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Supplementary material: Rethinking gold(II) porphyrins: an inherent wave distortion

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Not yet published

All-electron OLYP-D3/ZORA-STO-TZ2P Cartesian coordinates (Å)

1. Ag[P], D_{4h}, $q = 0$, $S = \frac{1}{2}$

Ag	0.000000000	0.000000000	0.000000000
C	0.684172000	4.283104000	0.000000000
C	0.684172000	−4.283104000	0.000000000
C	1.113133000	2.898576000	0.000000000
C	1.113133000	−2.898576000	0.000000000
C	2.438144000	2.438144000	0.000000000
C	2.438144000	−2.438144000	0.000000000
C	2.898576000	1.113133000	0.000000000
C	2.898576000	−1.113133000	0.000000000
C	4.283104000	0.684172000	0.000000000
C	4.283104000	−0.684172000	0.000000000
C	−0.684172000	4.283104000	0.000000000
C	−0.684172000	−4.283104000	0.000000000
C	−1.113133000	2.898576000	0.000000000
C	−1.113133000	−2.898576000	0.000000000
C	−2.438144000	2.438144000	0.000000000
C	−2.438144000	−2.438144000	0.000000000
C	−2.898576000	1.113133000	0.000000000
C	−2.898576000	−1.113133000	0.000000000
C	−4.283104000	0.684172000	0.000000000
C	−4.283104000	−0.684172000	0.000000000
H	1.350310000	5.136920000	0.000000000
H	1.350310000	−5.136920000	0.000000000
H	3.206806000	3.206806000	0.000000000
H	3.206806000	−3.206806000	0.000000000
H	5.136920000	1.350310000	0.000000000
H	5.136920000	−1.350310000	0.000000000
H	−1.350310000	5.136920000	0.000000000
H	−1.350310000	−5.136920000	0.000000000
H	−3.206806000	3.206806000	0.000000000
H	−3.206806000	−3.206806000	0.000000000
H	−5.136920000	1.350310000	0.000000000
H	−5.136920000	−1.350310000	0.000000000
N	0.000000000	2.108309000	0.000000000
N	0.000000000	−2.108309000	0.000000000
N	2.108309000	0.000000000	0.000000000
N	−2.108309000	0.000000000	0.000000000

* Corresponding authors.

2. Au[P], C_{2h}, $q = 0$, $S = \frac{1}{2}$

Au	0.000000000	0.000000000	0.000000000
C	0.658662000	0.193687000	4.250871000
C	0.658662000	0.193687000	−4.250871000
C	1.066477000	0.324846000	2.880944000
C	1.066477000	0.324846000	−2.880944000
C	2.331524000	0.726180000	2.431456000
C	2.331524000	0.726180000	−2.431456000
C	2.750598000	0.871653000	1.115354000
C	2.750598000	0.871653000	−1.115354000
C	4.098329000	1.166101000	0.681880000
C	4.098329000	1.166101000	−0.681880000
C	−0.658662000	−0.193687000	4.250871000
C	−0.658662000	−0.193687000	−4.250871000
C	−1.066477000	−0.324846000	2.880944000
C	−1.066477000	−0.324846000	−2.880944000
C	−2.331524000	−0.726180000	2.431456000
C	−2.331524000	−0.726180000	−2.431456000
C	−2.750598000	−0.871653000	1.115354000
C	−2.750598000	−0.871653000	−1.115354000
C	−4.098329000	−1.166101000	0.681880000
C	−4.098329000	−1.166101000	−0.681880000
H	1.292206000	0.407335000	5.102080000
H	1.292206000	0.407335000	−5.102080000
H	3.077124000	0.909920000	3.199466000
H	3.077124000	0.909920000	−3.199466000
H	4.931621000	1.336772000	1.351574000
H	4.931621000	1.336772000	−1.351574000
H	−1.292206000	−0.407335000	5.102080000
H	−1.292206000	−0.407335000	−5.102080000
H	−3.077124000	−0.909920000	3.199466000
H	−3.077124000	−0.909920000	−3.199466000
H	−4.931621000	−1.336772000	1.351574000
H	−4.931621000	−1.336772000	−1.351574000
N	0.000000000	0.000000000	2.079285000
N	0.000000000	0.000000000	−2.079285000
N	1.959610000	0.733602000	0.000000000
N	−1.959610000	−0.733602000	0.000000000

3. Ag[TPP], C_{2h}, $q = 0$, $S = \frac{1}{2}$

Ag	0.000000000	0.000000000	0.000000000
C	0.682303000	−0.031591000	4.283793000
C	0.682303000	−0.031591000	−4.283793000
C	1.115195000	−0.043882000	2.902098000
C	1.115195000	−0.043882000	−2.902098000
C	2.456299000	−0.094639000	2.457111000
C	2.456299000	−0.094639000	−2.457111000
C	2.897303000	−0.128405000	1.114873000
C	2.897303000	−0.128405000	−1.114873000
C	3.518446000	−0.087581000	3.501102000
C	3.518446000	−0.087581000	−3.501102000
C	3.643179000	0.986492000	4.393859000
C	3.643179000	0.986492000	−4.393859000
C	4.277132000	−0.038257000	0.682426000
C	4.277132000	−0.038257000	−0.682426000
C	4.426035000	−1.151700000	3.600344000
C	4.426035000	−1.151700000	−3.600344000
C	4.647570000	0.996295000	5.360291000
C	4.647570000	0.996295000	−5.360291000
C	5.432437000	−1.142781000	4.564687000
C	5.432437000	−1.142781000	−4.564687000
C	5.547074000	−0.068127000	5.448601000
C	5.547074000	−0.068127000	−5.448601000
C	−0.682303000	0.031591000	4.283793000
C	−0.682303000	0.031591000	−4.283793000
C	−1.115195000	0.043882000	2.902098000
C	−1.115195000	0.043882000	−2.902098000
C	−2.456299000	0.094639000	2.457111000
C	−2.456299000	0.094639000	−2.457111000
C	−2.897303000	0.128405000	1.114873000
C	−2.897303000	0.128405000	−1.114873000
C	−3.518446000	0.087581000	3.501102000
C	−3.518446000	0.087581000	−3.501102000
C	−3.643179000	−0.986492000	4.393859000
C	−3.643179000	−0.986492000	−4.393859000
C	−4.277132000	0.038257000	0.682426000
C	−4.277132000	0.038257000	−0.682426000
C	−4.426035000	1.151700000	3.600344000
C	−4.426035000	1.151700000	−3.600344000
C	−4.647570000	−0.996295000	5.360291000
C	−4.647570000	−0.996295000	−5.360291000
C	−5.432437000	1.142781000	4.564687000
C	−5.432437000	1.142781000	−4.564687000
C	−5.547074000	0.068127000	5.448601000
C	−5.547074000	0.068127000	−5.448601000
H	1.339512000	−0.072433000	5.138948000
H	1.339512000	−0.072433000	−5.138948000
H	2.948181000	1.817337000	4.317279000
H	2.948181000	1.817337000	−4.317279000
H	4.335144000	−1.985442000	2.910336000
H	4.335144000	−1.985442000	−2.910336000
H	4.732986000	1.840585000	6.040807000
H	4.732986000	1.840585000	−6.040807000
H	5.128119000	0.044492000	1.341333000
H	5.128119000	0.044492000	−1.341333000
H	6.126221000	−1.978081000	4.628602000

H	6.126221000	−1.978081000	−4.628602000
H	6.331953000	−0.060703000	6.201347000
H	6.331953000	−0.060703000	−6.201347000
H	−1.339512000	0.072433000	5.138948000
H	−1.339512000	0.072433000	−5.138948000
H	−2.948181000	−1.817337000	4.317279000
H	−2.948181000	−1.817337000	−4.317279000
H	−4.335144000	1.985442000	2.910336000
H	−4.335144000	1.985442000	−2.910336000
H	−4.732986000	−1.840585000	6.040807000
H	−4.732986000	−1.840585000	−6.040807000
H	−5.128119000	−0.044492000	1.341333000
H	−5.128119000	−0.044492000	−1.341333000
H	−6.126221000	1.978081000	4.628602000
H	−6.126221000	1.978081000	−4.628602000
H	−6.331953000	0.060703000	6.201347000
H	−6.331953000	0.060703000	−6.201347000
N	0.000000000	0.000000000	2.108992000
N	0.000000000	0.000000000	−2.108992000
N	2.105009000	−0.186863000	0.000000000
N	−2.105009000	0.186863000	0.000000000

4. Au[TPP], C_{2h}, $q = 0$, $S = \frac{1}{2}$

Au	0.000000000	0.000000000	0.000000000
C	0.685308000	0.028447000	4.248800000
C	0.685308000	0.028447000	−4.248800000
C	1.116093000	0.049801000	2.881511000
C	1.116093000	0.049801000	−2.881511000
C	2.459455000	0.096615000	2.451026000
C	2.459455000	0.096615000	−2.451026000
C	2.881995000	0.086033000	1.117388000
C	2.881995000	0.086033000	−1.117388000
C	3.512331000	0.213120000	3.495578000
C	3.512331000	0.213120000	−3.495578000
C	3.531098000	1.297709000	4.386465000
C	3.531098000	1.297709000	−4.386465000
C	4.233918000	0.350036000	0.681203000
C	4.233918000	0.350036000	−0.681203000
C	4.520707000	−0.757284000	3.599360000
C	4.520707000	−0.757284000	−3.599360000
C	4.528030000	1.407237000	5.355804000
C	4.528030000	1.407237000	−5.355804000
C	5.520359000	−0.648361000	4.566394000
C	5.520359000	−0.648361000	−4.566394000
C	5.527365000	0.434406000	5.449439000
C	5.527365000	0.434406000	−5.449439000
C	−0.685308000	−0.028447000	4.248800000
C	−0.685308000	−0.028447000	−4.248800000
C	−1.116093000	−0.049801000	2.881511000
C	−1.116093000	−0.049801000	−2.881511000
C	−2.459455000	−0.096615000	2.451026000
C	−2.459455000	−0.096615000	−2.451026000
C	−2.881995000	−0.086033000	1.117388000
C	−2.881995000	−0.086033000	−1.117388000
C	−3.512331000	−0.213120000	3.495578000
C	−3.512331000	−0.213120000	−3.495578000
C	−3.531098000	−1.297709000	4.386465000
C	−3.531098000	−1.297709000	−4.386465000
C	−4.233918000	−0.350036000	0.681203000
C	−4.233918000	−0.350036000	−0.681203000
C	−4.520707000	0.757284000	3.599360000
C	−4.520707000	0.757284000	−3.599360000
C	−4.528030000	−1.407237000	5.355804000
C	−4.528030000	−1.407237000	−5.355804000
C	−5.520359000	0.648361000	4.566394000
C	−5.520359000	0.648361000	−4.566394000
C	−5.527365000	−0.434406000	5.449439000
C	−5.527365000	−0.434406000	−5.449439000
H	1.346730000	0.026717000	5.101110000
H	1.346730000	0.026717000	−5.101110000
H	2.758340000	2.056536000	4.307387000
H	2.758340000	2.056536000	−4.307387000
H	4.512758000	−1.597690000	2.911277000
H	4.512758000	−1.597690000	−2.911277000
H	4.529620000	2.257674000	6.034129000
H	4.529620000	2.257674000	−6.034129000
H	5.061519000	0.550073000	1.344497000
H	5.061519000	0.550073000	−1.344497000
H	6.292317000	−1.411857000	4.632564000
H	6.292317000	−1.411857000	−4.632564000
H	6.305946000	0.520105000	6.203983000
H	6.305946000	0.520105000	−6.203983000
H	−1.346730000	−0.026717000	5.101110000
H	−1.346730000	−0.026717000	−5.101110000
H	−2.758340000	−2.056536000	4.307387000
H	−2.758340000	−2.056536000	−4.307387000
H	−4.512758000	1.597690000	2.911277000
H	−4.512758000	1.597690000	−2.911277000
H	−4.529620000	−2.257674000	6.034129000
H	−4.529620000	−2.257674000	−6.034129000
H	−5.061519000	−0.550073000	1.344497000
H	−5.061519000	−0.550073000	−1.344497000
H	−6.292317000	1.411857000	4.632564000
H	−6.292317000	1.411857000	−4.632564000
H	−6.305946000	−0.520105000	6.203983000
H	−6.305946000	−0.520105000	−6.203983000
N	0.000000000	0.000000000	2.075039000

N	0.000000000	0.000000000	−2.075039000
N	2.092465000	−0.094551000	0.000000000
N	−2.092465000	0.094551000	0.000000000

5. Ag[TPFPP], D_{4h}, $q = 0$, $S = \frac{1}{2}$

Ag	0.000000000	0.000000000	0.000000000
C	0.682520000	4.281765000	0.000000000
C	0.682520000	−4.281765000	0.000000000
C	1.110665000	2.896644000	0.000000000
C	1.110665000	−2.896644000	0.000000000
C	2.442674000	2.442674000	0.000000000
C	2.442674000	−2.442674000	0.000000000
C	2.896644000	1.110665000	0.000000000
C	2.896644000	−1.110665000	0.000000000
C	3.497160000	3.497160000	0.000000000
C	3.497160000	−3.497160000	0.000000000
C	4.008318000	4.008318000	1.192249000
C	4.008318000	4.008318000	−1.192249000
C	4.008318000	−4.008318000	1.192249000
C	4.008318000	−4.008318000	−1.192249000
C	4.281765000	0.682520000	0.000000000
C	4.281765000	−0.682520000	0.000000000
C	4.993940000	4.993940000	1.208008000
C	4.993940000	4.993940000	−1.208008000
C	4.993940000	−4.993940000	1.208008000
C	4.993940000	−4.993940000	−1.208008000
C	5.487556000	5.487556000	0.000000000
C	5.487556000	−5.487556000	0.000000000
C	−0.682520000	4.281765000	0.000000000
C	−0.682520000	−4.281765000	0.000000000
C	−1.110665000	2.896644000	0.000000000
C	−1.110665000	−2.896644000	0.000000000
C	−2.442674000	2.442674000	0.000000000
C	−2.442674000	−2.442674000	0.000000000
C	−2.896644000	1.110665000	0.000000000
C	−2.896644000	−1.110665000	0.000000000
C	−3.497160000	3.497160000	0.000000000
C	−3.497160000	−3.497160000	0.000000000
C	−4.008318000	4.008318000	1.192249000
C	−4.008318000	4.008318000	−1.192249000
C	−4.008318000	−4.008318000	1.192249000
C	−4.008318000	−4.008318000	−1.192249000
C	−4.281765000	0.682520000	0.000000000
C	−4.281765000	−0.682520000	0.000000000
C	−4.993940000	4.993940000	1.208008000
C	−4.993940000	4.993940000	−1.208008000
C	−4.993940000	−4.993940000	1.208008000
C	−4.993940000	−4.993940000	−1.208008000
C	−5.487556000	5.487556000	0.000000000
C	−5.487556000	−5.487556000	0.000000000
F	3.546462000	3.546462000	2.362216000
F	3.546462000	3.546462000	−2.362216000
F	3.546462000	−3.546462000	2.362216000
F	3.546462000	−3.546462000	−2.362216000
F	5.467755000	5.467755000	2.365135000
F	5.467755000	5.467755000	−2.365135000
F	5.467755000	−5.467755000	2.365135000
F	5.467755000	−5.467755000	−2.365135000
F	6.432554000	6.432554000	0.000000000
F	6.432554000	−6.432554000	0.000000000
F	−3.546462000	3.546462000	2.362216000
F	−3.546462000	3.546462000	−2.362216000
F	−3.546462000	−3.546462000	2.362216000
F	−3.546462000	−3.546462000	−2.362216000
F	−5.467755000	5.467755000	2.365135000
F	−5.467755000	5.467755000	−2.365135000
F	−5.467755000	−5.467755000	2.365135000
F	−5.467755000	−5.467755000	−2.365135000
F	−6.432554000	6.432554000	0.000000000
F	−6.432554000	−6.432554000	0.000000000
H	1.344580000	5.136049000	0.000000000
H	1.344580000	−5.136049000	0.000000000
H	5.136049000	1.344580000	0.000000000
H	5.136049000	−1.344580000	0.000000000
H	−1.344580000	5.136049000	0.000000000
H	−1.344580000	−5.136049000	0.000000000
H	−5.136049000	1.344580000	0.000000000
H	−5.136049000	−1.344580000	0.000000000
N	0.000000000	2.104153000	0.000000000
N	0.000000000	−2.104153000	0.000000000
N	2.104153000	0.000000000	0.000000000
N	−2.104153000	0.000000000	0.000000000

6. Au[TPFPP], C_{2h}, $q = 0$, $S = \frac{1}{2}$

Au	0.000000000	0.000000000	0.000000000
C	0.686023000	0.003282000	4.240754000
C	0.686023000	0.003282000	−4.240754000
C	1.112989000	−0.006460000	2.874975000
C	1.112989000	−0.006460000	−2.874975000
C	2.448320000	−0.033304000	2.436153000
C	2.448320000	−0.033304000	−2.436153000
C	2.875962000	−0.080529000	1.114505000
C	2.875962000	−0.080529000	−1.114505000
C	3.496135000	0.081312000	3.486439000
C	3.496135000	0.081312000	−3.486439000
C	3.842864000	1.326038000	4.014585000

C	3.842864000	1.326038000	−4.014585000
C	4.167163000	−1.037640000	3.981709000
C	4.167163000	−1.037640000	−3.981709000
C	4.247420000	0.048892000	0.680033000
C	4.247420000	0.048892000	−0.680033000
C	4.821818000	1.462849000	4.996202000
C	4.821818000	1.462849000	−4.996202000
C	5.154380000	−0.929791000	4.960984000
C	5.154380000	−0.929791000	−4.960984000
C	5.481189000	0.327806000	5.468317000
C	5.481189000	0.327806000	−5.468317000
C	−0.686023000	−0.003282000	4.240754000
C	−0.686023000	−0.003282000	−4.240754000
C	−1.112989000	0.006460000	2.874975000
C	−1.112989000	0.006460000	−2.874975000
C	−2.448320000	0.033304000	2.436153000
C	−2.448320000	0.033304000	−2.436153000
C	−2.875962000	0.080529000	1.114505000
C	−2.875962000	0.080529000	−1.114505000
C	−3.496135000	−0.081312000	3.486439000
C	−3.496135000	−0.081312000	−3.486439000
C	−3.842864000	−1.326038000	4.014585000
C	−3.842864000	−1.326038000	−4.014585000
C	−4.167163000	1.037640000	3.981709000
C	−4.167163000	1.037640000	−3.981709000
C	−4.247420000	−0.048892000	0.680033000
C	−4.247420000	−0.048892000	−0.680033000
C	−4.821818000	−1.462849000	4.996202000
C	−4.821818000	−1.462849000	−4.996202000
C	−5.154380000	0.929791000	4.960984000
C	−5.154380000	0.929791000	−4.960984000
C	−5.481189000	−0.327806000	5.468317000
C	−5.481189000	−0.327806000	−5.468317000
F	3.230364000	2.431227000	3.568718000
F	3.230364000	2.431227000	−3.568718000
F	3.861635000	−2.257041000	3.517810000
F	3.861635000	−2.257041000	−3.517810000
F	5.138204000	2.667352000	5.481565000
F	5.138204000	2.667352000	−5.481565000
F	5.785519000	−2.015494000	5.421192000
F	5.785519000	−2.015494000	−5.421192000
F	6.425621000	0.445606000	6.404886000
F	6.425621000	0.445606000	−6.404886000
F	−3.230364000	−2.431227000	3.568718000
F	−3.230364000	−2.431227000	−3.568718000
F	−3.861635000	2.257041000	3.517810000
F	−3.861635000	2.257041000	−3.517810000
F	−5.138204000	−2.667352000	5.481565000
F	−5.138204000	−2.667352000	−5.481565000
F	−5.785519000	2.015494000	5.421192000
F	−5.785519000	2.015494000	−5.421192000
F	−6.425621000	−0.445606000	6.404886000
F	−6.425621000	−0.445606000	−6.404886000
H	1.350968000	−0.018479000	5.091773000
H	1.350968000	−0.018479000	−5.091773000
H	5.091808000	0.149586000	1.346385000
H	5.091808000	0.149586000	−1.346385000
H	−1.350968000	0.018479000	5.091773000
H	−1.350968000	0.018479000	−5.091773000
H	−5.091808000	−0.149586000	1.346385000
H	−5.091808000	−0.149586000	−1.346385000
N	0.000000000	0.000000000	2.065303000
N	0.000000000	0.000000000	−2.065303000
N	2.071178000	−0.201233000	0.000000000
N	−2.071178000	0.201233000	0.000000000

7. Ag[P], C_1, $q = -1$, $S = 0$

Ag	0.000205000	0.000438000	0.003506000
C	0.000341000	−3.438412000	0.080272000
C	1.232706000	2.806461000	−0.083865000
C	1.232920000	−2.806361000	0.036529000
C	2.507124000	3.471066000	−0.126238000
C	2.507225000	−3.471945000	0.018116000
C	2.806656000	−1.233219000	−0.033207000
C	2.806845000	1.232221000	−0.085206000
C	3.439445000	−0.000822000	−0.072934000
C	3.471415000	−2.508122000	−0.024621000
C	3.471607000	2.506629000	−0.124690000
C	−0.000184000	3.439335000	−0.068627000
C	−1.232631000	−2.805699000	0.088867000
C	−1.232770000	2.807135000	−0.029192000
C	−2.507217000	−3.470229000	0.128082000
C	−2.507287000	3.472693000	−0.017896000
C	−2.806484000	−1.231442000	0.082649000
C	−2.806524000	1.234045000	0.034517000
C	−3.439175000	0.001496000	0.070976000
C	−3.471432000	−2.505614000	0.122906000
C	−3.471514000	2.508890000	0.023855000
H	0.000671000	−4.522991000	0.107850000
H	2.627397000	4.546120000	−0.152345000
H	2.627687000	−4.547172000	0.036314000
H	4.524016000	−0.001468000	−0.097249000
H	4.546452000	−2.629225000	−0.047784000
H	4.546718000	2.626893000	−0.149098000
H	−0.000626000	4.523950000	−0.090103000
H	−2.627571000	4.547825000	−0.039484000

H	−2.627665000	−4.545247000	0.155355000
H	−4.523781000	0.001869000	0.092283000
H	−4.546617000	−2.625526000	0.146625000
H	−4.546628000	2.629750000	0.043742000
N	1.448784000	1.448420000	−0.063482000
N	1.448895000	−1.448456000	0.004797000
N	−1.448467000	1.449424000	0.005986000
N	−1.448614000	−1.447872000	0.057602000

8. Au[P], D_{4h}**,** $q = -1$**,** $S = 0$

Au	0.000000000	0.000000000	0.000000000
C	0.682498000	4.221480000	0.000000000
C	0.682498000	−4.221480000	0.000000000
C	1.111767000	2.850969000	0.000000000
C	1.111767000	−2.850969000	0.000000000
C	2.430464000	2.430464000	0.000000000
C	2.430464000	−2.430464000	0.000000000
C	2.850969000	1.111767000	0.000000000
C	2.850969000	−1.111767000	0.000000000
C	4.221480000	0.682498000	0.000000000
C	4.221480000	−0.682498000	0.000000000
C	−0.682498000	4.221480000	0.000000000
C	−0.682498000	−4.221480000	0.000000000
C	−1.111767000	2.850969000	0.000000000
C	−1.111767000	−2.850969000	0.000000000
C	−2.430464000	2.430464000	0.000000000
C	−2.430464000	−2.430464000	0.000000000
C	−2.850969000	1.111767000	0.000000000
C	−2.850969000	−1.111767000	0.000000000
C	−4.221480000	0.682498000	0.000000000
C	−4.221480000	−0.682498000	0.000000000
H	1.358824000	5.066024000	0.000000000
H	1.358824000	−5.066024000	0.000000000
H	3.197646000	3.197646000	0.000000000
H	3.197646000	−3.197646000	0.000000000
H	5.066024000	1.358824000	0.000000000
H	5.066024000	−1.358824000	0.000000000
H	−1.358824000	5.066024000	0.000000000
H	−1.358824000	−5.066024000	0.000000000
H	−3.197646000	3.197646000	0.000000000
H	−3.197646000	−3.197646000	0.000000000
H	−5.066024000	1.358824000	0.000000000
H	−5.066024000	−1.358824000	0.000000000
N	0.000000000	2.034381000	0.000000000
N	0.000000000	−2.034381000	0.000000000
N	2.034381000	0.000000000	0.000000000
N	−2.034381000	0.000000000	0.000000000

9. Ag[TPP], C_1**,** $q = -1$**,** $S = 0$

Ag	0.007022000	0.010046000	0.032369000
C	0.002161000	7.762193000	0.115046000
C	0.006165000	4.955977000	0.041028000
C	0.006525000	3.476348000	0.006596000
C	0.127684000	−7.086893000	−0.888377000
C	0.129867000	−5.692368000	−0.942034000
C	0.711903000	7.088742000	−0.883371000
C	0.719938000	5.695446000	−0.916961000
C	1.230027000	−2.807240000	0.024190000
C	1.244648000	2.812818000	0.017613000
C	2.471525000	−3.477578000	−0.253087000
C	2.510284000	3.450413000	0.254802000
C	2.805241000	−1.243654000	−0.140206000
C	2.813888000	1.234085000	−0.065379000
C	3.434157000	−2.517063000	−0.372608000
C	3.469430000	−0.006143000	−0.146493000
C	3.472882000	2.483582000	0.197866000
C	4.947526000	−0.005538000	−0.221735000
C	5.607024000	0.727511000	−1.222583000
C	5.712094000	−0.730639000	0.707747000
C	6.998865000	0.729189000	−1.295862000
C	7.103800000	−0.720893000	0.638117000
C	7.750707000	0.007043000	−0.364672000
C	−0.001884000	−3.453007000	0.177827000
C	−0.004132000	−4.942036000	0.233020000
C	−0.007540000	−7.741043000	0.338906000
C	−0.142272000	−6.995569000	1.512700000
C	−0.142875000	−5.600773000	1.460995000
C	−0.706603000	7.035235000	1.076008000
C	−0.710850000	5.642186000	1.035882000
C	−1.233867000	2.817550000	−0.041878000
C	−1.235322000	−2.797074000	0.254106000
C	−2.496845000	3.464400000	−0.285930000
C	−2.503112000	−3.448771000	0.458259000
C	−2.804792000	1.240773000	−0.041630000
C	−2.807365000	−1.226870000	0.171739000
C	−3.457238000	0.005702000	0.037609000
C	−3.461171000	2.497966000	−0.278593000
C	−3.468836000	−2.485696000	0.400204000
C	−4.945191000	−0.002541000	−0.035841000
C	−5.583832000	0.162164000	−1.271725000
C	−5.714162000	−0.184305000	1.120236000
C	−6.976880000	0.144548000	−1.349902000
C	−7.107494000	−0.200817000	1.039865000
C	−7.741145000	−0.036918000	−0.194440000
H	0.000827000	8.848989000	0.143650000
H	0.228178000	−7.661830000	−1.805646000

H	0.234308000	−5.180277000	−1.894721000
H	1.256263000	7.649931000	−1.638668000
H	1.266375000	5.169527000	−1.694112000
H	2.572291000	−4.546378000	−0.363861000
H	2.631412000	4.501380000	0.467331000
H	4.479992000	−2.644598000	−0.605670000
H	4.535567000	2.588103000	0.354412000
H	5.019716000	1.284333000	−1.946549000
H	5.207410000	−1.287763000	1.491276000
H	7.497070000	1.290111000	−2.082578000
H	7.684409000	−1.275796000	1.370630000
H	8.836488000	0.011668000	−0.419733000
H	−0.009028000	−8.827322000	0.379754000
H	−0.245824000	−7.499072000	2.470590000
H	−0.247808000	−5.018167000	2.372259000
H	−1.253730000	7.554003000	1.859259000
H	−1.257512000	5.074639000	1.783057000
H	−2.612088000	4.523893000	−0.455762000
H	−2.620429000	−4.510509000	0.614420000
H	−4.523463000	2.608130000	−0.434458000
H	−4.537583000	−2.598801000	0.500346000
H	−4.985998000	0.302644000	−2.168121000
H	−5.218043000	−0.312188000	2.078496000
H	−7.464354000	0.270133000	−2.313603000
H	−7.698262000	−0.338236000	1.942160000
H	−8.826502000	−0.049728000	−0.255378000
N	1.460436000	1.465762000	−0.192121000
N	1.468849000	−1.451488000	0.116422000
N	−1.454149000	1.470559000	0.128878000
N	−1.454769000	−1.452141000	0.058617000

10. Au[TPP], D_{4h}, $q = -1$, $S = 0$

Au	0.000000000	0.000000000	0.000000000
C	0.000000000	3.459549000	0.000000000
C	0.000000000	4.950884000	0.000000000
C	0.000000000	5.654045000	1.210032000
C	0.000000000	5.654045000	−1.210032000
C	0.000000000	7.049941000	1.209141000
C	0.000000000	7.049941000	−1.209141000
C	0.000000000	7.750025000	0.000000000
C	0.000000000	−3.459549000	0.000000000
C	0.000000000	−4.950884000	0.000000000
C	0.000000000	−5.654045000	1.210032000
C	0.000000000	−5.654045000	−1.210032000
C	0.000000000	−7.049941000	1.209141000
C	0.000000000	−7.049941000	−1.209141000
C	0.000000000	−7.750025000	0.000000000
C	1.226981000	2.803043000	0.000000000
C	1.226981000	−2.803043000	0.000000000
C	2.500892000	3.465433000	0.000000000
C	2.500892000	−3.465433000	0.000000000
C	2.803043000	1.226981000	0.000000000
C	2.803043000	−1.226981000	0.000000000
C	3.459549000	0.000000000	0.000000000
C	3.465433000	2.500892000	0.000000000
C	3.465433000	−2.500892000	0.000000000
C	4.950884000	0.000000000	0.000000000
C	5.654045000	0.000000000	1.210032000
C	5.654045000	0.000000000	−1.210032000
C	7.049941000	0.000000000	1.209141000
C	7.049941000	0.000000000	−1.209141000
C	7.750025000	0.000000000	0.000000000
C	−1.226981000	2.803043000	0.000000000
C	−1.226981000	−2.803043000	0.000000000
C	−2.500892000	3.465433000	0.000000000
C	−2.500892000	−3.465433000	0.000000000
C	−2.803043000	1.226981000	0.000000000
C	−2.803043000	−1.226981000	0.000000000
C	−3.459549000	0.000000000	0.000000000
C	−3.465433000	2.500892000	0.000000000
C	−3.465433000	−2.500892000	0.000000000
C	−4.950884000	0.000000000	0.000000000
C	−5.654045000	0.000000000	1.210032000
C	−5.654045000	0.000000000	−1.210032000
C	−7.049941000	0.000000000	1.209141000
C	−7.049941000	0.000000000	−1.209141000
C	−7.750025000	0.000000000	0.000000000
H	0.000000000	5.105809000	2.148539000
H	0.000000000	5.105809000	−2.148539000
H	0.000000000	7.589747000	2.153012000
H	0.000000000	7.589747000	−2.153012000
H	0.000000000	8.837287000	0.000000000
H	0.000000000	−5.105809000	2.148539000
H	0.000000000	−5.105809000	−2.148539000
H	0.000000000	−7.589747000	2.153012000
H	0.000000000	−7.589747000	−2.153012000
H	0.000000000	−8.837287000	0.000000000
H	2.615880000	4.539034000	0.000000000
H	2.615880000	−4.539034000	0.000000000
H	4.539034000	2.615880000	0.000000000
H	4.539034000	−2.615880000	0.000000000
H	5.105809000	0.000000000	2.148539000
H	5.105809000	0.000000000	−2.148539000
H	7.589747000	0.000000000	2.153012000
H	7.589747000	0.000000000	−2.153012000
H	8.837287000	0.000000000	0.000000000
H	−2.615880000	4.539034000	0.000000000
H	−2.615880000	−4.539034000	0.000000000

H	−4.539034000	2.615880000	0.000000000
H	−4.539034000	−2.615880000	0.000000000
H	−5.105809000	0.000000000	2.148539000
H	−5.105809000	0.000000000	−2.148539000
H	−7.589747000	0.000000000	2.153012000
H	−7.589747000	0.000000000	−2.153012000
H	−8.837287000	0.000000000	0.000000000
N	1.436187000	1.436187000	0.000000000
N	1.436187000	−1.436187000	0.000000000
N	−1.436187000	1.436187000	0.000000000
N	−1.436187000	−1.436187000	0.000000000

11. Ag[TPFPP], C_1, $q = -1$, $S = 0$

Ag	0.003978000	−0.017343000	−0.009459000
C	0.003115000	−3.473197000	−0.013625000
C	0.004308000	−4.961839000	−0.020758000
C	0.004424000	3.436378000	−0.011572000
C	0.008437000	−7.771906000	−0.043222000
C	0.138045000	−5.672581000	−1.214788000
C	0.139668000	7.044018000	−1.187562000
C	0.152004000	−7.065903000	−1.240135000
C	0.154044000	5.650517000	−1.183310000
C	1.238123000	−2.826061000	−0.005882000
C	1.238910000	2.790707000	−0.009872000
C	2.511363000	3.454780000	0.076551000
C	2.513419000	−3.488859000	−0.067850000
C	2.810327000	1.218268000	0.000218000
C	2.810674000	−1.251634000	0.003079000
C	3.456663000	−0.016487000	0.006427000
C	3.474299000	2.491528000	0.082440000
C	3.475600000	−2.524772000	−0.066843000
C	4.943475000	−0.009718000	0.005719000
C	5.654107000	0.128812000	−1.187322000
C	5.669492000	−0.121679000	1.192789000
C	7.046785000	0.148638000	−1.208951000
C	7.063162000	−0.102064000	1.200709000
C	7.751265000	0.027340000	−0.008421000
C	−0.001223000	4.922006000	−0.003500000
C	−0.044612000	7.729506000	0.015977000
C	−0.126776000	−5.690960000	1.162506000
C	−0.137214000	−7.084903000	1.164621000
C	−0.177057000	5.629000000	1.186893000
C	−0.206837000	7.021468000	1.209812000
C	−1.229652000	2.789614000	−0.012715000
C	−1.232172000	−2.826503000	−0.019202000
C	−2.502170000	3.453437000	−0.098388000
C	−2.507144000	−3.489575000	0.045103000
C	−2.801450000	1.217703000	−0.009345000
C	−2.804851000	−1.251953000	−0.015287000
C	−3.449935000	−0.016232000	−0.008706000
C	−3.465197000	2.490656000	−0.095556000
C	−3.469446000	−2.525270000	0.051752000
C	−4.936082000	0.002197000	0.017178000
C	−5.619877000	0.205147000	1.217325000
C	−5.688519000	−0.137890000	−1.150017000
C	−7.010408000	0.271832000	1.263886000
C	−7.081338000	−0.084518000	−1.130958000
C	−7.741674000	0.123208000	0.082647000
F	0.012385000	−9.100048000	−0.053418000
F	0.263576000	−5.003816000	−2.368426000
F	0.292592000	7.719088000	−2.324706000
F	0.299178000	−7.723810000	−2.388800000
F	0.307276000	5.001467000	−2.345429000
F	4.987621000	0.243123000	−2.343996000
F	5.017687000	−0.236327000	2.357847000
F	7.704759000	0.280744000	−2.358282000
F	7.738771000	−0.199699000	2.344262000
F	9.079448000	0.037245000	−0.016950000
F	−0.065607000	9.057902000	0.027329000
F	−0.249568000	−5.042331000	2.328305000
F	−0.280146000	−7.761597000	2.302642000
F	−0.316878000	4.957952000	2.338378000
F	−0.386275000	7.677195000	2.353970000
F	−4.925986000	0.342166000	2.355536000
F	−5.064863000	−0.308080000	−2.323573000
F	−7.641486000	0.474221000	2.418057000
F	−7.781752000	−0.222784000	−2.254840000
F	−9.068423000	0.178546000	0.114270000
H	2.631878000	4.526444000	0.134435000
H	2.637329000	−4.560470000	−0.117254000
H	4.545533000	2.612442000	0.146055000
H	4.547862000	−2.645009000	−0.116472000
H	−2.623072000	4.524565000	−0.163591000
H	−2.630783000	−4.561443000	0.088993000
H	−4.536325000	2.612166000	−0.158617000
H	−4.541623000	−2.645427000	0.102563000
N	1.452605000	−1.467613000	0.063980000
N	1.453684000	1.433310000	−0.082850000
N	−1.444523000	1.432611000	0.063039000
N	−1.446920000	−1.467649000	−0.084842000

12. Au[TPFPP], D_{4h}, $q = -1$, $S = 0$

Au	0.000000000	0.000000000	0.000000000
C	0.000000000	3.451014000	0.000000000
C	0.000000000	4.938851000	0.000000000
C	0.000000000	5.656444000	1.196349000

C	0.000000000	5.656444000	−1.196349000
C	0.000000000	7.050196000	1.211222000
C	0.000000000	7.050196000	−1.211222000
C	0.000000000	7.746527000	0.000000000
C	0.000000000	−3.451014000	0.000000000
C	0.000000000	−4.938851000	0.000000000
C	0.000000000	−5.656444000	1.196349000
C	0.000000000	−5.656444000	−1.196349000
C	0.000000000	−7.050196000	1.211222000
C	0.000000000	−7.050196000	−1.211222000
C	0.000000000	−7.746527000	0.000000000
C	1.229452000	2.802778000	0.000000000
C	1.229452000	−2.802778000	0.000000000
C	2.502972000	3.465495000	0.000000000
C	2.502972000	−3.465495000	0.000000000
C	2.802778000	1.229452000	0.000000000
C	2.802778000	−1.229452000	0.000000000
C	3.451014000	0.000000000	0.000000000
C	3.465495000	2.502972000	0.000000000
C	3.465495000	−2.502972000	0.000000000
C	4.938851000	0.000000000	0.000000000
C	5.656444000	0.000000000	1.196349000
C	5.656444000	0.000000000	−1.196349000
C	7.050196000	0.000000000	1.211222000
C	7.050196000	0.000000000	−1.211222000
C	7.746527000	0.000000000	0.000000000
C	−1.229452000	2.802778000	0.000000000
C	−1.229452000	−2.802778000	0.000000000
C	−2.502972000	3.465495000	0.000000000
C	−2.502972000	−3.465495000	0.000000000
C	−2.802778000	1.229452000	0.000000000
C	−2.802778000	−1.229452000	0.000000000
C	−3.451014000	0.000000000	0.000000000
C	−3.465495000	2.502972000	0.000000000
C	−3.465495000	−2.502972000	0.000000000
C	−4.938851000	0.000000000	0.000000000
C	−5.656444000	0.000000000	1.196349000
C	−5.656444000	0.000000000	−1.196349000
C	−7.050196000	0.000000000	1.211222000
C	−7.050196000	0.000000000	−1.211222000
C	−7.746527000	0.000000000	0.000000000
F	0.000000000	4.993685000	2.360559000
F	0.000000000	4.993685000	−2.360559000
F	0.000000000	7.718086000	2.362937000
F	0.000000000	7.718086000	−2.362937000
F	0.000000000	9.075466000	0.000000000
F	0.000000000	−4.993685000	2.360559000
F	0.000000000	−4.993685000	−2.360559000
F	0.000000000	−7.718086000	2.362937000
F	0.000000000	−7.718086000	−2.362937000
F	0.000000000	−9.075466000	0.000000000
F	4.993685000	0.000000000	2.360559000
F	4.993685000	0.000000000	−2.360559000
F	7.718086000	0.000000000	2.362937000
F	7.718086000	0.000000000	−2.362937000
F	9.075466000	0.000000000	0.000000000
F	−4.993685000	0.000000000	2.360559000
F	−4.993685000	0.000000000	−2.360559000
F	−7.718086000	0.000000000	2.362937000
F	−7.718086000	0.000000000	−2.362937000
F	−9.075466000	0.000000000	0.000000000
H	2.624561000	4.538473000	0.000000000
H	2.624561000	−4.538473000	0.000000000
H	4.538473000	2.624561000	0.000000000
H	4.538473000	−2.624561000	0.000000000
H	−2.624561000	4.538473000	0.000000000
H	−2.624561000	−4.538473000	0.000000000
H	−4.538473000	2.624561000	0.000000000
H	−4.538473000	−2.624561000	0.000000000
N	1.437342000	1.437342000	0.000000000
N	1.437342000	−1.437342000	0.000000000
N	−1.437342000	1.437342000	0.000000000
N	−1.437342000	−1.437342000	0.000000000