

Supporting information

Formation Mechanism of ZnTPyP Fibers Fabricated by Surfactant-Assisted Method

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Table S1. Cartesian coordinates for ZnTPyP and ZnTPP dimers (**1 - 3**) calculated by B97D method.

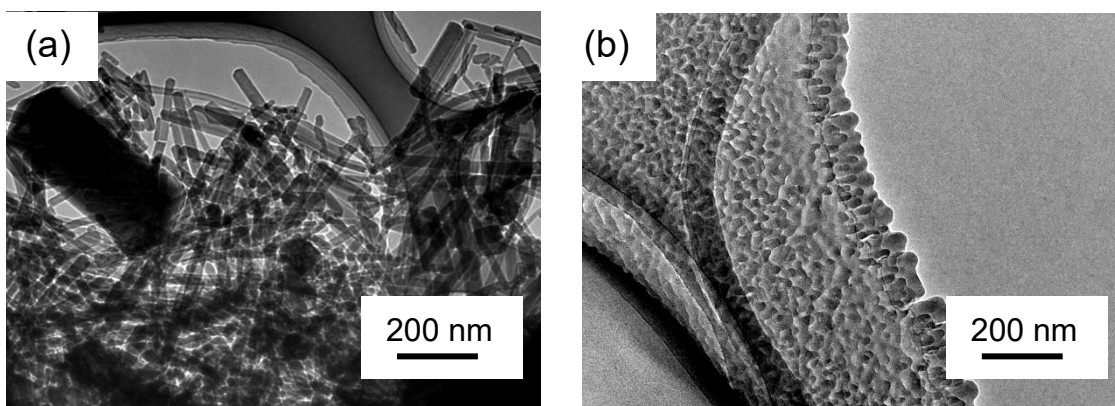


Figure S1. TEM images of ZnTPyP (a) before and (b) after washing with water.

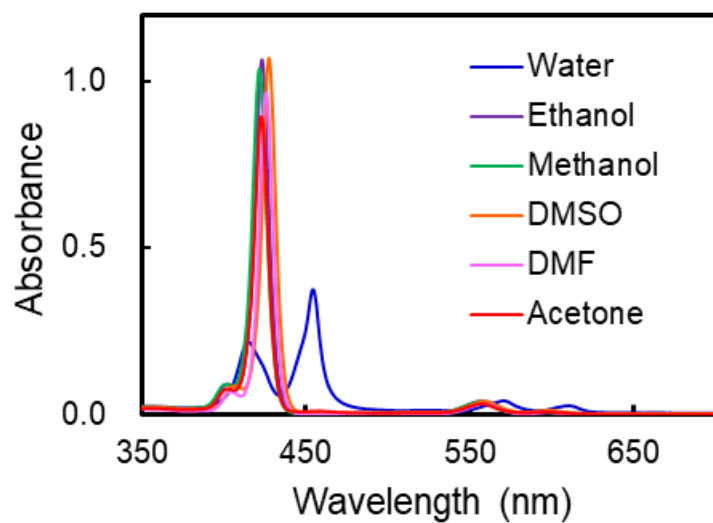
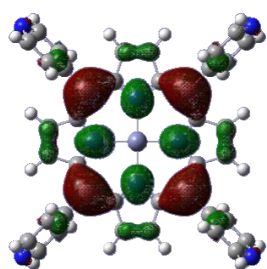
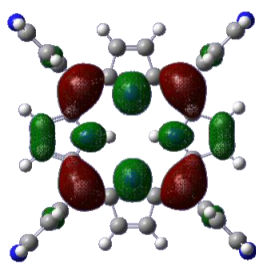


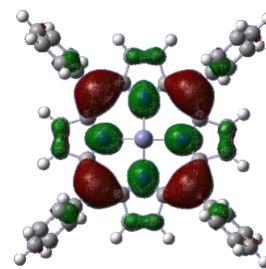
Figure S2. Absorption spectra of ZnTPyP fibers after being added into various solvents.



ZnTPyP
(63.5°)



TPyP
(90.0°)



ZnTPP
(73.5°)

Figure S3. Electron densities in HOMO of ZnTPyP, TPyP, and ZnTPP calculated by functional of B3LYP/6-311G(d)/LANL2DZ. Values in parentheses show dihedral angles between porphyrin macrocycle and phenyl or 4-pyridyl group.

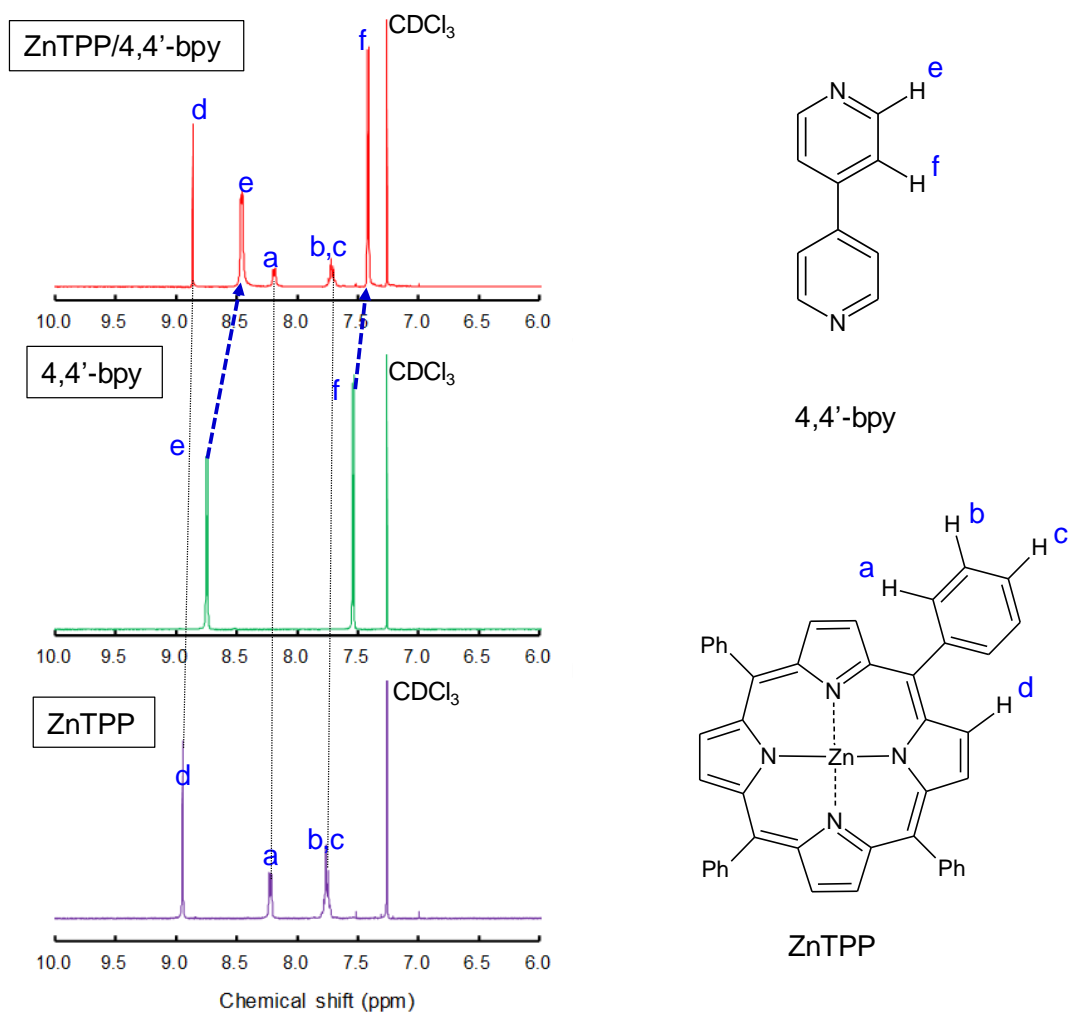


Figure S4. $^1\text{H-NMR}$ spectra of 4,4'-bpy, ZnTPP and ZnTPP/4,4'-bpy in CDCl_3 .

Table S1. Cartesian coordinates for ZnTPyP and ZnTPP dimers (**1 - 3**) calculated by B97D method.ZnTPyP dimer (Zn-N), **1**

N	0.17515100	4.60029900	-2.07018100
N	-0.68501200	6.46273700	0.05898300
N	1.04918800	5.04856500	1.98535500
N	1.85437400	3.16725400	-0.12115000
C	-0.75193100	5.32871300	-2.77461900
C	-1.31856800	7.04915500	-1.00823200
C	-0.85417000	7.28488700	1.14474700
C	0.48933500	5.96952200	2.83786900
C	1.83393100	4.21012600	2.74277100
C	2.67290700	2.72051500	0.88431000
C	2.14849100	2.43609100	-1.24284200
C	0.53584900	3.52715700	-2.85136500
C	-0.21535800	3.56313900	-4.09193100
C	-1.00309900	4.68159100	-4.04953100
C	-1.88467600	8.31985400	-0.58898800
C	-1.59924400	8.46471000	0.74000500
C	0.90387100	5.67766800	4.19820200
C	1.73077900	4.58893500	4.13966900
C	3.58046300	1.71768800	0.35698200
C	3.25011800	1.53544700	-0.95724500
N	-1.76202800	-6.38738300	-0.37506100
N	1.09091000	-6.01452800	0.26659300
N	0.65054300	-3.12189300	0.50552500
N	-2.16409700	-3.47442800	-0.28869200
C	-1.35011700	-7.69870700	-0.46259300
C	1.06415600	-7.39003800	0.21227800
C	2.35383600	-5.64530000	0.67389300
C	2.01072800	-3.14795500	0.72658400
C	0.27074200	-1.80098800	0.45517200
C	-2.17413300	-2.11191800	-0.09505300
C	-3.45387700	-3.85420900	-0.58539800
C	-3.07938500	-6.34353400	-0.77428100
C	-3.51107400	-7.67706100	-1.14479700
C	-2.44578500	-8.51228800	-0.95173600
C	2.35397100	-7.91051200	0.62197600
C	3.14845800	-6.83472600	0.90762000

C	2.51150800	-1.79017500	0.78188600
C	1.43874500	-0.95927800	0.61660500
C	-3.52389600	-1.61186500	-0.25786200
C	-4.31406200	-2.68648100	-0.56118300
Zn	-0.54905000	-4.75208500	0.03505400
Zn	0.36692900	4.66131300	0.03143400
C	-3.88242300	-5.17858900	-0.84462000
C	-0.05278600	-8.17832100	-0.15797300
C	2.80243800	-4.31451300	0.85667400
C	-1.04615700	-1.32651500	0.23351800
C	-1.40403700	6.50358600	-2.31418100
C	1.46812400	2.52447800	-2.48407700
C	2.61373000	3.13974900	2.23769800
C	-0.36332900	7.03635300	2.45183300
H	-4.49182100	-7.93534700	-1.52750200
H	-2.39691000	-9.57723500	-1.14778600
H	-5.38473900	-2.69317300	-0.73080300
H	-3.83023200	-0.57878400	-0.13434900
H	1.46071300	0.12081200	0.56534900
H	3.54925700	-1.50303600	0.89988200
H	4.17155200	-6.84507700	1.26590500
H	2.60931500	-8.96089800	0.70351800
H	-1.70539300	5.02239800	-4.80214400
H	-0.16092200	2.82653700	-4.88563300
H	-2.40454900	9.01991900	-1.23329700
H	-1.84382100	9.30382200	1.38150300
H	3.71563900	0.86487200	-1.67057000
H	4.36936900	1.22720800	0.91590600
H	2.21752000	4.08465800	4.96707400
H	0.59194100	6.22212200	5.08240000
C	-1.21650400	0.14967800	0.32871400
C	-0.88184400	0.83960500	1.50950900
C	-1.61586900	0.91712200	-0.77840900
C	-0.85121100	2.23166400	1.50039400
H	-0.59431200	0.28892100	2.40301200
C	-1.55937600	2.30885800	-0.69595300
H	-1.89129000	0.43439200	-1.71407000
N	-1.14279400	2.96373500	0.40623500
H	-0.52272100	2.79548000	2.37318500

H	-1.78957700	2.92985300	-1.56003500
C	-5.31279000	-5.36322800	-1.22958700
C	-6.18689800	-6.14228000	-0.45181900
C	-5.84321100	-4.76342600	-2.38499800
C	-7.52039400	-6.27839000	-0.85630500
H	-5.82994200	-6.62406700	0.45771300
C	-7.19209700	-4.96683600	-2.69993000
H	-5.20738900	-4.15689400	-3.02889300
N	-8.03476300	-5.70803900	-1.95972600
H	-8.21485800	-6.87498600	-0.25944900
H	-7.61875200	-4.51265000	-3.59776500
C	0.15885900	-9.65361200	-0.24138600
C	-0.56330400	-10.54538500	0.57039300
C	1.08828600	-10.20935600	-1.13771100
C	-0.32552300	-11.91993200	0.45026200
H	-1.29031300	-10.16752600	1.28835700
C	1.24544400	-11.59990000	-1.17998700
H	1.66878300	-9.56352900	-1.79545200
N	0.55959200	-12.45901200	-0.40607500
H	-0.87348400	-12.62689300	1.07827400
H	1.95845300	-12.04904700	-1.87587900
C	4.23554700	-4.11095100	1.21877400
C	4.59988000	-3.44033400	2.40035300
C	5.27823200	-4.55684000	0.38830600
C	5.95605900	-3.24290200	2.68504900
H	3.83196900	-3.08263900	3.08501800
C	6.60326700	-4.30944300	0.76810700
H	5.05482800	-5.07270400	-0.54483400
N	6.95760900	-3.66284400	1.89215900
H	6.25382000	-2.71741200	3.59569600
H	7.42558000	-4.64253800	0.12992100
C	1.72937100	1.42763900	-3.45778500
C	2.19505800	1.66515300	-4.76298100
C	1.51244000	0.08537100	-3.09083900
C	2.41027700	0.57759300	-5.61829500
H	2.39844500	2.68211900	-5.09592500
C	1.75848400	-0.92621900	-4.02510500
H	1.15796200	-0.16054600	-2.09099700
N	2.19930500	-0.70592900	-5.27646000

H	2.77850000	0.74590700	-6.63356700
H	1.59104500	-1.97189000	-3.75322500
C	-2.26606700	7.22270100	-3.29508200
C	-1.75116800	7.69280400	-4.51687700
C	-3.62981400	7.45943600	-3.04404200
C	-2.60241500	8.36003400	-5.40526300
H	-0.69936100	7.54605900	-4.75930200
C	-4.39358800	8.13465400	-4.00319100
H	-4.08347900	7.11081000	-2.11703800
N	-3.90733900	8.58672900	-5.17252600
H	-2.21482200	8.73701700	-6.35517900
H	-5.45608200	8.31955200	-3.82509000
C	-0.77217200	7.99630500	3.51780200
C	-2.12629900	8.21362400	3.82941900
C	0.17783100	8.72864800	4.25208000
C	-2.45681100	9.12792200	4.83653800
H	-2.90452700	7.66910700	3.29595000
C	-0.26108100	9.62075900	5.23737800
H	1.24043100	8.60774000	4.04516300
N	-1.55382000	9.83170900	5.54168200
H	-3.50460500	9.30293400	5.09402200
H	0.46501400	10.20222700	5.81131300
C	3.42864200	2.35532300	3.20981200
C	3.23157300	0.96969400	3.36019200
C	4.42853900	2.94642400	4.00160800
C	4.02444800	0.26164000	4.26909400
H	2.47224100	0.45407400	2.77486800
C	5.16884800	2.14298100	4.87824700
H	4.63392800	4.01292800	3.91862100
N	4.98652400	0.81851700	5.02526000
H	3.87755500	-0.81397500	4.39758800
H	5.95702000	2.58638600	5.49186800

ZnTPyP dimer (π - π), **2**

N	0.03366800	0.96783200	-1.58615000
N	-0.62720600	3.49194600	-0.25787400
N	1.79224800	3.27165800	1.38794700
N	2.50263800	0.77623200	-0.00555300

C	-1.19217800	1.18866500	-2.17117400
C	-1.67190000	3.44576300	-1.15059700
C	-0.69954000	4.70028200	0.39781300
C	1.26560000	4.41324300	1.94592200
C	2.94748500	2.97816800	2.07039800
C	3.64630800	0.95614600	0.73667600
C	2.74688600	-0.24208300	-0.89676200
C	0.52190400	-0.21799300	-2.08837100
C	-0.47194500	-0.80683700	-2.96586600
C	-1.52492200	0.06276200	-3.01718900
C	-2.41330700	4.69130800	-1.08061100
C	-1.81938000	5.45878100	-0.11641700
C	2.10052200	4.83756000	3.05226400
C	3.13200900	3.94314700	3.13813400
C	4.66325500	0.03198100	0.28067000
C	4.11493100	-0.69666500	-0.73666500
N	-1.77102900	-3.27064300	-1.38858300
N	0.64833000	-3.49103500	0.25738200
N	-0.01255700	-0.96690100	1.58561700
N	-2.48151000	-0.77533000	0.00505300
C	-1.24430200	-4.41215100	-1.94662500
C	0.72075800	-4.69929300	-0.39843300
C	1.69304700	-3.44485000	1.15008100
C	1.21328200	-1.18776300	2.17065900
C	-0.50073800	0.21898200	2.08777000
C	-2.72578900	0.24295400	0.89627100
C	-3.62519600	-0.95529700	-0.73715700
C	-2.92630600	-2.97721700	-2.07099200
C	-3.11075900	-3.94214300	-3.13878600
C	-2.07918700	-4.83646200	-3.05300400
C	1.84066900	-5.45775700	0.11568800
C	2.43454800	-4.69033500	1.07995500
C	1.54607600	-0.06184200	3.01661300
C	0.49317100	0.80783500	2.96520300
C	-4.09387400	0.69744200	0.73624500
C	-4.64218800	-0.03121100	-0.28109100
Zn	-0.82186600	-2.03294800	-0.00924600
Zn	0.84302700	2.03387400	0.00869500
C	-3.81504000	-1.92275600	-1.75426800

C	-0.11640900	-5.10964600	-1.46079500
C	2.00201900	-2.35311300	2.00131100
C	-1.79438600	0.75289200	1.83619700
C	-1.98092300	2.35400400	-2.00178700
C	1.81553000	-0.75191500	-1.83677700
C	3.83617600	1.92364800	1.75374600
C	0.13774000	5.11078100	1.46005400
H	-3.92655300	-3.94083700	-3.85271900
H	-1.90329300	-5.70890200	-3.67249400
H	-5.65270600	0.02663600	-0.66814900
H	-4.58188300	1.45203300	1.34147500
H	0.41237900	1.76911300	3.45637200
H	2.47192900	0.07184900	3.55988700
H	3.28831400	-4.95123100	1.69424300
H	2.13080800	-6.44852600	-0.21495400
H	-2.45077200	-0.07094300	-3.56046700
H	-0.39104500	-1.76805800	-3.45713600
H	-3.26705400	4.95219500	-1.69492800
H	-2.10944800	6.44960700	0.21411700
H	4.60289500	-1.45133000	-1.34183900
H	5.67374700	-0.02593100	0.66778300
H	3.94779000	3.94182400	3.85208100
H	1.92473100	5.71007300	3.67167700
C	-2.23095100	1.89001700	2.69541400
C	-2.13567500	1.81492600	4.09896900
C	-2.76734900	3.07431900	2.16208000
C	-2.54199700	2.90601900	4.87375800
H	-1.75111600	0.91402500	4.57415300
C	-3.14302200	4.10716500	3.02567700
H	-2.86735900	3.19640400	1.08936300
H	-2.46937100	2.85965600	5.96319600
H	-3.53272900	5.04126000	2.61617000
C	-5.07993800	-1.83389100	-2.53978500
C	-6.00527200	-2.89238700	-2.57624800
C	-5.40433500	-0.67496400	-3.26511900
C	-7.18087200	-2.74164600	-3.32133100
H	-5.81384800	-3.80946100	-2.02033900
C	-6.60828000	-0.62639000	-3.97881200
H	-4.73026200	0.17711700	-3.26980500

H	-7.91361700	-3.55208000	-3.35441600
H	-6.86655000	0.27438000	-4.53868900
C	0.21110400	-6.41182800	-2.11768700
C	0.01247200	-7.62991700	-1.44717500
C	0.73147600	-6.46639800	-3.42001500
C	0.34012700	-8.82478800	-2.09964000
H	-0.39496500	-7.64097400	-0.43653000
C	1.03213000	-7.71666200	-3.97599200
H	0.92850600	-5.55576200	-3.98065500
H	0.18752400	-9.78294000	-1.59624700
H	1.45393700	-7.77609700	-4.98210600
C	3.24780700	-2.46146900	2.81199400
C	3.23184100	-2.34042300	4.21384800
C	4.49927000	-2.68900500	2.21031600
C	4.43522300	-2.42663700	4.92353900
H	2.29111300	-2.18266000	4.73866400
C	5.64249200	-2.76391200	3.01228300
H	4.57564100	-2.77411700	1.12974500
H	4.43648900	-2.32588600	6.01140900
H	6.62175600	-2.92156700	2.55412900
C	2.25227000	-1.88875900	-2.69630000
C	2.15761400	-1.81291500	-4.09985500
C	2.78839200	-3.07334300	-2.16333500
C	2.56454300	-2.90348500	-4.87505600
H	1.77315400	-0.91180000	-4.57471600
C	3.16475900	-4.10561900	-3.02734300
H	2.88776500	-3.19603400	-1.09062900
H	2.49248000	-2.85652000	-5.96450400
H	3.55436300	-5.03991900	-2.61820900
C	-3.22676300	2.46236300	-2.81237100
C	-3.21096500	2.34132300	-4.21422900
C	-4.47814100	2.68993900	-2.21054200
C	-4.41443200	2.42756900	-4.92376900
H	-2.27030000	2.18356300	-4.73915900
C	-5.62146500	2.76485800	-3.01236200
H	-4.55433600	2.77509300	-1.12996100
H	-4.41583900	2.32680600	-6.01163800
H	-6.60066600	2.92256900	-2.55409100
C	-0.18941300	6.41329600	2.11649900

C	-0.70931600	6.46869200	3.41898500
C	0.00924800	7.63101300	1.44528400
C	-1.00950400	7.71934200	3.97437600
H	-0.90643400	5.55845000	3.98023100
C	-0.31790800	8.82630100	2.09720900
H	0.41633300	7.64144800	0.43449000
H	-1.43092300	7.77939200	4.98061900
H	-0.16529100	9.78414700	1.59323700
C	5.10104500	1.83478000	2.53930000
C	5.42539200	0.67588800	3.26471300
C	6.02639000	2.89326800	2.57576300
C	6.62930600	0.62733300	3.97846200
H	4.75130300	-0.17618000	3.26942300
C	7.20195600	2.74254700	3.32089900
H	5.83499100	3.81032600	2.01981800
H	6.88753300	-0.27340900	4.53840300
H	7.93470000	3.55298200	3.35399200
N	-7.49649700	-1.63579300	-4.01866800
N	0.84580200	-8.88844500	-3.34373600
N	5.63453800	-2.62857600	4.35022200
N	-3.03237500	4.05042000	4.36475600
N	-0.82314800	8.89074200	3.34145100
N	7.51754000	1.63672000	4.01829900
N	-5.61367500	2.62952600	-4.35030300
N	3.05493900	-4.04805800	-4.36645300

ZnTPP dimer (π - π), **3**

N	0.22211000	0.90199400	-1.49122300
N	-0.55077900	3.35594800	-0.07129800
N	2.02355200	3.32730100	1.36105800
N	2.76864600	0.84425400	-0.03421600
C	-1.04879600	1.04689000	-2.00019700
C	-1.58754700	3.28537700	-0.97336100
C	-0.61739000	4.58866800	0.53907100
C	1.46283000	4.43453900	1.94900800
C	3.18758400	3.04975400	2.03735300
C	3.92948900	1.07550400	0.66344700
C	3.02885500	-0.14781400	-0.95012100

C	0.74539500	-0.26332000	-2.00687200
C	-0.26704700	-0.92223600	-2.80865900
C	-1.37283900	-0.11138900	-2.80272300
C	-2.32115800	4.53790800	-0.95113200
C	-1.72594000	5.33670000	-0.01363900
C	2.28386700	4.85291500	3.06861800
C	3.34481200	3.99076600	3.12919800
C	4.97860900	0.22411200	0.14587000
C	4.43010700	-0.51603600	-0.86399300
N	-2.00195300	-3.32605900	-1.36198000
N	0.57238600	-3.35455400	0.07036200
N	-0.20097800	-0.90102600	1.49083900
N	-2.74736900	-0.84337900	0.03354800
C	-1.44139300	-4.43352200	-1.94963600
C	0.63887700	-4.58739900	-0.53977600
C	1.60899100	-3.28404200	0.97261100
C	1.07006800	-1.04565500	1.99951700
C	-0.72423800	0.26436200	2.00627500
C	-3.00769400	0.14861300	0.94951900
C	-3.90806700	-1.07447100	-0.66438600
C	-3.16602300	-3.04864500	-2.03826600
C	-3.32341100	-3.98997400	-3.12982600
C	-2.26256000	-4.85222000	-3.06902800
C	1.74726000	-5.33550100	0.01315800
C	2.34244000	-4.53667400	0.95065100
C	1.39418000	0.11283500	2.80170300
C	0.28829500	0.92356600	2.80770000
C	-4.40897300	0.51676100	0.86326600
C	-4.95727700	-0.22316900	-0.14686100
Zn	-1.01814600	-2.00360500	-0.08038000
Zn	1.03973600	2.00502700	0.07946100
C	-4.08313300	-2.02793000	-1.69778100
C	-0.25301900	-5.07465600	-1.52642700
C	1.90324700	-2.17839100	1.81315700
C	-2.05628400	0.72308800	1.82960000
C	-1.88186500	2.17971100	-1.81386600
C	2.07738000	-0.72221000	-1.83016800
C	4.10471700	2.02908700	1.69670600
C	0.27445800	5.07575300	1.52587100

H	-4.13537700	-3.98513400	-3.84849000
H	-2.04273600	-5.68459900	-3.72851700
H	-5.98394100	-0.21869400	-0.49503000
H	-4.91223000	1.23082800	1.50417700
H	0.17949600	1.88606100	3.29298700
H	2.35028400	0.30686100	3.27063100
H	3.18176100	-4.78335500	1.59033700
H	2.01035600	-6.35152100	-0.25917500
H	-2.32881900	-0.30512200	-3.27201900
H	-0.15821200	-1.88465000	-3.29410100
H	-3.16058900	4.78455400	-1.59068900
H	-1.98914400	6.35264600	0.25885900
H	4.93319900	-1.23029700	-1.50482200
H	6.00533600	0.21969100	0.49384500
H	4.15671300	3.98576700	3.84793300
H	2.06388900	5.68500500	3.72842000
C	-2.52009700	1.85165200	2.68516300
C	-2.39400000	1.78560900	4.08832000
C	-3.15138300	2.97896700	2.12502700
C	-2.90076500	2.80327200	4.90383400
H	-1.91322300	0.91567900	4.53387000
C	-3.67779200	3.98574200	2.93902300
H	-3.21835000	3.06457800	1.04479000
H	-2.79959200	2.72802100	5.98710500
H	-4.16496000	4.84591700	2.47879700
C	-5.35453400	-1.95689500	-2.47388600
C	-6.25082100	-3.04298700	-2.50941200
C	-5.67970300	-0.78648800	-3.18534100
C	-7.44197400	-2.96080800	-3.23985000
H	-6.00961600	-3.94669700	-1.95032500
C	-6.86759200	-0.70668400	-3.92018000
H	-4.99658600	0.05921200	-3.16296400
H	-8.13034400	-3.80691700	-3.24971200
H	-7.09338800	0.20666100	-4.47027400
C	0.05531100	-6.39540200	-2.15038900
C	-0.84756500	-7.47009400	-2.02898200
C	1.24482000	-6.59150800	-2.87585200
C	-0.56476800	-8.70996000	-2.61381600
H	-1.76871600	-7.32522500	-1.46505500

C	1.52606200	-7.82942500	-3.46536400
H	1.93050600	-5.75629300	-2.99228300
H	-1.27085400	-9.53399300	-2.50362900
H	2.44777800	-7.96012500	-4.03447200
C	3.15263500	-2.26643300	2.62321300
C	3.11201900	-2.15293900	4.02831500
C	4.39690300	-2.52224600	2.01233500
C	4.27160600	-2.30945800	4.79643400
H	2.15571700	-1.96358900	4.51377800
C	5.55550000	-2.68514200	2.77808500
H	4.44752900	-2.57506400	0.92850300
H	4.21489400	-2.22683800	5.88226700
H	6.50826700	-2.87239600	2.28186500
C	2.54119100	-1.85066000	-2.68591200
C	2.41566200	-1.78401900	-4.08909100
C	3.17194400	-2.97836000	-2.12595700
C	2.92243000	-2.80151800	-4.90479200
H	1.93532700	-0.91375500	-4.53447000
C	3.69812000	-3.98516300	-2.94012000
H	3.23873100	-3.06425300	-1.04573600
H	2.82178800	-2.72580600	-5.98808100
H	4.18481500	-4.84567700	-2.48004200
C	-3.13129400	2.26783100	-2.62389800
C	-3.09070500	2.15463300	-4.02901900
C	-4.37555900	2.52343900	-2.01293300
C	-4.25033700	2.31120000	-4.79707200
H	-2.13440700	1.96545600	-4.51455700
C	-5.53419900	2.68636300	-2.77860900
H	-4.42614600	2.57607200	-0.92909300
H	-4.19365600	2.22881100	-5.88292400
H	-6.48696900	2.87342800	-2.28232300
C	-0.03403400	6.39629000	2.15018100
C	-1.22388800	6.59231500	2.87512000
C	0.86902900	7.47092900	2.02961200
C	-1.50526300	7.83005700	3.46492300
H	-1.90979000	5.75718900	2.99090900
C	0.58610600	8.71062400	2.61475100
H	1.79043800	7.32615700	1.46608400
H	-2.42724700	7.96066800	4.03361600

H	1.29235600	9.53459900	2.50519800
C	5.37631900	1.95831400	2.47249300
C	5.70207300	0.78796600	3.18378600
C	6.27229300	3.04468600	2.50781700
C	6.89023100	0.70848900	3.91822800
H	5.01920400	-0.05794100	3.16163300
C	7.46369400	2.96283700	3.23787600
H	6.03064200	3.94835000	1.94885300
H	7.11650100	-0.20481100	4.46820200
H	8.15181100	3.80915300	3.24757200
C	-7.75316700	-1.79243700	-3.95014400
H	-8.68054200	-1.72950800	-4.52091800
C	0.62380400	-8.89403800	-3.33439100
H	0.84307700	-9.85942600	-3.79215700
C	5.49643400	-2.58753500	4.17471700
H	6.39824100	-2.72001100	4.77327100
C	-3.55565300	3.90318600	4.33300000
H	-3.96111900	4.69124400	4.96877100
C	-5.47517200	2.58903300	-4.17525900
H	-6.37700600	2.72155800	-4.77376100
C	3.57653100	-3.90197100	-4.33409600
H	3.98186400	-4.68994000	-4.97005100
C	7.77548000	1.79450700	3.94798000
H	8.70305600	1.73182800	4.51845400
C	-0.60279700	8.89460400	3.33479600
H	-0.82218500	9.85986000	3.79278300