

Supporting information for:

Molecular Magnetic Properties of Heteroporphyrins: A Theoretical Analysis.

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P ($E_{el}=-989.551252$ h)

6	0.000000	2.440953	2.421928
6	0.000000	2.855487	1.084817
6	0.000000	2.440953	-2.421928
6	0.000000	4.257827	-0.678156
6	0.000000	2.855487	-1.084817
7	0.000000	2.029286	0.000000
6	0.000000	4.257827	0.678156
6	0.000000	-2.440953	-2.421928
6	0.000000	0.686032	-4.260413
6	0.000000	1.130120	-2.895977
6	0.000000	-0.686032	-4.260413
6	0.000000	-1.130120	-2.895977
7	0.000000	0.000000	-2.117108
6	0.000000	-2.440953	2.421928
6	0.000000	-0.686032	4.260413
6	0.000000	-1.130120	2.895977
6	0.000000	0.686032	4.260413
6	0.000000	1.130120	2.895977
7	0.000000	0.000000	2.117108
6	0.000000	-4.257827	0.678156
6	0.000000	-2.855487	1.084817
7	0.000000	-2.029286	0.000000
6	0.000000	-2.855487	-1.084817
6	0.000000	-4.257827	-0.678156
1	0.000000	-5.106481	-1.351498
1	0.000000	-5.106481	1.351498
1	0.000000	-1.347201	5.116997
1	0.000000	1.347201	5.116997
1	0.000000	5.106481	1.351498
1	0.000000	-1.347201	-5.116997
1	0.000000	0.000000	-1.101667
1	0.000000	0.000000	1.101667
1	0.000000	-3.219588	-3.179391
1	0.000000	-3.219588	3.179391
1	0.000000	3.219588	3.179391
1	0.000000	3.219588	-3.179391
1	0.000000	5.106481	-1.351498
1	0.000000	1.347201	-5.116997

2OP ($E_{el}=-1029.2126869$ h)

6	0.000000	2.401006	2.412014
6	0.000000	1.106213	2.919285
6	0.000000	-2.401006	2.412014
6	0.000000	-0.688600	4.274270
6	0.000000	-1.106213	2.919285
6	0.000000	0.688600	4.274270
6	0.000000	-2.401006	-2.412014
6	0.000000	-4.241334	0.676757
6	0.000000	-2.824454	1.076333
6	0.000000	-4.241334	-0.676757
6	0.000000	-2.824454	-1.076333
7	0.000000	-2.006043	0.000000
6	0.000000	2.401006	-2.412014
6	0.000000	4.241334	-0.676757
6	0.000000	2.824454	-1.076333
6	0.000000	4.241334	0.676757
6	0.000000	2.824454	1.076333
7	0.000000	2.006043	0.000000
6	0.000000	0.688600	-4.274270
6	0.000000	1.106213	-2.919285
6	0.000000	-1.106213	-2.919285
6	0.000000	-0.688600	-4.274270
1	0.000000	-1.354202	-5.127039
1	0.000000	1.354202	-5.127039
1	0.000000	5.090524	-1.349987
1	0.000000	5.090524	1.349987
1	0.000000	1.354202	5.127039
1	0.000000	-1.354202	5.127039
1	0.000000	-5.090524	-1.349987
1	0.000000	-5.090524	1.349987
1	0.000000	-3.178031	-3.172196
1	0.000000	-3.178031	3.172196
1	0.000000	3.178031	3.172196
1	0.000000	3.178031	-3.172196
8	0.000000	0.000000	2.119556
8	0.000000	0.000000	-2.119556

2SP ($E_{el}=-1675.174353$ h)

6	-2.619359	-2.401986	0.000000
6	-1.261175	-2.740282	0.000000
6	2.619359	-2.401986	0.000000
6	0.689371	-4.046987	0.000000
6	1.261175	-2.740282	0.000000
6	-0.689371	-4.046987	0.000000
6	2.619359	2.401986	0.000000
6	4.534765	-0.680408	0.000000
6	3.128299	-1.089549	0.000000
6	4.534765	0.680408	0.000000
6	3.128299	1.089549	0.000000
7	2.324507	0.000000	0.000000
6	-2.619359	2.401986	0.000000
6	-4.534765	0.680408	0.000000
6	-3.128299	1.089549	0.000000
6	-4.534765	-0.680408	0.000000
6	-3.128299	-1.089549	0.000000
7	-2.324507	0.000000	0.000000
6	-0.689371	4.046987	0.000000
6	-1.261175	2.740282	0.000000
6	1.261175	2.740282	0.000000
6	0.689371	4.046987	0.000000
1	1.299293	4.945082	0.000000
1	-1.299293	4.945082	0.000000
1	-5.389758	1.345823	0.000000
1	-5.389758	-1.345823	0.000000
1	-1.299293	-4.945082	0.000000
1	1.299293	-4.945082	0.000000
1	5.389758	1.345823	0.000000
1	5.389758	-1.345823	0.000000
1	3.334455	3.222311	0.000000
1	3.334455	-3.222311	0.000000
1	-3.334455	-3.222311	0.000000
1	-3.334455	3.222311	0.000000
16	0.000000	-1.524965	0.000000
16	0.000000	1.524965	0.000000

2SeP ($E_{el}=-5677.5625721$ h)

6	0.000000	2.420045	2.662512
6	0.000000	2.763113	1.308422
6	0.000000	2.420045	-2.662512
6	0.000000	4.051644	-0.691529
6	0.000000	2.763113	-1.308422
6	0.000000	4.051644	0.691529
6	0.000000	-2.420045	-2.662512
6	0.000000	0.681519	-4.559941
6	0.000000	1.095523	-3.159366
6	0.000000	-0.681519	-4.559941
6	0.000000	-1.095523	-3.159366
7	0.000000	0.000000	-2.356090
6	0.000000	-2.420045	2.662512
6	0.000000	-0.681519	4.559941
6	0.000000	-1.095523	3.159366
6	0.000000	0.681519	4.559941
6	0.000000	1.095523	3.159366
7	0.000000	0.000000	2.356090
6	0.000000	-4.051644	0.691529
6	0.000000	-2.763113	1.308422
6	0.000000	-2.763113	-1.308422
6	0.000000	-4.051644	-0.691529
1	0.000000	-4.966064	-1.279000
1	0.000000	-4.966064	1.279000
1	0.000000	-1.346181	5.415461
1	0.000000	1.346181	5.415461
1	0.000000	4.966064	1.279000
1	0.000000	4.966064	-1.279000
1	0.000000	-1.346181	-5.415461
1	0.000000	1.346181	-5.415461
1	0.000000	-3.227207	-3.393698
1	0.000000	3.227207	-3.393698
1	0.000000	3.227207	3.393698
1	0.000000	-3.227207	3.393698
34	0.000000	1.427514	0.000000
34	0.000000	-1.427514	0.000000

TPP ($E_{el}=-1913.751047$ h)

C	0.01371800	-0.00099100	0.17785900
C	-0.16792300	0.01950400	1.57127900
C	0.98147700	0.00517700	5.00854600
C	-1.14579400	0.07029500	3.62072000
C	0.27726100	0.02190800	3.79239800
C	-1.41491400	0.06915800	2.27805000
C	5.76151400	0.26288200	4.05331300
C	3.06993800	-0.09115300	6.42181600
C	2.38750500	0.02894700	5.13676600
C	4.39580400	-0.02069500	6.15694000
C	4.51775400	0.14316100	4.71131100
N	3.28756300	0.15123900	4.11553800
C	4.79349800	0.25355600	-0.77810800
C	2.72431400	-0.03384400	-2.19481800
C	3.39255100	0.13288500	-0.90746000
C	1.39843800	-0.10355000	-1.92956000
C	1.26245600	0.02027900	-0.48124900
N	2.48591500	0.14370400	0.11529400
C	6.90271500	0.52082600	0.61293200
C	5.49272000	0.32414900	0.43924200
C	5.93839800	0.32883700	2.66035900
C	7.17214500	0.52358700	1.95562000
H	8.13233100	0.66048900	2.42977000
H	7.60561700	0.65516600	-0.19543000
H	3.21253600	-0.10640100	-3.15587100
H	0.58843900	-0.24432000	-2.63061500
H	-2.38452400	0.11155400	1.80528000
H	-1.85826200	0.11353500	4.43071300
H	5.21601300	-0.09101600	6.85667300
H	2.59202100	-0.23048800	7.38072500
C	-1.22869500	-0.04382900	-0.65807500
C	-2.07497900	-1.16399800	-0.63516400
C	-1.57516000	1.03923300	-1.48177800
C	-3.23263000	-1.20072600	-1.41346000
H	-1.81355800	-2.01306000	-0.00971500
C	-2.73327700	1.00371900	-2.25891900
H	-0.93186400	1.91433000	-1.50329300
C	-3.56596300	-0.11653500	-2.22726800
H	-3.87135600	-2.07976900	-1.38705300
H	-2.98671400	1.85425300	-2.88636500
H	-4.46777300	-0.14474300	-2.83304000
C	5.61855800	0.31496800	-2.02697000

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C	6.52087000	-0.71300600	-2.34438100
C	5.50879400	1.40338600	-2.90726100
C	7.28909700	-0.65582700	-3.50779100
H	6.60907200	-1.56561000	-1.67674900
C	6.27779000	1.46182400	-4.06994800
H	4.81954200	2.20868100	-2.66948500
C	7.17039900	0.43228500	-4.37430600
H	7.97675400	-1.46513400	-3.73914000
H	6.18168600	2.31520600	-4.73616400
H	7.76864400	0.47747900	-5.28042600
C	7.00282300	0.32859700	4.88893400
C	7.96252500	-0.69502100	4.83355900
C	7.23496700	1.41660900	5.74571500
C	9.11893600	-0.63348600	5.61196900
H	7.79073800	-1.54801200	4.18295000
C	8.39199300	1.47954000	6.52288700
H	6.50311400	2.21800100	5.79307700
C	9.33790800	0.45460500	6.45866100
H	9.84634900	-1.43943700	5.56003000
H	8.55564100	2.33272400	7.17604700
H	10.23867100	0.50320100	7.06468300
C	0.15669100	-0.03684100	6.25842800
C	0.15025400	1.04889200	7.14877000
C	-0.62765600	-1.15961600	6.56739400
C	-0.61769100	1.01297300	8.31305400
H	0.74797300	1.92609900	6.91785000
C	-1.39448300	-1.19687700	7.73268300
H	-0.62389500	-2.01061200	5.89190900
C	-1.39229400	-0.11027900	8.60911100
H	-0.61316500	1.86544600	8.98730700
H	-1.98963500	-2.07812400	7.95754300
H	-1.98957900	-0.13870500	9.51655700
N	0.82094400	0.00174000	2.52822300
H	1.81585300	0.02274200	2.32834400
N	4.95578400	0.22400800	1.70247100
H	3.96474000	0.13370600	1.90225500

2OTPP ($E_{el}=-1953.411962$ h)

C	0.03422700	0.00412200	0.21863100
C	-0.17875000	0.13518000	1.59976300
C	0.98429000	0.00596500	4.96795100
C	-1.12894800	0.38788400	3.62210600
C	0.25625300	0.13546800	3.77485500
C	-1.39861900	0.38798800	2.27329500
C	5.74007700	0.26746500	4.01362800

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C	3.07439400	-0.40372400	6.34795600
C	2.39136100	-0.06650900	5.08913300
C	4.39794700	-0.32919900	6.08248700
C	4.50398700	0.05121000	4.66521800
N	3.28058500	0.17966500	4.09692200
C	4.79072900	0.25639900	-0.73551100
C	2.75344700	-0.34117500	-2.12516500
C	3.39875500	0.04117500	-0.85950200
C	1.42978900	-0.41163000	-1.85935800
C	1.28592000	-0.07119900	-0.43516600
N	2.48962900	0.17391700	0.13655500
C	6.85513700	0.82750800	0.61857300
C	5.50266100	0.43879200	0.46026500
C	5.93702400	0.44455500	2.63526100
C	7.12449200	0.83156500	1.96752000
H	8.05123400	1.09698200	2.45325600
H	7.52393300	1.08920100	-0.18725900
H	3.25492600	-0.55308100	-3.05902800
H	0.63197700	-0.69274300	-2.53238200
H	-2.34799300	0.56694100	1.79179300
H	-1.82045100	0.56693100	4.43139800
H	5.22154100	-0.53757900	6.75095600
H	2.59861900	-0.68562400	7.27679800
C	-1.20294400	-0.03934800	-0.62360100
C	-2.15710100	-1.05740000	-0.46058800
C	-1.43226400	0.94029500	-1.60414000
C	-3.30387100	-1.09589900	-1.25410700
H	-1.98621200	-1.82995700	0.28387300
C	-2.58087200	0.90442600	-2.39472000
H	-0.70536000	1.73643700	-1.73577300
C	-3.52029900	-0.11414600	-2.22297100
H	-4.02530300	-1.89751800	-1.11891200
H	-2.74312500	1.67554400	-3.14325900
H	-4.41415500	-0.14335400	-2.84035900
C	5.60861400	0.31595800	-1.98832700
C	6.64527600	-0.60318300	-2.22063100
C	5.35020500	1.29259800	-2.96445800
C	7.39923900	-0.54897100	-3.39311600
H	6.84673200	-1.37287200	-1.48091900
C	6.10692100	1.34979500	-4.13490900
H	4.55519800	2.01252600	-2.79362100
C	7.13363400	0.42907500	-4.35341800
H	8.19072300	-1.27528000	-3.55849100
H	5.89569600	2.11705800	-4.87514000
H	7.72163800	0.47261300	-5.26630800
C	6.97703200	0.33408600	4.85474400
C	8.02483700	-0.58442600	4.67631500
C	7.11283300	1.31776800	5.84838600
C	9.17204400	-0.52285300	5.46769600
H	7.92749600	-1.35943900	3.92122900

C	8.26180700	1.38239300	6.63674100
H	6.31250800	2.03782200	5.99186100
C	9.29498800	0.46201700	6.44966400
H	9.96739600	-1.24882000	5.32035800
H	8.35071000	2.15532200	7.39565300
H	10.18905800	0.51126800	7.06547400
C	0.16620200	-0.03923200	6.22090100
C	0.33159800	0.93779000	7.21680900
C	-0.77926100	-1.05631200	6.43378200
C	-0.42686100	0.90051800	8.38685700
H	1.05443600	1.73346100	7.06183700
C	-1.53481900	-1.09624500	7.60581700
H	-0.90794500	-1.82667600	5.67866400
C	-1.36257100	-0.11656900	8.58557100
H	-0.28868000	1.66969300	9.14220300
H	-2.25415700	-1.89717000	7.75548900
H	-1.95202500	-0.14653600	9.49806200
O	0.81564400	0.00486000	2.53200200
O	4.96017600	0.23047500	1.70003600

2STPP ($E_{el}=-2599.383385$ h)

C	-2.39418500	2.66785000	-0.00439100
C	-2.72727800	1.29518500	0.01825700
C	-2.44930000	-2.61709900	-0.01138400
C	-4.04111300	-0.64668400	0.16388500
C	-2.75388500	-1.23774300	0.01337000
C	-4.02657000	0.73073300	0.16737800
C	2.39418500	-2.66785000	-0.00439100
C	-0.72651100	-4.52606600	-0.16344600
C	-1.12311600	-3.12223900	-0.03805900
C	0.63258500	-4.54022500	-0.16158900
C	1.05798000	-3.14508100	-0.03527300
N	-0.02414900	-2.33030200	0.02388400
C	2.44930000	2.61709900	-0.01138400
C	0.72651100	4.52606600	-0.16344600
C	1.12311600	3.12223900	-0.03805900
C	-0.63258500	4.54022500	-0.16158900
C	-1.05798000	3.14508100	-0.03527300
N	0.02414900	2.33030200	0.02388400
C	4.04111300	0.64668400	0.16388500
C	2.75388500	1.23774300	0.01337000
C	2.72727800	-1.29518500	0.01825700
C	4.02657000	-0.73073300	0.16737800
H	4.91315800	-1.34016500	0.29292900
H	4.94042900	1.23769700	0.28742500

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H	1.39445100	5.37037000	-0.26374400
H	-1.28347600	5.39805400	-0.25902200
H	-4.91315800	1.34016500	0.29292900
H	-4.94042900	-1.23769700	0.28742500
H	1.28347600	-5.39805400	-0.25902200
H	-1.39445100	-5.37037000	-0.26374400
S	-1.52910000	0.01601400	-0.08858800
S	1.52910000	-0.01601400	-0.08858800
C	-3.50517400	3.66631700	0.01293500
C	-4.46804900	3.69169800	-1.01000500
C	-3.60967000	4.60475200	1.05325800
C	-5.50183400	4.62788200	-0.99418600
H	-4.39175600	2.98084600	-1.82788400
C	-4.64634700	5.53798300	1.07068100
H	-2.87818800	4.58902800	1.85597400
C	-5.59545000	5.55342800	0.04692100
H	-6.23165100	4.63691500	-1.79951100
H	-4.71393600	6.25122300	1.88796400
H	-6.40178100	6.28182600	0.05996500
C	3.58105600	3.59171600	-0.00255800
C	4.54235400	3.58943900	-1.02740800
C	3.70728100	4.53520700	1.03082200
C	5.59545000	4.50389700	-1.02024500
H	4.44805000	2.87578500	-1.84092000
C	4.76335200	5.44655100	1.03963800
H	2.97839100	4.53932800	1.83604900
C	5.71046300	5.43473400	0.01402300
H	6.32340500	4.49231800	-1.82723000
H	4.84796500	6.16353100	1.85206000
H	6.53201900	6.14600500	0.02041500
C	3.50517400	-3.66631700	0.01293500
C	4.46804900	-3.69169800	-1.01000500
C	3.60967000	-4.60475200	1.05325800
C	5.50183400	-4.62788200	-0.99418600
H	4.39175600	-2.98084600	-1.82788400
C	4.64634700	-5.53798300	1.07068100
H	2.87818800	-4.58902800	1.85597400
C	5.59545000	-5.55342800	0.04692100
H	6.23165100	-4.63691500	-1.79951100
H	4.71393600	-6.25122300	1.88796400
H	6.40178100	-6.28182600	0.05996500
C	-3.58105600	-3.59171600	-0.00255800
C	-3.70728100	-4.53520700	1.03082200
C	-4.54235400	-3.58943900	-1.02740800
C	-4.76335200	-5.44655100	1.03963800
H	-2.97839100	-4.53932800	1.83604900
C	-5.59545000	-4.50389700	-1.02024500
H	-4.44805000	-2.87578500	-1.84092000
C	-5.71046300	-5.43473400	0.01402300
H	-4.84796500	-6.16353100	1.85206000

H	-6.32340500	-4.49231800	-1.82723000
H	-6.53201900	-6.14600500	0.02041500

2SeTPP ($E_{el}=-6601.776141$ h)

C	3.47741000	1.03476600	-0.01078600
C	2.37912900	1.91702200	-0.00444400
C	-1.36279800	3.36216900	-0.00984800
C	1.12684600	3.93749400	0.11792900
C	0.01211600	3.05516600	-0.00391600
C	2.37231700	3.33862700	0.11761400
C	-3.47741000	-1.03476600	-0.01078600
C	-3.81773000	2.59117400	-0.12824100
C	-2.37912900	2.36125800	-0.03488900
C	-4.40776400	1.36432400	-0.12870200
C	-3.33007800	0.38402100	-0.03537400
N	-2.13008900	1.02418900	0.00403300
C	1.36279800	-3.36216900	-0.00984800
C	3.81773000	-2.59117400	-0.12824100
C	2.37912900	-2.36125800	-0.03488900
C	4.40776400	-1.36432400	-0.12870200
C	3.33007800	-0.38402100	-0.03537400
N	2.13008900	-1.02418900	0.00403300
C	-1.12684600	-3.93749400	0.11792900
C	-0.01211600	-3.05516600	-0.00391600
C	-2.37912900	-1.91702200	-0.00444400
C	-2.37231700	-3.33862700	0.11761400
H	-3.28932100	-3.90748800	0.22657700
H	-0.99864200	-5.00895400	0.22710700
H	4.30310200	-3.55418200	-0.20459500
H	5.46305400	-1.14234900	-0.20546600
H	3.28932100	3.90748800	0.22657700
H	0.99864200	5.00895400	0.22710700
H	-5.46305400	1.14234900	-0.20546600
H	-4.30310200	3.55418200	-0.20459500
C	4.85560600	1.60767600	0.01871700
C	5.29445500	2.47356600	-0.99703400
C	5.74209800	1.29934700	1.06420200
C	6.58141900	3.01058300	-0.97057900
H	4.62403200	2.70977700	-1.81840700
C	7.02761200	1.84000500	1.09200200
H	5.41120000	0.64200000	1.86295400
C	7.45221800	2.69646700	0.07447700
H	6.90519400	3.67104400	-1.77069900

Supplementary Material (ESI) for PCCP
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H	7.69630700	1.59470500	1.91292100
H	8.45440400	3.11604900	0.09585800
C	1.77583300	-4.79636200	0.02056500
C	1.37258600	-5.68084500	-0.99393100
C	2.57111400	-5.29527400	1.06583900
C	1.75674500	-7.02137800	-0.96649100
H	0.76869000	-5.30551900	-1.81512200
C	2.95155700	-6.63693300	1.09461400
H	2.87858200	-4.62558300	1.86369100
C	2.54680600	-7.50438600	0.07830700
H	1.44228700	-7.68746500	-1.76566300
H	3.56143800	-7.00525500	1.91535600
H	2.84488300	-8.54915600	0.10043300
C	-4.85560600	-1.60767600	0.01871700
C	-5.29445500	-2.47356600	-0.99703400
C	-5.74209800	-1.29934700	1.06420200
C	-6.58141900	-3.01058300	-0.97057900
H	-4.62403200	-2.70977700	-1.81840700
C	-7.02761200	-1.84000500	1.09200200
H	-5.41120000	-0.64200000	1.86295400
C	-7.45221800	-2.69646700	0.07447700
H	-6.90519400	-3.67104400	-1.77069900
H	-7.69630700	-1.59470500	1.91292100
H	-8.45440400	-3.11604900	0.09585800
C	-1.77583300	4.79636200	0.02056500
C	-2.57111400	5.29527400	1.06583900
C	-1.37258600	5.68084500	-0.99393100
C	-2.95155700	6.63693300	1.09461400
H	-2.87858200	4.62558300	1.86369100
C	-1.75674500	7.02137800	-0.96649100
H	-0.76869000	5.30551900	-1.81512200
C	-2.54680600	7.50438600	0.07830700
H	-3.56143800	7.00525500	1.91535600
H	-1.44228700	7.68746500	-1.76566300
H	-2.84488300	8.54915600	0.10043300
Se	0.61887200	1.28662800	-0.10039400
Se	-0.61887200	-1.28662800	-0.10039400

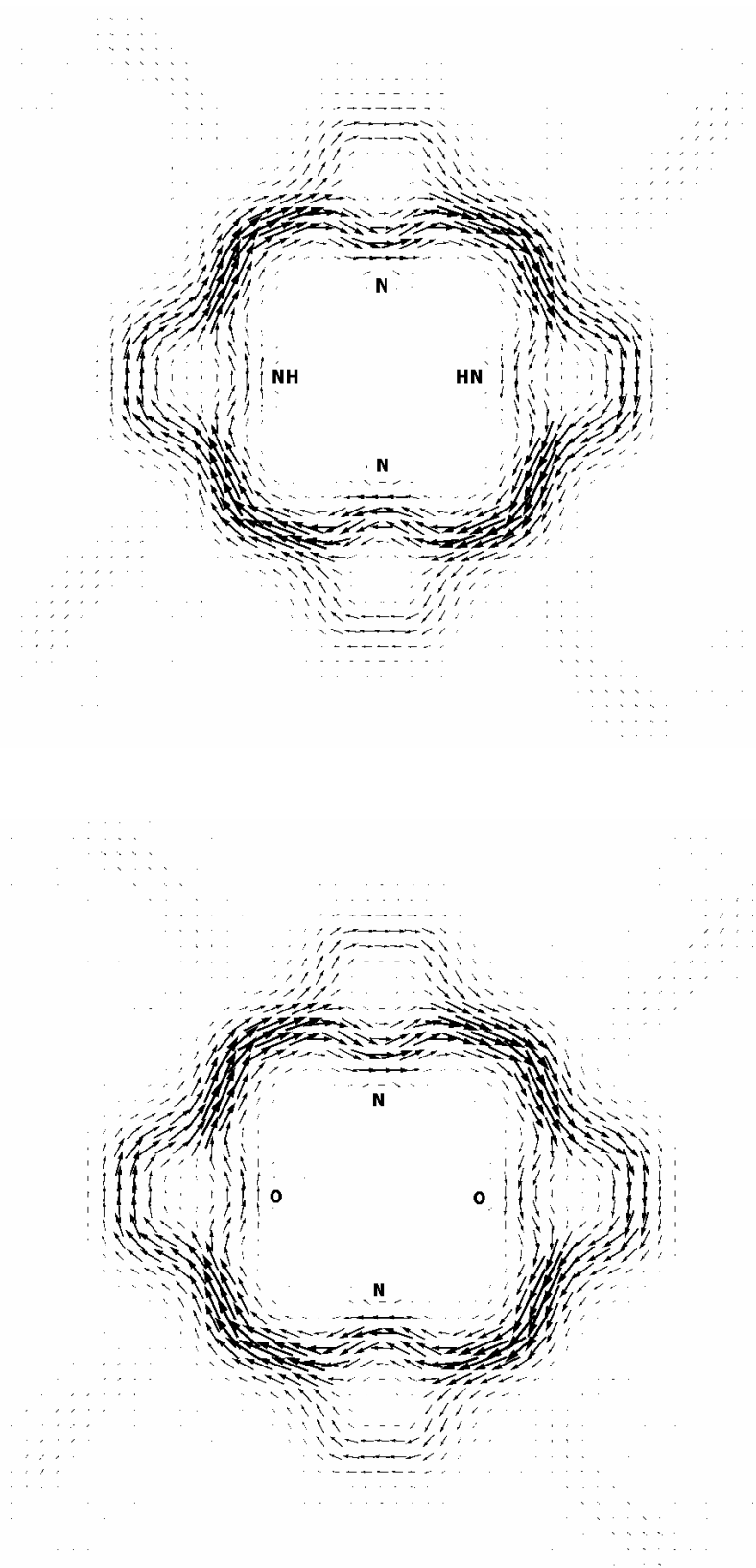


Figure 1S: Current density maps for the π electron distribution of **TPP** and **2OTPP**

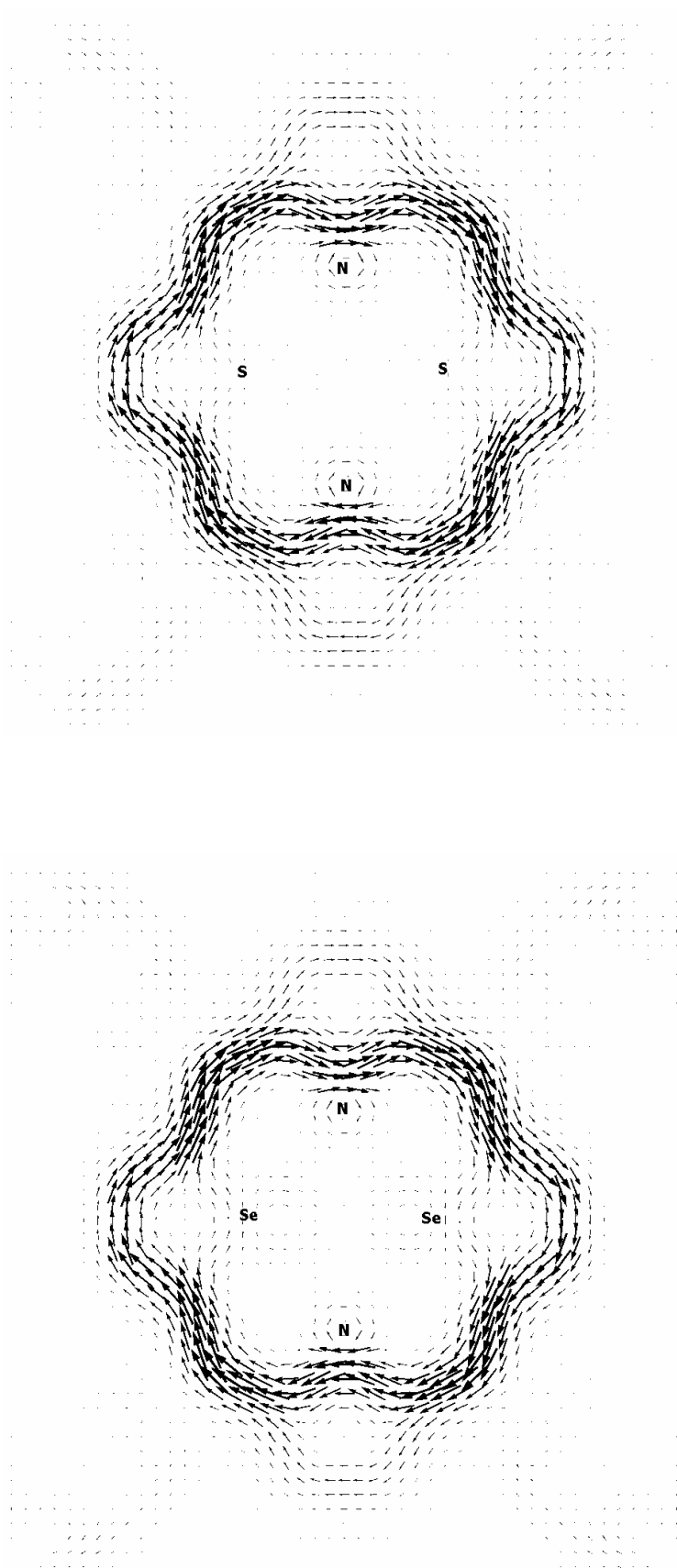


Figure 2S: Current density maps for the π electron distribution of **2STPP** and **2SeTPP**