

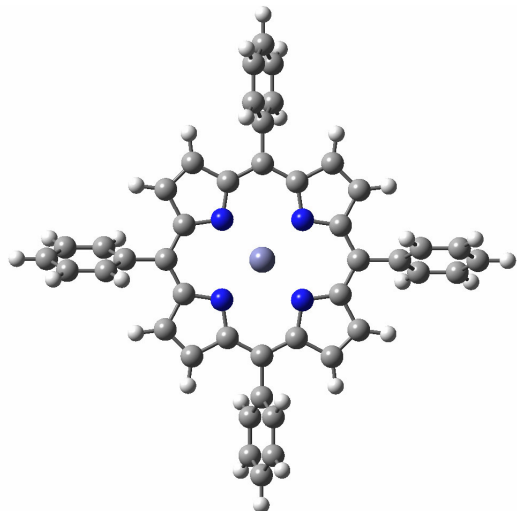
# Structural and Photophysical Studies of *trans*-AB<sub>2</sub>C-substituted Porphyrin Ligands and their Zinc and Copper Complexes

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## Supplementary Information

- Cartesian Coordinates of DFT optimised ZnTPP, **2a**, **2b**, **2c** and **2d**
- Energies of frontier orbitals of ZnTPP, **2a**, **2b**, **2c** and **2d** in eV
- Normal coordinate structural decomposition (NSD) analysis for **1a**, **2a**, **3a** and CuTPP
- Full <sup>1</sup>H and <sup>13</sup>C NMR data tables.

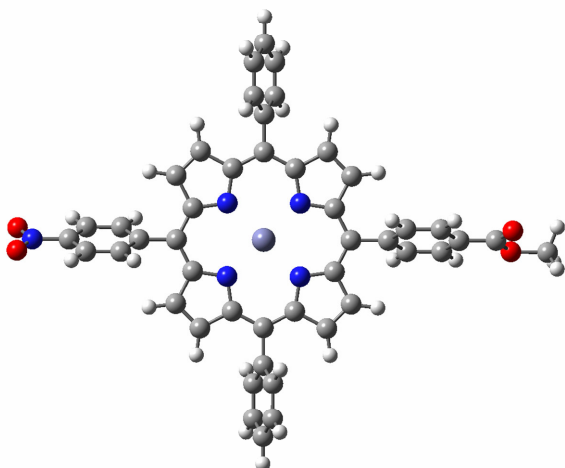
## Cartesian Coordinates of ZnTPP



Zn	0.00010200	0.00006100	-0.00009300
N	-2.06398100	0.12366700	-0.00057100
N	0.12562700	2.06395000	0.00234100
N	-0.12552700	-2.06391700	0.00041400
N	2.06407400	-0.12361200	-0.00238600
C	-2.96027300	-0.94582500	-0.00003000
C	-4.32256000	-0.42758900	0.01299800
C	-4.23909800	0.94477000	0.01163000
C	-2.82407900	1.29399700	0.00878900
H	-5.21655300	-1.03333200	0.02537600
H	-5.05304300	1.65456400	0.01052700
C	-2.31818400	2.61616000	0.00127000
C	-2.61798200	-2.31976600	0.00012300
C	-0.42823000	4.32191500	-0.01523200
C	0.94421200	4.23985300	-0.01572000
C	1.29521900	2.82515400	0.00011700
C	-0.94481200	2.95922700	-0.00714500
H	-1.03510700	5.21525700	-0.01685900
H	1.65267000	5.05474800	-0.03102000
C	2.61819800	2.31994800	0.00022200
C	0.94482100	-2.95928900	-0.00753500
C	0.42809200	-4.32200300	-0.01165500
C	-0.94433900	-4.23977600	-0.01430600
C	-1.29515000	-2.82502700	0.00028100
H	1.03494800	-5.21536500	-0.01082300
H	-1.65306900	-5.05447500	-0.02808100
C	4.32265800	0.42744600	0.01446600
C	4.23904200	-0.94490100	0.01504900
C	2.82406800	-1.29402200	0.00848700
C	2.96044000	0.94586000	0.00029900
H	5.21681800	1.03288800	0.02833800
H	5.05298900	-1.65468100	0.01615000
C	2.31818200	-2.61621400	0.00078800
C	-3.31584900	3.74249300	0.00086700
C	-3.50594600	4.53691900	-1.15229600
C	-4.44061200	5.58928800	-1.15443600
C	-5.19643600	5.86767300	0.00103500
C	-5.01182600	5.08367200	1.15652800
C	-4.08075500	4.02813100	1.15430800
H	-2.92767800	4.32195700	-2.04771800
H	-4.57834200	6.18640500	-2.05295500
H	-5.91710400	6.68209600	0.00105800
H	-5.58741100	5.29314800	2.05522900
H	-3.93705300	3.42838800	2.04987900
C	-3.74408100	-3.31692600	-0.00078900
C	-4.00240000	-4.11452500	1.13712300

C	-5.05827000	-5.04504200	1.13874800
C	-5.87014300	-5.19721200	-0.00214300
C	-5.61924300	-4.40911100	-1.14223200
C	-4.56685700	-3.47463500	-1.13914300
H	-3.38162600	-3.99584100	2.02193900
H	-5.24639000	-5.64546800	2.02583900
H	-6.23777600	-4.52159600	-2.02970100
H	-4.37318900	-2.87179000	-2.02311700
C	3.31577900	-3.74260400	0.00120000
C	4.08062700	-4.02798600	1.15473200
C	5.01149600	-5.08370200	1.15731700
C	5.19601600	-5.86810300	0.00208000
C	4.44030100	-5.58993800	-1.15351300
C	3.50582300	-4.53740400	-1.15173200
H	3.93696300	-3.42799300	2.05014400
H	5.58699200	-5.29301500	2.05611300
H	5.91656900	-6.68262700	0.00238400
H	4.57796000	-6.18735700	-2.05184200
H	2.92760300	-4.32262500	-2.04722700
C	3.74414000	3.31699500	-0.00072100
C	3.99530100	4.12303100	1.13293300
C	5.05110400	5.05356300	1.13448400
C	5.87023700	5.19751300	-0.00227100
C	5.62658500	4.40107500	-1.13814000
C	4.57426800	3.46660200	-1.13494100
H	3.36910800	4.01070200	2.01474300
H	5.23354700	5.66039500	2.01839100
H	6.25066900	4.50717000	-2.02249800
H	4.38614000	2.85754600	-2.01583700
H	6.68478600	5.91803100	-0.00290000
H	-6.68473300	-5.91768700	-0.00269000

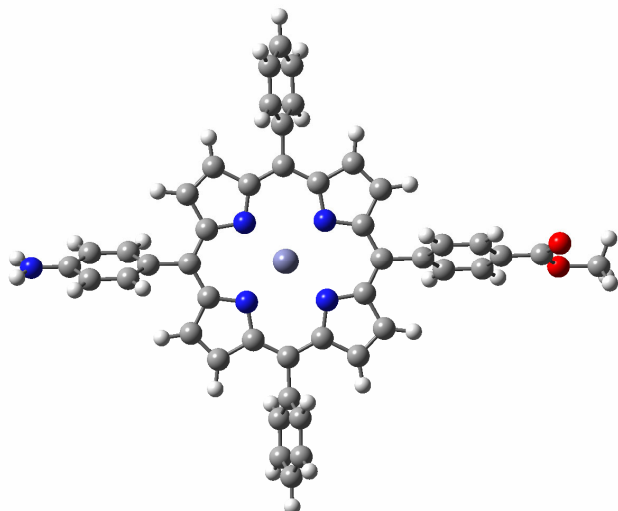
## Cartesian Coordinates of 2a



Zn	-0.23858600	0.00883000	0.02310900
N	1.23702800	-1.43991800	0.04131900
N	-1.68899400	-1.46647200	0.01021400
N	1.21031100	1.48414700	0.04148500
N	-1.71551800	1.45742700	-0.00120100
C	2.61474100	-1.22137700	0.05482000
C	3.30219400	-2.50686700	0.07357900
C	2.33870200	-3.48688800	0.05883400
C	1.04235200	-2.82138200	0.04578200
H	4.37327800	-2.64109300	0.09907700
H	2.48838200	-4.55616400	0.05541100
C	-0.20663900	-3.48759500	0.02548100
C	3.25622100	0.04060400	0.06899500
C	-2.75015000	-3.53480100	-0.00825600
C	-3.73235700	-2.57376000	-0.02234700
C	-3.06987100	-1.27447700	-0.00242800
C	-1.46688200	-2.84494800	0.00531700
H	-2.87981300	-4.60669300	-0.00594000
H	-4.79992500	-2.73329800	-0.05096100
C	-3.73304900	-0.02297200	-0.02048500
C	0.99084600	2.86184800	0.03186700
C	2.27481600	3.55077200	0.05370500
C	3.25595000	2.58841300	0.06519900
C	2.59165500	1.29064800	0.06544500
H	2.40510000	4.62256300	0.06175000
H	4.32471000	2.74207200	0.06957800
C	-3.77881600	2.52744100	-0.01986300
C	-2.81415300	3.50614700	-0.01051600
C	-1.51861800	2.83972000	0.00824100
C	-3.09256200	1.24041900	-0.02262200
H	-4.84946100	2.66766000	-0.01717300
H	-2.96307500	4.57552400	-0.01657100
C	-0.27016800	3.50525400	0.01955100
C	-0.19256900	-4.99229400	0.02509700
C	-0.57454900	-5.71623000	-1.12703800
C	-0.55837000	-7.12348000	-1.12959000
C	-0.16619600	-7.82942400	0.02435200
C	0.21299200	-7.11686300	1.17858700
C	0.20308900	-5.70956500	1.17677200
H	-0.87187900	-5.17533000	-2.02226100
H	-0.84864500	-7.66433300	-2.02725400
H	-0.15633400	-8.91675000	0.02416500
H	0.51316500	-7.65265300	2.07602200
H	0.49080000	-5.16370400	2.07211200
C	4.75921400	0.05442200	0.09075900
C	5.46062400	0.50470100	1.23389700
C	6.86261800	0.51457600	1.25748900

C	7.59423700	0.08043200	0.13046000
C	6.90470500	-0.36724400	-1.01730700
C	5.50152500	-0.38230200	-1.03117000
H	4.90193800	0.83293600	2.10621100
H	7.40520600	0.85189000	2.13593400
H	7.47037600	-0.69546800	-1.88267900
H	4.97355600	-0.72040000	-1.91878800
C	-0.28339200	5.00990100	0.01915800
C	-0.70918500	5.72721300	1.16002900
C	-0.71851300	7.13451300	1.16180300
C	-0.30836900	7.84700300	0.01818800
C	0.11445700	7.14101400	-1.12487200
C	0.13004600	5.73378900	-1.12209800
H	-1.02033800	5.18136500	2.04751300
H	-1.04229600	7.67034000	2.05096100
H	-0.31792500	8.93432800	0.01781900
H	0.42903700	7.68188100	-2.01429500
H	0.45152000	5.19284700	-2.00890000
C	-5.23435500	-0.03674600	-0.03860100
C	-5.96536500	-0.52912100	1.06956900
C	-7.36711800	-0.54238500	1.06463800
C	-8.04162000	-0.06306200	-0.07210800
C	-7.34929700	0.42915800	-1.19250900
C	-5.94780700	0.44222500	-1.16396000
H	-5.42783400	-0.88622200	1.94303500
H	-7.93562400	-0.90823300	1.91227700
H	-7.90415700	0.78450800	-2.05355700
H	-5.39644500	0.80957600	-2.02446700
C	9.08015500	0.11170300	0.19763300
O	9.74516800	0.49445100	1.17988000
O	9.67585500	-0.33798400	-0.96826800
N	-9.51568600	-0.07707700	-0.08973600
C	11.14853200	-0.34402600	-0.99788000
H	11.40843000	-0.71772400	-1.98929600
H	11.53361700	0.66897500	-0.84434900
H	11.53892900	-1.00066400	-0.21395300
O	-10.11273500	0.36689800	-1.13189900
O	-10.12890600	-0.53261700	0.93793200

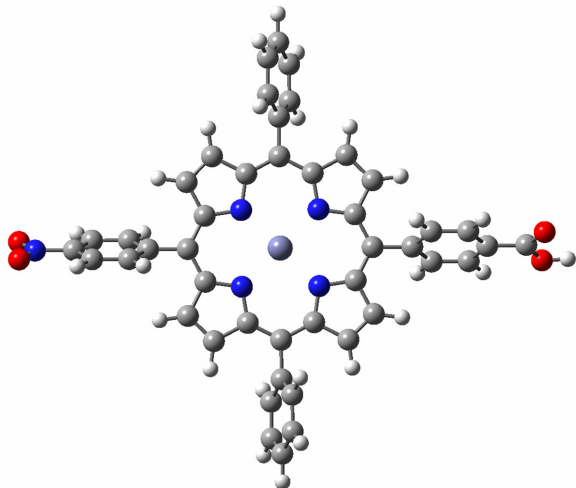
## Cartesian Coordinates of 2b



Zn	-0.60316900	0.00398200	0.01897800
N	0.87971000	-1.43855300	0.04456300
N	-2.04727200	-1.47597300	0.00888700
N	0.84223200	1.48406900	0.03563100
N	-2.08449900	1.44628000	-0.01394300
C	2.25641700	-1.21553700	0.06139400
C	2.94759100	-2.49916500	0.08927900
C	1.98715400	-3.48235000	0.07617000
C	0.68838500	-2.82157700	0.05458700
H	4.01900700	-2.63032200	0.11968300
H	2.14057200	-4.55121200	0.07908200
C	-0.55743700	-3.49080700	0.02987100
C	2.89375200	0.04882500	0.07117200
C	-3.10204100	-3.54661600	-0.02866100
C	-4.08699300	-2.58760500	-0.05294300
C	-3.43025200	-1.28720800	-0.01949400
C	-1.82146200	-2.85265900	0.00186400
H	-3.22803500	-4.61903100	-0.03247800
H	-5.15449100	-2.74217000	-0.09725600
C	-4.10562700	-0.04097900	-0.03172300
C	0.61603100	2.86174400	0.01974800
C	1.89755300	3.55554300	0.03770600
C	2.88275200	2.59727100	0.05409600
C	2.22409900	1.29636000	0.06103100
H	2.02380000	4.62795700	0.04007700
H	3.95088600	2.75577500	0.05728900
C	-4.15292700	2.50532300	-0.01124100
C	-3.19255400	3.48923000	-0.00808400
C	-1.89425700	2.82831600	-0.00131200
C	-3.46242200	1.22219600	-0.02514700
H	-5.22483400	2.63255500	0.00294600
H	-3.34590000	4.55809200	-0.00830200
C	-0.64675300	3.49879100	0.00720700
C	-0.53819800	-4.99561800	0.03160800
C	-0.90569100	-5.72339900	-1.12289600
C	-0.88379700	-7.13060200	-1.12358400
C	-0.49968800	-7.83377300	0.03484100
C	-0.13483600	-7.11788200	1.19162700
C	-0.15119800	-5.71054700	1.18772700
H	-1.19703000	-5.18440600	-2.02119600
H	-1.16307700	-7.67369600	-2.02354300
H	-0.48482600	-8.92117300	0.03602000
H	0.15940100	-7.65110100	2.09270600
H	0.12553500	-5.16178600	2.08474000
C	4.39636900	0.06823800	0.09493600

C	5.09589800	0.53798200	1.23180700
C	6.49769600	0.55354200	1.25721500
C	7.23288100	0.10493900	0.13793800
C	6.54593200	-0.36256900	-1.00372600
C	5.14298800	-0.38248600	-1.01900900
H	4.53454000	0.87684300	2.09827300
H	7.03762900	0.90600500	2.13138200
H	7.11366700	-0.70176900	-1.86354100
H	4.61704100	-0.73531800	-1.90203100
C	-0.66604500	5.00354400	0.00479600
C	-1.08807800	5.72180000	1.14655100
C	-1.10235000	7.12908800	1.14656300
C	-0.70036600	7.84170000	0.00004500
C	-0.28125300	7.13526000	-1.14409900
C	-0.26148400	5.72799400	-1.13933700
H	-1.39324100	5.17564000	2.03588600
H	-1.42331300	7.66495500	2.03688100
H	-0.71310900	8.92912200	-0.00160000
H	0.02742800	7.67579500	-2.03594300
H	0.05717300	5.18633900	-2.02670700
C	-5.60655400	-0.06031600	-0.05268400
C	-6.34838700	-0.56345700	1.04084800
C	-7.75049700	-0.58002500	1.03186700
C	-8.46923600	-0.09722100	-0.09183000
C	-7.73273700	0.40428800	-1.19564600
C	-6.33091100	0.42394700	-1.16626800
H	-5.81896700	-0.93088900	1.91691200
H	-8.29250300	-0.96387300	1.89443200
H	-8.26070300	0.77438600	-2.07281000
H	-5.78746900	0.80532100	-2.02767700
C	8.71768000	0.14235500	0.20627900
O	9.38221600	0.54212700	1.18245300
O	9.31732300	-0.32326200	-0.95257100
N	-9.86364300	-0.11515700	-0.11085000
C	10.78946300	-0.32390100	-0.97898400
H	11.05314700	-0.71375100	-1.96325900
H	11.17072000	0.69305000	-0.84237000
H	11.18138700	-0.96506500	-0.18300700
H	-10.38776200	-0.47302200	0.67279500
H	-10.37526000	0.22982400	-0.90841500

## Cartesian Coordinates of 2c

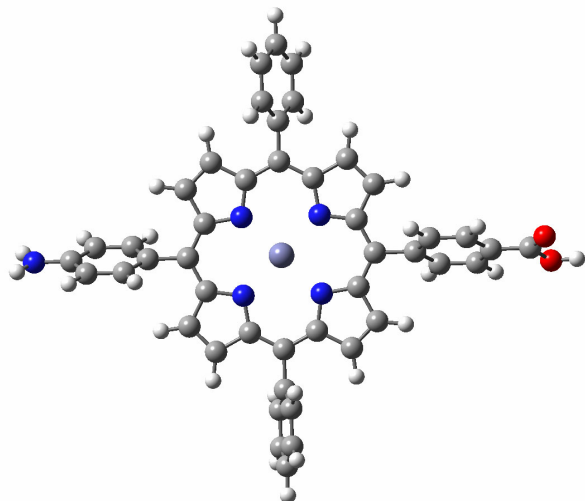


Zn	0.00821000	0.00170600	-0.00450800
N	-1.45667300	-1.45822200	-0.00605800
N	1.46972900	-1.46260200	-0.00558100
N	-1.45214400	1.46606600	-0.00898800
N	1.47421700	1.46150400	0.00321500
C	-2.83597500	-1.25024600	-0.00440600
C	-3.51375300	-2.54108700	-0.01524400
C	-2.54267800	-3.51363000	-0.01079600
C	-1.25137700	-2.83825700	-0.01211000
H	-4.58389700	-2.68427300	-0.02925000
H	-2.68422500	-4.58398900	-0.00533400
C	0.00269200	-3.49496100	-0.00462600
C	-3.48672100	0.00705500	-0.01242700
C	2.54677900	-3.52275200	0.00282100
C	3.52173400	-2.55428400	0.00675200
C	2.84919100	-1.26011400	-0.00713100
C	1.25820200	-2.84265600	0.00228300
H	2.68452200	-4.59361800	-0.00049100
H	4.59071200	-2.70567400	0.02463200
C	3.50296600	-0.00365100	0.00314700
C	-1.24267500	2.84546900	-0.00246300
C	-2.53187500	3.52481000	-0.01058400
C	-3.50593700	2.55528200	-0.01070100
C	-2.83207100	1.26234400	-0.01759200
H	-2.67016500	4.59558400	-0.01767400
H	-4.57567100	2.70191100	-0.00288100
C	3.52957300	2.54693000	-0.00028400
C	2.55756400	3.51836200	-0.00047300
C	1.26693400	2.84219400	-0.00549400
C	2.85302800	1.25481800	0.01066200
H	4.59906600	2.69508300	-0.01377500
H	2.69852300	4.58880900	0.00336200
C	0.01340800	3.49834800	-0.00422100
C	0.00006900	-4.99974400	-0.00360700
C	0.39928300	-5.72024800	1.14482600
C	0.39385600	-7.12756800	1.14794100
C	-0.00466600	-7.83688600	-0.00174700
C	-0.40096600	-7.12770000	-1.15230200
C	-0.40177400	-5.72037900	-1.15102900
H	0.70156900	-5.17680100	2.03684500
H	0.69733400	-7.66586800	2.04275100
H	-0.00631500	-8.92424500	-0.00111100
H	-0.70616300	-7.66612900	-2.04644400
H	-0.70260100	-5.17710000	-2.04362900
C	-4.98978700	0.00950300	-0.01624700
C	-5.70792200	0.45875700	-1.14992800
C	-7.10965800	0.45860300	-1.15724300



C	-7.82311500	0.01464000	-0.02191400
C	-7.11786400	-0.43233100	1.11663400
C	-5.71488100	-0.43688700	1.11331500
H	-5.16162000	0.79390300	-2.02730000
H	-7.66484700	0.79502400	-2.02814400
H	-7.67099600	-0.76761400	1.98751400
H	-5.17349200	-0.77385400	1.99308700
C	0.01534100	5.00311300	-0.00551900
C	0.42201000	5.72218700	-1.15222600
C	0.42064600	7.12950900	-1.15565700
C	0.01882400	7.84023000	-0.00799300
C	-0.38488100	7.13246000	1.14085600
C	-0.38978400	5.72515300	1.13986400
H	0.72671200	5.17769200	-2.04277800
H	0.72967300	7.66671800	-2.04921200
H	0.02016900	8.92758600	-0.00894000
H	-0.69279400	7.67200100	2.03339800
H	-0.69643100	5.18292000	2.03112300
C	5.00451600	-0.00597900	0.00628800
C	5.72825000	-0.49231400	-1.10923900
C	7.13007200	-0.49471700	-1.11808000
C	7.81191400	-0.01048600	0.01215000
C	7.12691800	0.47597900	1.13951000
C	5.72514700	0.47808400	1.12480900
H	5.18498700	-0.85345600	-1.97749600
H	7.69304000	-0.85596900	-1.97137100
H	7.68748000	0.83545800	1.99513200
H	5.17943400	0.84101200	1.99078300
C	-9.30493300	0.03443800	-0.06731300
O	-9.99914100	0.41263300	-1.02869500
O	-9.89135000	-0.42579600	1.10862400
N	9.28627500	-0.01292100	0.01526500
O	9.88991100	0.43534400	1.05171700
O	9.89280200	-0.46318300	-1.01861900
H	-10.87163000	-0.39341600	1.03368700

## Cartesian Coordinates of 2d



Zn	0.37175200	0.00103100	-0.00386100
C	-2.47525600	-1.24823100	-0.00996400
C	-3.15330900	-2.53912900	-0.02928300
C	-2.18259500	-3.51215300	-0.02754700
C	-0.89064800	-2.83787800	-0.02209800
N	-1.09633400	-1.45681900	-0.01026100
H	-4.22349600	-2.68210200	-0.04707300
H	-2.32486200	-4.58254600	-0.02827100
C	0.36213600	-3.49414100	-0.01222100
C	-3.12541700	0.00971900	-0.01297500
C	2.90767600	-3.52356200	0.01549400
C	3.88288500	-2.55447300	0.02775900
C	3.21239300	-1.26094500	0.00172300
N	1.83120700	-1.46392600	-0.00999000
C	1.61976900	-2.84278900	0.00022500
H	3.04457800	-4.59463200	0.01819100
H	4.95235500	-2.69793300	0.05957600
C	3.87501900	-0.00779300	0.00542900
N	-1.08902000	1.46606300	-0.00458900
C	-0.87651600	2.84607300	0.00786300
C	-2.16508900	3.52681700	0.00567300
C	-3.14064700	2.55869800	0.00195900
C	-2.46896300	1.26438400	-0.01271600
H	-2.30206600	4.59789900	0.00467600
H	-4.21017200	2.70717500	0.01272600
C	3.89573000	2.53883200	-0.01702700
C	2.92531100	3.51275300	-0.00954200
C	1.63397100	2.83840400	-0.00101500
N	1.83848900	1.45850200	0.01033900
C	3.21869200	1.24865600	0.00576900
H	4.96603900	2.67697700	-0.04362100
H	3.06749500	4.58313800	-0.01163500
C	0.37956800	3.49605900	0.00466800
C	0.35854300	-4.99906600	-0.01330400
C	0.74821600	-5.72244400	1.13668800
C	0.74100700	-7.12979200	1.13801000
C	0.34966200	-7.83736600	-0.01530700
C	-0.03716800	-7.12581300	-1.16762600
C	-0.03549800	-5.71838900	-1.16431400
H	1.04521900	-5.18011300	2.03111000
H	1.03721800	-7.66959600	2.03450100
H	0.34605500	-8.92484100	-0.01598700
H	-0.33713200	-7.66246800	-2.06474600
H	-0.32908300	-5.17293700	-2.05797600
C	-4.62809500	0.01356400	-0.01716500
C	-5.34689300	0.48164200	-1.14326800

C	-6.74849500	0.48296100	-1.15111900
C	-7.46322800	0.02107400	-0.02346700
C	-6.75798600	-0.44498100	1.10774700
C	-5.35516900	-0.45038300	1.10452200
H	-4.79974400	0.82991500	-2.01491900
H	-7.30293000	0.83379700	-2.01682000
H	-7.31135800	-0.79376000	1.97317100
H	-4.81392700	-0.80139800	1.97880800
C	0.38348200	5.00097100	0.00536300
C	0.78308400	5.72204700	-1.14266200
C	0.78275900	7.12940700	-1.14443100
C	0.38851100	7.83925000	0.00649400
C	-0.00816300	7.12997800	1.15686900
C	-0.01340800	5.72256800	1.15396400
H	1.08221600	5.17800200	-2.03532700
H	1.08639500	7.66745700	-2.03947800
H	0.39006600	8.92672700	0.00676700
H	-0.31056300	7.66841500	2.05210300
H	-0.31468000	5.17882400	2.04611200
C	5.37613400	-0.01156900	0.00900700
C	6.11063500	-0.50841400	-1.09236500
C	7.51284000	-0.51029000	-1.09937700
C	8.23921800	-0.01862100	0.01554100
C	7.51019400	0.47663500	1.12713700
C	6.10803300	0.48167800	1.11371800
H	5.57522900	-0.88240200	-1.96198700
H	8.04895100	-0.88949100	-1.96763200
H	8.04420800	0.85326200	1.99780300
H	5.57052400	0.85836700	1.98087700
C	-8.94412500	0.04259400	-0.06876400
O	-9.63980600	0.43603900	-1.02354200
O	-9.53264900	-0.43618800	1.09969900
H	-10.51261000	-0.40097700	1.02224300
N	9.63377900	-0.02194200	0.01865800
H	10.15267700	-0.37573800	-0.77030700
H	10.15083200	0.32883100	0.81017900

### Energies of frontier orbitals of ZnTPP, 2a, 2b, 2c and 2d in eV

	HOMO-1	HOMO	LUMO	LUMO+1	LUMO+2
ZnTPP	-5,42	-5,14	-2,39	-2,39	-0,86
2a	-5,77	-5,51	-3,20	-2,74	-2,72
2b	-5,40	-5,05	-2,39	-2,37	-1,60
2c	-5,81	-5,55	-3,23	-2,78	-2,75
2d	-5,44	-5,09	-2,43	-2,40	-1,76

## Normal coordinate structural decomposition (NSD) analysis for 1a, 2a, 3a and CuTPP

NSD analyses of the compounds was accomplished using the web-based NSD program (<http://jasheln.unm.edu/>). The results of the NSD decomposition are given below.

NSD result generated from file 1a.PDB at Tue Apr 10 17:53:41 CEST 2007

Summary of the NSD (in Å):

basis	Doop	doop	B2u	B1u	A2u	Eg(x)	Eg(y)	A1u
min.	0,2588	0,0384	-0,0693	0,0741	-0,0044	0,0724	0,2267	-0,0066
ext.	0,3416	0,0060	-0,0690	0,0741	-0,0043	0,0711	0,2350	-0,0066
			0,0151	-0,0045	0,0021	-0,0327	0,2201	0,0005
comp.	0,3434	0,0000	0,0709	0,0743	0,0048	0,0846	0,3165	0,0066

NSD result generated from file 2a.PDB at Tue Apr 10 17:47:18 CEST 2007

Summary of the NSD (in Å):

basis	Doop	doop	B2u	B1u	A2u	Eg(x)	Eg(y)	A1u
min.	0,3392	0,0210	-0,2076	0,0204	0,1238	-0,2159	0,0959	0,0200
ext.	0,3608	0,0032	-0,2072	0,0204	0,1240	-0,2203	0,0971	0,0200
			0,0225	-0,0058	0,0039	-0,1172	0,0295	0,0021
comp.	0,3613	0,0000	0,2088	0,0212	0,1240	0,2459	0,1011	0,0201

NSD result generated from file 3a.PDB at Tue Apr 10 17:56:18 CEST 2007

Summary of the NSD (in Å):

basis	Doop	doop	B2u	B1u	A2u	Eg(x)	Eg(y)	A1u
min.	0,9525	0,0077	0,8607	0,3243	-0,2356	-0,0511	0,0551	-0,0063
ext.	0,9533	0,0035	0,8601	0,3243	-0,2361	-0,0516	0,0556	-0,0063
			-0,0330	0,0024	-0,0120	-0,0120	0,0136	-0,0059
comp.	0,9536	0,0000	0,8614	0,3246	0,2359	0,0541	0,0581	0,0086

NSD result generated from file CuTPP.PDB at Tue Apr 10 17:43:51 CEST 2007

Summary of the NSD (in Å):

basis	Doop	doop	B2u	B1u	A2u	Eg(x)	Eg(y)	A1u
min.	1,1964	0,0185	-0,1822	-1,1825	0,0000	0,0000	0,0000	0,0000
ext.	1,2028	0,0056	-0,1798	-1,1825	0,0000	0,0000	0,0000	0,0000
			0,1239	-0,0056	0,0000	0,0000	0,0000	0,0000
comp.	1,2033	0,0000	0,2227	1,1825	0,0000	0,0000	0,0000	0,0000

Full  $^1\text{H}$  and  $^{13}\text{C}$  NMR data tables. $^1\text{H}$  NMR data of **1a** – **1d** and **2a** – **2d** in  $[\text{D}]_8\text{-THF}$  (atom numbering according to Scheme 3)

	<b>1a</b>	<b>1b</b>	<b>1c</b>	<b>1d</b>	<b>2a</b>	<b>2b</b>	<b>2c</b>	<b>2d</b>
$\text{NH}_{\text{pyrrol}}$	-2.72 (s, 2H)	-2.66 (s, 2H)	-2.72 (s, 2H)	-2.67 (s, 2H)	–	–	–	–
$\text{NH}_2$	–	5.00 (br.s, 2H)	–	5.04 (br.s, 2H)	–	4.88 (br.s)	–	5.35 (br.s)
$\text{CH}_3$	4.04 (s, 3H)	4.04 (s, 3H)	–	–	4.04 (s, 3H)	4.04 (s, 3H)	–	–
$5_2$	8.45 (d, 2H, $^3J_{\text{HH}} = 8.5 \text{ Hz}$ )	7.88 (d, 2H, $^3J_{\text{HH}} = 8.3 \text{ Hz}$ )	8.46 (d, 2H, $^3J_{\text{HH}} = 8.4 \text{ Hz}$ )	7.87 (d, 2H, $^3J_{\text{HH}} = 8.2 \text{ Hz}$ )	8.43 (d, 2H, $^3J_{\text{HH}} = 8.6 \text{ Hz}$ )	7.86 (d, 2H, $^3J_{\text{HH}} = 6.7 \text{ Hz}$ )	8.43 (d, 2H, $^3J_{\text{HH}} = 8.5 \text{ Hz}$ )	7.99 (d, 2H, $^3J_{\text{HH}} = 8.2 \text{ Hz}$ )
$5_3$	8.66 (d, 2H, $^3J_{\text{HH}} = 8.5 \text{ Hz}$ )	6.99 (d, 2H, $^3J_{\text{HH}} = 8.3 \text{ Hz}$ )	8.67 (d, 2H, $^3J_{\text{HH}} = 8.4 \text{ Hz}$ )	6.99 (d, 2H, $^3J_{\text{HH}} = 8.2 \text{ Hz}$ )	8.64 (d, 2H, $^3J_{\text{HH}} = 8.6 \text{ Hz}$ )	6.95 (d, 2H, $^3J_{\text{HH}} = 6.7 \text{ Hz}$ )	8.64 (d, 2H, $^3J_{\text{HH}} = 8.5 \text{ Hz}$ )	7.24 (d, 2H, $^3J_{\text{HH}} = 8.2 \text{ Hz}$ )
$15_2$	8.32 (d, 2H, $^3J_{\text{HH}} = 8.0 \text{ Hz}$ )	8.31 (d, 2H, $^3J_{\text{HH}} = 8.1 \text{ Hz}$ )	8.29 (d, 2H, $^3J_{\text{HH}} = 7.8 \text{ Hz}$ )	8.26 (d, 2H, $^3J_{\text{HH}} = 7.8 \text{ Hz}$ )	8.30 (d, 2H, $^3J_{\text{HH}} = 8.1 \text{ Hz}$ )	8.30 (d, 2H, $^3J_{\text{HH}} = 8.0 \text{ Hz}$ )	8.28 (d, 2H, $^3J_{\text{HH}} = 8.0 \text{ Hz}$ )	8.30 (m, 2H)
$15_3$	8.44 (d, 2H, $^3J_{\text{HH}} = 8.0 \text{ Hz}$ )	8.42 (d, 2H, $^3J_{\text{HH}} = 8.1 \text{ Hz}$ )	8.45 (d, 2H, $^3J_{\text{HH}} = 7.8 \text{ Hz}$ )	8.47 (d, 2H, $^3J_{\text{HH}} = 7.8 \text{ Hz}$ )	8.41 (d, 2H, $^3J_{\text{HH}} = 8.1 \text{ Hz}$ )	8.39 (d, 2H, $^3J_{\text{HH}} = 8.0 \text{ Hz}$ )	8.42 (d, 2H, $^3J_{\text{HH}} = 8.0 \text{ Hz}$ )	8.42 (m, 2H)
$10_2/20_2$	8.19 (m, 4H)	8.20 (m, 4H)	8.20 (m, 4H)	8.16 (m, 4H)	8.19 (m, 4H)	8.19 (m, 4H)	8.18 (m, 4H)	8.20 (m, 4H)
$10_3/20_3/$ $10_4/20_4$	7.77 (m, 6H)	7.76 (m, 6H)	7.77 (m, 6H)	7.72 (m, 6H)	7.74 (m, 6H)	7.73 (m, 6H)	7.74 (m, 6H)	7.76 (m, 6H)
$2,3,7,8,12,$ $13,17,18$	8.78-8.83 (m, 4H)	8.78 (m, 6H) 8.96 (d, 2H, $^3J_{\text{HH}} = 4.6 \text{ Hz}$ )	8.84 (m, 8H)	8.78 (m, 6H) 8.95 (d, 2H, $^3J_{\text{HH}} = 4.5 \text{ Hz}$ )	8.81 (m, 4H) 8.86 (d, 2H, $^3J_{\text{HH}} = 4.6 \text{ Hz}$ ) 8.88 (d, 2H, $^3J_{\text{HH}} = 4.6 \text{ Hz}$ )	8.77 (d, 2H, $^3J_{\text{HH}} = 4.5 \text{ Hz}$ ) 8.80 (d, 2H, $^3J_{\text{HH}} = 4.5 \text{ Hz}$ ) 8.83 (d, 2H, $^3J_{\text{HH}} = 4.5 \text{ Hz}$ ) 8.98 (d, 2H, $^3J_{\text{HH}} = 4.5 \text{ Hz}$ )	8.81 (d, 2H, $^3J_{\text{HH}} = 4.6 \text{ Hz}$ ) 8.84 (d, 2H, $^3J_{\text{HH}} = 4.6 \text{ Hz}$ ) 8.87 (d, 2H, $^3J_{\text{HH}} = 4.6 \text{ Hz}$ ) 8.89 (d, 2H, $^3J_{\text{HH}} = 4.6 \text{ Hz}$ )	8.89 (m, 8H)

 $^{13}\text{C}$  NMR data of **1a** – **1d** and **2a** – **2d** in  $[\text{D}]_8\text{-THF}$  (atom numbering according to Scheme 3)

	<b>1a</b>	<b>1b</b>	<b>1c</b>	<b>1d</b>	<b>2a</b>	<b>2b</b>	<b>2c</b>	<b>2d</b>
$\text{CH}_3$	52.2 (s)	51.9 (s)	–	–	52.2 (s)	52.2 (s)	–	–
$\text{CO}$	167.0 (s)	167.3 (s)	167.6 (s)	169.6 (s)	167.0 (s)	167.3 (s)	168.9 (s)	167.4 (s)
$5$	118.4 (s)	122.8 (s)	121.4 (s)	120.7 (s)	118.9 (s)	123.1 (s)	118.5 (s)	124.2 (s)
$5_1$	149.5 (s)	130.6 (s)	149.6 (s)	128.9 (s)	149.9 (s)	132.0 (s)	150.3 (s)	140.5 (s)
$5_2$	135.3 (s)	136.1 (s)	135.9 (s)	136.3 (s)	135.8 (s)	136.2 (s)	135.7 (s)	135.5 (s)
$5_3$	122.5 (s)	112.9 (s)	122.3 (s)	113.0 (s)	122.0 (s)	112.7 (s)	122.1 (s)	119.1 (s)
$5_4$	148.9 (s)	149.7 (s)	148.5 (s)	143.4 (s)	148.6 (s)	148.7 (s)	148.6 (s)	150.9 (s)
$15$	120.2 (s)	118.3 (s)	120.8 (s)	119.8 (s)	120.2 (s)	119.2 (s)	120.8 (s)	119.7 (s)
$15_1$	147.7 (s)	148.0 (s)	147.4 (s)	142.2 (s)	148.8 (s)	149.5 (s)	148.4 (s)	148.7 (s)
$15_2$	135.3 (s)	134.9 (s)	135.3 (s)	134.9 (s)	135.2 (s)	135.2 (s)	135.0 (s)	134.9 (s)
$15_3$	128.5 (s)	128.1 (s)	128.6 (s)	128.5 (s)	127.9 (s)	128.0 (s)	128.1 (s)	128.0 (s)
$15_4$	130.8 (s)	130.4 (s)	131.6 (s)	131.3 (s)	130.3 (s)	130.0 (s)	131.2 (s)	130.7 (s)
$10/20$	121.3 (s)	120.9 (s)	121.4 (s)	123.0 (s)	121.9 (s)	121.7 (s)	121.7 (s)	121.6 (s)
$10_1/20_1$	142.6 (s)	143.4 (s)	142.8 (s)	141.9 (s)	143.8 (s)	144.5 (s)	144.2 (s)	144.4 (s)
$10_2/20_2$	135.3 (s)	135.2 (s)	134.9 (s)	135.1 (s)	134.9 (s)	135.2 (s)	135.0 (s)	134.9 (s)
$10_3/20_3$	127.4 (s)	127.5 (s)	127.5 (s)	127.4 (s)	127.0 (s)	127.1 (s)	127.1 (s)	126.5 (s)
$10_4/20_4$	128.6 (s)	128.5 (s)	128.8 (s)	128.5 (s)	128.1 (s)	128.3 (s)	128.0 (s)	128.2 (s)
$2,3,7,8,12,$ $13,17,18$	131.1 (s)	131.2 (s)	n.o.	131.0 (s)	131.5 (s)	131.3 (s)	131.4 (s)	131.5 (s)
					132.6 (s)	131.7 (s)	132.1 (s)	131.8 (s)
					132.8 (s)	132.0 (s)	132.3 (s)	131.9 (s)
						132.6 (s)	132.6 (s)	132.5 (s)
$1,4,6,9,11,$ $14,16,19$	n.o.	n.o.	n.o.	n.o.	150.3 (s)	150.1 (s)	149.9 (s)	150.5 (s)
					150.7 (s)	150.8 (s)	150.1 (s)	150.6 (s)
					151.4 (s)	151.0 (s)	150.3 (s)	151.0 (s)
					151.5 (s)	151.4 (s)	150.7 (s)	151.1 (s)