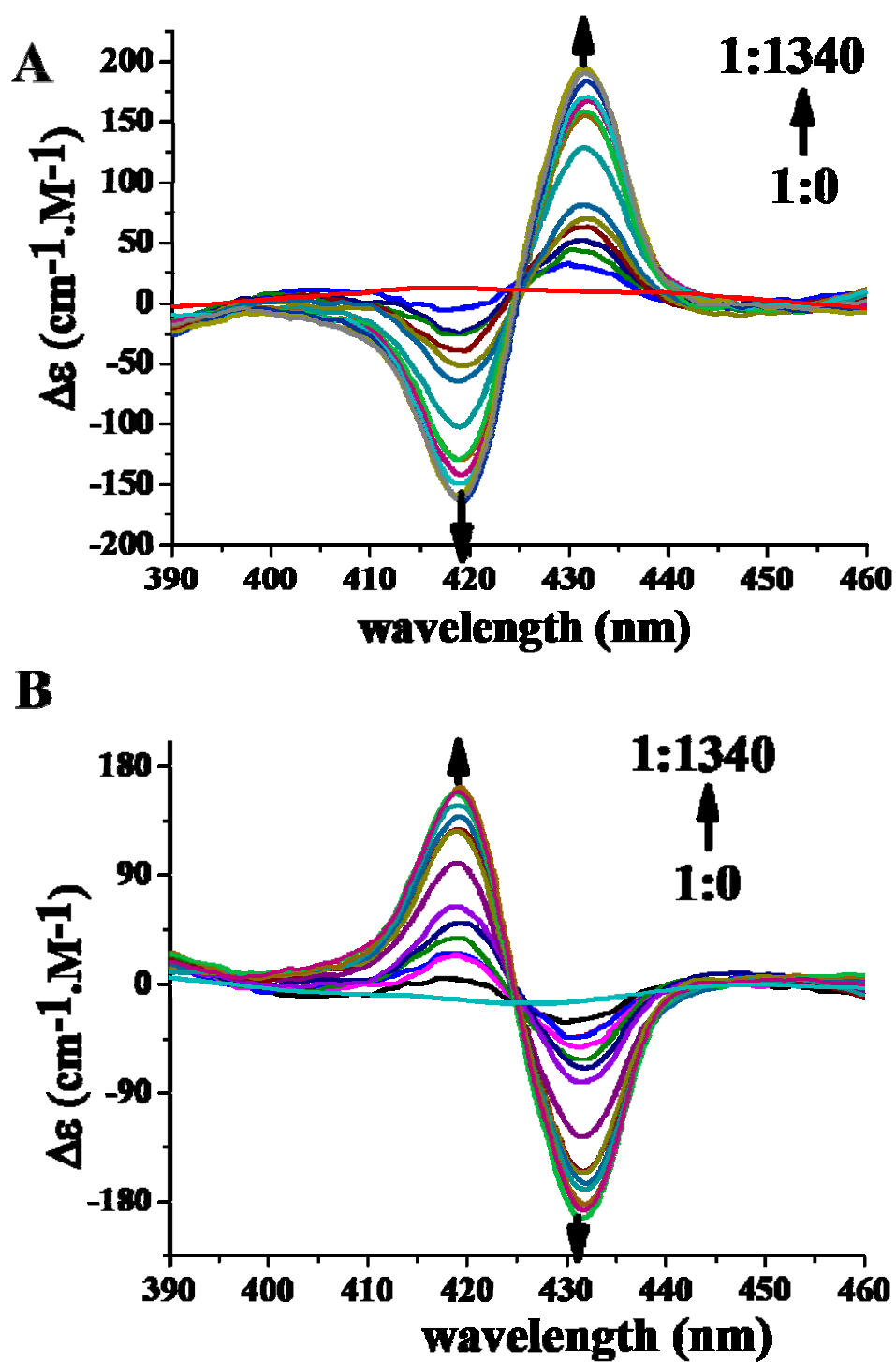


Figure S4. Circular dichroism spectra of a solution of $[\text{Zn}_2\text{-III}]$ (1.75×10^{-6} M) and from 1: 0 to 1:1340 equivalents of (A) 4R, (B) 4S in methylene chloride at 25°C.

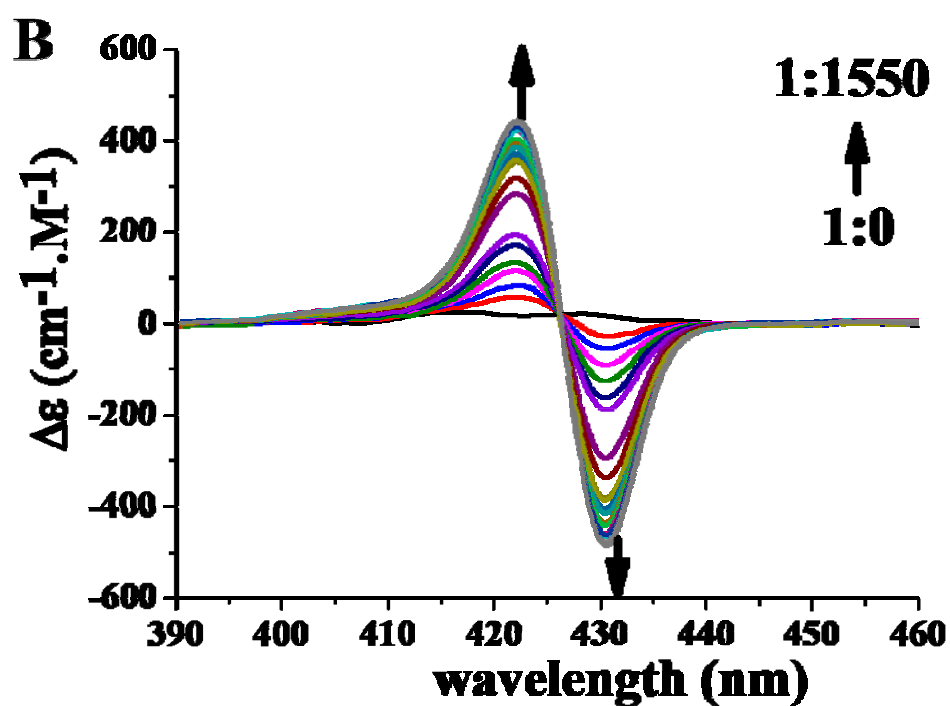
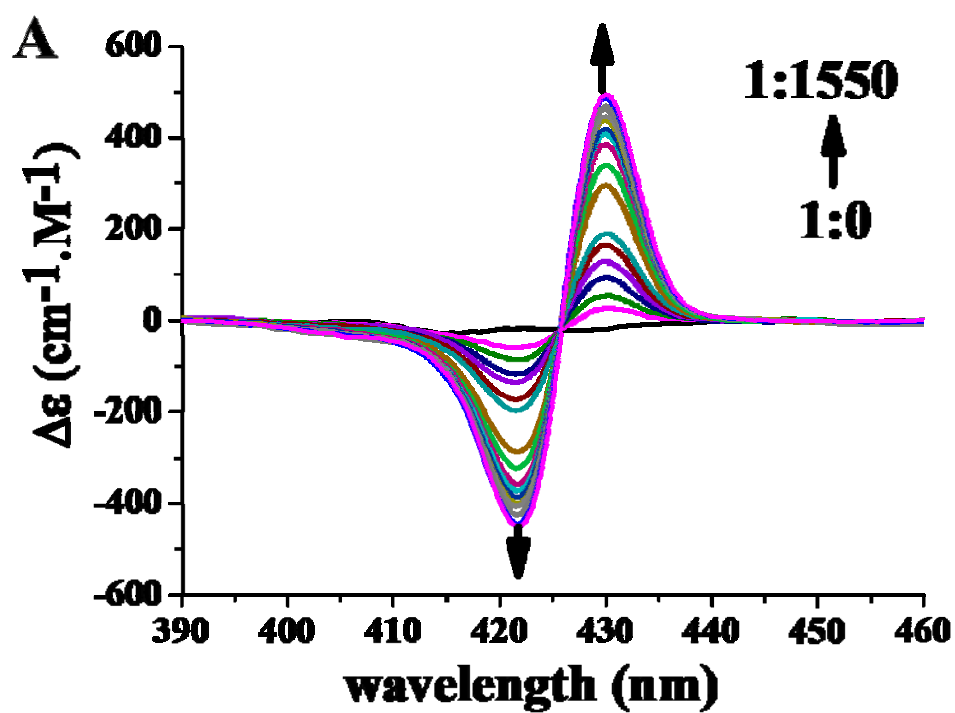


Figure S5. Circular dichroism spectra of a solution of $[\text{Zn}_2\text{-III}]$ (1.75×10^{-6} M) and from 1: 0 to 1:1550 equivalents of (A) 5R, (B) 5S in methylene chloride at 25°C.

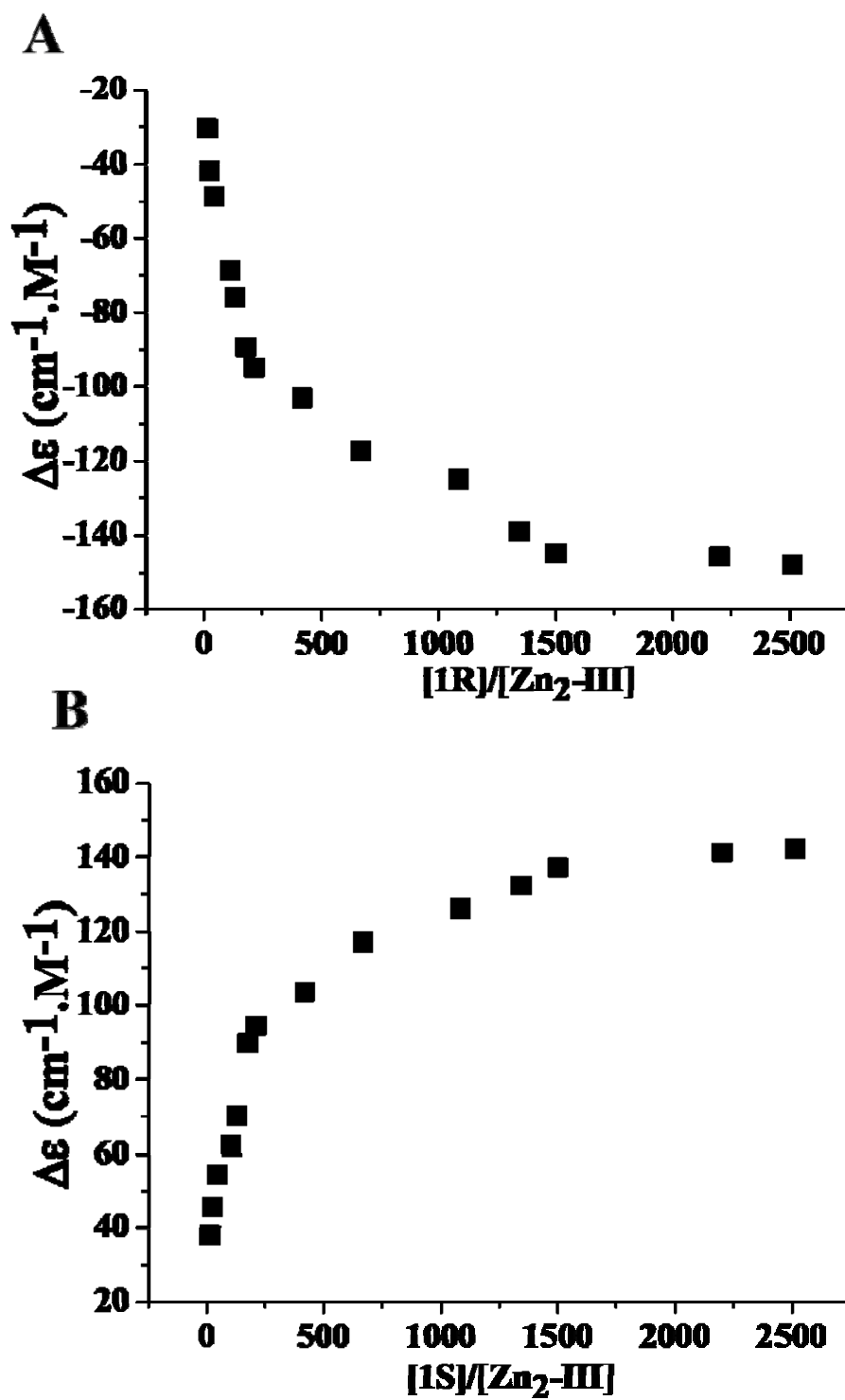


Figure S6. Plots of CD intensity at 431 nm as the function of the equivalents of (A) 1R, (B) 1S.

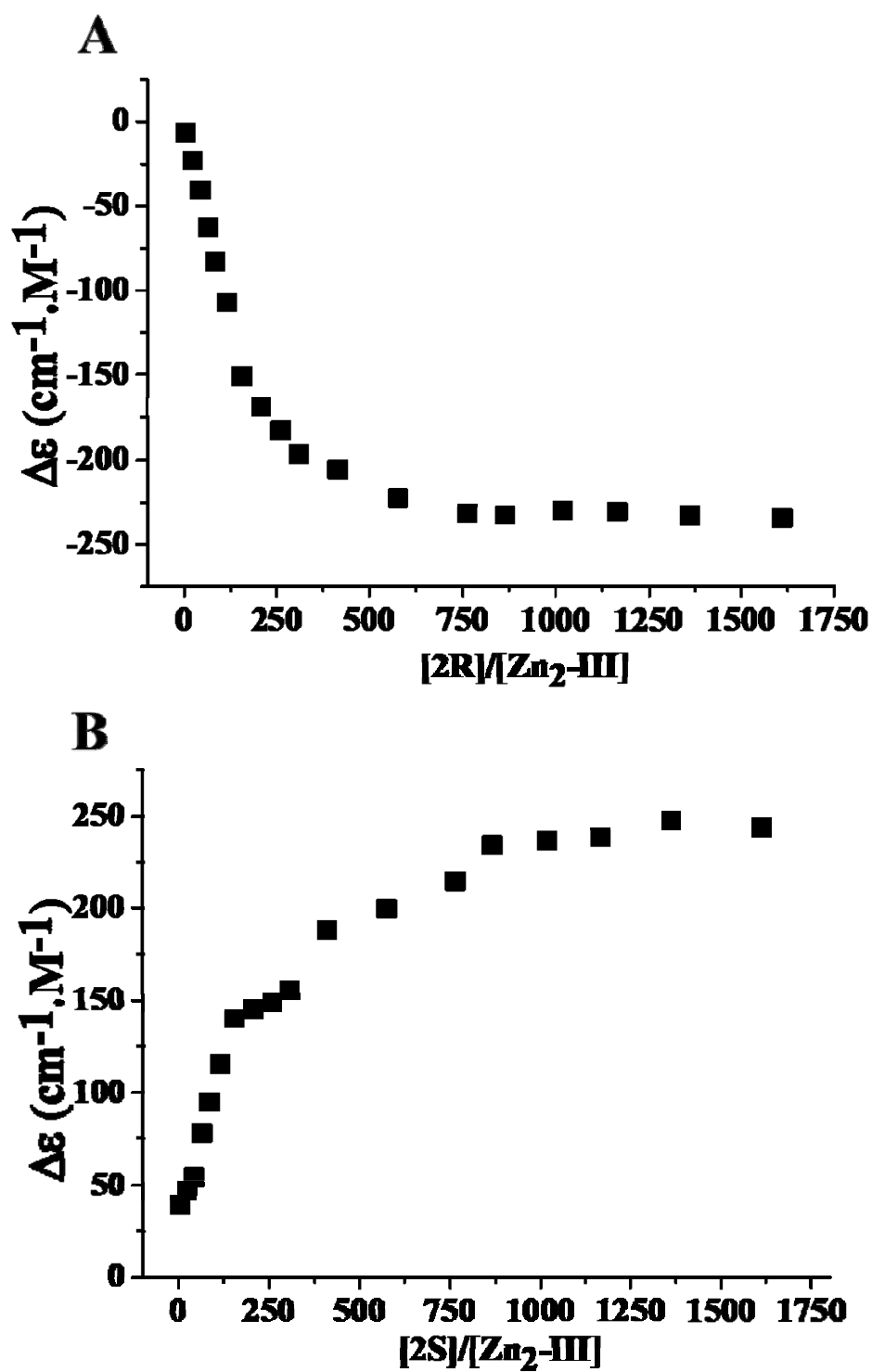


Figure S7. Plots of CD intensity at 431 nm as the function of the equivalents of (A) 2R, (B) 2S.

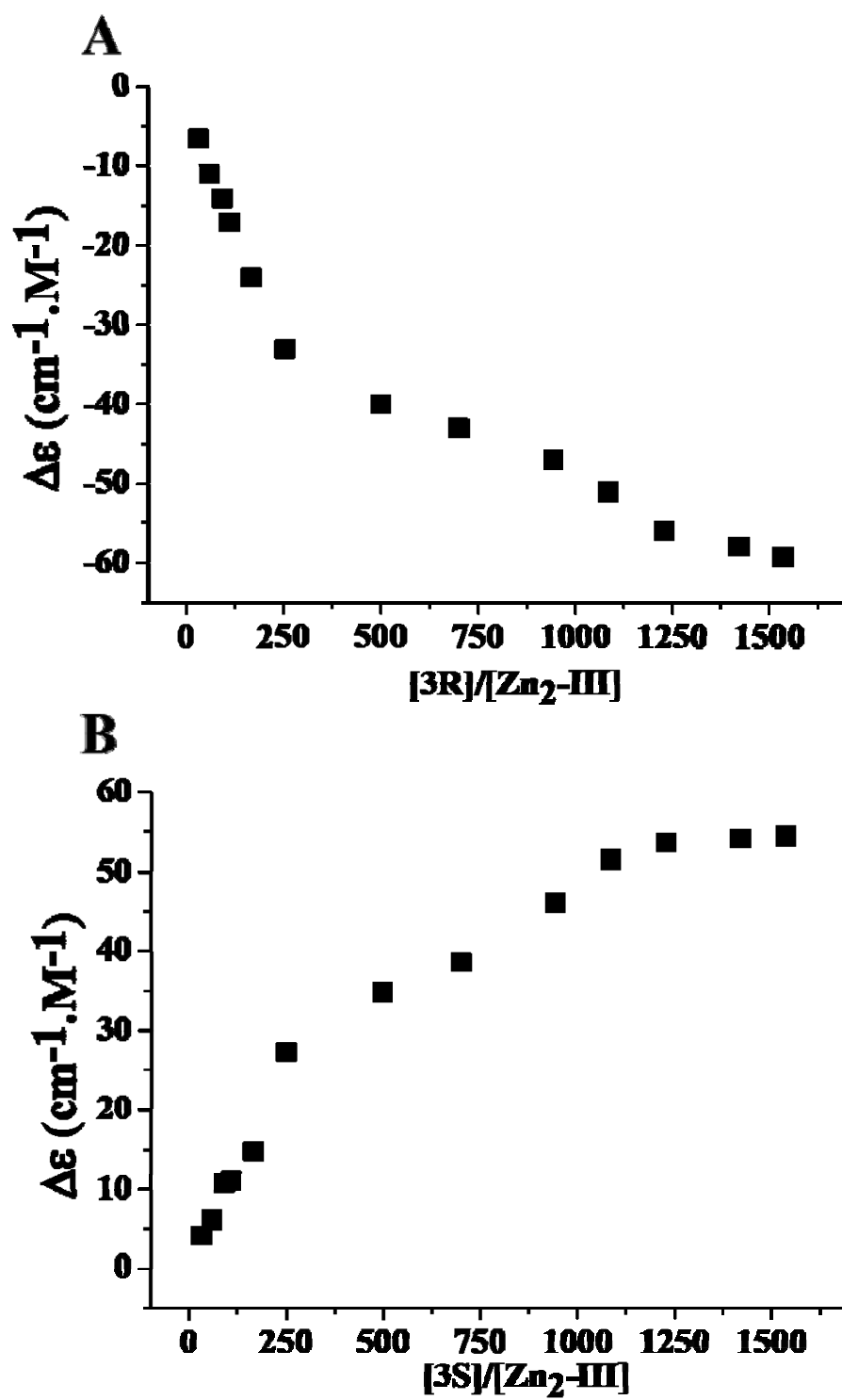


Figure S8. Plots of CD intensity at 432 nm as the function of the equivalents of (A) 3R, (B) 3S.

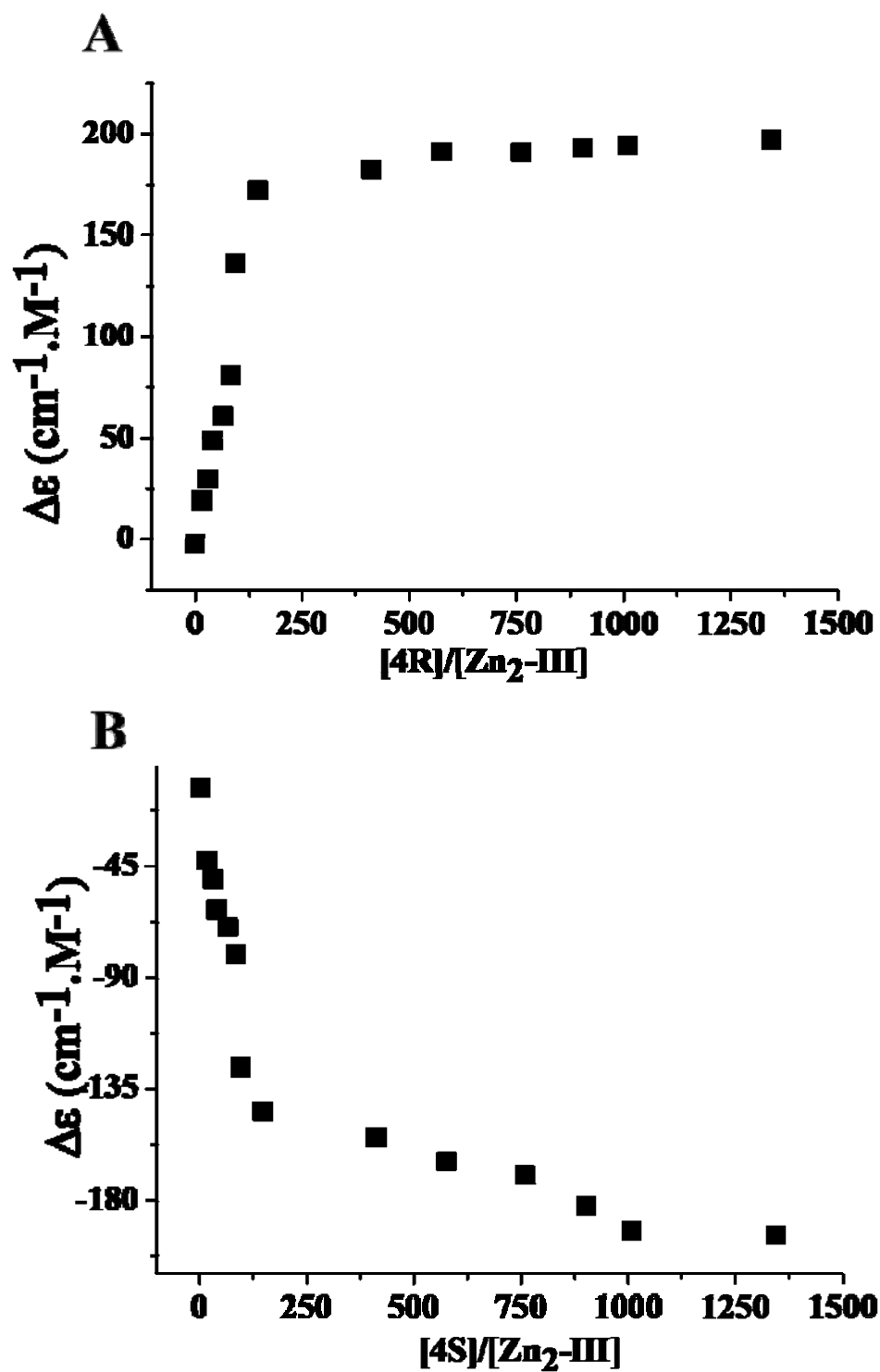


Figure S9. Plots of CD intensity at 432 nm as the function of the equivalents of (A) 4R, (B) 4S.

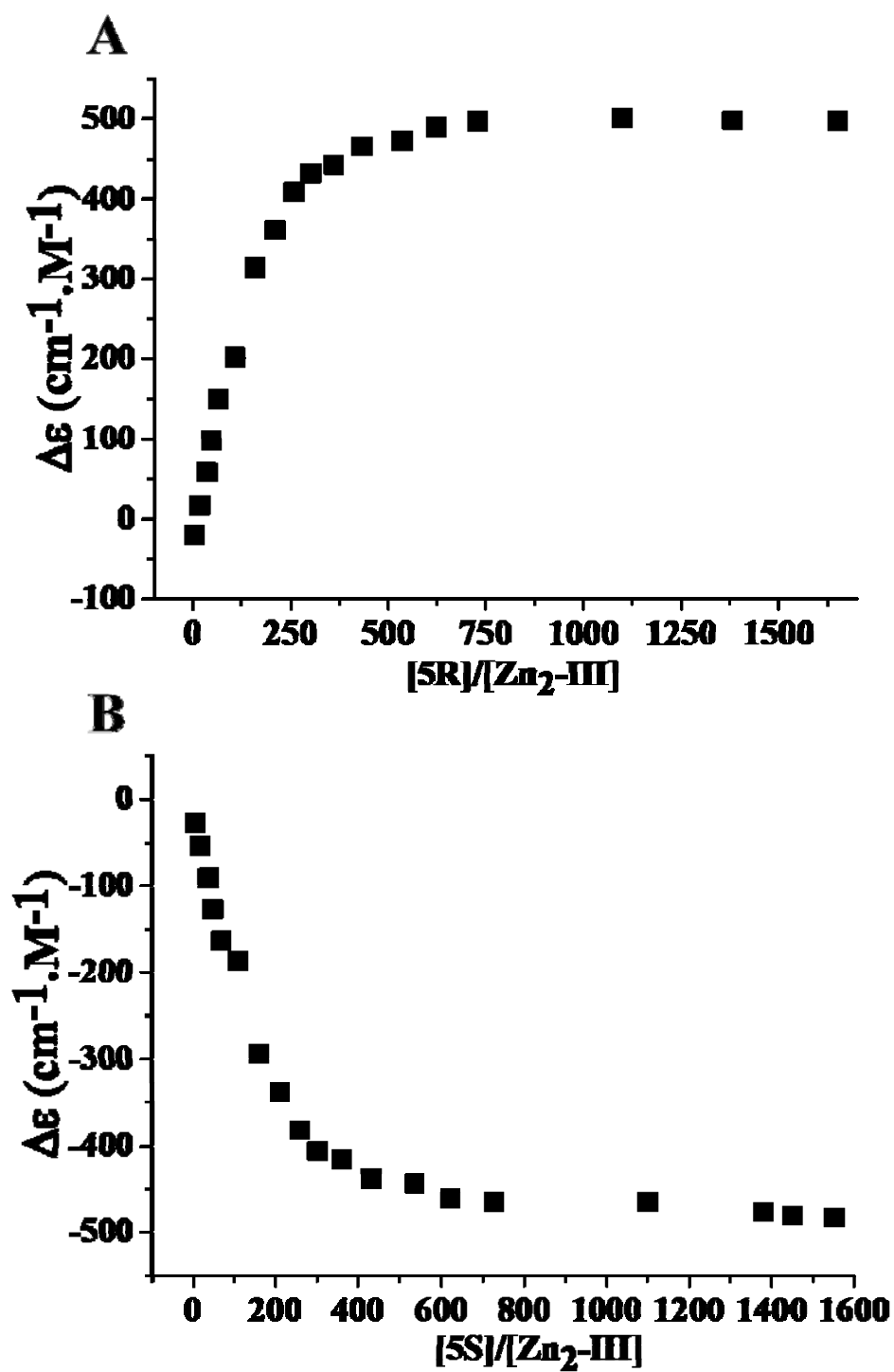


Figure S10. Plots of CD intensity at 430 nm as the function of the equivalents of (A) 5R, (B) 5S.

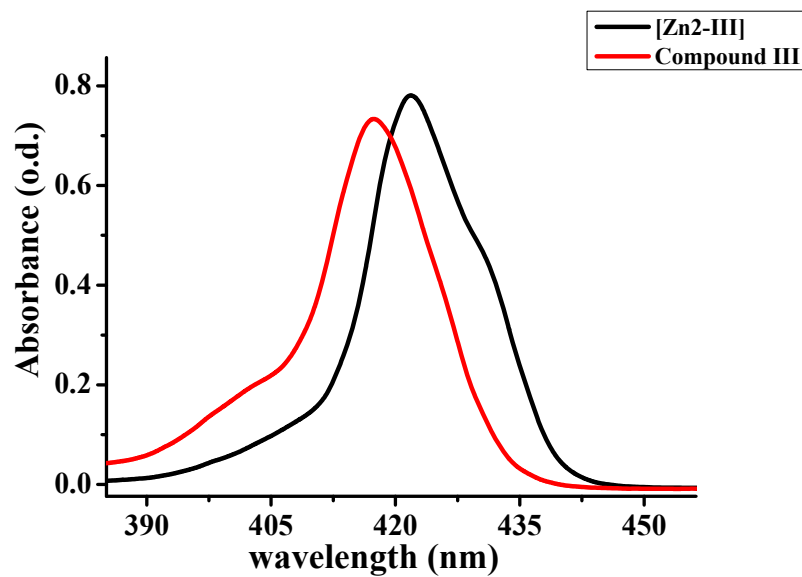


Figure S11. Comparison of metal free bisporphyrin III and [Zn₂-III] in UV-vis spectra.

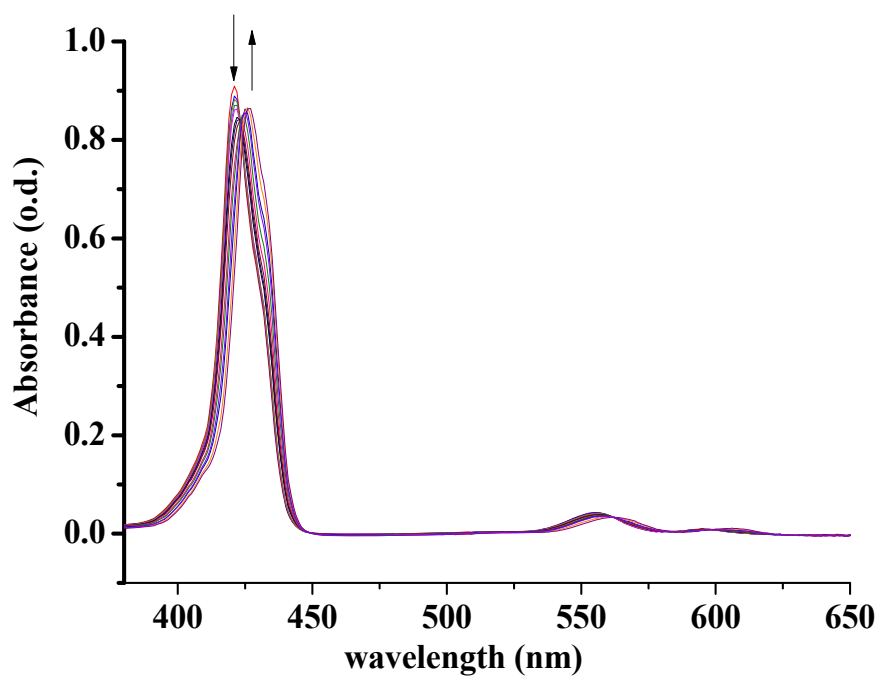


Figure S12. UV-vis spectral change of [Zn₂-III] (1.58×10^{-6} M) upon addition of 2R as the host:guest molar ratios are from 1:0 to 1: 850.

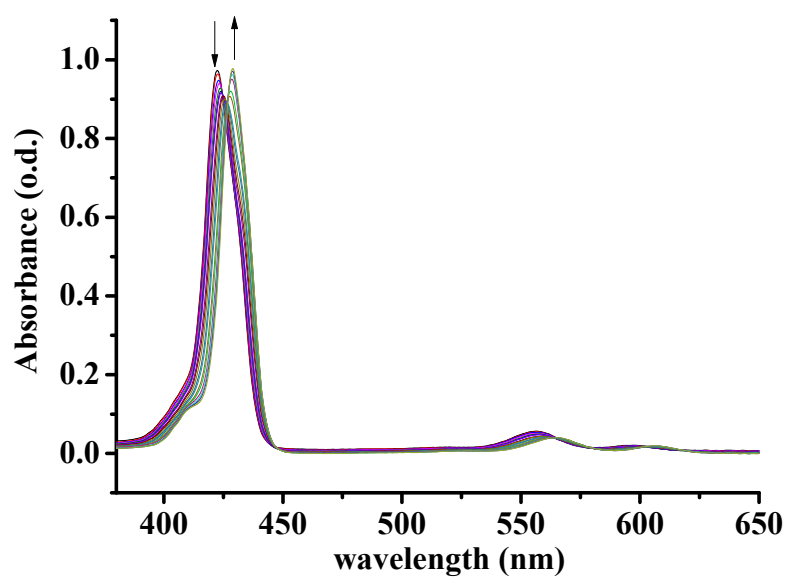


Figure S13. UV-vis spectral change of $[\text{Zn}_2\text{-III}]$ (1.62×10^{-6} M) upon addition of 3R as the host:guest molar ratios are from 1:0 to 1: 850.

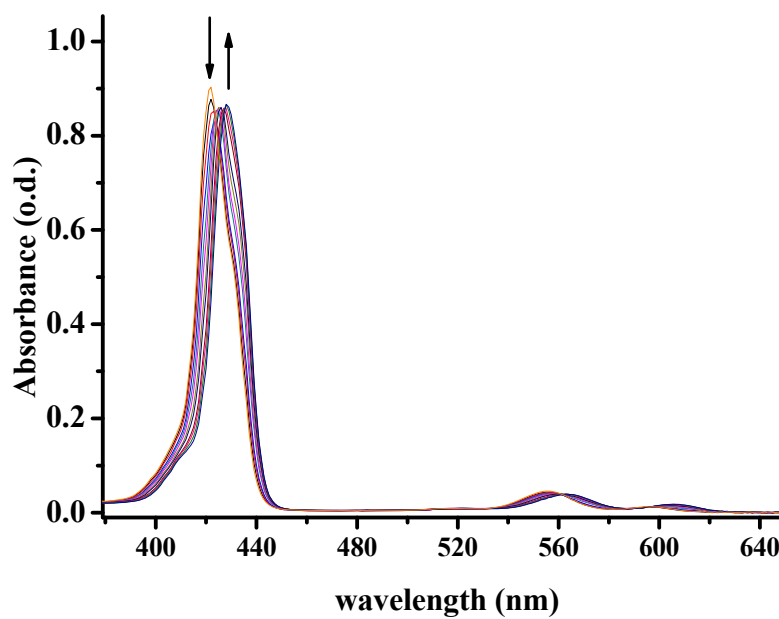


Figure S14. UV-vis spectral change of $[\text{Zn}_2\text{-III}]$ (1.58×10^{-6} M) upon addition of 4R as the host:guest molar ratios are from 1:0 to 1: 850.

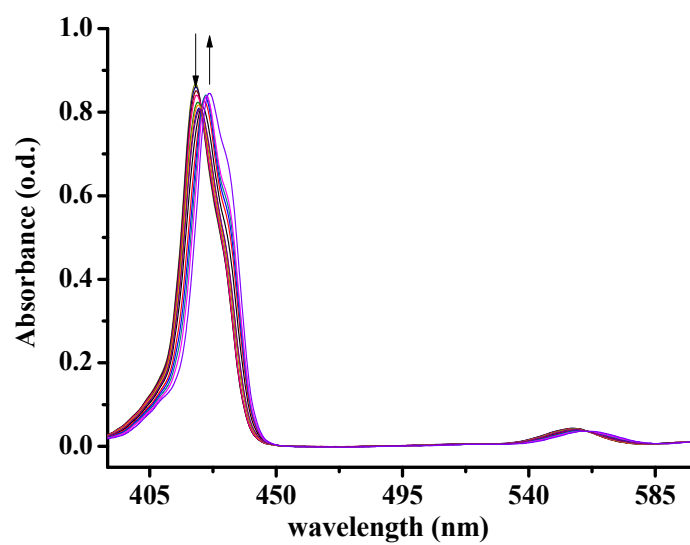


Figure S15. UV-vis spectral change of [Zn₂-III] (1.58×10^{-6} M) upon addition of 5R as the host:guest molar ratios are from 1:0 to 1: 850.

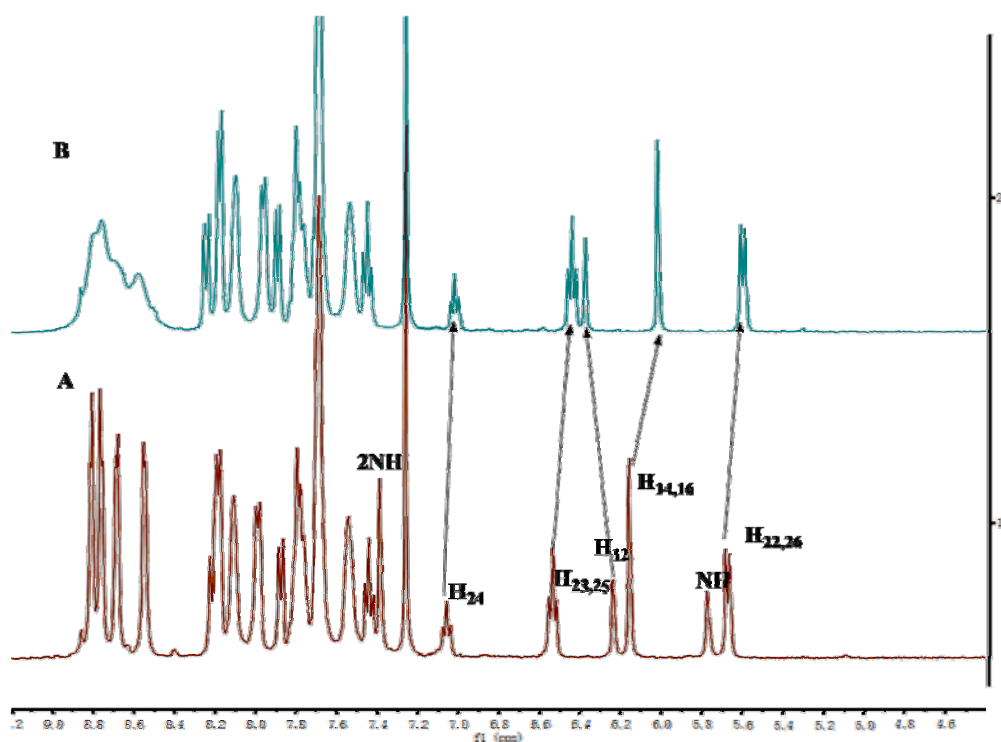


Figure S16. ^1H NMR for free base bisporphyrin III (3.58×10^{-3} M) A) before and B) after addition of D_2O .

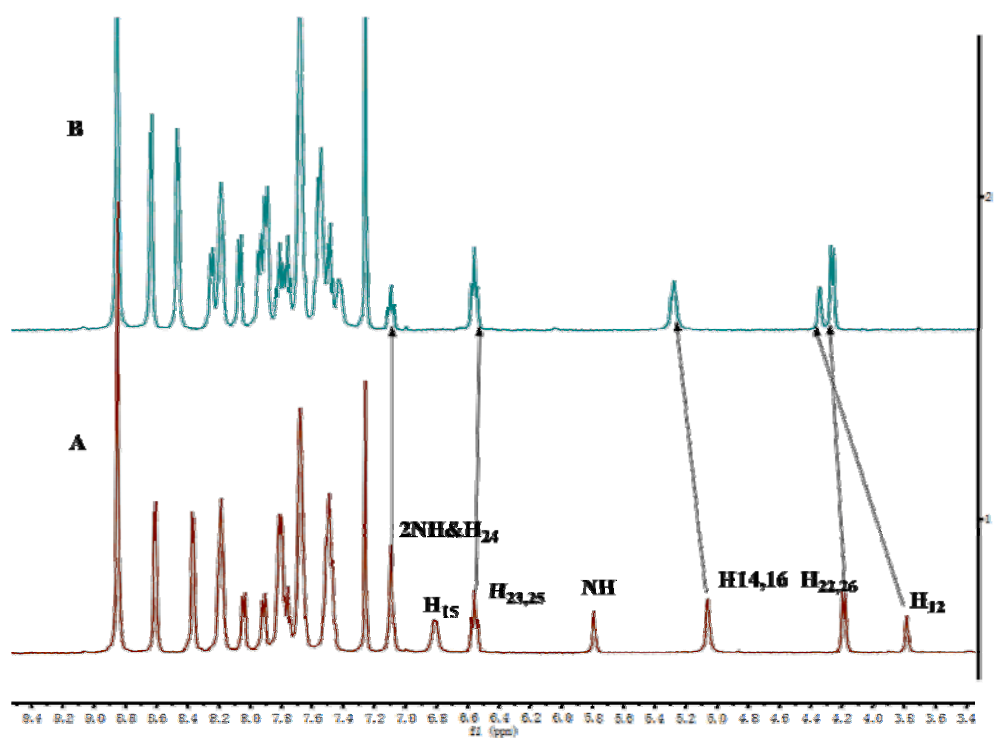


Figure S17. ^1H NMR for $[\text{Zn}_2\text{-III}]$ (3.46×10^{-3} M) A) before and B) after addition of D_2O .

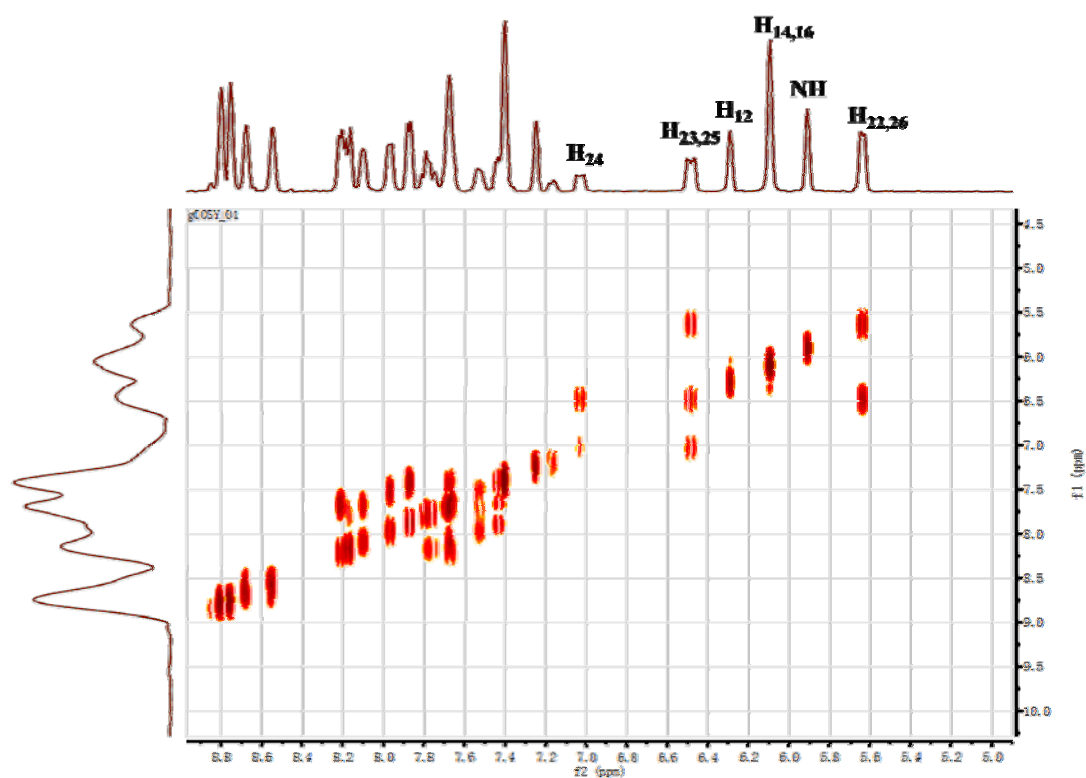


Figure S18. ^1H - ^1H COSY NMR spectrum for the free base bisporphyrin III.

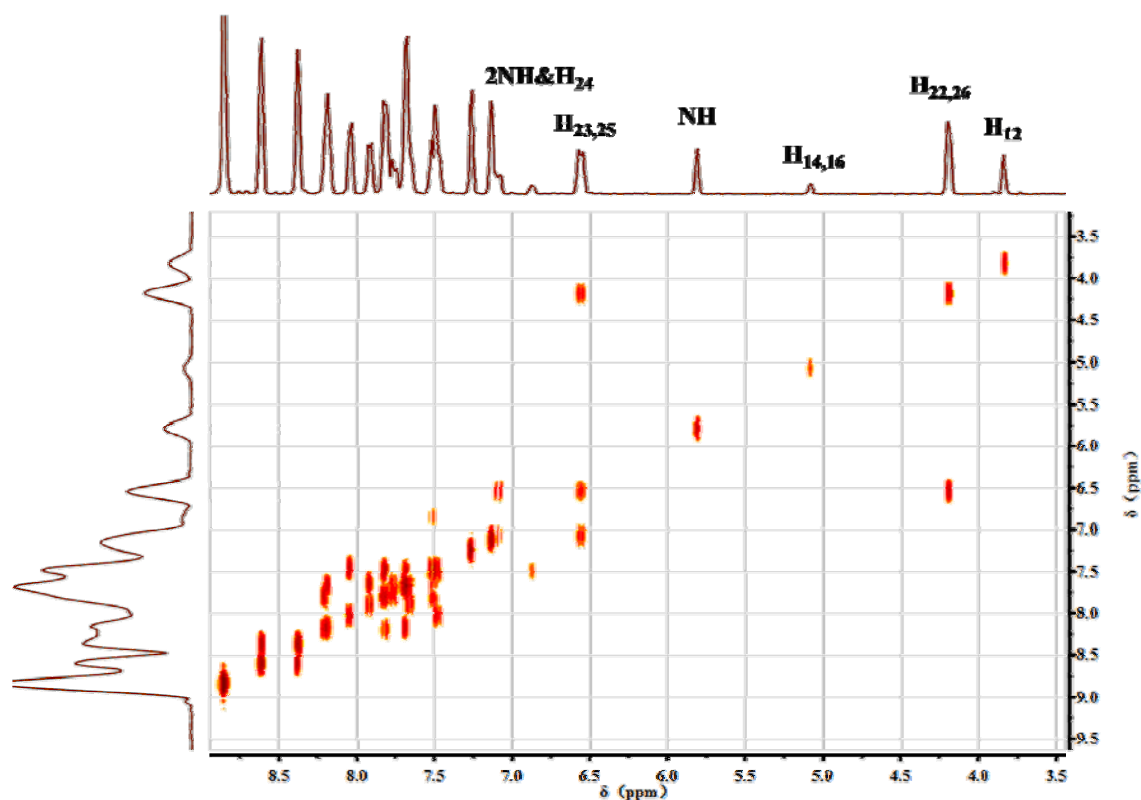


Figure S19. ^1H - ^1H COSY NMR spectrum for $[\text{Zn}_2\text{-III}]$.

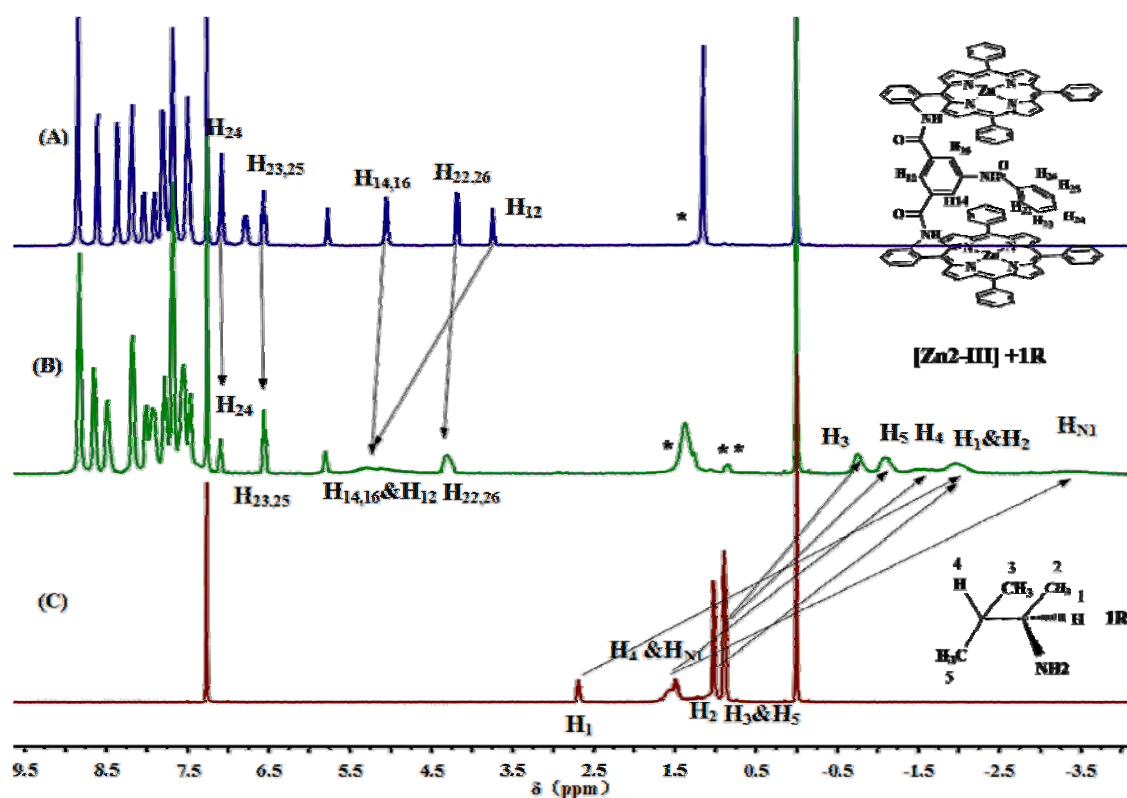


Figure S20. ^1H NMR spectra in CDCl_3 (at 298 K) of (A) $[\text{Zn}_2\text{-III}]$ (4.36×10^{-3} M), (B) the mixture of $[\text{Zn}_2\text{-III}]$ (4.36×10^{-3} M) and 1R (0.95 eq.), (C) 1R. Inset shows the proton numbering scheme of $[\text{Zn}_2\text{-III}]$ and 1R. *: Impurity from water; **: impurity from petroleum ether.

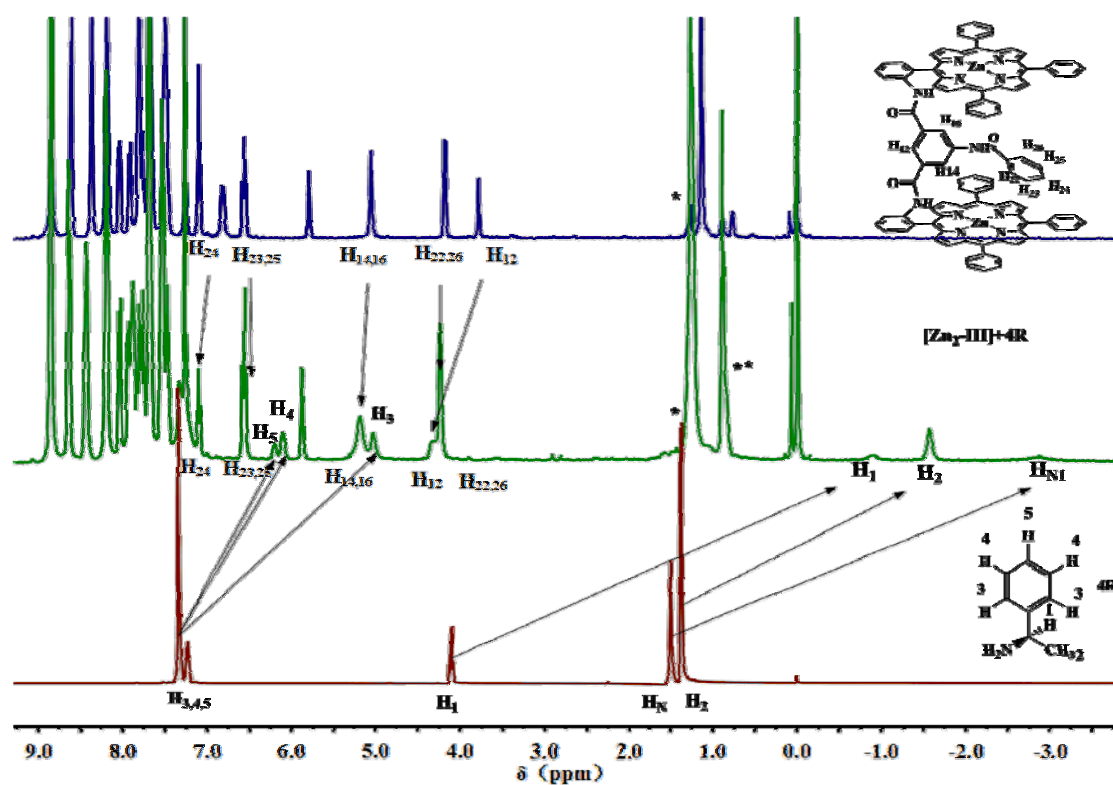


Figure S21. ^1H NMR spectra in CDCl_3 (at 298 K) of (A) $[\text{Zn}_2\text{-III}]$ (4.8×10^{-3} M), (B) the mixture of $[\text{Zn}_2\text{-III}]$ (4.8×10^{-3} M) and 4R (0.3 eq.), (C) 4R. Inset shows the proton numbering scheme of $[\text{Zn}_2\text{-III}]$ and 4R. *: Impurity from water; **: impurity from petroleum ether.

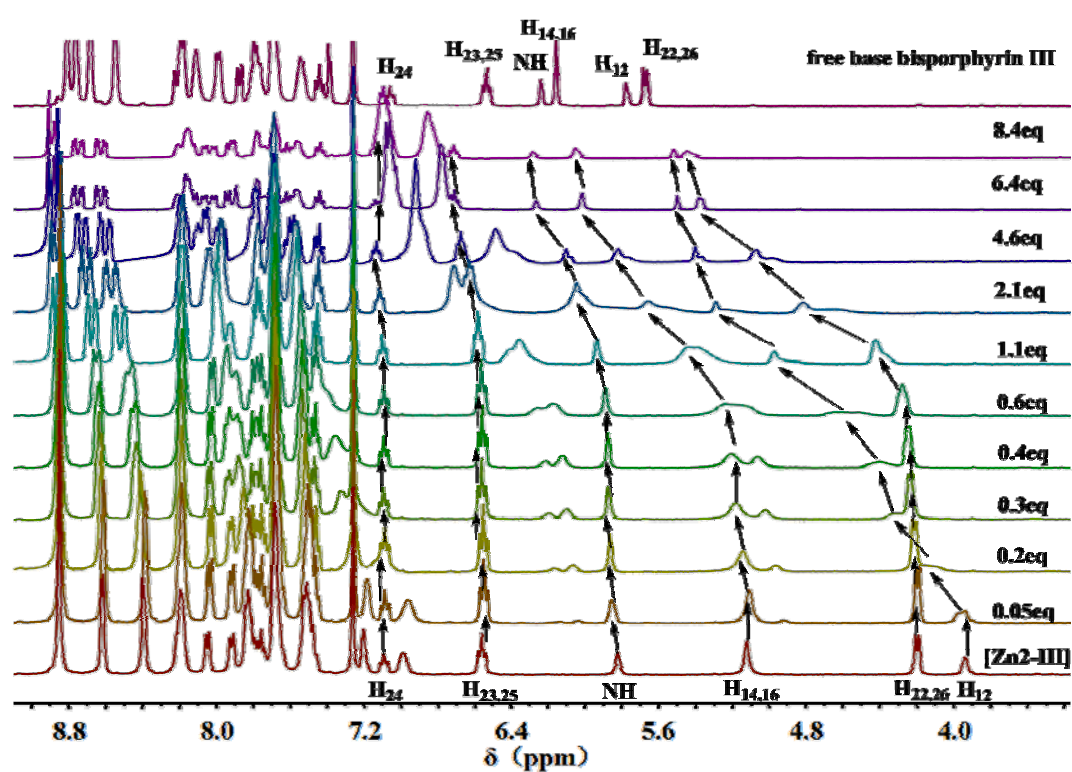


Figure S22. ^1H NMR spectral changes of $[\text{Zn}_2\text{-III}]$ (4.8×10^{-3} M) upon addition of 4R in CDCl_3 at 298 K as the host:guest molar ratios are from 1:0 to 1:8.4.

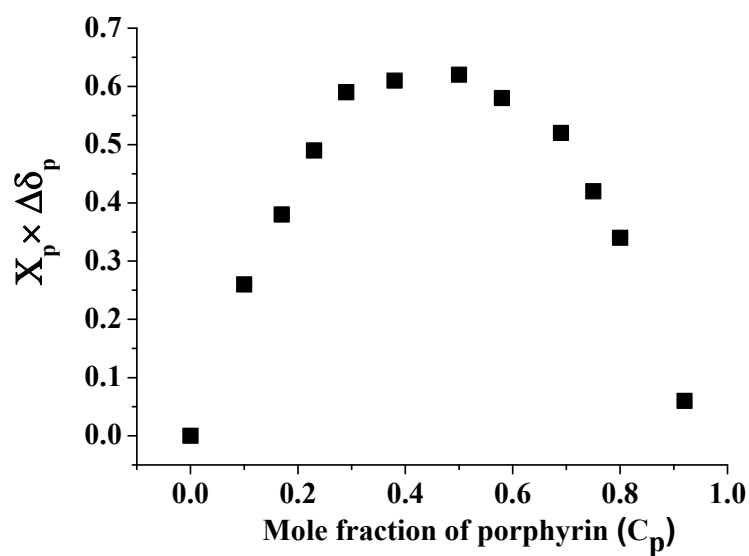


Figure S23. Job's continuous plot of $[Zn_2\text{-III}]$ with 1R (following the changes in chemical shift of H12 of $[Zn_2\text{-III}]$).

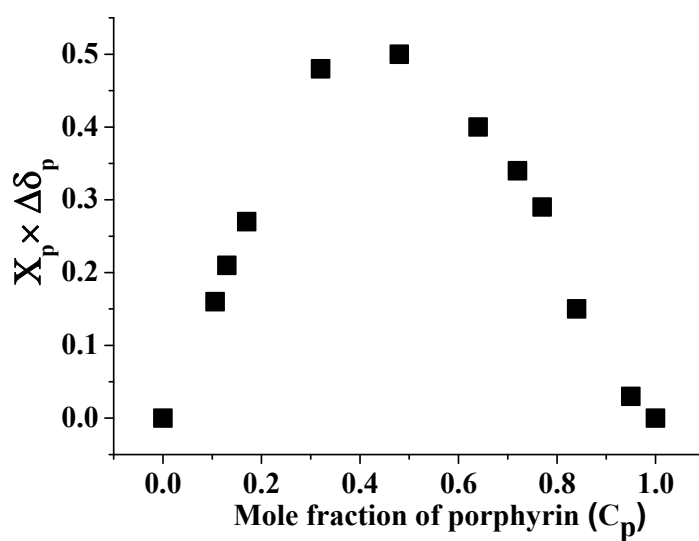


Figure S24. Job's continuous plot of $[Zn_2\text{-III}]$ with 4R (following the changes in chemical shift of H12 of $[Zn_2\text{-III}]$).

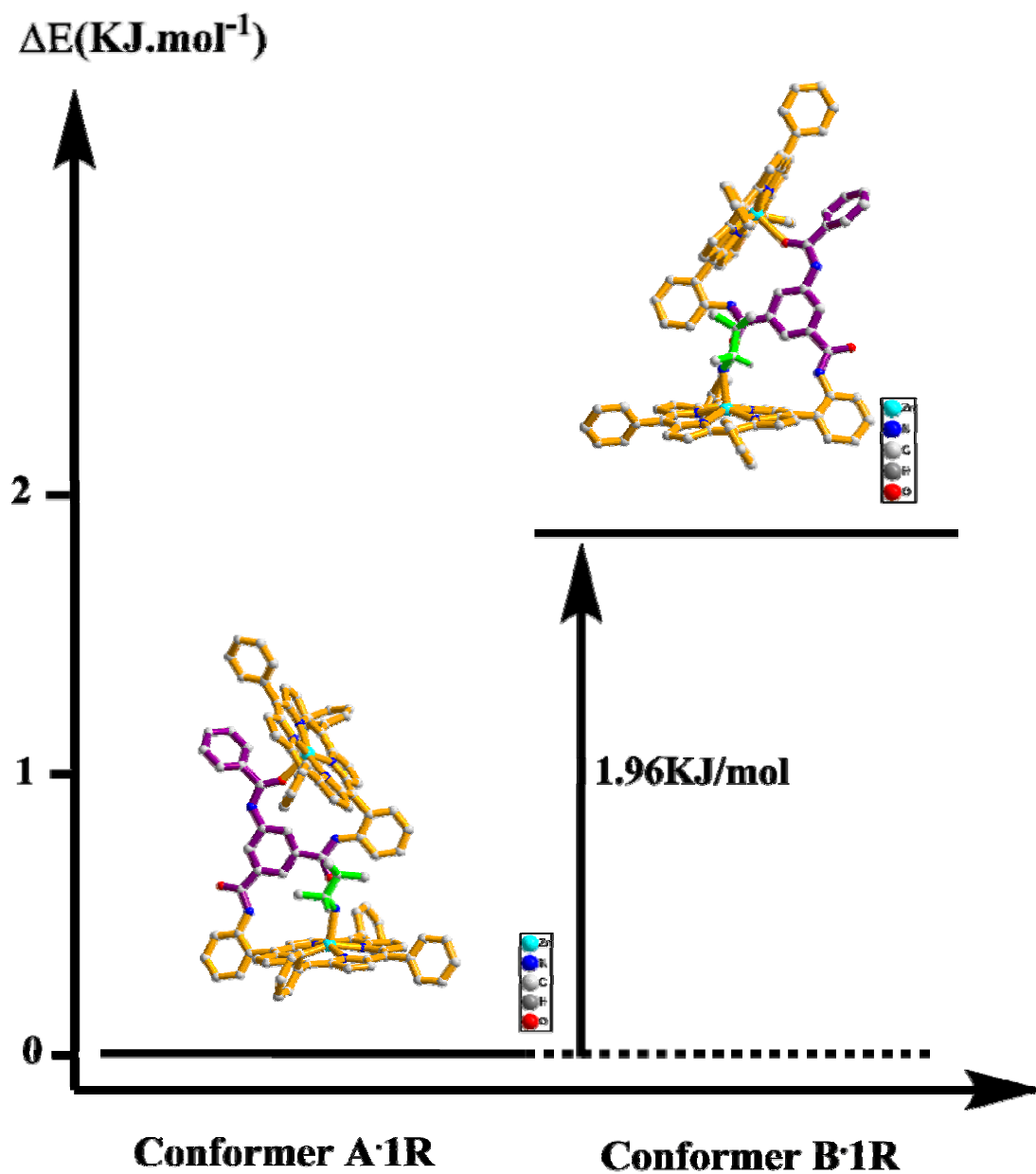


Figure S25. Relative energies of DFT-optimized conformer A·1R and conformer B·1R.

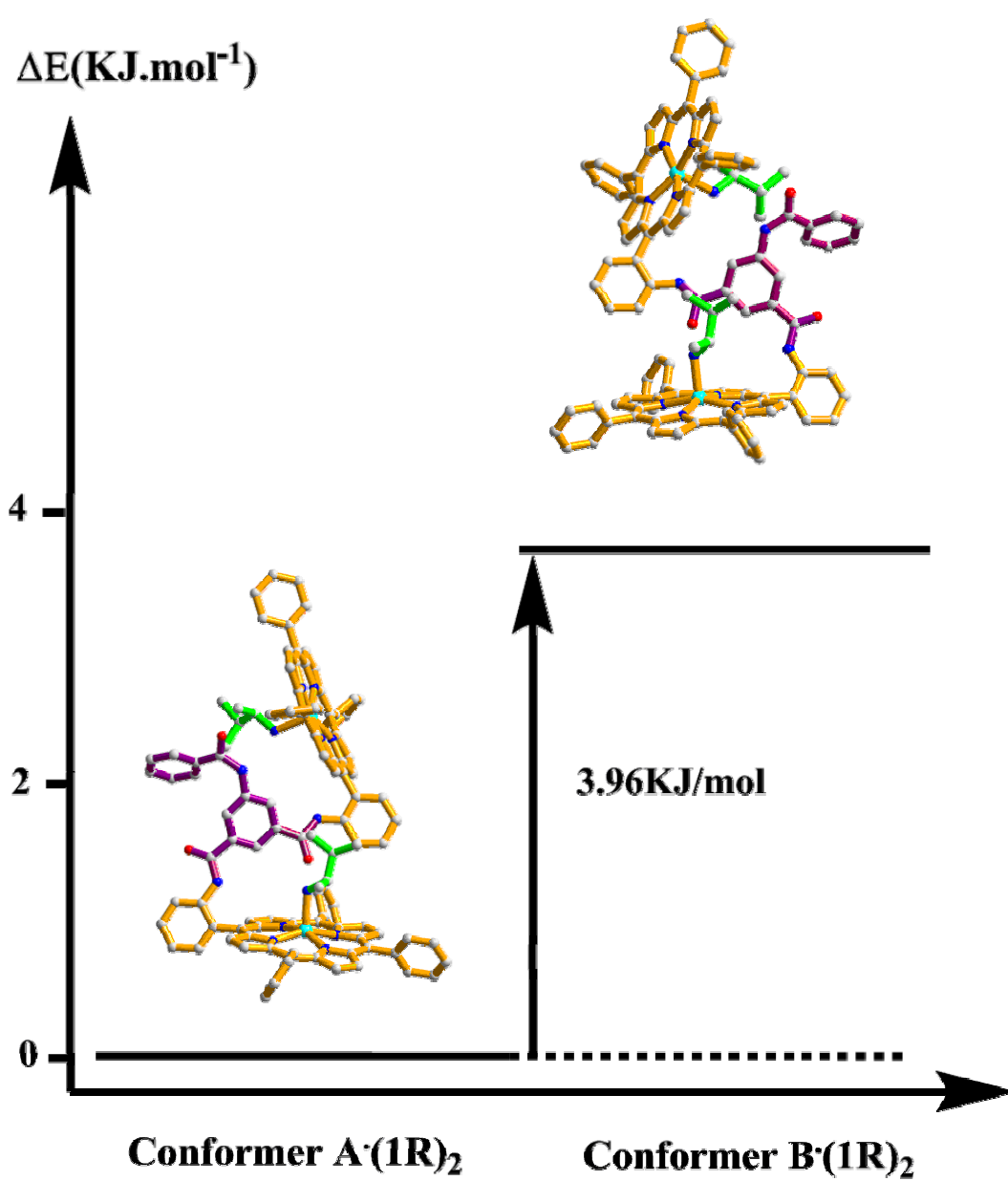


Figure S26. Relative energies of DFT-optimized conformer A·(1R)₂ and conformer B·(1R)₂.

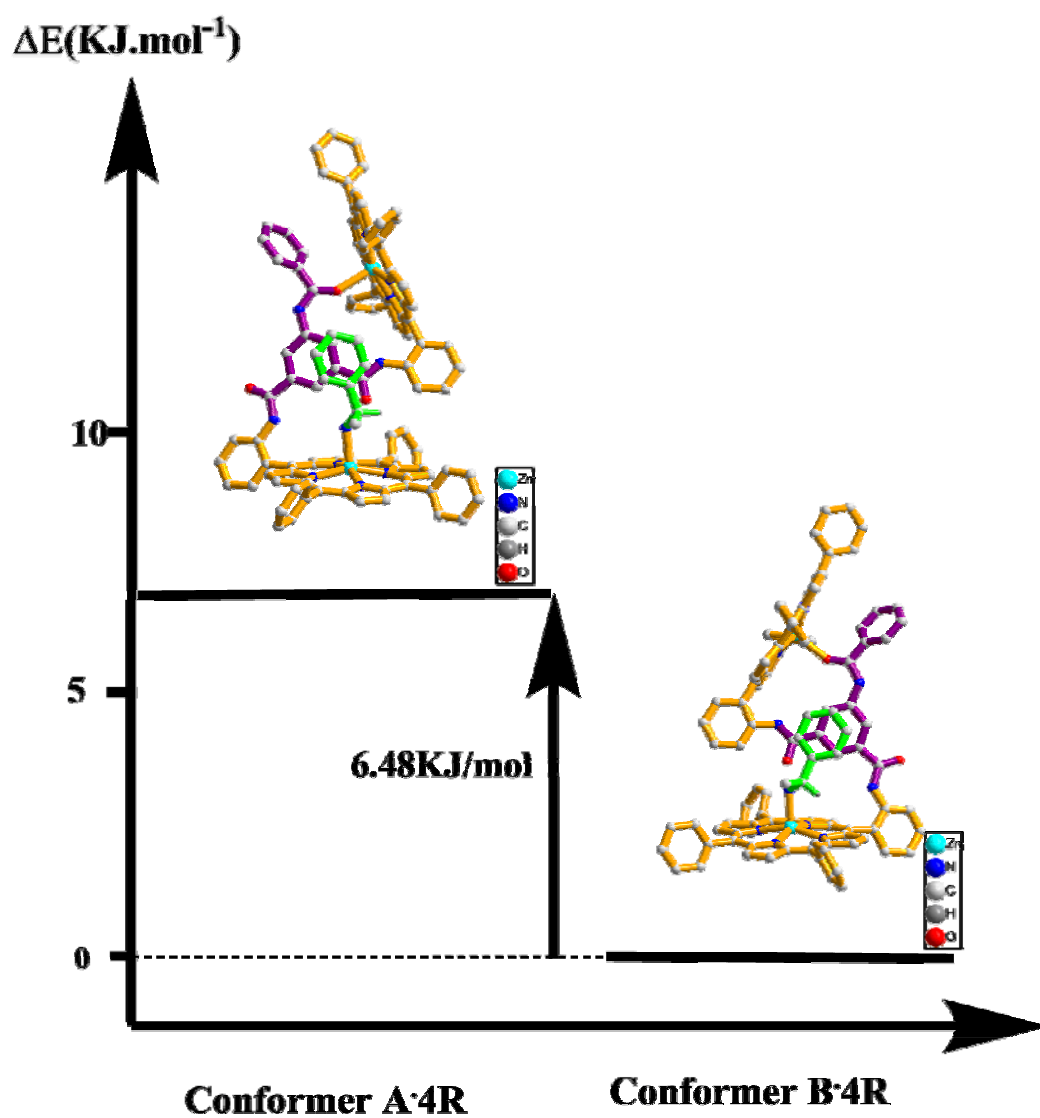


Figure S27. Relative energies of DFT-optimized conformer A·4R and conformer B·4R.

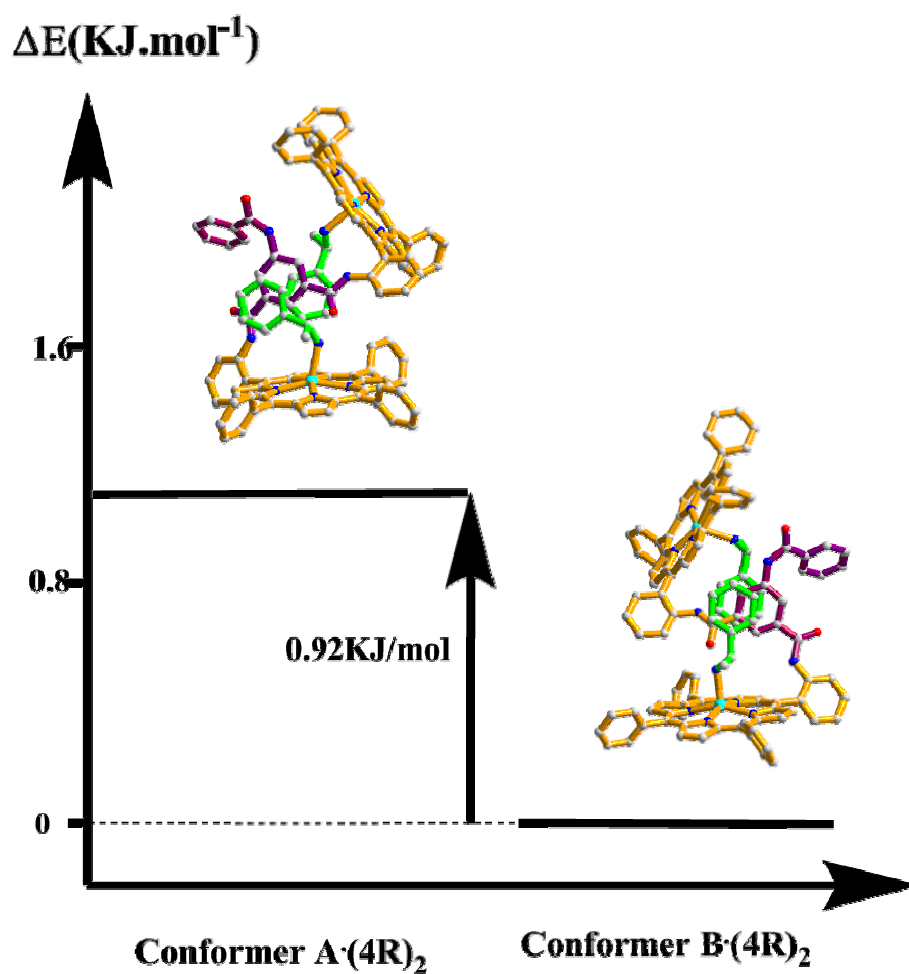
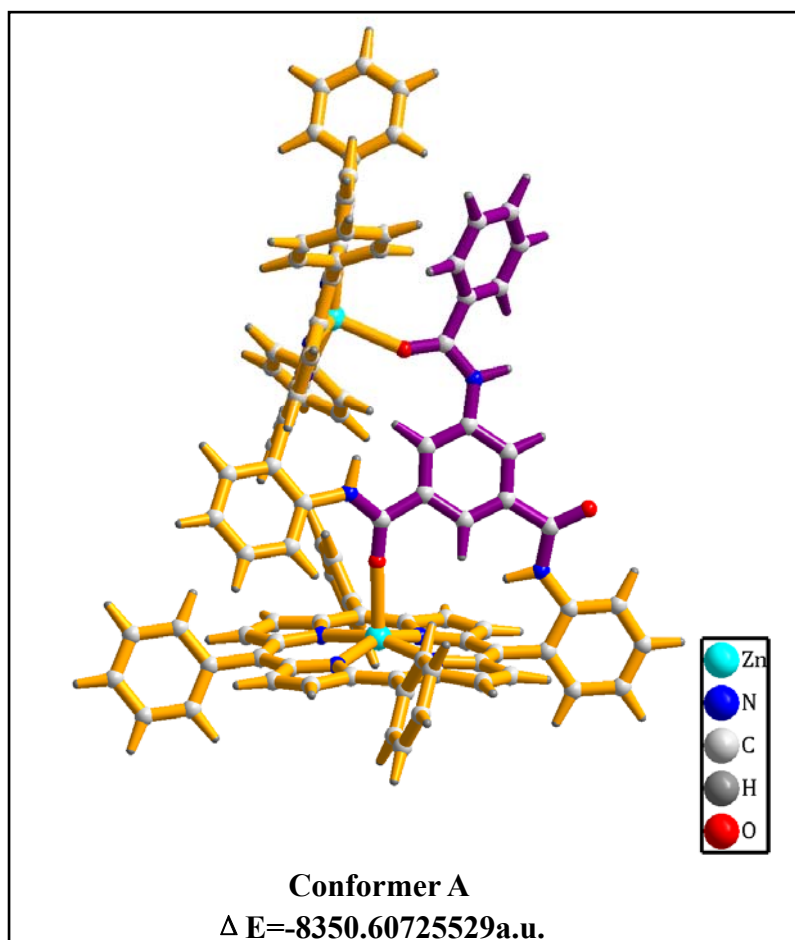


Figure S28. Relative energies of DFT-optimized conformer A·(4R)₂ and conformer B·(4R)₂.

Table S1. Selected bond distances (Å) for [Zn₂-III]•1R

Zn(1)-N(11)	2.070(3)	Zn(2)-N(24)	2.047(2)
Zn(1)-N(13)	2.074(2)	Zn(2)-N(23)	2.054(2)
Zn(1)-N(12)	2.074(2)	Zn(2)-N(22)	2.054(2)
Zn(1)-N(14)	2.083(3)	Zn(2)-N(21)	2.055(2)
Zn(1)-N(1)	2.105(3)	Zn(1)-O(013)	2.246(2)



Cartesian coordinates for Geometry Optimized Conformer A

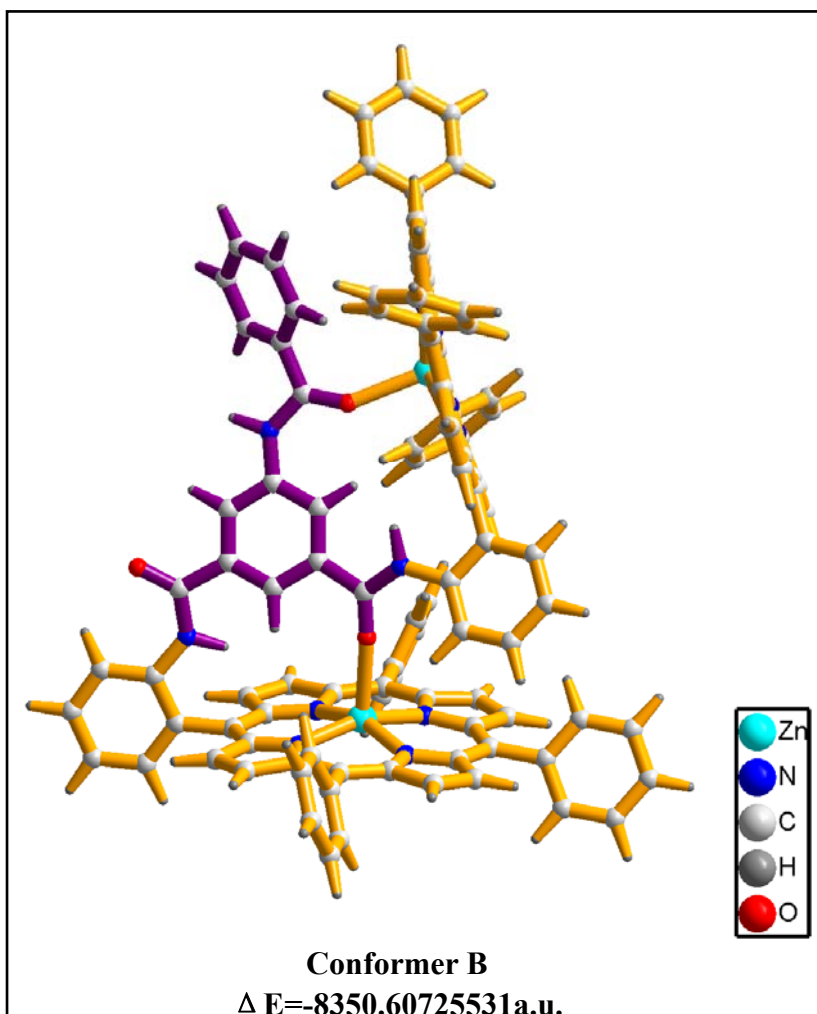
Atoms	x	y	z
Zn	-4.91225100	-0.22507700	-0.04586700
N	-4.93761600	-2.09290000	0.87570900
N	-5.72740500	0.56307600	1.69528100
N	-5.66923300	1.42651500	-1.05457300
N	-4.74980000	-1.19754600	-1.86041800
C	-5.56989000	-1.41584500	3.17744600
C	-6.21007400	2.85715900	0.89408000
C	-5.32690900	0.66643700	-3.38880500
C	-4.22949300	-3.48153900	-1.04717400
C	-4.52158200	-3.27756500	0.31373800
C	-5.15398300	-2.35064300	2.20923100
C	-5.83664800	-0.05796700	2.91689100
C	-6.09575100	1.87389600	1.89260800
C	-6.24299900	3.61441400	-1.51595800
H	-6.52171900	4.64446900	-1.34822100

C	-5.66816800	1.62492900	-2.41451100
C	-4.90230400	-0.64576000	-3.11078800
C	-4.38496100	-2.50694100	-2.05333600
C	-4.45435000	-4.30615700	1.33062400
H	-4.14832400	-5.32903500	1.16692300
C	-4.85778300	-3.73721500	2.49829400
H	-4.95368000	-4.20599400	3.46776300
C	-6.27335000	0.89181900	3.91700500
H	-6.45071200	0.66393600	4.95832000
C	-6.43552000	2.08431000	3.28393800
H	-6.77637100	3.01725700	3.70894500
C	-6.03422800	2.62301900	-0.48411500
C	-6.03255900	2.99374500	-2.70929400
H	-6.11043000	3.42181400	-3.69836800
C	-4.61949900	-1.64083000	-4.12254100
H	-4.69116500	-1.48600800	-5.18910000
C	-4.28997400	-2.78695800	-3.47002700
H	-4.04336300	-3.74554400	-3.90257500
C	-4.38404500	-1.83940800	5.35845200
C	-5.59327800	-1.85625800	4.61811100
C	-6.76609300	-2.24059700	5.27087800
H	-7.69555200	-2.25665700	4.70844400
C	-6.75546500	-2.58769900	6.62473800
H	-7.67843300	-2.88214600	7.11614300
C	-5.55787900	-2.54785200	7.33936900
H	-5.54419200	-2.81118200	8.39366000
C	-4.36573200	-2.17803900	6.71575100
H	-3.42847200	-2.14381800	7.25642400
C	-6.59192000	4.24045500	1.32705700
C	-5.68967800	5.03528400	2.05104900
H	-4.70624200	4.63806400	2.28703000
C	-6.04006600	6.32269900	2.46039400
H	-5.32534000	6.92408200	3.01627200
C	-7.30097000	6.83765200	2.15440500
H	-7.57454700	7.83988300	2.47342700
C	-8.20909500	6.05609800	1.43767700
H	-9.19573100	6.44565900	1.20040200
C	-7.85758500	4.76904200	1.02848500
H	-8.56952900	4.15984600	0.47852900
C	-5.44669200	1.06801200	-4.82783700
C	-6.70668000	1.31780500	-5.39490000
H	-7.59439000	1.21344300	-4.77727300
C	-6.82772100	1.68522400	-6.73555000
H	-7.81287700	1.86852500	-7.15668800

C	-5.68950700	1.81026000	-7.53441900
H	-5.78295700	2.09584200	-8.57887200
C	-4.43068000	1.56553300	-6.98274200
H	-3.53829300	1.66385100	-7.59565000
C	-4.30995600	1.19719800	-5.64180100
H	-3.32830400	1.01788100	-5.21353500
C	-3.77855400	-4.84355600	-1.47857500
C	-4.64339500	-5.94797000	-1.41686600
H	-5.65469200	-5.80814000	-1.04535600
C	-4.22323300	-7.20966400	-1.83987000
H	-4.91023400	-8.05049900	-1.78898700
C	-2.93091700	-7.38943000	-2.33658600
H	-2.60554600	-8.37133200	-2.67028200
C	-2.06117800	-6.29939500	-2.40605600
H	-1.05262700	-6.42548100	-2.79054900
C	-2.48161900	-5.03882200	-1.97940700
H	-1.80073000	-4.19353600	-2.03135100
Zn	4.52554600	0.44447800	-0.74918300
N	3.77977600	2.34787100	-1.10858900
N	2.91446900	-0.33321100	-1.79686900
N	5.50657400	-1.35649500	-1.06019700
N	6.36319100	1.31346700	-0.34132100
C	1.57998200	1.73471300	-2.06423500
C	3.59680700	-2.71116600	-1.86786600
C	7.79264400	-0.71161500	-0.35644300
C	5.65338900	3.68729200	-0.20471300
C	2.50902300	2.64911200	-1.53198700
C	4.33957600	3.52869700	-0.68244800
C	1.79602800	0.34923600	-2.20473100
C	2.69317600	-1.65735300	-2.09051200
C	4.91414600	-2.55065000	-1.39459200
C	6.81041900	-1.64563900	-0.73513500
C	7.56841200	0.66776200	-0.18977400
C	6.59854900	2.64593300	-0.09871500
C	2.24974400	4.06207900	-1.34857200
H	1.32669600	4.56626800	-1.59741900
C	3.37835500	4.60375400	-0.81717900
H	3.54924400	5.63431500	-0.54218300
C	0.84407200	-0.56963700	-2.79281000
H	-0.11088800	-0.29471800	-3.21812400
C	1.39733100	-1.80989700	-2.71872900
H	0.98319800	-2.74105500	-3.07781500
C	5.86278900	-3.63097800	-1.23387500
H	5.65658400	-4.67675800	-1.40933000

C	7.03737800	-3.07040600	-0.83753500
H	7.97063300	-3.57179100	-0.62571200
C	8.59635300	1.62600200	0.15070700
H	9.64203000	1.39542100	0.29487000
C	7.99609700	2.84612200	0.21732900
H	8.45950600	3.80034400	0.42249200
C	-0.89536700	2.06972600	-1.65544900
C	-2.15465200	2.53558400	-2.04478400
H	-3.01122500	2.37889600	-1.40331500
C	-2.28907300	3.20853100	-3.25936300
H	-3.26935300	3.57033100	-3.55214000
C	-1.18197300	3.42139400	-4.08100200
H	-1.29228400	3.94943200	-5.02396900
C	0.07092900	2.94876900	-3.68789900
H	0.93916900	3.09892100	-4.32324000
C	0.23707200	2.26374100	-2.48022800
C	3.13474300	-4.10068100	-2.18840600
C	2.16727800	-4.73060200	-1.39056200
H	1.75576800	-4.19815600	-0.53755200
C	1.74143800	-6.02957100	-1.67388400
H	0.99689300	-6.50235700	-1.03901200
C	2.27202600	-6.71848500	-2.76669500
H	1.94378300	-7.73097900	-2.98675400
C	3.22908100	-6.09978300	-3.57365900
H	3.64258100	-6.62581600	-4.43020200
C	3.65719500	-4.80322100	-3.28598000
H	4.39963600	-4.32285600	-3.91714600
C	9.18714700	-1.22218100	-0.14788200
C	9.95244000	-1.66190500	-1.23976700
H	9.52168800	-1.62441500	-2.23647300
C	11.25310700	-2.13354000	-1.05794800
H	11.83092400	-2.46417600	-1.91712800
C	11.81160700	-2.17635100	0.22084800
H	12.82437400	-2.54385300	0.36347100
C	11.06011900	-1.74462500	1.31514400
H	11.48504600	-1.77991300	2.31521400
C	9.75992000	-1.27118800	1.13209700
H	9.17287000	-0.94651500	1.98607600
C	6.09992100	5.06630700	0.17491500
C	6.24213100	6.07149800	-0.79508200
H	6.02857800	5.83732800	-1.83421400
C	6.66177300	7.35396800	-0.43971000
H	6.77007800	8.11656200	-1.20658200
C	6.94730900	7.65542000	0.89322600

H	7.27349300	8.65433100	1.17029100
C	6.81193500	6.66514100	1.86780200
H	7.02818400	6.89116300	2.90880000
C	6.39336200	5.38280700	1.51075600
H	6.28310700	4.61615500	2.27290500
C	-1.10729500	-0.73252300	3.85672200
C	0.27235400	-0.86901300	3.97677400
H	0.66877000	-1.24821300	4.91537500
C	1.11772200	-0.53228600	2.91185400
C	0.57598400	-0.05558200	1.71052200
H	1.25064300	0.13629000	0.88717100
C	-0.81241500	0.13440100	1.60908800
C	-1.64329800	-0.20083900	2.67776400
H	-2.70301100	-0.00296100	2.56579200
C	-1.96190900	-1.17971300	5.02078700
C	-1.48471900	0.71148500	0.38595200
C	3.58271800	-0.32555000	2.38539400
N	-3.23860900	-1.47002300	4.63409900
H	-3.41098300	-1.42595500	3.63971500
N	-0.66233800	1.44417700	-0.40670300
H	0.30576200	1.49083200	-0.11697500
N	2.50304600	-0.69930400	3.13821200
H	2.72977000	-1.00600300	4.07533000
O	-1.51481600	-1.28633400	6.15872900
O	-2.69462900	0.54904800	0.16748700
O	3.47410600	0.18415700	1.26109600
C	4.89594100	-0.53304500	3.07221300
C	5.87414100	0.46271900	2.95428800
H	5.68059500	1.33118700	2.33504400
C	7.08013800	0.33890000	3.64228500
H	7.82733400	1.12194300	3.55442000
C	7.32666000	-0.78682700	4.43177400
H	8.26804900	-0.88130500	4.96614200
C	6.36576700	-1.79592800	4.52940800
H	6.56281900	-2.68331100	5.12388300
C	5.15077900	-1.66777900	3.85887600
H	4.41784500	-2.46866800	3.91875900



Cartesian coordinates for Geometry Optimized Conformer B

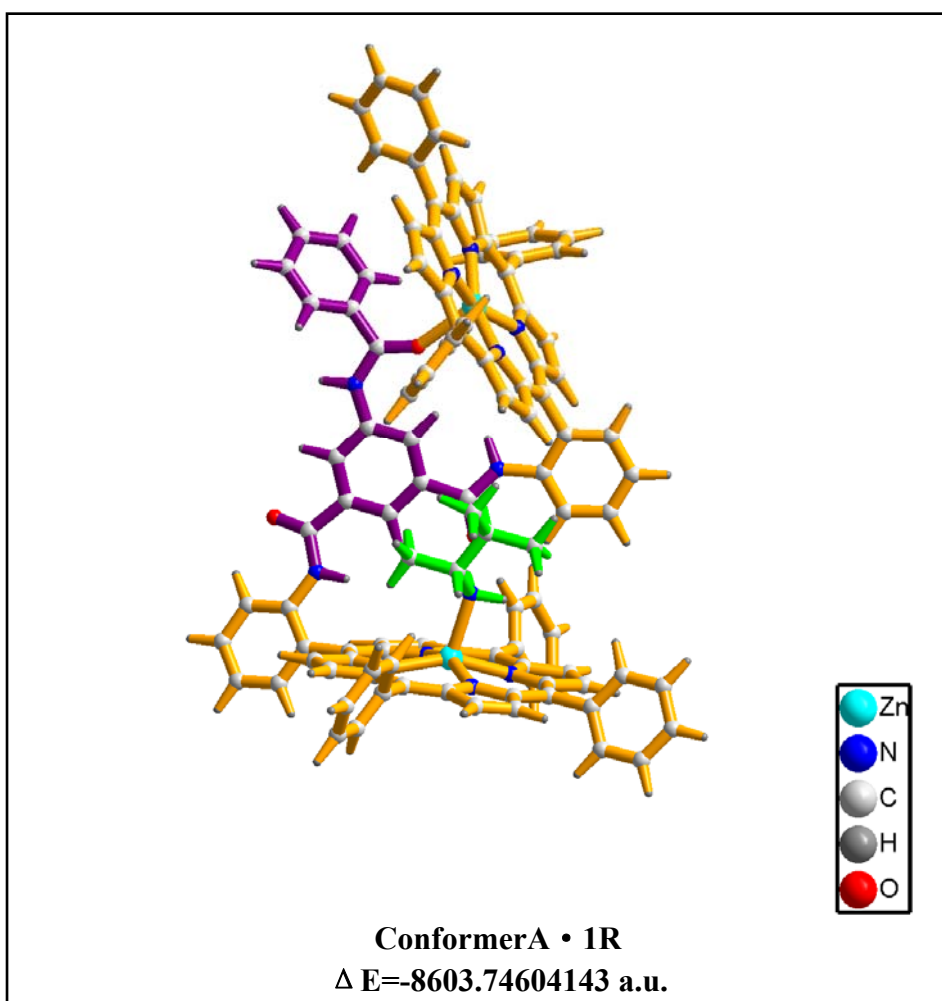
Atoms	x	y	z
Zn	4.91227400	-0.22508500	-0.04586100
N	4.93762800	-2.09288800	0.87575200
N	5.72741100	0.56310400	1.69527500
N	5.66924400	1.42649400	-1.05459300
N	4.74982800	-1.19758800	-1.86039300
C	5.56989500	-1.41578900	3.17747700
C	6.21006400	2.85717800	0.89403600
C	5.32694000	0.66636700	-3.38881200
C	4.22950500	-3.48156200	-1.04710600
C	4.52159000	-3.27756200	0.31380300
C	5.15399000	-2.35060600	2.20927900
C	5.83665100	-0.05791500	2.91689700
C	6.09574600	1.87393100	1.89258000
C	6.24299600	3.61438800	-1.51601700
H	6.52170600	4.64444900	-1.34829800
C	5.66818700	1.62488100	-2.41453500

C	4.90233700	-0.64582600	-3.11077300
C	4.38498200	-2.50698400	-2.05328700
C	4.45435100	-4.30613400	1.33070800
H	4.14832200	-5.32901400	1.16702700
C	4.85778800	-3.73717200	2.49836700
H	4.95368400	-4.20593400	3.46784600
C	6.27334600	0.89189100	3.91699500
H	6.45070700	0.66402800	4.95831500
C	6.43551000	2.08437200	3.28390700
H	6.77635400	3.01732900	3.70889900
C	6.03422700	2.62301100	-0.48415600
C	6.03257200	2.99369400	-2.70934200
H	6.11044700	3.42174300	-3.69842500
C	4.61952800	-1.64091400	-4.12250700
H	4.69119600	-1.48611000	-5.18906900
C	4.28999600	-2.78702700	-3.46997200
H	4.04338000	-3.74562000	-3.90250300
C	4.38404700	-1.83929800	5.35849100
C	5.59328100	-1.85617100	4.61815200
C	6.76609300	-2.24050500	5.27092700
H	7.69555300	-2.25658200	4.70849400
C	6.75546000	-2.58758100	6.62479300
H	7.67842600	-2.88202500	7.11620500
C	5.55787400	-2.54771400	7.33942200
H	5.54418300	-2.81102300	8.39371800
C	4.36573000	-2.17790400	6.71579600
H	3.42847000	-2.14366700	7.25646600
C	6.59189600	4.24048500	1.32698900
C	5.68964200	5.03531900	2.05096100
H	4.70620900	4.63809200	2.28694600
C	6.04001400	6.32274500	2.46028300
H	5.32528000	6.92413100	3.01614700
C	7.30091400	6.83770500	2.15429000
H	7.57448000	7.83994600	2.47329300
C	8.20905100	6.05614700	1.43758000
H	9.19568300	6.44571500	1.20030100
C	7.85755600	4.76908000	1.02841100
H	8.56950800	4.15988100	0.47846900
C	5.44672900	1.06791500	-4.82785100
C	6.70672100	1.31770000	-5.39491100
H	7.59442700	1.21335200	-4.77727700
C	6.82776800	1.68509400	-6.73556800
H	7.81292700	1.86838900	-7.15670400
C	5.68955900	1.81011200	-7.53444500

H	5.78301400	2.09567400	-8.57890300
C	4.43072900	1.56539300	-6.98277100
H	3.53834500	1.66369800	-7.59568700
C	4.30999800	1.19708300	-5.64182400
H	3.32834300	1.01777200	-5.21356000
C	3.77855500	-4.84358300	-1.47848100
C	4.64338400	-5.94800500	-1.41674600
H	5.65468100	-5.80817900	-1.04523300
C	4.22321100	-7.20970300	-1.83972600
H	4.91020200	-8.05054500	-1.78882300
C	2.93089500	-7.38946500	-2.33644500
H	2.60551600	-8.37137100	-2.67012300
C	2.06116800	-6.29942200	-2.40594200
H	1.05261800	-6.42550500	-2.79043700
C	2.48162100	-5.03884500	-1.97931600
H	1.80074100	-4.19355300	-2.03128100
Zn	-4.52555000	0.44446000	-0.74919700
N	-3.77977500	2.34784600	-1.10863100
N	-2.91448000	-0.33324900	-1.79687800
N	-5.50658600	-1.35651300	-1.06018000
N	-6.36319100	1.31346300	-0.34134200
C	-1.57998600	1.73466600	-2.06427500
C	-3.59682600	-2.71120200	-1.86783700
C	-7.79265300	-0.71161500	-0.35643300
C	-5.65338000	3.68728700	-0.20476900
C	-2.50902200	2.64907600	-1.53203800
C	-4.33956900	3.52867900	-0.68250500
C	-1.79603600	0.34918800	-2.20475100
C	-2.69319100	-1.65739700	-2.09049800
C	-4.91416500	-2.55067500	-1.39456400
C	-6.81043300	-1.64564700	-0.73511500
C	-7.56841400	0.66776500	-0.18978300
C	-6.59854300	2.64593200	-0.09875400
C	-2.24973700	4.06204500	-1.34864200
H	-1.32668800	4.56622600	-1.59749900
C	-3.37834400	4.60373100	-0.81725500
H	-3.54922900	5.63429700	-0.54227300
C	-0.84408200	-0.56969900	-2.79281200
H	0.11087900	-0.29478900	-3.21813100
C	-1.39734700	-1.80995400	-2.71871500
H	-0.98321800	-2.74111900	-3.07778700
C	-5.86281200	-3.63099600	-1.23383300
H	-5.65661300	-4.67677900	-1.40927700
C	-7.03739900	-3.07041400	-0.83750300

H	-7.97065800	-3.57179100	-0.62567800
C	-8.59635000	1.62601200	0.15068900
H	-9.64202800	1.39543700	0.29485900
C	-7.99609000	2.84613100	0.21729100
H	-8.45949500	3.80035800	0.42244200
C	0.89536500	2.06968400	-1.65549700
C	2.15465000	2.53553100	-2.04484500
H	3.01122400	2.37885400	-1.40337400
C	2.28907100	3.20844900	-3.25944000
H	3.26935300	3.57023700	-3.55222700
C	1.18197100	3.42129600	-4.08108200
H	1.29228200	3.94931400	-5.02406100
C	-0.07093200	2.94868300	-3.68796700
H	-0.93917200	3.09882300	-4.32331000
C	-0.23707400	2.26368300	-2.48027900
C	-3.13476900	-4.10072400	-2.18835900
C	-2.16731000	-4.73064000	-1.39050500
H	-1.75579800	-4.19818600	-0.53750100
C	-1.74147700	-6.02961600	-1.67380900
H	-0.99693600	-6.50239800	-1.03893000
C	-2.27206700	-6.71854000	-2.76661300
H	-1.94383000	-7.73103900	-2.98665900
C	-3.22911700	-6.09984300	-3.57358700
H	-3.64261800	-6.62588400	-4.43012400
C	-3.65722300	-4.80327500	-3.28592500
H	-4.39966000	-4.32291200	-3.91709800
C	-9.18715700	-1.22217100	-0.14786300
C	-9.95245800	-1.66189500	-1.23974200
H	-9.52171100	-1.62441000	-2.23645000
C	-11.25312600	-2.13352300	-1.05791400
H	-11.83095000	-2.46415900	-1.91709000
C	-11.81162000	-2.17632700	0.22088500
H	-12.82438800	-2.54382400	0.36351500
C	-11.06012300	-1.74460100	1.31517600
H	-11.48504600	-1.77988400	2.31524700
C	-9.75992300	-1.27117100	1.13212000
H	-9.17286700	-0.94649900	1.98609400
C	-6.09990500	5.06630800	0.17484100
C	-6.24210700	6.07148800	-0.79517000
H	-6.02855300	5.83730300	-1.83429800
C	-6.66174400	7.35396500	-0.43981600
H	-6.77004300	8.11654900	-1.20669700
C	-6.94728200	7.65543500	0.89311600
H	-7.27346100	8.65435200	1.17016700

C	-6.81191600	6.66516800	1.86770500
H	-7.02816600	6.89120500	2.90869900
C	-6.39334900	5.38282800	1.51067600
H	-6.28310000	4.61618400	2.27283600
C	1.10729700	-0.73244300	3.85673600
C	-0.27235200	-0.86893000	3.97679300
H	-0.66876700	-1.24811000	4.91540200
C	-1.11772100	-0.53222700	2.91186500
C	-0.57598300	-0.05554900	1.71052300
H	-1.25064400	0.13630800	0.88716900
C	0.81241600	0.13443300	1.60908300
C	1.64329900	-0.20078500	2.67776600
H	2.70301200	-0.00291000	2.56579000
C	1.96191200	-1.17961000	5.02080900
C	1.48471700	0.71149000	0.38593400
C	-3.58271800	-0.32550900	2.38539900
N	3.23861500	-1.46992100	4.63412700
H	3.41099200	-1.42586800	3.63974200
N	0.66233600	1.44416500	-0.40673600
H	-0.30576600	1.49082000	-0.11701300
N	-2.50304500	-0.69923800	3.13822800
H	-2.72976900	-1.00591100	4.07535600
O	1.51482000	-1.28621000	6.15875300
O	2.69462800	0.54905000	0.16747100
O	-3.47410700	0.18416300	1.26108500
C	-4.89593900	-0.53298300	3.07222600
C	-5.87413900	0.46277900	2.95427600
H	-5.68059400	1.33123100	2.33500900
C	-7.08013400	0.33897900	3.64227800
H	-7.82733000	1.12201900	3.55439500
C	-7.32665600	-0.78672800	4.43179800
H	-8.26804500	-0.88119100	4.96616900
C	-6.36576300	-1.79582600	4.52945700
H	-6.56281500	-2.68319400	5.12395500
C	-5.15077600	-1.66769600	3.85891900
H	-4.41784300	-2.46858400	3.91882200



Cartesian coordinates for Geometry Optimized ConformerA · 5R

Atoms	x	y	z
Zn	-5.71881600	0.19186200	0.35985500
N	-6.13573900	-1.42033900	1.61426700
N	-5.15660900	1.27312200	2.04947600
N	-6.06682000	2.04124700	-0.59605500
N	-7.02517700	-0.66610000	-1.03823600
C	-5.13012400	-0.56684400	3.71124200
C	-4.96359300	3.53122700	1.04133100
C	-7.23769500	1.22862800	-2.62198600
C	-7.24157900	-2.91583500	-0.02194700
C	-6.63938600	-2.63736900	1.21986900
C	-5.68930600	-1.57845400	2.90297100
C	-4.92285400	0.76805100	3.30398100
C	-4.82633200	2.60517300	2.09340500
C	-5.77241500	4.23352900	-1.25364600
H	-5.47353400	5.27093500	-1.21346700
C	-6.59588900	2.21876800	-1.85063000

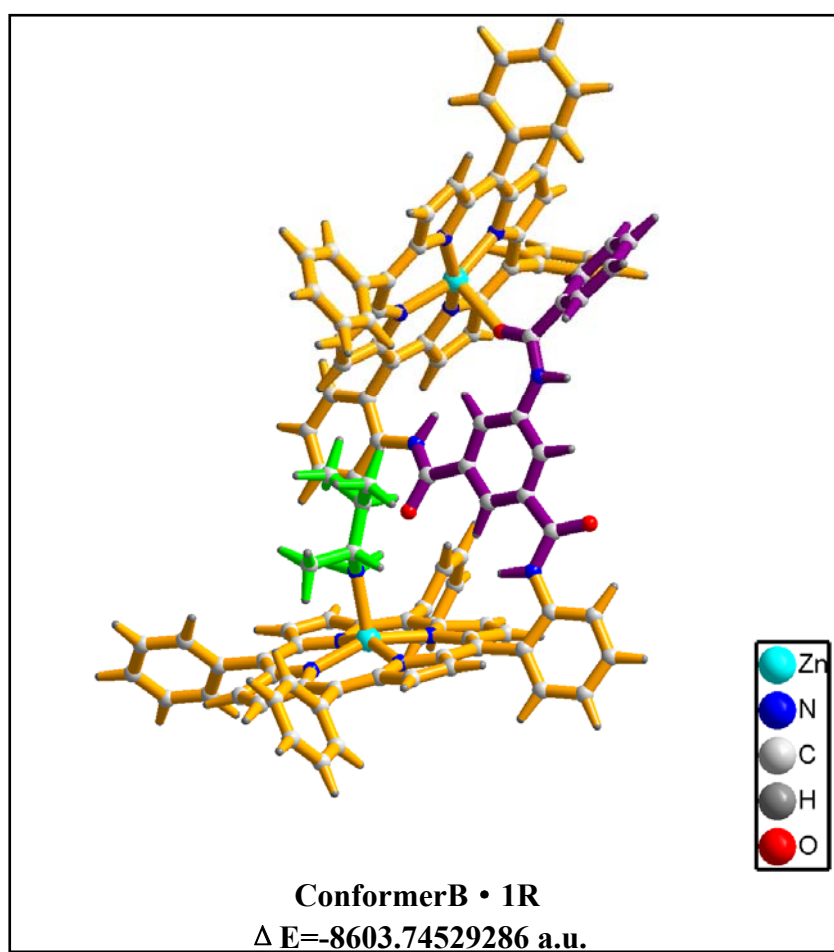
C	-7.44745600	-0.10539100	-2.21916400
C	-7.43795800	-1.97448400	-1.05447700
C	-6.46856100	-3.60417900	2.28478500
H	-6.76018200	-4.64348400	2.24038300
C	-5.88675700	-2.94937900	3.32582300
H	-5.61609700	-3.35220500	4.29125200
C	-4.43468000	1.81895500	4.17387400
H	-4.20310800	1.70585400	5.22378800
C	-4.36896400	2.95188500	3.42381300
H	-4.07220100	3.93972000	3.74517500
C	-5.56825400	3.25703900	-0.20296400
C	-6.42125800	3.59535200	-2.26538000
H	-6.75852400	4.01518500	-3.20212100
C	-8.14489000	-1.09831300	-3.01042700
H	-8.58383900	-0.92956400	-3.98306400
C	-8.14698700	-2.25028400	-2.28703100
H	-8.59520700	-3.19651800	-2.55343000
C	-3.47506600	-1.06775500	5.59908600
C	-4.80608400	-0.92328700	5.13528400
C	-5.85192700	-1.12804300	6.04395600
H	-6.87087700	-1.01111900	5.68642200
C	-5.61098400	-1.46794700	7.37423600
H	-6.44196200	-1.61786000	8.05765800
C	-4.29514900	-1.60940200	7.81217000
H	-4.08701200	-1.87538600	8.84516200
C	-3.22860100	-1.41390500	6.93704400
H	-2.20746400	-1.53010600	7.26990100
C	-4.43603000	4.91353100	1.27529000
C	-3.05293300	5.12525500	1.39581400
H	-2.38264300	4.27414300	1.31020200
C	-2.54333900	6.40591600	1.61422300
H	-1.46936800	6.55102600	1.69896100
C	-3.40805900	7.49699700	1.71979800
H	-3.01173800	8.49440300	1.89112600
C	-4.78544600	7.29880100	1.60590500
H	-5.46672200	8.14121000	1.69440700
C	-5.29493200	6.01815000	1.38591900
H	-6.36774300	5.86543500	1.30724000
C	-7.75461200	1.63456200	-3.97061900
C	-9.13169500	1.78328200	-4.19738700
H	-9.82453600	1.60418300	-3.37984600
C	-9.61277200	2.16207500	-5.45151800
H	-10.68279000	2.27501500	-5.60597600
C	-8.72440500	2.40026700	-6.50184300

H	-9.09874100	2.69547800	-7.47851200
C	-7.35211600	2.25744400	-6.28926200
H	-6.65252000	2.43792500	-7.10144600
C	-6.87255600	1.87825900	-5.03457400
H	-5.80387900	1.76428600	-4.87331900
C	-7.74313200	-4.30931200	-0.25517900
C	-8.84944800	-4.80528600	0.45260700
H	-9.34585800	-4.16280900	1.17445100
C	-9.31732300	-6.10141200	0.23194200
H	-10.17824200	-6.46478000	0.78720900
C	-8.68716200	-6.92604100	-0.70185700
H	-9.05144800	-7.93537600	-0.87422900
C	-7.58678900	-6.44513800	-1.41378300
H	-7.08782100	-7.08045100	-2.14117500
C	-7.12047700	-5.14857200	-1.19239400
H	-6.26177200	-4.77793800	-1.74561300
Zn	5.41994000	0.07484900	-1.01442500
N	5.05293700	2.11633300	-1.14699900
N	3.66960100	-0.25704400	-2.07391200
N	6.02248700	-1.83638100	-1.55498800
N	7.39877300	0.52542400	-0.60023000
C	2.76446500	2.04842200	-2.08487800
C	3.86597400	-2.70287100	-2.40826200
C	8.40540800	-1.72191000	-0.88847900
C	7.17069400	2.96280100	-0.18968400
C	3.86122400	2.70319000	-1.49534700
C	5.84243600	3.11450300	-0.62876200
C	2.70437900	0.67062700	-2.37497300
C	3.18803400	-1.47352200	-2.49429500
C	5.19759100	-2.85286600	-1.97373600
C	7.24958400	-2.40488600	-1.31190800
C	8.45863900	-0.35142700	-0.57229600
C	7.89507900	1.75345300	-0.23194200
C	3.89063500	4.11316900	-1.16775400
H	3.08316900	4.81141200	-1.33834000
C	5.11203100	4.36571100	-0.62514100
H	5.48944500	5.30956200	-0.25967700
C	1.58498800	0.02377600	-3.02579100
H	0.70326400	0.52564200	-3.39865500
C	1.88267800	-1.30190700	-3.09630700
H	1.29101500	-2.09035100	-3.53850600
C	5.91552800	-4.10846800	-1.95038600
H	5.50101900	-5.07151500	-2.21054600
C	7.18671600	-3.82977400	-1.55349100

H	8.00583500	-4.52244100	-1.42540700
C	9.66184600	0.34985600	-0.18262100
H	10.64625300	-0.08981900	-0.11249000
C	9.31236900	1.64668700	0.03886400
H	9.95764800	2.46608900	0.32088500
C	0.42581100	2.80707200	-1.50431000
C	-0.75691600	3.49332100	-1.80584500
H	-1.59720900	3.43836500	-1.12730100
C	-0.83532200	4.24021300	-2.98147400
H	-1.75564600	4.77102700	-3.20874600
C	0.25355000	4.31723200	-3.84978900
H	0.18975700	4.90525400	-4.76094700
C	1.42739600	3.62523100	-3.54648300
H	2.27608500	3.66175100	-4.22369100
C	1.53166500	2.85440000	-2.38468800
C	3.12568000	-3.93104000	-2.84350700
C	2.04415500	-4.41240900	-2.08893300
H	1.75666900	-3.88725500	-1.18219700
C	1.34622800	-5.55383200	-2.48562900
H	0.51585600	-5.91430000	-1.88391900
C	1.71567400	-6.23291800	-3.64815600
H	1.17214700	-7.12117700	-3.95886700
C	2.78713200	-5.76283500	-4.40984700
H	3.07814500	-6.28113000	-5.31983800
C	3.48598200	-4.62254300	-4.01076600
H	4.31462400	-4.25479900	-4.60948100
C	9.67831400	-2.50914600	-0.80017500
C	10.30052300	-2.98289000	-1.96636400
H	9.84867700	-2.76856200	-2.93083700
C	11.48864100	-3.71127500	-1.89767800
H	11.95748600	-4.06412300	-2.81257700
C	12.07546800	-3.98166300	-0.66006200
H	13.00074800	-4.54909500	-0.60567800
C	11.46514400	-3.51923100	0.50711200
H	11.91182900	-3.73057200	1.47547400
C	10.27757800	-2.78922400	0.43736800
H	9.79764000	-2.44088200	1.34706300
C	7.88722200	4.17951200	0.31202000
C	8.20847500	5.23704700	-0.55392300
H	7.93580100	5.16318100	-1.60293700
C	8.87847800	6.36748200	-0.08440900
H	9.12202400	7.17303300	-0.77225300
C	9.24007300	6.46155600	1.26076700
H	9.76117100	7.34213700	1.62680900

C	8.92910000	5.41638800	2.13236800
H	9.20342400	5.48165500	3.18212300
C	8.26038800	4.28592200	1.66110400
H	8.01449900	3.47710600	2.34384800
N	-3.87386000	-0.12281600	-0.72228500
H	-4.09704900	0.45419900	-1.53223600
H	-3.09525600	0.35817300	-0.25844400
C	-3.44049100	-1.46995100	-1.18035300
H	-4.34365000	-1.96021700	-1.56861000
C	-2.94468400	-2.24944500	0.04123700
H	-2.75037600	-3.29712100	-0.20262000
H	-2.01407300	-1.81404400	0.42835300
H	-3.69420700	-2.22538200	0.83637600
C	-2.07220200	-2.83147000	-2.84834300
H	-1.60881400	-3.46200600	-2.08375500
H	-2.98032800	-3.33904800	-3.20040800
H	-1.37619400	-2.78097400	-3.69317700
C	-2.39799600	-1.42006600	-2.33020100
H	-1.47296500	-0.98371400	-1.92295300
C	-2.86147800	-0.53702000	-3.50287700
H	-2.15049000	-0.60165000	-4.33429600
H	-3.84080400	-0.85993600	-3.88094100
H	-2.93161100	0.52231300	-3.23119000
C	-0.23244000	-0.54098200	3.66851500
C	1.09423000	-0.97249700	3.70077600
H	1.41735600	-1.54717300	4.56441800
C	1.97884500	-0.66034400	2.66401600
C	1.53223300	0.09431400	1.57219800
H	2.22236400	0.27714700	0.76041600
C	0.21279900	0.56919600	1.55913800
C	-0.66782800	0.24794700	2.59911400
H	-1.66852600	0.66493900	2.55644700
C	-1.07997100	-0.93271100	4.85767500
C	-0.33341600	1.43511600	0.45205300
C	4.42456800	-0.86838000	2.06021400
N	-2.43287800	-0.84556300	4.67046100
H	-2.75648700	-0.59643100	3.74446400
N	0.60137800	2.06674100	-0.31122800
H	1.57142700	1.89217100	-0.08502600
N	3.30706400	-1.12305700	2.80757100
H	3.48574800	-1.58461600	3.69000100
O	-0.54088300	-1.31042000	5.89580700
O	-1.55011400	1.56510400	0.28382300
O	4.39561400	-0.21175200	1.00901600

C	5.68724300	-1.40054800	2.66171300
C	6.83672100	-0.60147600	2.60985900
H	6.80066600	0.35330800	2.09771700
C	8.01173000	-1.03010700	3.22524600
H	8.89354200	-0.39729100	3.19006500
C	8.05439100	-2.26581500	3.87523800
H	8.97193700	-2.59846600	4.35282600
C	6.91894700	-3.07878800	3.90507100
H	6.95435100	-4.05023000	4.38954900
C	5.73641300	-2.64621700	3.30792900
H	4.86483100	-3.29629100	3.31344800



Cartesian coordinates for Geometry Optimized ConformerB·5R

Atoms	x	y	z
Zn	5.86412900	0.23702500	0.32667800
N	6.48751600	-1.39536900	1.46861600
N	4.96625300	0.99594100	2.06787700
N	5.90105800	2.21227300	-0.39632200
N	7.44544000	-0.17169200	-0.97927200

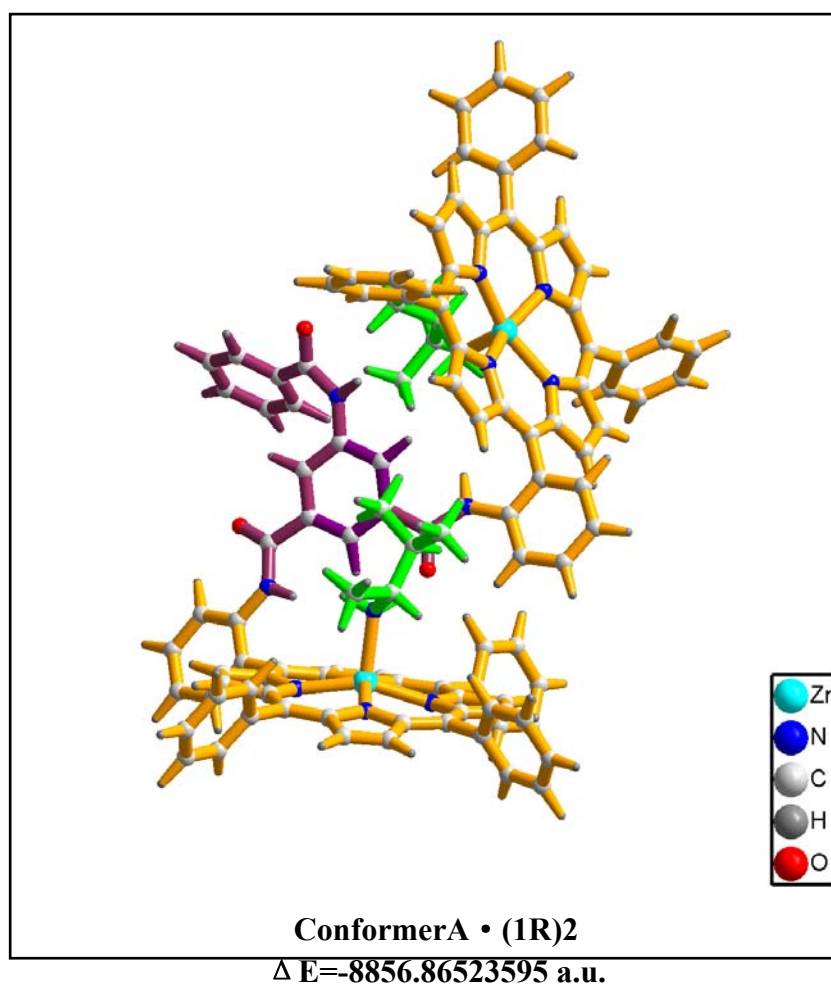
C	5.14846400	-1.01008100	3.51622900
C	4.43145600	3.28608600	1.28173300
C	7.34478600	1.87329900	-2.37872600
C	8.10778500	-2.39834000	-0.11427700
C	7.27991500	-2.42747400	1.02530700
C	5.93909200	-1.80479800	2.65900200
C	4.75992000	0.32008700	3.24489100
C	4.42984000	2.24923800	2.23515300
C	5.07376400	4.29432000	-0.94918900
H	4.51072700	5.21309400	-0.87014000
C	6.41449400	2.60264800	-1.60866800
C	7.85739900	0.60590200	-2.03379500
C	8.20892800	-1.31204000	-1.00936600
C	7.17453500	-3.54941000	1.93512700
H	7.67208100	-4.50101700	1.81688700
C	6.34765100	-3.16483300	2.94469300
H	6.04618800	-3.74214500	3.80674000
C	4.08581700	1.18165400	4.19511900
H	3.83541600	0.91695100	5.21299600
C	3.88026400	2.37233000	3.57008300
H	3.42792700	3.26318200	3.98099000
C	5.10453400	3.23942800	0.04268600
C	5.88138400	3.89914400	-1.97147500
H	6.09800100	4.43370300	-2.88489800
C	8.93637100	-0.05591000	-2.73689300
H	9.47256100	0.34788600	-3.58346200
C	9.15522700	-1.23929200	-2.10278800
H	9.90199700	-1.98446500	-2.33563300
C	3.47429500	-1.92452300	5.23252600
C	4.79978000	-1.58586900	4.86032000
C	5.82367200	-1.80449800	5.79213000
H	6.83721900	-1.53526500	5.51001400
C	5.56937600	-2.34456300	7.05146000
H	6.38442500	-2.49814200	7.75301400
C	4.26096600	-2.67996200	7.39554100
H	4.04209400	-3.10503400	8.37150400
C	3.21564800	-2.47568500	6.49754700
H	2.20032000	-2.73727200	6.75728700
C	3.68612200	4.53842500	1.62441800
C	2.29115800	4.51703600	1.78537200
H	1.76138700	3.58037000	1.64056700
C	1.59084800	5.67940000	2.11017900
H	0.51034600	5.64300900	2.22313900
C	2.27303700	6.88508500	2.28302400

H	1.72821700	7.79049500	2.53725200
C	3.66015300	6.92031800	2.12715900
H	4.20103500	7.85297000	2.26582600
C	4.35977800	5.75813700	1.80032600
H	5.44008600	5.78688700	1.68916000
C	7.85569800	2.50356000	-3.63725800
C	8.61153400	3.68678600	-3.59867600
H	8.83081100	4.14256800	-2.63733400
C	9.09012900	4.26937200	-4.77267900
H	9.67861100	5.18172500	-4.71929300
C	8.82176300	3.68022800	-6.00965800
H	9.19432200	4.13396700	-6.92423800
C	8.07345500	2.50289900	-6.06334200
H	7.85669300	2.03747200	-7.02147500
C	7.59682400	1.92044800	-4.88845100
H	7.01203300	1.00591500	-4.93442700
C	8.96717800	-3.59592300	-0.38278600
C	10.00433900	-3.95193100	0.49463400
H	10.18334100	-3.34194700	1.37550100
C	10.80623300	-5.06528700	0.24064100
H	11.60741700	-5.31980000	0.92975000
C	10.58565700	-5.84545100	-0.89595000
H	11.20997500	-6.71281300	-1.09363900
C	9.55882800	-5.50286800	-1.77749700
H	9.37690800	-6.10564500	-2.66362400
C	8.75891300	-4.38824000	-1.52328600
H	7.95769700	-4.12760800	-2.20917900
Zn	-5.56843100	0.19468800	-0.99726400
N	-5.02464000	2.19273100	-0.81862800
N	-3.94425000	-0.08153700	-2.25601700
N	-6.38677400	-1.53588400	-1.79838300
N	-7.46003800	0.72168900	-0.33675300
C	-2.83210000	2.11266800	-1.96320000
C	-4.39322000	-2.40726400	-2.98001500
C	-8.69645100	-1.34545700	-0.92272600
C	-6.97213900	3.02064200	0.46157300
C	-3.81435700	2.73664100	-1.17248400
C	-5.67407100	3.14265000	-0.06749000
C	-2.92356100	0.80706700	-2.48548800
C	-3.61295000	-1.23806300	-2.92029100
C	-5.69595900	-2.52545500	-2.45633700
C	-7.64359400	-2.03473600	-1.55324600
C	-8.59505200	-0.05526000	-0.36971600
C	-7.80878100	1.90005500	0.27962200

C	-3.68636100	4.06507200	-0.61119400
H	-2.83346600	4.71702200	-0.73852400
C	-4.83189400	4.31252200	0.07903200
H	-5.08985100	5.20398300	0.63190100
C	-1.92449900	0.20077900	-3.33881100
H	-1.03106600	0.68979000	-3.70024400
C	-2.34976400	-1.06378600	-3.60632400
H	-1.87215000	-1.80284700	-4.23316600
C	-6.52816900	-3.70180700	-2.58525000
H	-6.22822700	-4.63452000	-3.04012600
C	-7.73614800	-3.39337000	-2.04055600
H	-8.60820100	-4.02662100	-1.96454700
C	-9.69432200	0.66032400	0.23918300
H	-10.70882900	0.29712600	0.31773200
C	-9.20653600	1.86252700	0.65129800
H	-9.74777600	2.66793400	1.12640900
C	-0.40761300	2.60174300	-1.44508600
C	0.80740200	3.24010300	-1.72406400
H	1.67766500	3.02770500	-1.11877300
C	0.87736600	4.14712000	-2.78139000
H	1.82431900	4.63664800	-2.99127000
C	-0.24920700	4.43070700	-3.55305100
H	-0.19061700	5.14200600	-4.37197900
C	-1.45594200	3.78662300	-3.27298700
H	-2.33709800	3.98588200	-3.87639400
C	-1.55531200	2.86011200	-2.23117600
C	-3.80686200	-3.59218600	-3.68513500
C	-2.70210500	-4.26711200	-3.14174100
H	-2.28413200	-3.92419800	-2.19909800
C	-2.14506700	-5.36900200	-3.79179200
H	-1.29260400	-5.87998600	-3.35171800
C	-2.68196100	-5.81508900	-5.00071600
H	-2.24838100	-6.67250100	-5.50850300
C	-3.77829100	-5.15125200	-5.55436800
H	-4.19886500	-5.48664800	-6.49884100
C	-4.33535300	-4.05013700	-4.90259300
H	-5.18247800	-3.53011600	-5.34100000
C	-10.03215700	-2.02544200	-0.87167800
C	-10.77735600	-2.20851500	-2.04757600
H	-10.37396100	-1.84977200	-2.99039200
C	-12.02474200	-2.83287700	-2.01361500
H	-12.58850300	-2.95989000	-2.93416700
C	-12.54892800	-3.28844700	-0.80250900
H	-13.52042100	-3.77482500	-0.77550800

C	-11.81649400	-3.11593300	0.37314900
H	-12.21412600	-3.47319100	1.31980600
C	-10.56954200	-2.48969200	0.33841400
H	-9.99520000	-2.36795100	1.25178800
C	-7.52965400	4.18061400	1.22891200
C	-7.81897200	5.39735300	0.59063400
H	-7.63824500	5.49100000	-0.47652400
C	-8.34214100	6.47412800	1.30756700
H	-8.56389600	7.40585000	0.79367000
C	-8.58580100	6.35429400	2.67705700
H	-8.99262100	7.19302400	3.23562100
C	-8.30475600	5.14958300	3.32395400
H	-8.48786300	5.04750800	4.39051000
C	-7.78320400	4.07306400	2.60541800
H	-7.56021200	3.13865200	3.11332800
C	0.24891400	-1.33794200	3.28951800
C	-1.08105300	-1.76097200	3.28057500
H	-1.40392400	-2.42426900	4.07823400
C	-1.97029800	-1.32466900	2.29366900
C	-1.52321300	-0.46129900	1.28592200
H	-2.21499900	-0.18197700	0.50322500
C	-0.19836100	-0.00298000	1.31482400
C	0.68366400	-0.44053000	2.30967400
H	1.68539500	-0.02434100	2.30422800
C	1.09565000	-1.85475300	4.43099900
C	0.35486500	0.96962500	0.30446200
C	-4.44043600	-1.35531600	1.76720700
N	2.44628700	-1.67978300	4.29364800
H	2.77521800	-1.27327000	3.42783500
N	-0.57585200	1.70154200	-0.36731400
H	-1.54503000	1.53378200	-0.13138000
N	-3.30303600	-1.78523300	2.39685700
H	-3.46689200	-2.38536200	3.19494300
O	0.55684100	-2.39406300	5.39544300
O	1.57285300	1.08894100	0.13593700
O	-4.42889600	-0.51786100	0.85377700
C	-5.69488700	-1.94324300	2.33307500
C	-6.79481300	-1.09941700	2.53454700
H	-6.73598600	-0.06136100	2.22696200
C	-7.94812700	-1.59359000	3.14195000
H	-8.78976800	-0.92795500	3.30918700
C	-8.02075000	-2.93426400	3.52749600
H	-8.92181900	-3.31705600	3.99884100
C	-6.93738100	-3.78617500	3.30088700

H	-6.99841400	-4.83440100	3.57866900
C	-5.77371800	-3.29203700	2.71446800
H	-4.94156300	-3.96462500	2.52138900
H	4.07584700	-2.37974900	-0.13455300
C	3.81037500	-1.83172600	-1.04773000
N	4.09881800	-0.39651200	-0.75842800
H	4.12498900	0.12375200	-1.63664600
H	3.31652700	0.01600700	-0.23964800
C	2.30108400	-2.08685400	-1.30826100
H	1.77622300	-1.67716900	-0.43353900
C	1.98143300	-3.58883800	-1.36135800
H	0.89707800	-3.74869000	-1.38163100
H	2.39679600	-4.06248900	-2.25867900
H	2.38086700	-4.11724000	-0.48687000
C	1.75496700	-1.36194600	-2.54787300
H	1.94633600	-0.28393100	-2.50573900
H	2.19312500	-1.75287000	-3.47417600
H	0.66922300	-1.49248800	-2.61797500
C	4.73295100	-2.31087000	-2.17006300
H	5.77749900	-2.13506100	-1.90434100
H	4.60226000	-3.38162300	-2.35355000
H	4.52968400	-1.78177700	-3.10929700



Cartesian coordinates for Geometry Optimized ConformerA·(5R)₂

Atoms	x	y	z
Zn	6.23070700	0.35285600	-0.34828400
N	7.79046800	0.70025700	0.99172000
N	7.03218000	-1.55868500	-0.66402400
N	5.31905200	0.17048200	-2.23498300
N	6.07262600	2.42886700	-0.57504100
C	8.68410700	-1.60553900	1.17980200
C	5.69078400	-2.25052000	-2.62733100
C	4.57505400	2.51326400	-2.54601200
C	7.47306000	3.13501100	1.34037800
C	8.09725900	1.89636800	1.59369800
C	8.65159700	-0.23458100	1.51193600
C	7.90372100	-2.21000200	0.17484600
C	6.54724000	-2.50278300	-1.53512000
C	5.17786700	-0.98034100	-2.96920400
C	4.67140700	1.16201900	-2.92953700
C	5.21870300	3.08201000	-1.42800300

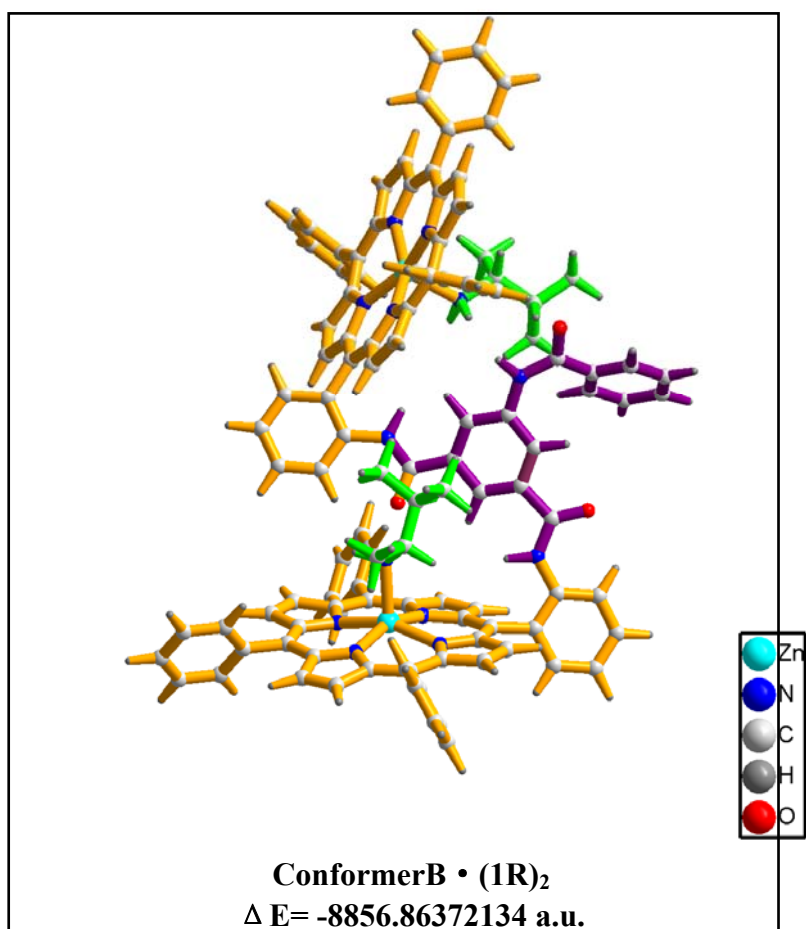
C	6.51783500	3.36273200	0.32761800
C	9.20215400	1.71270200	2.51088900
H	9.66950000	2.49450900	3.09185000
C	9.54668400	0.39772600	2.45783400
H	10.34718100	-0.09703100	2.98841600
C	7.92789800	-3.62272500	-0.14535700
H	8.51050800	-4.37248800	0.36995600
C	7.08971700	-3.80394700	-1.20127200
H	6.86259200	-4.72801100	-1.71304200
C	4.42586100	-0.70442000	-4.17687700
H	4.19947100	-1.42357200	-4.95185900
C	4.11396000	0.61999400	-4.15210400
H	3.58103800	1.18675100	-4.90184700
C	5.08508800	4.46598400	-1.02301800
H	4.46431200	5.20424400	-1.51004600
C	5.88474500	4.63832700	0.06509800
H	6.03636800	5.54343500	0.63516700
C	9.64380100	-2.47511100	1.93364800
C	10.74691300	-3.05738300	1.28866000
H	10.90200800	-2.86546700	0.23069100
C	11.64344700	-3.86363300	1.99104600
H	12.49399400	-4.29993200	1.47361300
C	11.45315300	-4.10410400	3.35306800
H	12.15089800	-4.73224100	3.90055400
C	10.36104400	-3.53122100	4.00733400
H	10.20208200	-3.71525300	5.06682700
C	9.46632900	-2.72369900	3.30415300
H	8.61510400	-2.28330000	3.81604800
C	5.37813200	-3.40346700	-3.53977300
C	6.38898400	-3.92956800	-4.35457200
H	7.37251000	-3.47085800	-4.31060700
C	6.15739600	-5.00874100	-5.20604600
H	6.96024400	-5.39381800	-5.82832700
C	4.88768800	-5.58292000	-5.24693900
H	4.68912400	-6.42761800	-5.90132200
C	3.85616700	-5.08566900	-4.45315200
H	2.87228000	-5.53170600	-4.47352500
C	4.09121300	-3.99426500	-3.60249000
C	3.74520200	3.41704700	-3.40546600
C	2.35231800	3.25589300	-3.47622000
H	1.88510600	2.47612500	-2.88244300
C	1.57745000	4.09288100	-4.28036000
H	0.49936300	3.95769200	-4.31658000
C	2.18137100	5.10393800	-5.03013700

H	1.57786700	5.75502000	-5.65721900
C	3.56588300	5.27389700	-4.96899500
H	4.04593900	6.05486500	-5.55317800
C	4.34035600	4.43834800	-4.16317800
H	5.41843300	4.56713100	-4.12347000
C	7.88696500	4.30037300	2.18488100
C	8.56106000	5.39782400	1.62455500
H	8.78798900	5.39234100	0.56224100
C	8.94999600	6.47917300	2.41595400
H	9.47638000	7.31544100	1.96303000
C	8.67199600	6.48468700	3.78417500
H	8.97495800	7.32689800	4.40064600
C	8.00403500	5.39995700	4.35518800
H	7.78036300	5.39554800	5.41894400
C	7.61720300	4.31849700	3.56290200
H	7.09461600	3.47736200	4.01000900
N	4.46940200	-0.07789800	0.84163800
H	3.71017800	0.38227300	0.32846500
H	4.28861200	-1.07843500	0.74808200
C	5.23752600	-0.70653700	3.09124700
H	6.26384100	-0.74046600	2.71888400
H	4.81642600	-1.71729700	3.02251900
H	5.26938500	-0.42938800	4.14939900
C	4.41073500	0.29748900	2.28540000
H	4.89663200	1.27857500	2.35581100
Zn	-5.78038400	0.80061600	0.83042800
N	-6.64308800	-0.48067400	2.20683400
N	-7.70317200	1.47023100	0.33872300
N	-5.04676900	2.58876300	-0.00728600
N	-4.00224100	0.69147500	1.91859800
C	-9.02422000	-0.23459600	1.56138100
C	-7.09117800	3.30125200	-1.21659300
C	-2.73782400	2.56786000	0.88872800
C	-4.60700400	-1.17623600	3.43741600
C	-6.91868900	-2.10732200	3.82139500
C	-7.97270600	-0.81397100	2.30039200
C	-8.87688800	0.82193100	0.63870700
C	-8.00415300	2.40397100	-0.62203700
C	-5.72196800	3.39185700	-0.89647500
C	-3.61567700	4.20194500	-0.83398700
C	-2.88073500	1.47255200	1.76951100
C	-3.71179600	-0.23379800	2.89562300
C	-5.97929700	-1.25160000	3.12983500
C	-8.15054000	-1.83185500	3.31521400

H	-9.09704100	-2.25690700	3.61549600
C	-9.95189300	1.35654300	-0.17127900
C	-9.41187400	2.32954600	-0.95391000
H	-9.91637200	2.93866400	-1.68970200
C	-4.82553100	4.40132200	-1.42192800
H	-5.09625000	5.17245100	-2.12844200
C	-3.76358800	3.07188200	0.06127000
C	-1.84530500	1.01767500	2.67353000
H	-0.87184700	1.47348800	2.78984300
C	-2.35064700	-0.04954400	3.35311100
H	-1.86637500	-0.63194000	4.12374000
C	-10.40394400	-0.77507800	1.78045400
C	-11.40265800	0.02116700	2.36400000
H	-11.16127900	1.03678400	2.66481300
C	-12.68812100	-0.48099400	2.56919600
H	-13.44507100	0.14969600	3.02812200
C	-12.99976000	-1.78901800	2.19344900
H	-14.00091200	-2.18020100	2.35342700
C	-12.01639000	-2.59156400	1.61216800
H	-12.24975500	-3.61010900	1.31303400
C	-10.73066800	-2.08910100	1.40876900
H	-9.96911900	-2.71544100	0.95227400
C	-7.62415900	4.25728800	-2.24098100
C	-7.24554400	4.15086200	-3.58844000
C	-7.73988100	5.03962500	-4.54403500
H	-7.43747400	4.93681200	-5.58297800
C	-8.62239500	6.05375800	-4.16813300
H	-9.00755300	6.74671100	-4.91133500
C	-9.00558300	6.17286100	-2.83087200
H	-9.68732100	6.96301800	-2.52725600
C	-8.51086800	5.28300400	-1.87668300
H	-8.80507000	5.38295900	-0.83569700
C	-1.43201600	3.31454400	0.89268600
C	-1.38250000	4.60105600	1.44576500
H	-2.29313200	5.01042600	1.87325500
C	-0.20554400	5.34834900	1.46105600
H	-0.19760700	6.34121600	1.90152800
C	0.95278900	4.80815100	0.90523100
H	1.87931900	5.37539200	0.89825600
C	0.94219100	3.53219100	0.34465900
H	1.83689100	3.11803000	-0.09626500
C	-0.24076900	2.77746900	0.34486700
C	-4.08155100	-2.12022500	4.48112200
C	-3.84056100	-1.67688800	5.79094700

H	-4.04085000	-0.63957400	6.04588700
C	-3.35521300	-2.55415900	6.76175100
H	-3.17728400	-2.19468100	7.77204200
C	-3.10416700	-3.88901000	6.43726400
H	-2.72601200	-4.57261100	7.19292400
C	-3.34263000	-4.33951000	5.13810400
H	-3.14861100	-5.37582700	4.87421200
C	-3.83013900	-3.46418000	4.16484400
H	-4.00566800	-3.82807800	3.15578900
N	-5.47421800	-0.31132000	-1.02985500
H	-5.38863600	0.48746200	-1.66071100
H	-4.57010600	-0.78446900	-1.05558600
C	-6.33928100	-2.60816500	-0.89470400
H	-6.30359000	-2.52677900	0.19541500
H	-5.40904800	-3.07960900	-1.23192500
H	-7.16201900	-3.28088300	-1.15384200
N	3.07662900	-3.43797600	-2.79229300
H	3.37508300	-2.63058800	-2.26097100
N	-2.23310600	-3.28231300	0.21290200
N	-0.30281000	1.46760500	-0.18939600
H	-1.23718700	1.08046900	-0.20803100
O	1.28904700	-4.84729500	-3.14156700
O	1.90122800	0.97317200	-0.59403400
C	0.33148400	-0.80903300	-0.77426700
C	1.19191600	-1.57646800	-1.57037700
C	0.92340200	-2.93207600	-1.77793300
C	-0.20854900	-3.52087200	-1.20143800
H	-0.37732200	-4.57476900	-1.37813400
C	-1.08620000	-2.75765200	-0.42559200
C	-0.79967800	-1.40105000	-0.20465800
H	-1.44846700	-0.83714100	0.46079100
C	0.71935200	0.62168800	-0.51552900
C	1.77383400	-3.83612800	-2.64096800
H	-2.71011700	4.77275600	-0.97973500
H	-6.66623400	-2.80266100	4.60867800
H	-10.97839100	1.02078900	-0.15114000
H	-6.56162900	3.36034800	-3.88583200
C	-2.95000300	-4.46294900	0.05551800
C	-2.95689300	-5.18717800	-1.25414300
C	-2.88776200	-4.53569100	-2.49428300
C	-3.15348300	-6.57509000	-1.21639000
C	-2.99755600	-5.26605300	-3.67676100
H	-2.75111500	-3.46049400	-2.53970400
C	-3.24346600	-7.30471500	-2.39922000

H	-3.23804900	-7.06366000	-0.25139100
C	-3.16665800	-6.65133500	-3.63138100
H	-2.94324700	-4.75347000	-4.63275200
H	-3.37914600	-8.38183400	-2.36040700
H	-3.23903700	-7.21974500	-4.55449500
O	-3.63619200	-4.86383700	0.99136000
H	2.03856600	-1.07846200	-2.03154800
C	2.95420800	0.47732000	2.79075200
H	2.47585600	1.16351600	2.07783600
C	2.91545700	1.15919100	4.16716900
H	1.88487000	1.40714900	4.44656300
H	3.31963900	0.51188000	4.95457300
H	3.49219300	2.09204400	4.16815100
C	2.13945400	-0.82567100	2.80018600
H	1.08589300	-0.61751400	3.01993200
H	2.17208500	-1.33762900	1.83146600
H	2.50025900	-1.52485600	3.56376200
C	-6.54157200	-1.23078800	-1.52764100
H	-7.48301200	-0.81598900	-1.15197500
C	-6.63956600	-1.22581500	-3.07613800
H	-6.74923500	-0.16638000	-3.35986500
C	-5.38930100	-1.76787000	-3.78519000
H	-5.25326900	-2.84003900	-3.60463700
H	-5.47298500	-1.62534800	-4.86849500
H	-4.47614300	-1.25278700	-3.46110500
C	-7.90559200	-1.94919700	-3.55981800
H	-8.80111000	-1.56233700	-3.05946900
H	-8.03994800	-1.81136200	-4.63858900
H	-7.85186000	-3.02794500	-3.37164500
H	-2.46980300	-2.83975300	1.09639200



Cartesian coordinates for Geometry Optimized ConformerB • (5R)₂

Atoms	x	y	z
Zn	5.92673200	0.84097100	0.75530100
N	4.10714100	0.57368200	1.79372700
N	5.12650400	2.63373100	0.02994400
N	7.82119500	1.62890300	0.42304400
N	6.78547800	-0.52362000	2.06692200
C	2.79087600	2.45487400	0.84249400
C	7.18389700	3.55834600	-0.99784100
C	9.17192900	-0.13631700	1.52279600
C	4.75371300	-1.35599300	3.21609700
C	3.83827800	-0.40634900	2.72230800
C	2.96187000	1.32495800	1.67361000
C	3.81532700	3.04154900	0.06829100
C	5.79481200	3.53307700	-0.76701500
C	8.11678600	2.67173900	-0.42091000
C	9.01270100	1.00884800	0.71621400
C	8.12181800	-0.82589200	2.16253700
C	6.12868200	-1.38225300	2.91452400

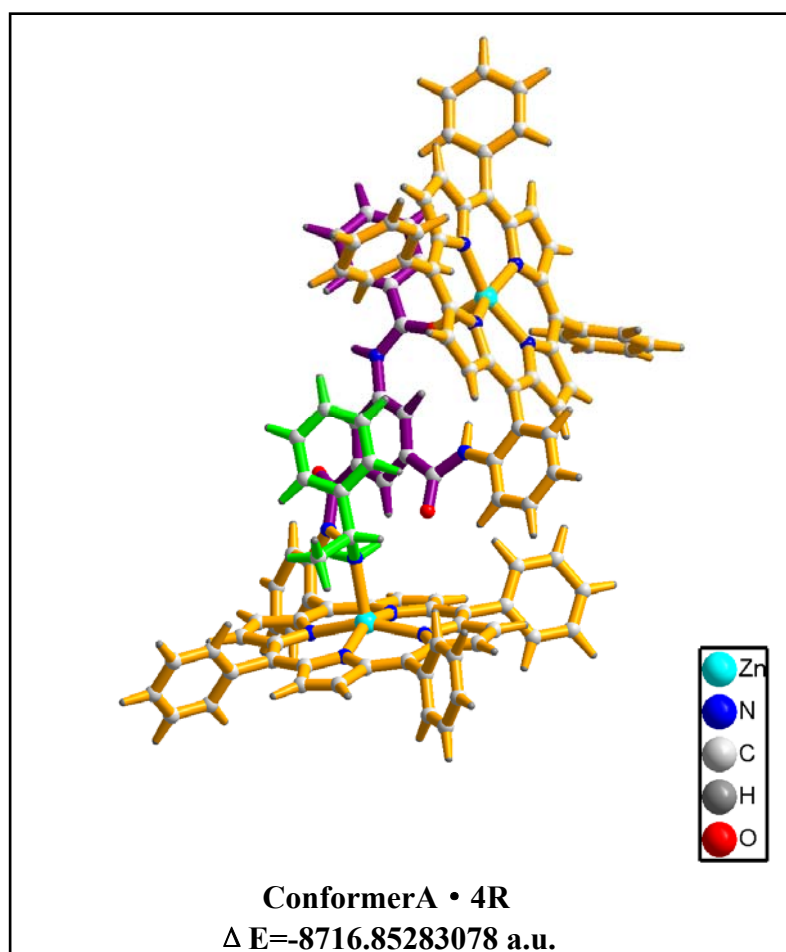
C	2.47054000	-0.28413100	3.18116900
H	2.00111600	-0.91524800	3.92223000
C	1.93613100	0.79810100	2.54935700
H	0.94862900	1.21749800	2.68168200
C	3.64205400	4.21135700	-0.76954900
H	2.71158300	4.73624100	-0.92950900
C	4.86476100	4.51767900	-1.27957100
H	5.12177600	5.34538100	-1.92443500
C	9.54159400	2.70719500	-0.67366400
H	10.04752900	3.41697700	-1.31168800
C	10.09474100	1.68214800	0.02964600
H	11.13611000	1.39825600	0.07118900
C	8.31065600	-1.92423800	3.08801900
H	9.26329400	-2.34941800	3.36819600
C	7.07903100	-2.27022100	3.54869800
H	6.83203700	-3.03491700	4.27078400
C	1.46897800	3.17228900	0.87838700
C	1.41077400	4.44448400	1.46558600
H	2.32212400	4.85208600	1.89278900
C	0.22832900	5.18045900	1.51435200
H	0.21723400	6.16148400	1.98053900
C	-0.93060500	4.64476800	0.95591700
H	-1.86168300	5.20457500	0.96873000
C	-0.91381700	3.38227400	0.36678500
H	-1.80906000	2.97104900	-0.07498600
C	0.27444600	2.63525300	0.33699000
C	7.71450200	4.63132500	-1.90037700
C	7.44416600	4.61126900	-3.27752400
H	6.84748900	3.80131800	-3.68836900
C	7.93705400	5.61010600	-4.11837700
H	7.72017900	5.57383900	-5.18284500
C	8.70930700	6.64888400	-3.59570200
H	9.09346600	7.42715100	-4.24964800
C	8.98387800	6.68227700	-2.22723500
H	9.57930400	7.49023800	-1.81008200
C	8.49073300	5.68274100	-1.38764400
H	8.69980300	5.71537700	-0.32200000
C	10.56367600	-0.64975500	1.73341500
C	11.50712800	0.09989500	2.45407400
H	11.21531500	1.06131400	2.86736800
C	12.80192400	-0.38135700	2.65144700
H	13.51590100	0.21160600	3.21712700
C	13.17750200	-1.62136200	2.13137500
H	14.18586100	-1.99613400	2.28534200

C	12.24884800	-2.37765500	1.41407700
H	12.53221200	-3.34316800	1.00316400
C	10.95391600	-1.89615500	1.21849300
H	10.23434900	-2.48573100	0.65705300
C	4.24521500	-2.36119600	4.21054400
C	4.01812200	-1.98867500	5.54482200
H	4.21784200	-0.96541400	5.85164500
C	3.54590100	-2.91704100	6.47350500
H	3.37816800	-2.61134700	7.50307200
C	3.29450100	-4.23392300	6.08247900
H	2.92645700	-4.95736000	6.80532300
C	3.51974700	-4.61460300	4.75896800
H	3.32602900	-5.63587700	4.44176200
C	3.99393000	-3.68733600	3.82780400
H	4.15948900	-4.00124900	2.80065800
Zn	-6.26039500	0.53082000	-0.25727000
N	-7.09122500	-1.37573000	-0.45627000
N	-7.80504600	0.98023200	1.07623500
N	-6.06917900	2.59601400	-0.59135400
N	-5.37664700	0.24078700	-2.14050500
C	-8.71721100	-1.30104300	1.41023100
C	-7.44993300	3.42564400	1.28873000
C	-4.56772900	2.54585500	-2.55954100
C	-5.82123300	-2.18278600	-2.42417800
C	-6.65171800	-2.36703800	-1.29876700
C	-7.96063300	-1.96890500	0.42806500
C	-8.66708100	0.08642400	1.66197200
C	-8.09023400	2.21211900	1.61329900
C	-6.49382700	3.58317200	0.26346500
C	-5.19736100	3.18566000	-1.47178200
C	-4.70607900	1.18222700	-2.88184500
C	-5.27898400	-0.94334600	-2.82749800
C	-7.21570400	-3.63893800	-0.89586400
H	-7.02345600	-4.58897600	-1.37316300
C	-8.02195800	-3.39326400	0.17194900
C	-9.54292100	0.78142500	2.58147700
H	-10.33972300	0.32644000	3.15182100
C	-9.18560400	2.09373900	2.55276100
H	-9.63804400	2.91239500	3.09333500
C	-5.82967800	4.82894500	-0.05931900
H	-5.96071800	5.76466700	0.46458000
C	-5.02984500	4.58376400	-1.13353400
H	-4.38843500	5.28187900	-1.65190000
C	-4.17888000	0.57284400	-4.08600700

H	-3.63673000	1.09155500	-4.86337900
C	-4.53545500	-0.73999800	-4.05477500
H	-4.34259500	-1.49644500	-4.80282400
C	-9.67266500	-2.11560300	2.22834100
C	-10.79806600	-2.71458800	1.63970000
H	-10.97441100	-2.57709200	0.57659400
C	-11.68969700	-3.46816800	2.40408300
H	-12.55783500	-3.91858500	1.92974500
C	-11.47208800	-3.63813500	3.77262900
H	-12.16613800	-4.22534700	4.36812900
C	-10.35776400	-3.04749100	4.37129100
H	-10.17788900	-3.17642000	5.43556100
C	-9.46800800	-2.29263900	3.60609200
H	-8.59968600	-1.83761600	4.07462400
C	-7.84121400	4.64198400	2.06977100
C	-8.49404600	5.72018800	1.45011100
H	-8.72145300	5.66113400	0.38954800
C	-8.86144500	6.85040200	2.18113100
H	-9.37164100	7.67085700	1.68302500
C	-8.58260600	6.92507400	3.54716800
H	-8.86871000	7.80541500	4.11662900
C	-7.93582100	5.86016600	4.17688900
H	-7.71184200	5.90932600	5.23944900
C	-7.57053800	4.72977200	3.44499100
H	-7.06474800	3.90392500	3.93753200
C	-3.70631900	3.38246800	-3.45485700
C	-4.26238900	4.39330600	-4.25496300
H	-5.33513300	4.56252800	-4.22414700
C	-3.45641900	5.16762200	-5.09048900
H	-3.90662000	5.94158100	-5.70686000
C	-2.07880900	4.94558700	-5.13963300
H	-1.45064300	5.54917100	-5.78957700
C	-1.51366200	3.94359200	-4.34856800
H	-0.44112200	3.76811700	-4.37571900
C	-2.32006300	3.16779100	-3.51464900
H	-1.88257100	2.39546800	-2.88901700
C	-5.59059300	-3.37500000	-3.31105900
C	-4.33541700	-4.02553400	-3.41020700
C	-4.18573200	-5.14734400	-4.24098900
H	-3.22412900	-5.63728900	-4.29128100
C	-5.27069100	-5.61688800	-4.97813600
H	-5.13733600	-6.48568100	-5.61734000
C	-6.51098300	-4.98535800	-4.89970800
H	-7.35603200	-5.34885100	-5.47749700

C	-6.65746700	-3.87582400	-4.06891500
H	-7.61677600	-3.37164100	-3.99728400
N	2.21573600	-3.47279200	0.03236100
H	2.49727000	-3.05625000	0.91537300
H	-3.50808300	-2.68231500	-2.11098000
O	-1.88471500	0.85339700	-0.57815700
O	-1.53970100	-4.96206400	-3.09751300
C	1.04573600	-2.91915800	-0.53912300
C	0.80547200	-1.55512900	-0.30682900
H	1.50420900	-1.00584100	0.31916600
C	-0.34194000	-0.93827000	-0.81388700
C	-1.26054900	-1.68776500	-1.56104800
H	-2.11938400	-1.17092800	-1.97592400
C	-1.04064900	-3.05030500	-1.77358000
C	0.10615900	-3.66468300	-1.25701000
H	0.23742400	-4.72399700	-1.43295500
C	-0.70313800	0.49504000	-0.53237100
C	-1.96578700	-3.93430000	-2.57753200
N	0.33026300	1.33448800	-0.22241100
N	-3.26336100	-3.49876900	-2.65618800
H	1.26287900	0.94388400	-0.25503100
C	2.89789000	-4.66662400	-0.17859100
O	3.62906400	-5.09005100	0.71235200
C	2.81102000	-5.38112200	-1.49077800
C	2.66447900	-4.72326700	-2.72071400
C	2.99272700	-6.77161700	-1.47192200
C	2.68255700	-5.44979000	-3.91048300
H	2.53827800	-3.64653500	-2.75199600
C	2.99324600	-7.49684200	-2.66082600
H	3.13648400	-7.26545900	-0.51672600
C	2.83897700	-6.83712000	-3.88223600
H	2.56532900	-4.93317800	-4.85879300
H	3.11858400	-8.57559900	-2.63548300
H	2.84012200	-7.40215100	-4.81025100
H	-8.60910100	-4.10617900	0.73241700
C	-4.41158700	-0.85440500	1.95498200
H	-4.88664800	-1.70842500	1.45600400
C	-2.94430400	-1.26424500	2.24977100
H	-2.48036600	-1.43277800	1.26711400
N	-4.50411800	0.28154300	0.99123400
H	-3.72312300	0.25083000	0.32786500
H	-4.38095400	1.16281500	1.49163000
C	-5.23449200	-0.51801600	3.20077800
H	-6.26535600	-0.28481800	2.92474700

H	-5.24964100	-1.36091600	3.89821500
H	-4.82154700	0.34896900	3.73121300
C	-2.12604700	-0.17659000	2.96241600
H	-2.49457200	0.01001700	3.97796000
H	-1.07843200	-0.48794700	3.04861500
H	-2.14103500	0.77212300	2.41390200
C	-2.87328500	-2.59623000	3.01279800
H	-3.46456400	-3.37512800	2.51630900
H	-1.83803000	-2.95101100	3.07264900
H	-3.24345700	-2.49759200	4.04005300
C	6.45296900	-1.31765400	-1.63066200
H	6.98401300	-1.81137900	-0.80766200
N	5.45919800	-0.41707200	-0.97370600
H	5.04256800	0.20258000	-1.67059700
H	4.68932900	-0.98105300	-0.60868000
C	7.45468300	-0.46874200	-2.41512100
H	8.20909100	-1.10256200	-2.89055900
H	6.95965900	0.11021600	-3.20454100
H	7.96788800	0.23231100	-1.75539600
C	5.77000600	-2.43079400	-2.46892000
H	5.01722400	-2.88665300	-1.80709200
C	5.03763700	-1.90219600	-3.71219700
H	4.48032300	-2.71066000	-4.19701300
H	4.31823600	-1.11125800	-3.46516100
H	5.73751600	-1.49823900	-4.45238600
C	6.75880200	-3.54402900	-2.84683400
H	7.28928500	-3.92315800	-1.96538300
H	6.22840300	-4.38658900	-3.30354700
H	7.50701000	-3.19476500	-3.56824500



Cartesian coordinates for Geometry Optimized ConformerA · 1R

Atoms	x	y	z
Zn	-5.89139900	0.40747300	0.06253600
N	-6.59509700	0.21905500	2.04163100
N	-4.93077900	2.17145400	0.69729300
N	-5.78930700	1.14306100	-1.87762700
N	-7.50491500	-0.76263700	-0.53177700
C	-5.19198600	1.93000500	3.15407700
C	-4.30062700	3.08840900	-1.51845900
C	-7.28164200	-0.49208000	-2.98491000
C	-8.24394700	-1.59371900	1.68467000
C	-7.43768400	-0.76774100	2.49270000
C	-6.05259100	0.81126000	3.15574300
C	-4.73435000	2.58780700	1.99120900
C	-4.32621800	3.10307800	-0.11046100
C	-4.98020100	2.17437300	-3.77630600
H	-4.42931100	2.86957400	-4.39314900
C	-6.32174500	0.53929300	-2.98933700
C	-7.85085900	-1.06030600	-1.82862500

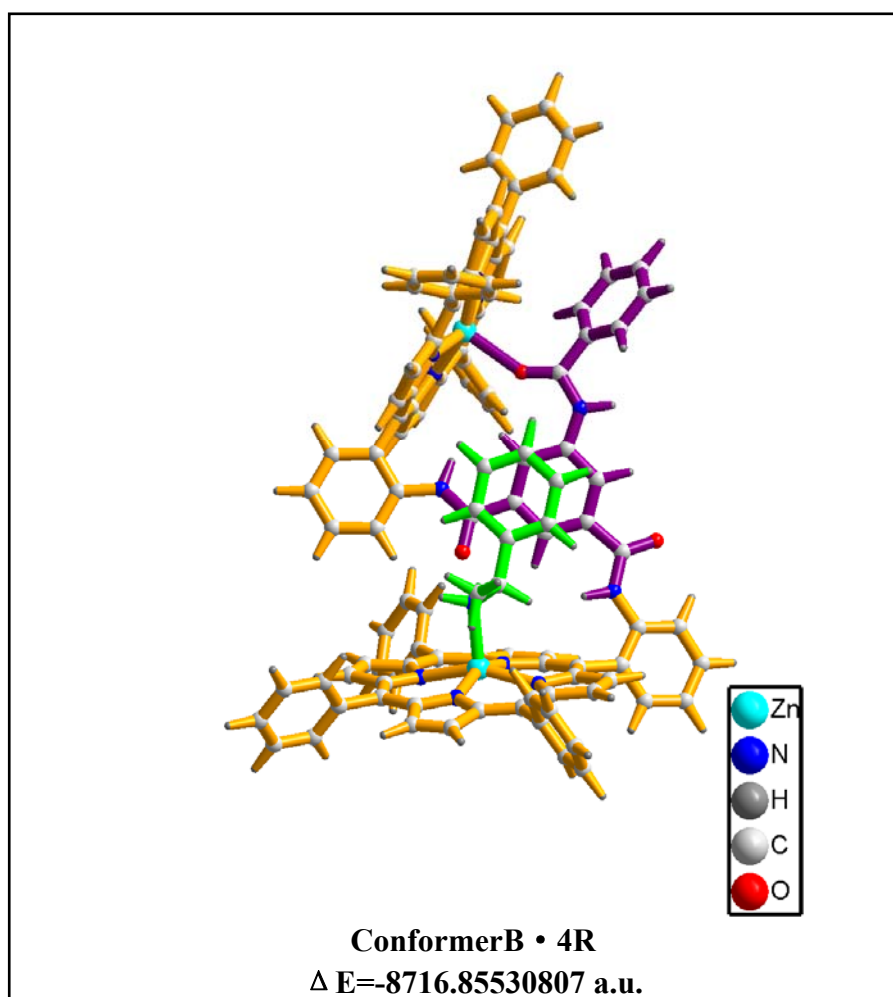
C	-8.28457300	-1.55403400	0.27561800
C	-7.38689600	-0.83181500	3.93928600
H	-7.93527300	-1.52933800	4.55574600
C	-6.53088000	0.14295800	4.34917400
H	-6.25091600	0.39221300	5.36250200
C	-3.98901900	3.83045600	2.00038100
H	-3.72668700	4.39658300	2.88331800
C	-3.73753800	4.14827000	0.70168300
H	-3.22612900	5.02133400	0.32309900
C	-4.98568100	2.16041600	-2.32792000
C	-5.81219300	1.17745400	-4.18464200
H	-6.07584600	0.90970500	-5.19773100
C	-8.88708400	-2.07082900	-1.83781800
H	-9.34698000	-2.48811200	-2.72182500
C	-9.16443400	-2.36565300	-0.53879700
H	-9.89986800	-3.06203200	-0.16300000
C	-3.49620500	2.45781300	5.00212600
C	-4.81669500	2.51308500	4.48766600
C	-5.80507100	3.12782300	5.26789300
H	-6.81399500	3.17740100	4.86906800
C	-5.52085700	3.67023300	6.51998200
H	-6.30780100	4.14404700	7.09987400
C	-4.21911300	3.59708600	7.01320400
H	-3.97849600	4.01078300	7.98894100
C	-3.20840400	2.99554800	6.26633000
H	-2.19881400	2.93115200	6.64559500
C	-3.50688400	4.16046600	-2.20145900
C	-2.10618200	4.17255600	-2.11103500
H	-1.61059900	3.38313400	-1.55449200
C	-1.35908300	5.17196800	-2.73553200
H	-0.27482700	5.16162800	-2.65743700
C	-1.99996700	6.17837400	-3.46046600
H	-1.41852400	6.95776800	-3.94599900
C	-3.39288900	6.17810800	-3.55717000
H	-3.90112500	6.96085900	-4.11449900
C	-4.13964600	5.17773000	-2.93324100
H	-5.22395400	5.18481100	-3.00226500
C	-7.75834400	-0.99494200	-4.31522000
C	-9.03866000	-0.67132600	-4.79058000
H	-9.68655500	-0.04611300	-4.18239400
C	-9.47898100	-1.13630300	-6.03060500
H	-10.47276000	-0.87187500	-6.38278600
C	-8.64559300	-1.93258900	-6.81838000
H	-8.98818700	-2.29443500	-7.78422500

C	-7.36917100	-2.26028700	-6.35793000
H	-6.71392600	-2.88191000	-6.96282500
C	-6.93026700	-1.79505200	-5.11734100
H	-5.93754400	-2.05459400	-4.75942900
C	-9.14210500	-2.57451100	2.37584400
C	-10.22731000	-2.13275100	3.14957300
H	-10.41468600	-1.06616900	3.23651300
C	-11.06489200	-3.04401500	3.79403400
H	-11.90258200	-2.68106400	4.38402300
C	-10.83242500	-4.41563000	3.67727000
H	-11.48441800	-5.12570400	4.17912700
C	-9.75752200	-4.86908400	2.91058800
H	-9.56620500	-5.93495300	2.81594800
C	-8.92131000	-3.95669000	2.26575900
H	-8.08351400	-4.31320200	1.67269700
Zn	5.58279300	-0.32168100	-0.85831900
N	4.69962800	1.27828900	-1.85125300
N	4.26805600	-1.58644900	-1.84485200
N	6.80901700	-1.96554600	-0.52796800
N	7.23413500	0.89375800	-0.53481800
C	2.78271600	0.10105900	-2.88465900
C	5.23563800	-3.76636300	-1.17790600
C	8.88679600	-0.81270000	0.17749200
C	6.22275400	3.08318800	-1.11894900
C	3.50954500	1.25439000	-2.53551000
C	5.05008200	2.60088200	-1.72679400
C	3.16275600	-1.21814600	-2.57158300
C	4.25366300	-2.95884500	-1.77996200
C	6.43884100	-3.28593200	-0.62611500
C	8.09331800	-1.95625200	-0.03694200
C	8.46456900	0.51168300	-0.05221400
C	7.24611400	2.26812700	-0.59555000
C	3.09171300	2.60505000	-2.84920300
H	2.19710700	2.87066200	-3.39532000
C	4.03786300	3.43770800	-2.33850500
H	4.06000300	4.51700100	-2.37930800
C	2.42847300	-2.39510700	-2.98305200
H	1.53436600	-2.39164100	-3.59026200
C	3.10397500	-3.47168100	-2.49547900
H	2.86777400	-4.51737300	-2.63040000
C	7.50849500	-4.13282300	-0.14559500
H	7.48175400	-5.21165900	-0.10135400
C	8.53948100	-3.31352200	0.19251100
H	9.51572500	-3.59951600	0.55509800

C	9.26678700	1.68445100	0.22089200
H	10.27549600	1.67751600	0.60751900
C	8.51373600	2.76834200	-0.11272200
H	8.79525200	3.81006900	-0.06037000
C	0.28492100	0.49830000	-2.84124200
C	-0.95272500	0.62725700	-3.48655000
H	-1.84698700	0.79377900	-2.90275000
C	-1.01216800	0.54682000	-4.87782000
H	-1.97694900	0.65116800	-5.36655200
C	0.14349100	0.34686800	-5.63195600
H	0.09208100	0.29096000	-6.71557100
C	1.37355200	0.21908600	-4.98335200
H	2.28181800	0.05745000	-5.55719900
C	1.46740600	0.28522600	-3.59076800
C	5.00493600	-5.24801700	-1.18309200
C	4.00908100	-5.81594800	-0.37361900
H	3.41585700	-5.16851500	0.26672100
C	3.78005400	-7.19259700	-0.37968900
H	3.00544900	-7.61311800	0.25633000
C	4.54403700	-8.02643600	-1.19799400
H	4.36604800	-9.09846700	-1.20433300
C	5.53640600	-7.47436200	-2.01026300
H	6.13164000	-8.11497900	-2.65577100
C	5.76386700	-6.09755700	-2.00348700
H	6.53022100	-5.66955200	-2.64362400
C	10.29236400	-1.01848500	0.65656400
C	11.37924200	-0.69221500	-0.17111900
H	11.18709100	-0.29354700	-1.16323200
C	12.69184600	-0.88300900	0.26161200
H	13.51783900	-0.62811200	-0.39726100
C	12.94391700	-1.40578000	1.53135000
H	13.96610200	-1.55534300	1.86862800
C	11.87329900	-1.73739600	2.36342600
H	12.05927200	-2.14457200	3.35412900
C	10.56032100	-1.54595000	1.93011300
H	9.72995200	-1.80195100	2.58143900
C	6.42683800	4.56758800	-1.06538300
C	6.69889400	5.30168600	-2.23042800
H	6.76412500	4.78033900	-3.18144600
C	6.89361500	6.68250400	-2.17542400
H	7.10716000	7.23276200	-3.08810600
C	6.82041100	7.35372600	-0.95344400
H	6.97167000	8.42901100	-0.91035000
C	6.55209800	6.63504400	0.21288800

H	6.48983100	7.14942000	1.16837200
C	6.35813000	5.25419400	0.15674300
H	6.14561200	4.69803400	1.06574700
C	-0.35075100	1.17673300	3.27723200
C	0.94661000	0.76132200	3.58220500
H	1.27562700	0.84738900	4.61402200
C	1.79883600	0.27569800	2.58631300
C	1.35020200	0.19071800	1.26371600
H	2.00798600	-0.23657500	0.51937600
C	0.05930600	0.63583100	0.94838600
C	-0.78586200	1.12539600	1.94987900
H	-1.75849600	1.49410700	1.64281600
C	-1.16229900	1.71711300	4.43292100
C	-0.49480200	0.61514300	-0.45181400
C	4.25393800	-0.23182600	2.27401300
N	-2.50392300	1.85685300	4.19545100
H	-2.84812500	1.53886800	3.29963400
N	0.44127600	0.58220300	-1.44023400
H	1.40872300	0.62890000	-1.14763700
N	3.09336000	-0.12187200	2.99460900
H	3.22522200	-0.12365900	3.99783300
O	-0.61021200	1.99393000	5.49557500
O	-1.71213000	0.65661600	-0.65828400
O	4.30390800	-0.08656400	1.04458300
C	5.45143200	-0.49602500	3.13337500
C	6.62445900	0.23216700	2.90041300
H	6.66328700	0.93589600	2.07670100
C	7.72581400	0.06211200	3.73786800
H	8.62713000	0.63983100	3.55770500
C	7.67281100	-0.85081400	4.79373000
H	8.53475300	-0.98280600	5.44205200
C	6.51377300	-1.59851000	5.01332100
H	6.47492800	-2.32344200	5.82133300
C	5.40182100	-1.41586400	4.19301100
H	4.50774300	-2.01247400	4.35602500
H	-1.07049000	-3.98878800	3.08536900
C	-1.15026200	-3.66495900	2.05067300
C	-2.36037800	-3.16077100	1.57537400
C	-0.04718400	-3.75694800	1.19900000
C	-2.49163800	-2.73768500	0.24404400
H	-3.21071900	-3.10207300	2.25186800
C	-0.16272500	-3.34096500	-0.12779400
H	0.89644900	-4.15086400	1.56828100
C	-1.37749200	-2.83589800	-0.59739900

H	0.69089700	-3.40126100	-0.79729700
H	-1.45932300	-2.50448500	-1.63014000
C	-3.81021800	-2.17240900	-0.27475700
H	-3.69216900	-1.96179500	-1.34292100
C	-4.97021800	-3.15703800	-0.09799900
H	-5.87468300	-2.77882600	-0.57784200
H	-4.71133700	-4.12452500	-0.54043000
H	-5.19402900	-3.32332100	0.96249800
N	-4.13440900	-0.85748900	0.35465800
H	-4.15369000	-0.97901900	1.36901100
H	-3.35070900	-0.22355200	0.16026200



Cartesian coordinates for Geometry Optimized ConformerB · 1R

Atoms	x	y	z
Zn	5.88106500	0.33535300	0.19882600
N	4.12133900	-0.72913400	-0.50883200
H	4.09575100	-0.59205300	-1.51990200
H	3.31783800	-0.19796000	-0.15673600
C	3.97133000	-2.17901900	-0.19472300

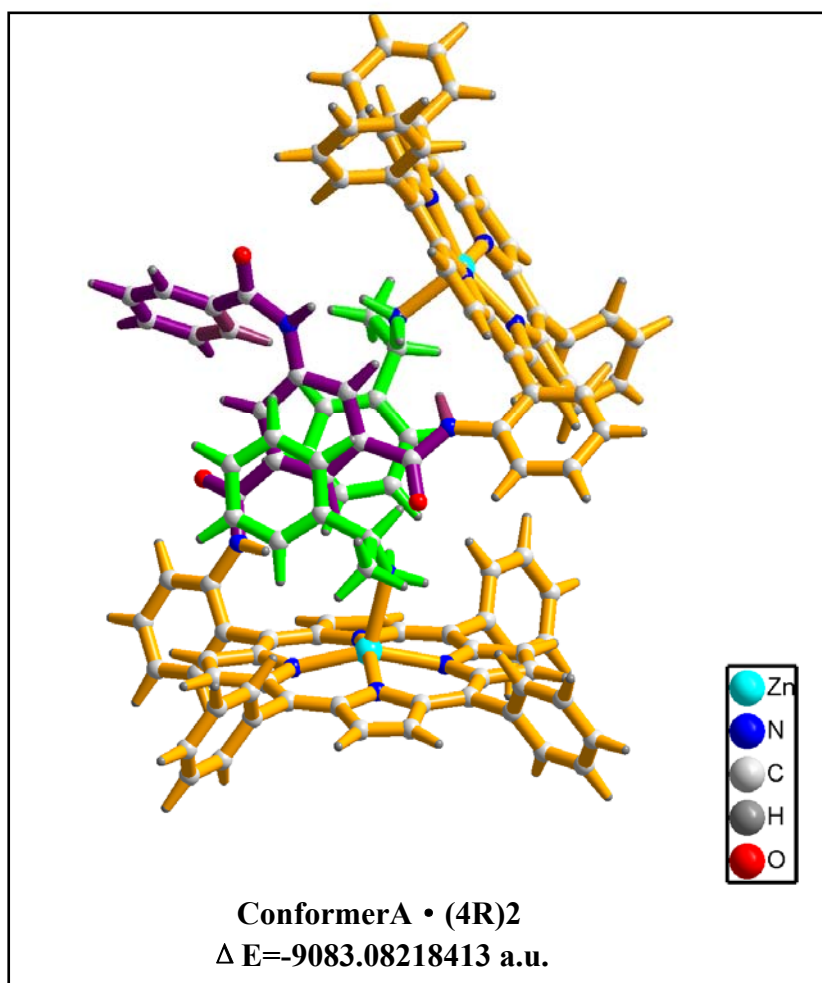
H	4.41306800	-2.32447200	0.79709900
C	4.78032600	-3.00578200	-1.20324900
H	4.74790900	-4.06591900	-0.93349700
H	5.82276700	-2.67817900	-1.22655200
H	4.35770400	-2.90729700	-2.21136200
C	2.52457100	-2.65226700	-0.13410200
C	1.61411300	-2.37459300	-1.16348500
H	1.92152400	-1.76117700	-2.00714100
C	0.30786700	-2.86085900	-1.11299400
H	-0.38916600	-2.62729400	-1.91303000
C	-0.10820800	-3.64099400	-0.03089500
H	-1.12539900	-4.02222200	0.00379100
C	0.78709800	-3.92250100	1.00094800
H	0.47296200	-4.52422100	1.85011900
C	2.09178000	-3.42742900	0.94831400
H	2.78560300	-3.64775100	1.75709200
N	6.51534600	-0.74254000	1.87618200
N	7.45229700	-0.54882700	-0.86110100
N	5.90240200	1.87369800	-1.22542700
N	4.98849600	1.69272400	1.52316600
C	5.97376300	-0.66633900	3.13589900
C	7.31000500	-1.86434000	1.85715400
C	8.21865100	-1.61457000	-0.45774900
C	7.85654700	-0.23340000	-2.13582700
C	6.41608600	1.77768100	-2.49529900
C	5.10588600	2.99077000	-1.20637900
C	4.43292100	2.90577300	1.19796000
C	4.77819000	1.51209600	2.86765200
C	6.39034800	-1.81155700	3.91857900
H	6.09664700	-2.01413700	4.93841100
C	7.21443000	-2.55179500	3.12846300
H	7.71613000	-3.47447100	3.38166300
C	9.15589200	-1.96708400	-1.50324700
H	9.90217000	-2.74559000	-1.43897300
C	8.93033000	-1.11600500	-2.54038100
H	9.45947900	-1.06766100	-3.48100300
C	5.88552200	2.84353900	-3.31947500
H	6.10532000	2.99625100	-4.36612700
C	5.07729900	3.59494300	-2.52205700
H	4.51611400	4.47718000	-2.79435500
C	3.86693400	3.51854900	2.38255100
H	3.39558200	4.48994700	2.41959000
C	4.08245500	2.65933000	3.41500300
H	3.82235900	2.79583500	4.45542800

C	5.17651800	0.38961400	3.62571800
C	8.12855900	-2.27411000	0.78651200
C	7.34265100	0.80904400	-2.93418000
C	4.42970800	3.49993000	-0.07845400
C	4.81867700	0.36222500	5.08565600
C	3.49342600	0.15644400	5.54529500
C	3.22145100	0.12341100	6.92214400
H	2.20667900	-0.04606200	7.25180900
C	4.25393400	0.30429300	7.83997100
H	4.02557100	0.27840400	8.90219700
C	5.56196200	0.51583800	7.40690400
H	6.36637500	0.66157500	8.12227900
C	5.82959600	0.54098700	6.03927300
H	6.84290100	0.70698000	5.68543600
C	8.99275800	-3.48040200	0.99269400
C	8.78415500	-4.65154600	0.24650200
H	7.97895000	-4.67807900	-0.48244200
C	9.58934600	-5.77522200	0.43661600
H	9.40698500	-6.67346800	-0.14780700
C	10.62186200	-5.74820600	1.37580400
H	11.25005200	-6.62267800	1.52350500
C	10.84329800	-4.58944200	2.12240300
H	11.64917900	-4.55567400	2.85105500
C	10.03613900	-3.46718500	1.93264100
H	10.21620500	-2.56411700	2.50894000
C	7.84921700	0.91497300	-4.33952900
C	8.61269300	2.01970800	-4.75116000
H	8.84088600	2.80146200	-4.03226500
C	9.08717000	2.11445700	-6.05984700
H	9.68155100	2.97511800	-6.35566100
C	8.80678400	1.10584900	-6.98358800
H	9.17606200	1.17951700	-8.00306900
C	8.05052700	0.00101800	-6.58820300
H	7.82435200	-0.78836800	-7.30047300
C	7.57819600	-0.09337400	-5.27864800
H	6.98737700	-0.95324500	-4.97528300
C	3.66756200	4.77868100	-0.24123100
C	2.26864500	4.79241800	-0.12248300
H	1.75107700	3.85776000	0.07096100
C	1.55176800	5.98088600	-0.26638500
H	0.46841100	5.97014200	-0.17765500
C	2.22136700	7.17737100	-0.52953600
H	1.66339200	8.10346700	-0.64044100
C	3.61248900	7.17715900	-0.64980500

H	4.14277500	8.10486200	-0.84927300
C	4.32897900	5.98811400	-0.50790200
H	5.41206600	5.99168400	-0.59353700
N	-4.75099900	1.92858200	-1.24188900
N	-7.30108900	1.00523000	-0.27367100
N	-6.74608500	-1.63955900	-1.30888800
N	-4.22488800	-0.69616200	-2.35366800
C	-3.57902600	2.21908200	-1.89554100
C	-5.16883000	3.09727700	-0.65400600
C	-7.34839700	2.28164600	0.23867700
C	-8.50151100	0.41215700	0.03952400
C	-8.05313200	-1.84295500	-0.93169500
C	-6.33422200	-2.79565200	-1.92662300
C	-4.13041400	-2.00026200	-2.77760400
C	-3.10675600	-0.05143400	-2.82157900
C	-3.24929700	3.61841000	-1.72179400
H	-2.39144400	4.11531400	-2.15315200
C	-4.23151200	4.16078400	-0.95355200
H	-4.33182600	5.18890800	-0.63726600
C	-8.59828100	2.48154800	0.93744500
H	-8.89026000	3.38428300	1.45376800
C	-9.31610000	1.33220200	0.80272400
H	-10.30236500	1.12285700	1.19075000
C	-8.47699400	-3.16731100	-1.33194800
H	-9.46725600	-3.57586200	-1.19504600
C	-7.41128200	-3.76078300	-1.93225900
H	-7.36701500	-4.74384300	-2.37793200
C	-2.90003800	-2.18699600	-3.51818500
H	-2.57159600	-3.11488500	-3.96337800
C	-2.27383000	-0.97895000	-3.55621600
H	-1.34229100	-0.72975700	-4.04443600
C	-2.79300600	1.30661700	-2.62357700
C	-6.35528000	3.26971800	0.08221900
C	-8.88349600	-0.90441500	-0.28917100
C	-5.09524300	-3.00157100	-2.56578100
C	-1.48376100	1.79608800	-3.17881100
C	-1.37993900	2.26814800	-4.48989600
H	-2.27659900	2.29925400	-5.10259700
C	-0.15387500	2.68357800	-5.01336200
H	-0.09418400	3.04614800	-6.03559900
C	0.98811400	2.62593200	-4.21512200
H	1.94966900	2.94512200	-4.60768300
C	0.91771900	2.16655900	-2.90009800
H	1.80070700	2.12759300	-2.27789700

C	-0.31617400	1.75407400	-2.37935300
C	-6.59280900	4.61072100	0.70658600
C	-7.61656600	5.45468200	0.24728500
H	-8.24143900	5.12796000	-0.57922300
C	-7.82862600	6.70416100	0.83130800
H	-8.62292000	7.34501900	0.45739000
C	-7.02027900	7.13307100	1.88580700
H	-7.18542400	8.10614400	2.34061200
C	-5.99712500	6.30493600	2.35060100
H	-5.36373600	6.62884600	3.17236500
C	-5.78510100	5.05613000	1.76513800
H	-4.99033200	4.41221900	2.13170800
C	-10.27829900	-1.32674600	0.05524500
C	-11.38305600	-0.68772700	-0.53194300
H	-11.21212300	0.11318600	-1.24556300
C	-12.68570600	-1.07714300	-0.21916900
H	-13.52554600	-0.57293000	-0.69010500
C	-12.91030200	-2.11443300	0.68789600
H	-13.92484400	-2.41848500	0.93132100
C	-11.82210600	-2.75976100	1.27792100
H	-11.98664900	-3.56762300	1.98652600
C	-10.51923200	-2.37062000	0.96389900
H	-9.67514900	-2.87174400	1.42840500
C	-4.81988000	-4.37116700	-3.10721600
C	-4.76087900	-4.60812600	-4.48985500
H	-4.92442000	-3.78200800	-5.17617400
C	-4.50749000	-5.88776500	-4.98545400
H	-4.47056700	-6.05126900	-6.05935500
C	-4.30936500	-6.95480200	-4.10721400
H	-4.11153500	-7.95119400	-4.49321800
C	-4.36978000	-6.73404900	-2.73013100
H	-4.21580100	-7.55832700	-2.03850100
C	-4.62448200	-5.45424300	-2.23567700
H	-4.66973500	-5.28430500	-1.16333900
C	0.30893900	-0.14487200	3.48099600
C	0.74399200	0.36348000	2.25408400
H	1.72446400	0.80912500	2.12488100
C	-0.10852200	0.35338700	1.14521600
C	-1.40515900	-0.16811900	1.25043400
H	-2.06911700	-0.23576900	0.39971300
C	-1.85167800	-0.64666100	2.48723700
C	-0.99394600	-0.63305400	3.59078300
H	-1.32134400	-0.98787000	4.56415300
C	1.13181400	-0.16001100	4.74789400

C	0.44969900	0.90844300	-0.13840700
N	2.48124700	-0.00329900	4.57297600
H	2.81908000	0.04491000	3.62084900
N	-3.14682000	-1.17450300	2.69802500
H	-3.28226500	-1.57396100	3.61772600
N	-0.48197100	1.29001600	-1.05569400
H	-1.45116600	1.21147900	-0.77639400
O	0.58269200	-0.31371400	5.83682100
O	1.66809900	1.02073300	-0.30946000
Zn	-5.59077800	0.04919300	-0.97544700
C	-5.41963000	-2.88806800	3.26490700
C	-5.49396100	-1.63271900	2.63994400
C	-6.69243200	-0.90960100	2.67586200
C	-7.79636400	-1.42662100	3.35212500
C	-7.71891700	-2.67415500	3.97537900
C	-6.53261100	-3.40942800	3.92228700
H	-4.50431500	-3.47203300	3.20887800
H	-6.74991600	0.05750300	2.18964800
H	-8.71797300	-0.85393000	3.38463000
H	-8.58271100	-3.07476700	4.49886000
H	-6.47371400	-4.38793100	4.39032900
C	-4.29917600	-1.02343600	1.97390300
O	-4.34640600	-0.41238600	0.89643300



Cartesian coordinates for Geometry Optimized ConformerA·(1R)₂

Atoms	x	y	z
Zn	6.08515900	0.52703400	-0.39392600
N	7.92082100	0.69859100	0.58315100
N	6.78610300	-1.22613300	-1.26176200
N	4.72460200	0.68123400	-1.97402200
N	5.88505600	2.62574100	-0.16119000
C	8.81716800	-1.56586000	0.11523500
C	5.01570800	-1.57596200	-2.95885200
C	3.91111500	2.99510200	-1.60625800
C	7.73279500	3.02162800	1.43758400
C	8.37196700	1.77113600	1.31444300
C	8.86243100	-0.29123100	0.71773200
C	7.83691500	-1.98688700	-0.80375400
C	6.12110800	-1.99115700	-2.18898400
C	4.41341000	-0.30276900	-2.87850100
C	3.90777300	1.74852900	-2.25865400
C	4.84289100	3.38933700	-0.62676800

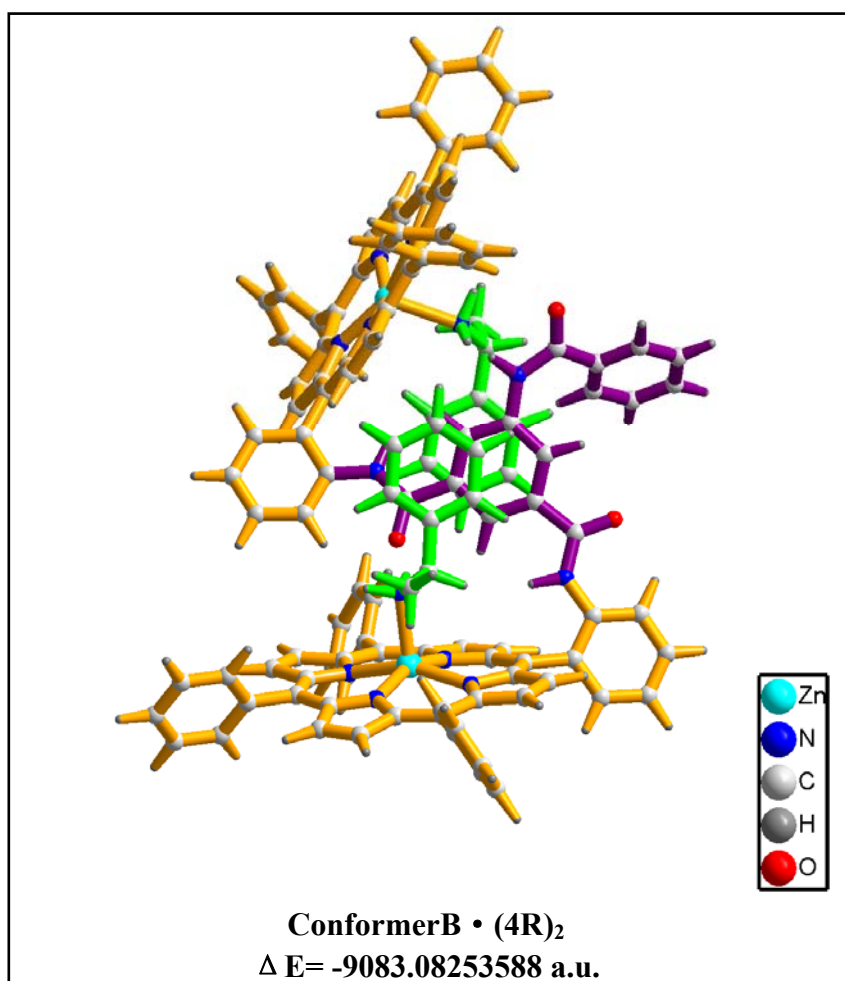
C	6.56622100	3.40348400	0.74304100
C	9.64791200	1.44905800	1.91894700
H	10.24332200	2.12196500	2.51861100
C	9.95086900	0.17578400	1.55010000
H	10.83924800	-0.38875700	1.79322400
C	7.80065000	-3.29298100	-1.42686000
H	8.49642200	-4.09714400	-1.23647000
C	6.74319400	-3.29478700	-2.28430300
H	6.41768600	-4.09800900	-2.92964500
C	3.37340300	0.16202800	-3.77337600
H	2.97231400	-0.39732400	-4.60722400
C	3.05738800	1.42781200	-3.38603400
H	2.34655300	2.10233200	-3.84159300
C	4.84549200	4.67898800	0.03002200
H	4.12751200	5.46868700	-0.13843900
C	5.90987600	4.68784600	0.87820100
H	6.22348100	5.48660200	1.53457200
C	9.91888800	-2.52637400	0.44669500
C	10.86496200	-2.89761900	-0.52211500
H	10.79327600	-2.47500200	-1.52039000
C	11.89365500	-3.78834500	-0.21289500
H	12.61909200	-4.05863800	-0.97589300
C	11.99475800	-4.32558400	1.07175100
H	12.79536400	-5.01983100	1.31286400
C	11.06154500	-3.96405600	2.04500800
H	11.12974800	-4.37934300	3.04720000
C	10.03429700	-3.07181300	1.73507100
H	9.30722600	-2.79601600	2.49388800
C	4.50775600	-2.52540700	-4.00662800
C	5.29493500	-2.77689300	-5.13814600
H	6.25139400	-2.26858200	-5.21882500
C	4.87534700	-3.64286900	-6.14634900
H	5.50477200	-3.81435600	-7.01493800
C	3.64074900	-4.27847200	-6.02464000
H	3.29631000	-4.95941900	-6.79851000
C	2.83235400	-4.05622200	-4.91186000
H	1.87787900	-4.55155400	-4.80985600
C	3.25504700	-3.17928200	-3.89963400
C	2.84799900	3.97789000	-1.99706200
C	1.51784800	3.76977800	-1.59931100
H	1.28329800	2.90225600	-0.99014500
C	0.51672900	4.67465500	-1.95757000
H	-0.50574200	4.50449100	-1.62848500
C	0.82983000	5.79969100	-2.72389000

H	0.05124000	6.50424600	-3.00447400
C	2.14954400	6.01704300	-3.12404500
H	2.40132900	6.88919900	-3.72199100
C	3.15123400	5.11436100	-2.76172600
H	4.17697800	5.28326800	-3.07804500
C	8.36230400	4.03204800	2.34726100
C	8.92332200	5.21275500	1.83395900
H	8.90129600	5.38563900	0.76169200
C	9.51437900	6.15118100	2.68066500
H	9.94835000	7.05554400	2.26202000
C	9.55510600	5.92733000	4.05815700
H	10.01547800	6.65810100	4.71777400
C	9.00213600	4.75760400	4.58228300
H	9.02639500	4.57499700	5.65354500
C	8.41273500	3.81921100	3.73419600
H	7.98118900	2.91119500	4.14656900
Zn	-5.88357600	0.82339200	0.84062000
N	-7.11891800	-0.60774000	1.69788600
N	-7.54515600	1.59166500	-0.14284700
N	-4.93273200	2.66918700	0.52301800
N	-4.55014900	0.52341400	2.43592500
C	-9.13420000	-0.26049200	0.29932400
C	-6.53374100	3.64625900	-1.09679700
C	-2.96539700	2.38440700	2.00132900
C	-5.62309500	-1.45048300	3.48488200
C	-7.89369500	-2.39832500	2.93262500
C	-8.38178600	-0.94302200	1.27720200
C	-8.73036000	0.92566500	-0.34774600
C	-7.56160500	2.68888800	-0.96970300
C	-5.31658600	3.62475000	-0.38697400
C	-3.28616000	4.27951600	0.35401900
C	-3.39750200	1.22744900	2.68562800
C	-4.59414400	-0.49827300	3.35407000
C	-6.80018000	-1.47602700	2.71405700
C	-8.87091400	-2.06971400	2.04587600
H	-9.84489700	-2.52440400	1.93841500
C	-9.51181400	1.61854100	-1.35109700
C	-8.79182900	2.70790500	-1.73240900
H	-9.06120000	3.45202500	-2.46779300
C	-4.28802000	4.63926800	-0.49436500
H	-4.33885000	5.51753800	-1.12146200
C	-3.70442900	3.05237500	1.00226000
C	-2.68296200	0.62276300	3.79145600
H	-1.76034300	0.99210100	4.21783100

C	-3.42007400	-0.44816400	4.19986300
H	-3.21021100	-1.12362000	5.01699300
C	-10.47695700	-0.82423500	-0.05253000
C	-11.65768500	-0.13341300	0.26403300
H	-11.59098900	0.82138900	0.77802500
C	-12.90590600	-0.66447800	-0.06311400
H	-13.80824100	-0.11653200	0.19553800
C	-12.99662500	-1.89687600	-0.71288600
H	-13.96873400	-2.31047200	-0.96763600
C	-11.83070800	-2.59542900	-1.03130100
H	-11.89082300	-3.55458200	-1.53904200
C	-10.58304400	-2.06399700	-0.70297600
H	-9.67736600	-2.60861100	-0.95543700
C	-6.75594400	4.77742800	-2.05595500
C	-6.02117400	4.86371100	-3.24882500
C	-6.22776900	5.91578000	-4.14210300
H	-5.65192600	5.96141900	-5.06281300
C	-7.17367100	6.90212600	-3.85719500
H	-7.33527000	7.72183500	-4.55210700
C	-7.91066400	6.82893100	-2.67371100
H	-8.64608400	7.59467100	-2.44098700
C	-7.70374900	5.77593100	-1.78159300
H	-8.27454400	5.72423000	-0.85858400
C	-1.65160000	2.99293200	2.40600400
C	-1.63608900	4.19439200	3.12566700
H	-2.58773200	4.63964400	3.40106100
C	-0.44168300	4.81897000	3.48246600
H	-0.46012600	5.75129500	4.03941900
C	0.76955600	4.23668400	3.11213100
H	1.71028200	4.71447100	3.37136300
C	0.79303600	3.03591300	2.40552600
H	1.72943600	2.58757700	2.10704000
C	-0.41041600	2.40448400	2.05773100
C	-5.47316300	-2.48554700	4.56268300
C	-5.72223100	-2.15760200	5.90455300
H	-6.03643700	-1.14783400	6.15505200
C	-5.57403000	-3.11385000	6.91027100
H	-5.77488600	-2.84375100	7.94388300
C	-5.17083700	-4.41214600	6.59001900
H	-5.05253300	-5.15573300	7.37390100
C	-4.92024000	-4.74829900	5.25883300
H	-4.59788000	-5.75128500	4.99331600
C	-5.07381900	-3.79339700	4.25166800
H	-4.87179500	-4.07309900	3.22247300

N	2.46848700	-2.91735600	-2.75425500
H	2.92573100	-2.35055800	-2.05050600
N	-2.14453900	-3.67189500	1.16304600
N	-0.44540900	1.16307800	1.38127000
H	-1.37449600	0.77411600	1.28834800
O	0.52604000	-4.07288200	-3.19795800
O	1.73137600	0.85156600	0.72235100
C	0.18390700	-0.92527700	0.32806000
C	0.88527000	-1.44635200	-0.76534700
C	0.56258600	-2.71572400	-1.24901100
C	-0.44020700	-3.47468900	-0.63406000
H	-0.65314700	-4.45618000	-1.03479100
C	-1.14586200	-2.96249000	0.45854300
C	-0.82513400	-1.67940300	0.93439500
H	-1.34772600	-1.29917200	1.80991000
C	0.57295000	0.43782200	0.82736900
C	1.18031400	-3.30729300	-2.49184900
H	-2.36355300	4.80803200	0.54618200
H	-7.91222100	-3.17570800	3.68282300
H	-10.47885200	1.30694600	-1.71779100
H	-5.28823600	4.09478100	-3.47816900
C	-2.81879700	-4.86838500	0.94048300
C	-3.05257700	-5.37873200	-0.44534800
C	-3.26648400	-4.53744300	-1.54588800
C	-3.17828600	-6.76650100	-0.60395200
C	-3.58293600	-5.08061200	-2.78996200
H	-3.18372400	-3.46123200	-1.43351600
C	-3.47743800	-7.30688900	-1.85185100
H	-3.04429700	-7.40442200	0.26333000
C	-3.68144700	-6.46434900	-2.94716600
H	-3.74657500	-4.42521900	-3.64082200
H	-3.55792300	-8.38384100	-1.96950100
H	-3.91774900	-6.88457400	-3.92086300
O	-3.28635200	-5.46095900	1.90937100
H	1.63508600	-0.82508400	-1.24297300
H	-2.24935600	-3.39853700	2.13525100
C	4.55868600	-0.70082200	2.43056700
H	3.86231300	-0.27038200	3.16510400
C	5.93167400	-0.82503300	3.10081400
H	6.31815800	0.16014600	3.38717800
H	5.85400800	-1.44052100	4.00313300
H	6.65719400	-1.28732400	2.42581100
N	4.64131000	0.23419300	1.26664400
H	3.70932000	0.29081300	0.84241200

H	4.80254500	1.16969900	1.64538800
C	3.99211800	-2.05274900	2.02841800
C	2.87423200	-2.56658700	2.69653500
C	4.58910400	-2.82955100	1.02585200
C	2.36366900	-3.82687900	2.37862300
H	2.39974600	-1.97506800	3.47690400
C	4.07583300	-4.08544800	0.69896500
H	5.45998800	-2.45386200	0.50054600
C	2.96235700	-4.58947300	1.37550000
H	1.49775300	-4.20983000	2.91247400
H	4.55562200	-4.67040400	-0.08099900
H	2.56658600	-5.56982300	1.12365600
C	-4.79785400	0.25683700	-2.09432700
H	-5.00891600	1.32591900	-2.00629200
C	-5.96603800	-0.39944200	-2.83169500
H	-6.04764700	0.00298000	-3.84566700
H	-5.83708500	-1.48596300	-2.91175700
H	-6.90549100	-0.20524200	-2.30634200
N	-4.75519400	-0.25638900	-0.68236400
H	-4.95018000	-1.25905100	-0.67180400
H	-3.80390200	-0.16055500	-0.32640400
C	-3.44613300	0.11415900	-2.78012900
C	-2.57989700	1.21599100	-2.81261200
C	-3.00372700	-1.09933700	-3.32591700
C	-1.30464200	1.10919500	-3.37120000
H	-2.90676700	2.16451300	-2.39059600
C	-1.72716200	-1.21504600	-3.87735100
H	-3.66173800	-1.96455900	-3.32571500
C	-0.87487500	-0.10825400	-3.90059700
H	-0.64615700	1.97387800	-3.38192200
H	-1.38791100	-2.17158400	-4.26495000
H	0.12310700	-0.19718400	-4.32031700



Cartesian coordinates for Geometry Optimized ConformerB • (1R)₂

Atoms	x	y	z
Zn	5.75764400	0.73929100	0.88685000
N	4.12114200	0.47673700	2.16197200
N	5.00517900	2.61589400	0.42650600
N	7.63817100	1.40315700	0.29994200
N	6.72801500	-0.78407500	1.97359200
C	2.75977500	2.43394800	1.45823200
C	6.95715700	3.51241400	-0.81183500
C	9.00459200	-0.53572100	1.02780400
C	4.85820000	-1.54252700	3.40944900
C	3.92577600	-0.54428100	3.06529600
C	2.98160300	1.24555400	2.18776200
C	3.72850500	3.07294100	0.65804600
C	5.62330400	3.55734200	-0.36380600
C	7.88308200	2.49743000	-0.49309500
C	8.79957100	0.66724900	0.32224700
C	8.03748300	-1.17527800	1.83019700

C	6.16999500	-1.62653700	2.90509100
C	2.60930600	-0.42780100	3.65543800
H	2.20085700	-1.09042800	4.40442800
C	2.02990700	0.68198000	3.11994400
H	1.05806700	1.09628600	3.34767000
C	3.52843900	4.33074600	-0.03070000
H	2.61867500	4.91292200	-0.02062600
C	4.70158400	4.63529000	-0.64883500
H	4.92966700	5.51533300	-1.23217700
C	9.23759500	2.44293200	-1.00032000
H	9.68959200	3.17002900	-1.65893800
C	9.80226500	1.31134200	-0.50004900
H	10.80202300	0.94124700	-0.67386100
C	8.30805100	-2.31057700	2.68732900
H	9.26342700	-2.80483600	2.78665300
C	7.15494300	-2.58681300	3.35361100
H	6.98591600	-3.35339900	4.09575200
C	1.42825300	3.11588500	1.60675900
C	1.35049700	4.32680600	2.30796900
H	2.26066400	4.72317200	2.74868800
C	0.14784200	5.01749900	2.44931100
H	0.11898400	5.95272200	3.00109300
C	-1.00847400	4.49629300	1.87128100
H	-1.95471300	5.02377900	1.95447500
C	-0.97125500	3.29217100	1.17135400
H	-1.86491800	2.89380700	0.71423000
C	0.23698200	2.58912700	1.04616500
C	7.43117400	4.63423500	-1.68611900
C	6.93835000	4.78528000	-2.99187900
H	6.20864100	4.07363000	-3.36855300
C	7.37940700	5.82964000	-3.80570900
H	6.98938800	5.92676700	-4.81556300
C	8.32077700	6.74263100	-3.32704700
H	8.66422600	7.55638500	-3.96014700
C	8.81812900	6.60410900	-2.02989800
H	9.54752300	7.31310500	-1.64692000
C	8.37735900	5.55902900	-1.21700400
H	8.76113200	5.45736500	-0.20564600
C	10.36310500	-1.16366000	0.95658600
C	11.48130100	-0.52876400	1.52071800
H	11.35144900	0.42796900	2.01871100
C	12.74465800	-1.11751200	1.45748500
H	13.59657300	-0.61255800	1.90534700
C	12.91363600	-2.35221700	0.82802800

H	13.89768600	-2.81056200	0.77842700
C	11.81007600	-2.99532400	0.26471600
H	11.93142000	-3.95586300	-0.22917200
C	10.54659900	-2.40674500	0.33063000
H	9.69055800	-2.90978300	-0.11091200
C	4.44401600	-2.55218100	4.44103800
C	4.33526100	-2.18244800	5.79114200
H	4.56292700	-1.16027600	6.08144900
C	3.94593800	-3.11233100	6.75598200
H	3.87107400	-2.80911400	7.79712700
C	3.65864400	-4.42780700	6.38558700
H	3.35460800	-5.15250600	7.13635700
C	3.76651200	-4.80591200	5.04638800
H	3.54445700	-5.82684100	4.74683800
C	4.15905000	-3.87790900	4.07853200
H	4.23345000	-4.18607700	3.03890600
Zn	-6.11365600	0.51411200	-0.34111300
N	-7.02226700	-1.29276900	-0.86673900
N	-7.77332400	0.90581400	0.86900800
N	-5.77696800	2.58617600	-0.38659800
N	-5.04259000	0.39111600	-2.13888100
C	-8.88339600	-1.30898200	0.76886500
C	-7.27517800	3.26241200	1.46297300
C	-4.12064400	2.68991500	-2.22352300
C	-5.53227400	-1.96911700	-2.72633700
C	-6.51340500	-2.21993200	-1.74385100
C	-8.03817000	-1.91561500	-0.18195700
C	-8.76816300	0.02482600	1.21545100
C	-8.02957000	2.07389800	1.54499300
C	-6.21812000	3.48250400	0.55541600
C	-4.80748700	3.22688100	-1.11585700
C	-4.27672100	1.37820400	-2.70933800
C	-4.91017400	-0.71875200	-2.93500200
C	-7.18752700	-3.48872100	-1.56060400
H	-6.97160600	-4.39735500	-2.10368300
C	-8.13190100	-3.29928200	-0.59970700
C	-9.69886500	0.66805400	2.11907800
H	-10.59579500	0.21785400	2.51887700
C	-9.23813400	1.93052900	2.32896600
H	-9.68916200	2.70626900	2.93063200
C	-5.46326100	4.71411300	0.45039200
H	-5.58670800	5.58217700	1.08159700
C	-4.59657700	4.55871800	-0.58838100
H	-3.88063400	5.27532700	-0.96439300

C	-3.65466800	0.87766500	-3.91805400
H	-3.02838000	1.45365200	-4.58387500
C	-4.04318000	-0.41890300	-4.05659000
H	-3.79602600	-1.10279200	-4.85659500
C	-9.99749900	-2.13498100	1.33515600
C	-11.04419300	-2.58888900	0.51601700
H	-11.04177000	-2.32649800	-0.53812800
C	-12.08344400	-3.35711400	1.04195500
H	-12.88659900	-3.69330100	0.39124700
C	-12.09624100	-3.68716500	2.39842200
H	-12.90545700	-4.28575300	2.80827400
C	-11.06305200	-3.24191600	3.22497900
H	-11.06154100	-3.49654200	4.28174500
C	-10.02514700	-2.47255500	2.69805600
H	-9.22071800	-2.13219300	3.34411800
C	-7.65769500	4.38519900	2.37704100
C	-8.17565200	5.58888400	1.87138900
H	-8.30685700	5.69847500	0.79863200
C	-8.53180600	6.63085400	2.72827600
H	-8.93630800	7.55180500	2.31626800
C	-8.37705100	6.48966400	4.10866800
H	-8.65405200	7.30137100	4.77613700
C	-7.86706100	5.29749500	4.62583100
H	-7.74159100	5.17789800	5.69894200
C	-7.51313100	4.25562100	3.76790500
H	-7.11424300	3.32992500	4.17355100
C	-3.16975200	3.58879700	-2.95307300
C	-3.64094600	4.69097300	-3.68366100
H	-4.70922900	4.88606400	-3.71654200
C	-2.75695900	5.52352400	-4.37154000
H	-3.14215200	6.36825100	-4.93687400
C	-1.38469800	5.26980400	-4.33867800
H	-0.69560300	5.91811400	-4.87350700
C	-0.90288600	4.17908400	-3.61211300
H	0.16573700	3.98178500	-3.57428800
C	-1.78727700	3.34506200	-2.92611000
H	-1.41530400	2.50389900	-2.34920300
C	-5.20673000	-3.08371300	-3.68054900
C	-3.94701900	-3.73510500	-3.68926100
C	-3.70364200	-4.78562000	-4.58815400
H	-2.74229100	-5.27811300	-4.56787600
C	-4.69557700	-5.18082200	-5.48306500
H	-4.48907800	-5.99461400	-6.17320700
C	-5.93606600	-4.54498100	-5.49667700

H	-6.70793000	-4.84914900	-6.19795100
C	-6.17786000	-3.50786500	-4.59744400
H	-7.13839800	-3.00098200	-4.59657300
N	2.32583700	-3.38592300	0.28661400
H	2.51881400	-3.07416100	1.23430600
H	-3.27270200	-2.51437400	-2.19582100
O	-1.87656100	0.86390400	-0.08528400
O	-1.18035800	-4.67345000	-3.19471200
C	1.16429300	-2.81770100	-0.29537500
C	0.85412300	-1.49974000	0.07058400
H	1.49135700	-0.99768400	0.79348400
C	-0.28387600	-0.86996700	-0.43724100
C	-1.12684200	-1.56187000	-1.31569600
H	-1.97776400	-1.02825300	-1.72535700
C	-0.83740600	-2.88274900	-1.66556400
C	0.30368400	-3.51054800	-1.14971300
H	0.49284300	-4.53614400	-1.43824600
C	-0.69177700	0.51934300	-0.03481600
C	-1.67021900	-3.70326000	-2.62251100
N	0.31910400	1.34460300	0.37653800
N	-2.96783500	-3.28380500	-2.77703800
H	1.26053800	0.98682600	0.27936100
C	3.07880100	-4.51490400	-0.01467000
O	3.76323100	-5.01973600	0.87200200
C	3.12435300	-5.05808500	-1.40778400
C	3.01939200	-4.25517100	-2.55250200
C	3.38880600	-6.42832000	-1.54894400
C	3.15809300	-4.82248900	-3.81836600
H	2.83059700	-3.19068500	-2.46292100
C	3.51130900	-6.99385600	-2.81550900
H	3.49942100	-7.03260000	-0.65474700
C	3.39585800	-6.19155300	-3.95308900
H	3.07006500	-4.19542200	-4.70109600
H	3.70069900	-8.05886400	-2.91584600
H	3.49123200	-6.63190200	-4.94184100
H	-8.82838300	-4.02646100	-0.20832100
C	-4.53427600	-1.33516000	1.74051300
H	-4.79376600	-2.06161800	0.96261700
C	-5.62819100	-1.37657600	2.81460000
H	-5.40973600	-0.66376700	3.61997600
H	-6.60226900	-1.13048600	2.38684500
H	-5.67962200	-2.37459100	3.26054800
N	-4.53818200	-0.00247300	1.07484900
H	-4.54964800	0.73300200	1.78287000

H	-3.66225400	0.13813300	0.55887500
C	-3.18572000	-1.73906700	2.32497200
C	-2.64707500	-2.99654200	2.02797200
C	-2.49047200	-0.91009300	3.21685600
C	-1.45307400	-3.42484200	2.61184100
H	-3.17261400	-3.65114100	1.33588600
C	-1.29622800	-1.33211100	3.80064500
C	-0.77421000	-2.59387100	3.50317800
H	-1.05550100	-4.40664000	2.36882100
H	-0.77731000	-0.67896900	4.49743000
H	0.15279000	-2.92577400	3.96341800
C	5.27556600	-0.80529000	-2.20156500
H	5.32495800	-1.85006400	-2.54192300
C	6.52624000	-0.08308900	-2.71695600
H	6.57827400	-0.16195300	-3.80763700
H	6.50358700	0.97584300	-2.44680000
H	7.43823300	-0.52320300	-2.29756300
N	5.27080200	-0.79606000	-0.70520800
H	4.40885800	-1.23795200	-0.37938000
H	6.01878400	-1.41502700	-0.38728400
C	3.99885600	-0.21005600	-2.77310700
C	3.40142100	-0.80058300	-3.89502300
C	3.42295000	0.95079200	-2.24169100
C	2.25025800	-0.25514300	-4.46671800
H	3.84548700	-1.69462200	-4.32818100
C	2.26924800	1.49524700	-2.80925000
H	3.88270100	1.43745200	-1.38924900
C	1.67578300	0.89359600	-3.92059400
H	1.79982000	-0.73188100	-5.33316500
H	1.84034900	2.39615200	-2.37835600
H	0.77526100	1.31747900	-4.35671000
H	-2.88353700	0.07379900	3.46336800