

Supporting Information

Tuning the hyperconjugative aromaticity of Au(III)-substituted indoliums

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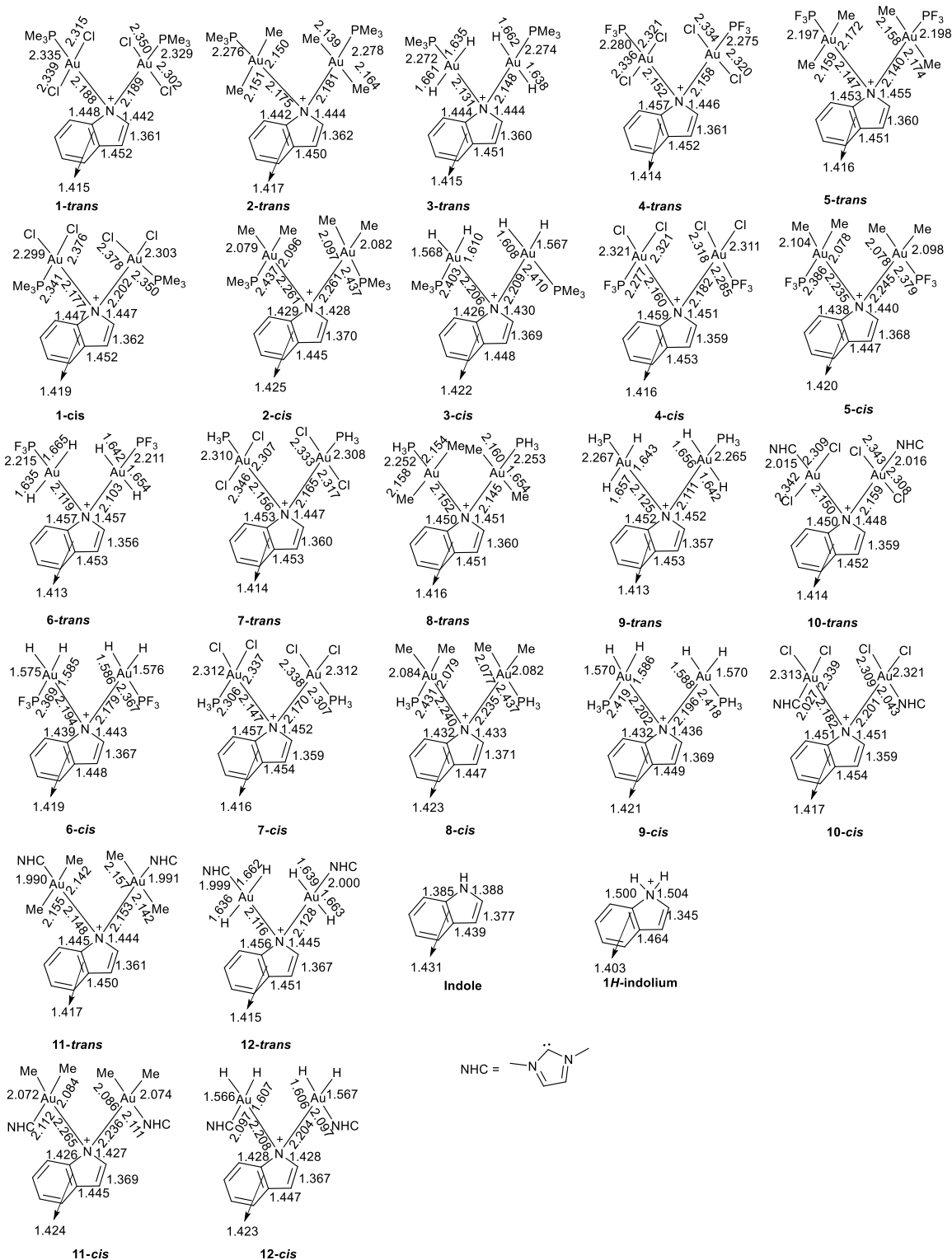


Fig. S1 The optimized structures of Au(III)-substituted indoliums (**1-trans** to **12-cis**), indole and **1H-indolium** with bond length (Å).

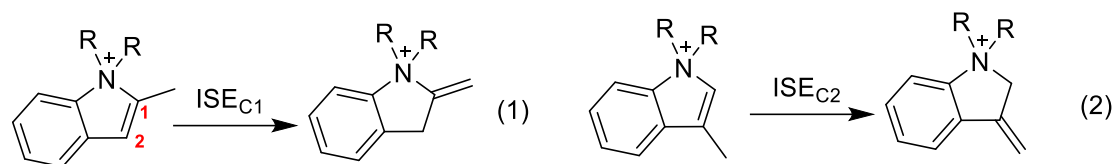


Fig. S2 The equation of methyl-methylene ISE calculation.

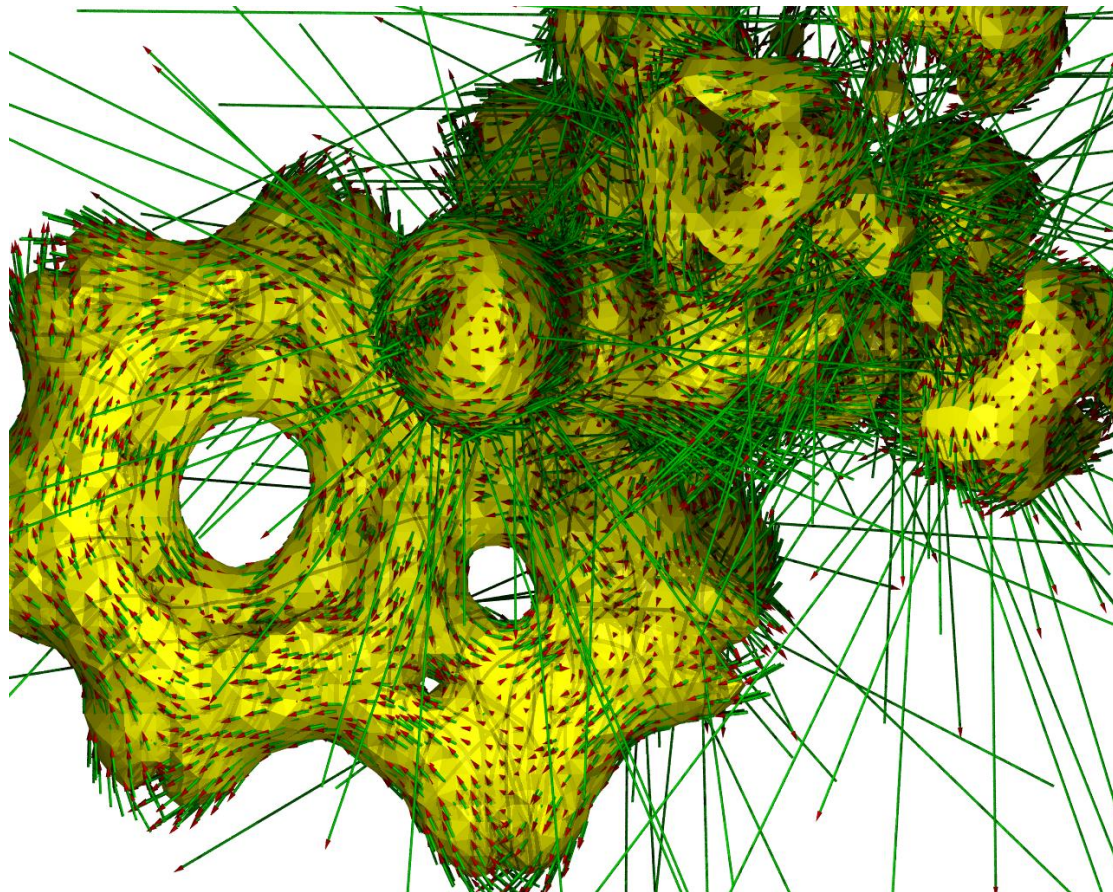


Fig. S3 The ACID graph of indolium **1-trans**. The magnetic field vectors are perpendicular to the ring and point forward. The iso-surface value of the current is 0.003 a.u..

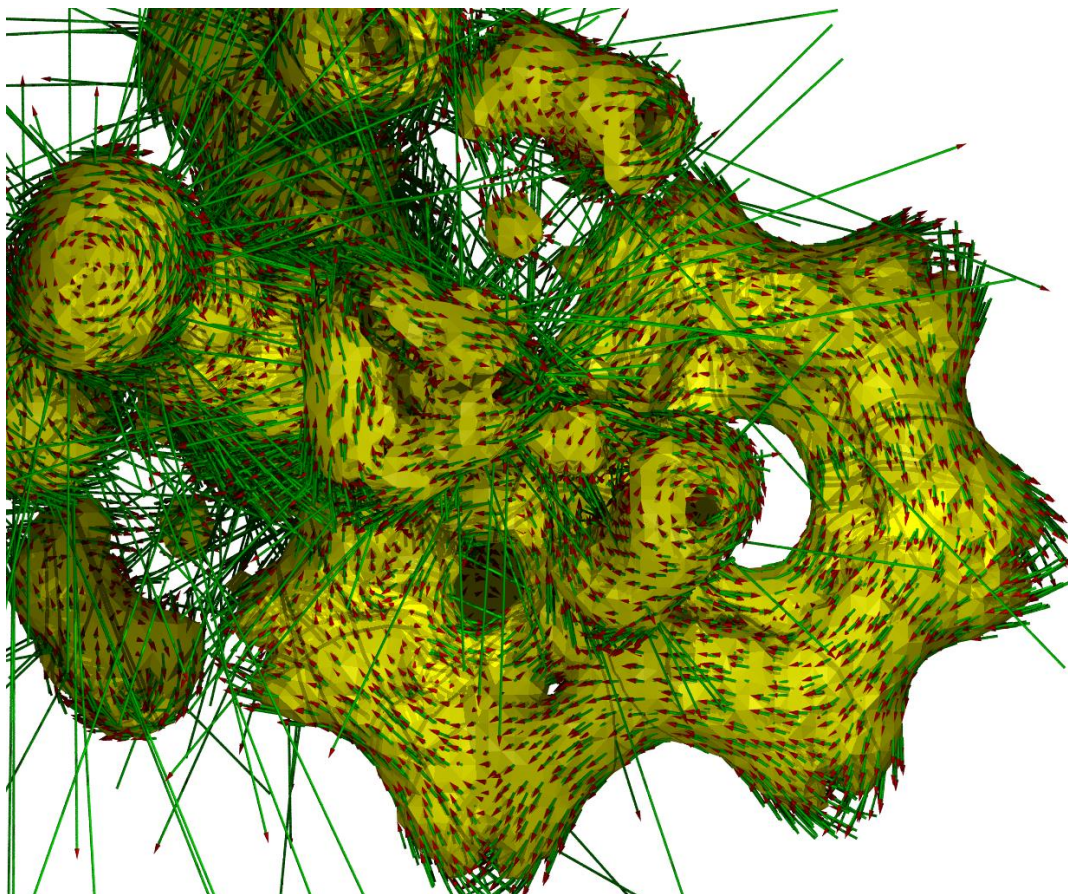


Fig. S4 The ACID graph of indolium **1-cis**. The magnetic field vectors are perpendicular to the ring and point forward. The iso-surface value of the current is 0.003 a.u..

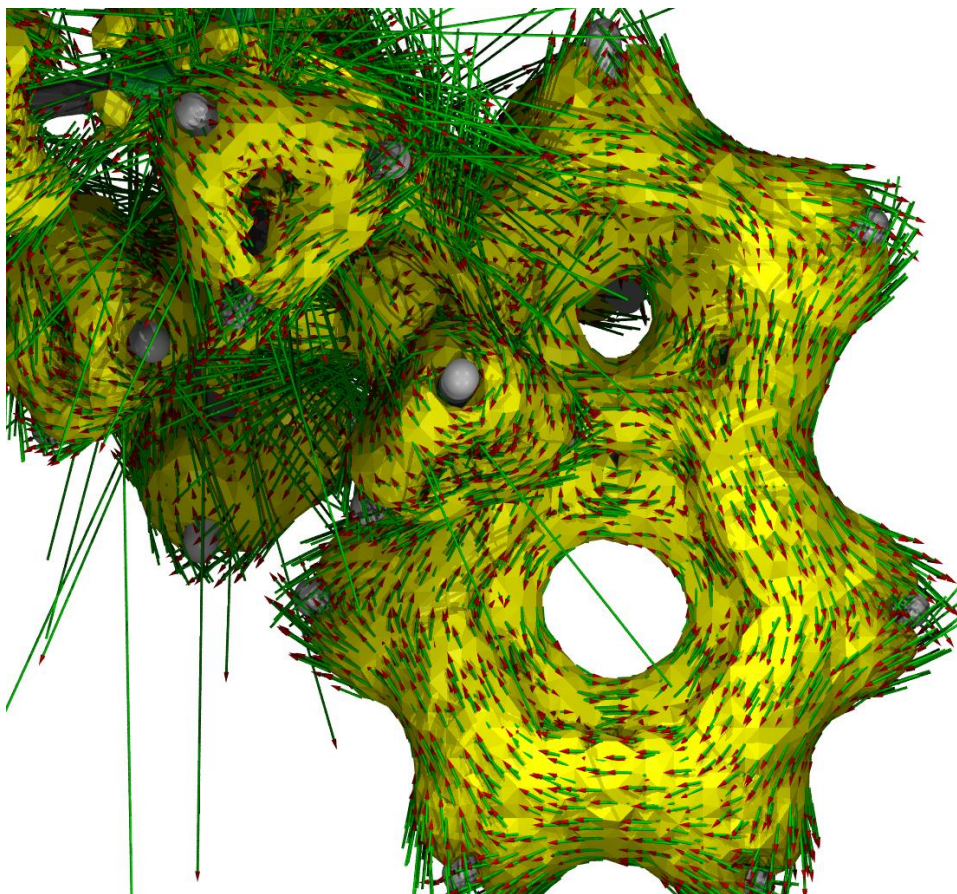


Fig. S5 The ACID graph of indolium **2-trans**. The magnetic field vectors are perpendicular to the ring and point forward. The iso-surface value of the current is 0.003 a.u..

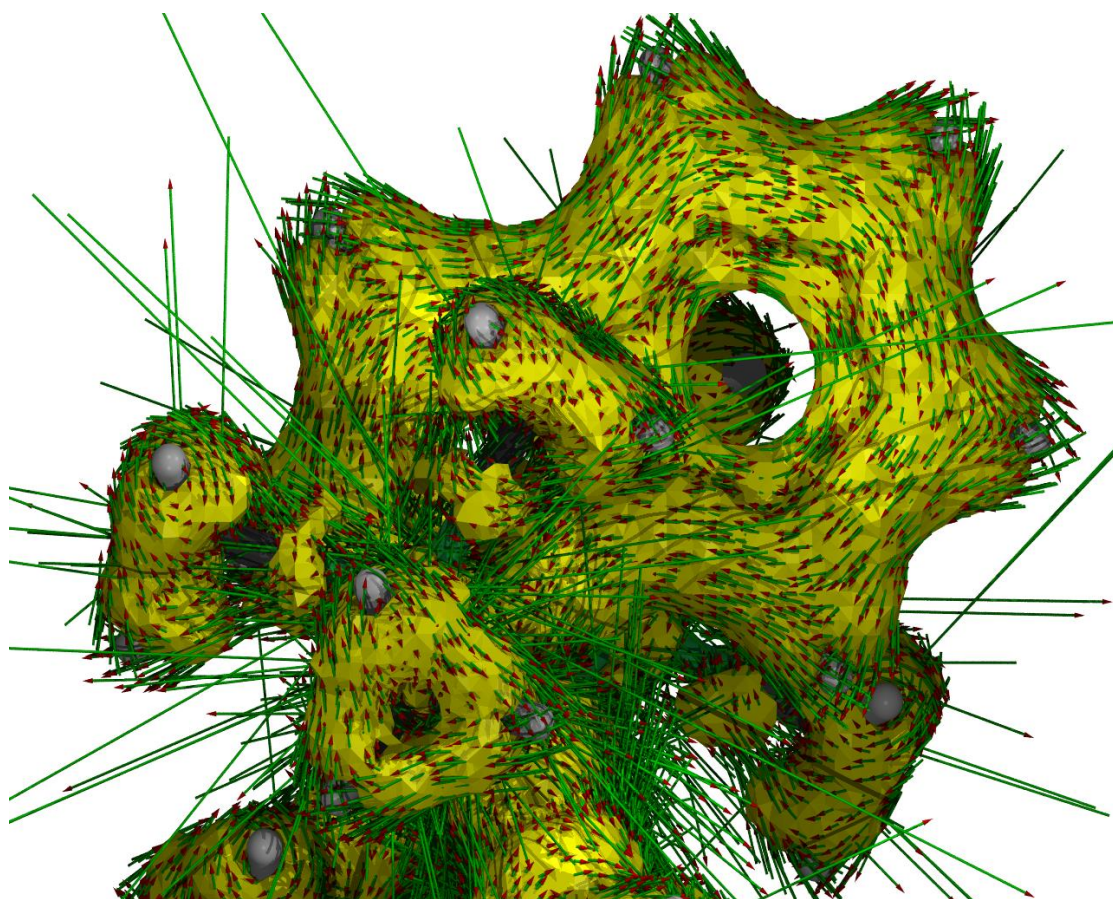


Fig. S6 The ACID graph of indolium **2-cis**. The magnetic field vectors are perpendicular to the ring and point forward. The iso-surface value of the current is 0.003 a.u..

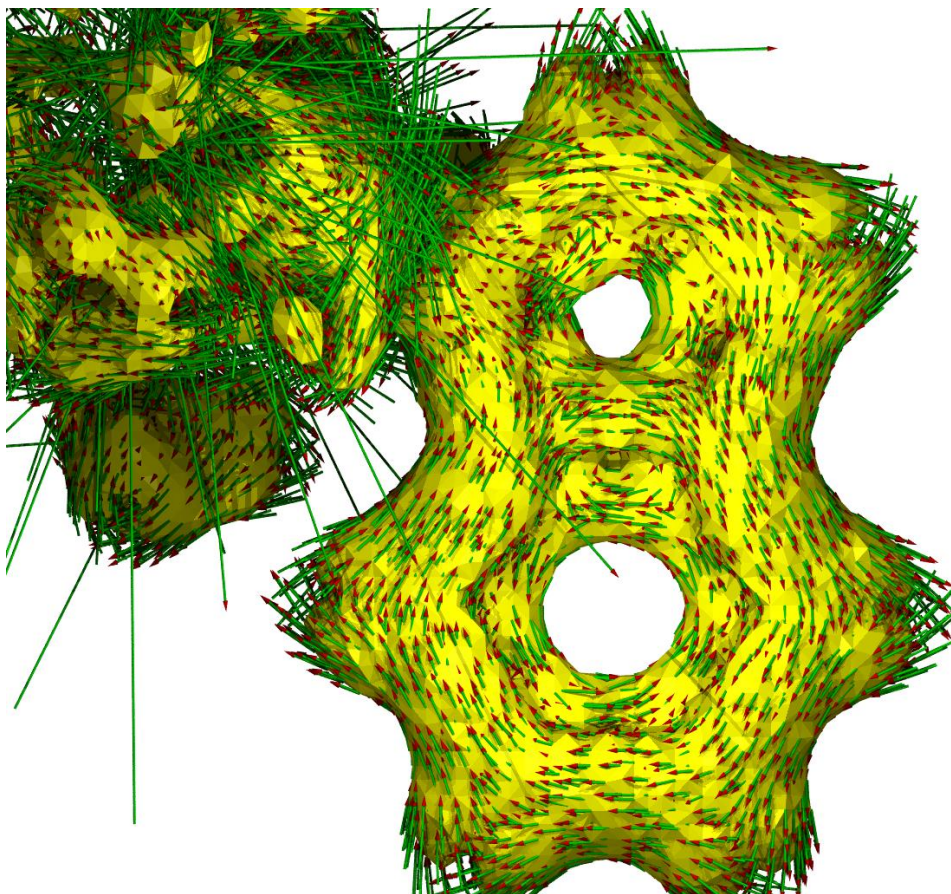


Fig. S7 The ACID graph of indolium **3-trans**. The magnetic field vectors are perpendicular to the ring and point forward. The iso-surface value of the current is 0.003 a.u..

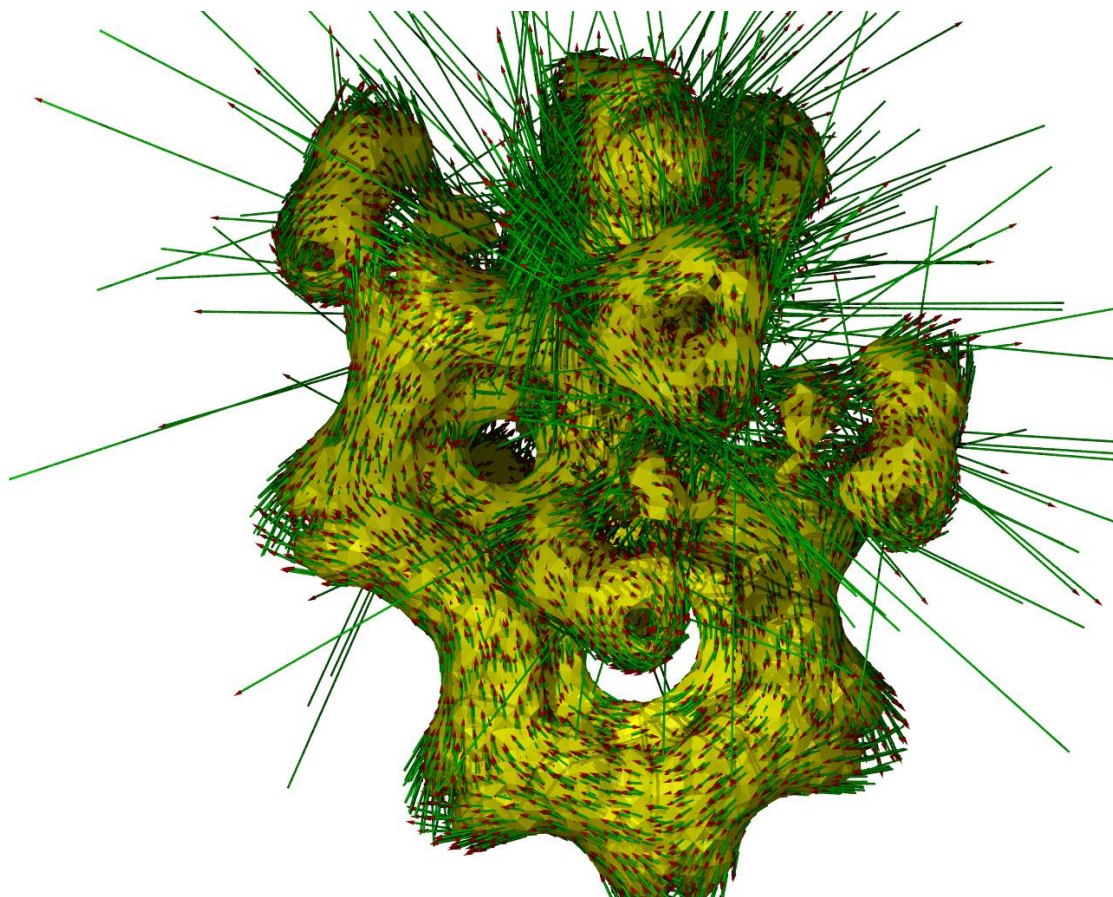


Fig. S8 The ACID graph of indolium **3-cis**. The magnetic field vectors are perpendicular to the ring and point forward. The iso-surface value of the current is 0.003 a.u..

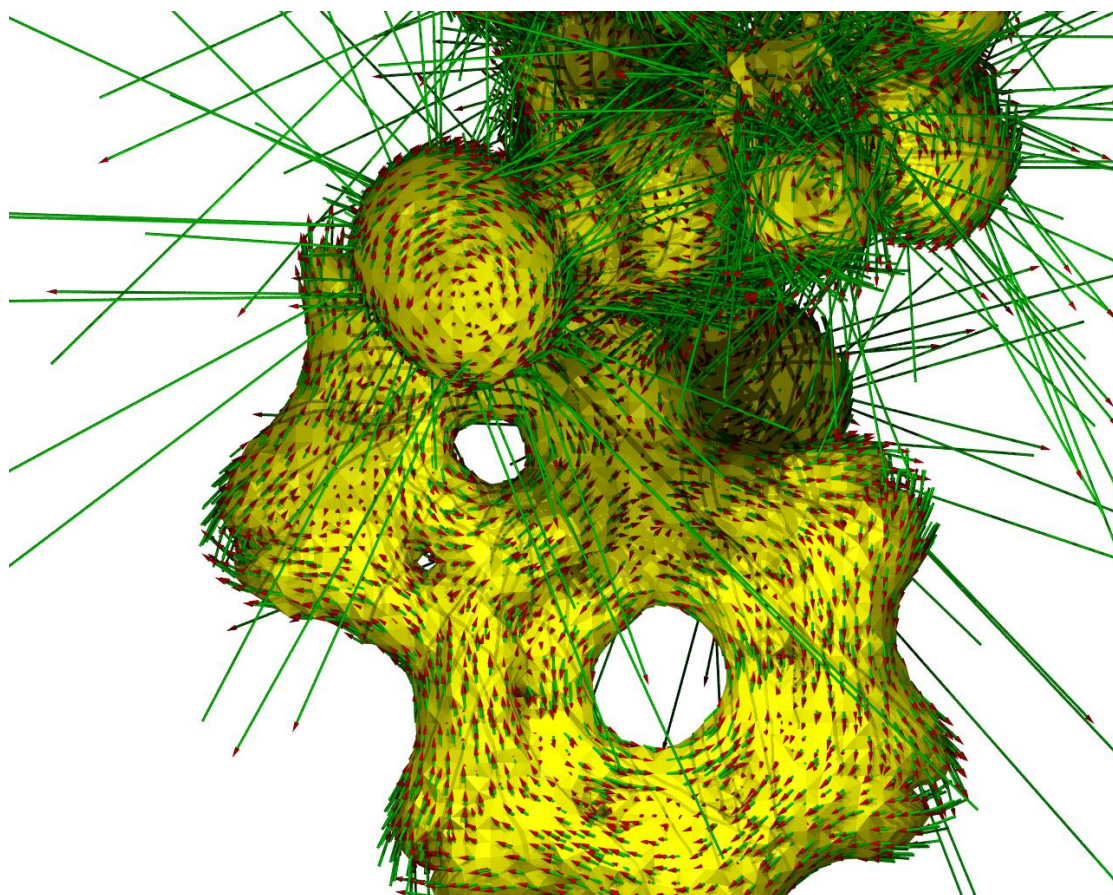


Fig. S9 The ACID graph of indolium *4-trans*. The magnetic field vectors are perpendicular to the ring and point forward. The iso-surface value of the current is 0.003 a.u..

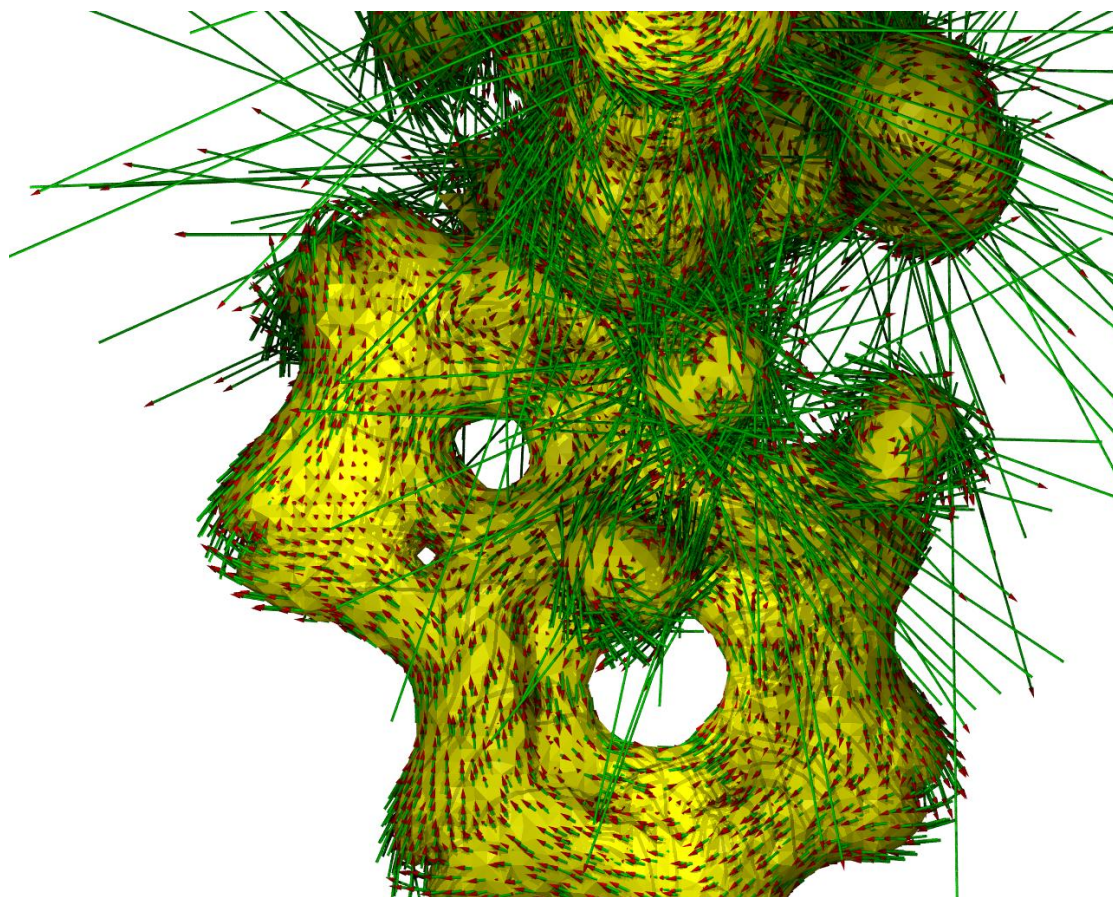


Fig. S10 The ACID graph of indolium *4-cis*. The magnetic field vectors are perpendicular to the ring and point forward. The iso-surface value of the current is 0.003 a.u..

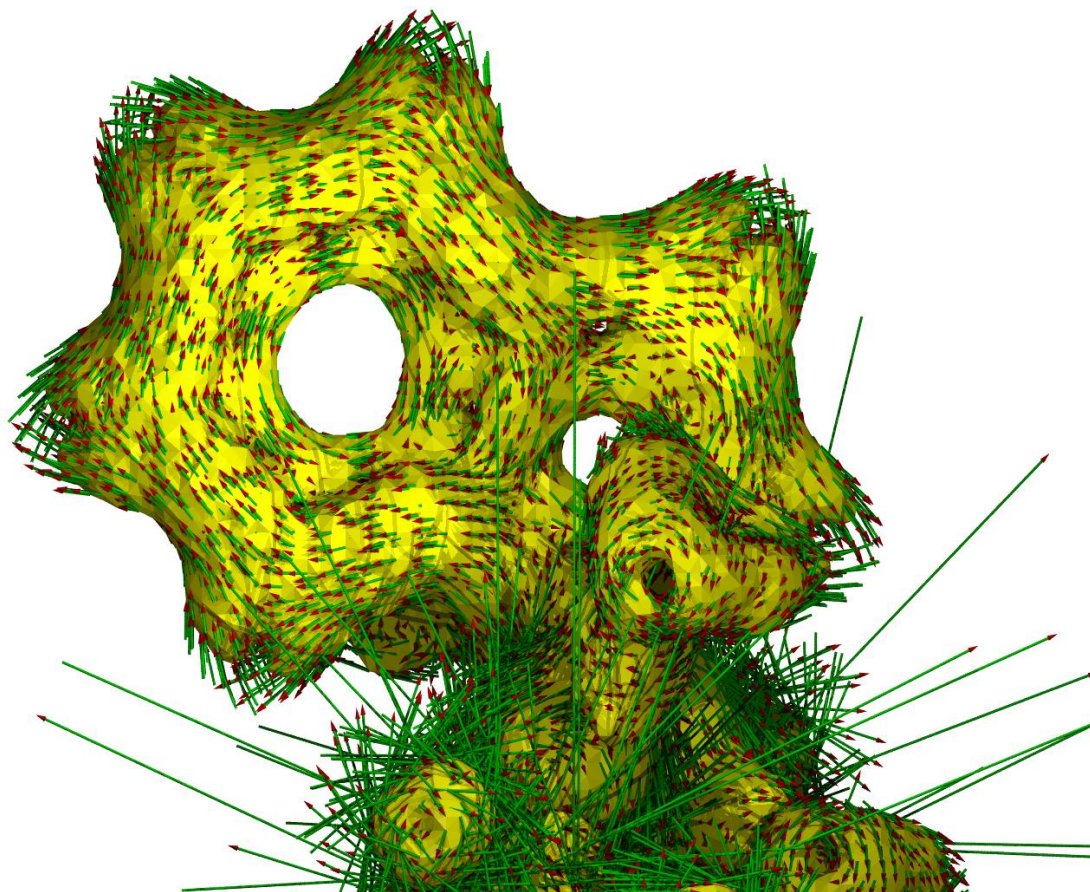


Fig. S11 The ACID graph of indolium **5-trans**. The magnetic field vectors are perpendicular to the ring and point forward. The iso-surface value of the current is 0.003 a.u..

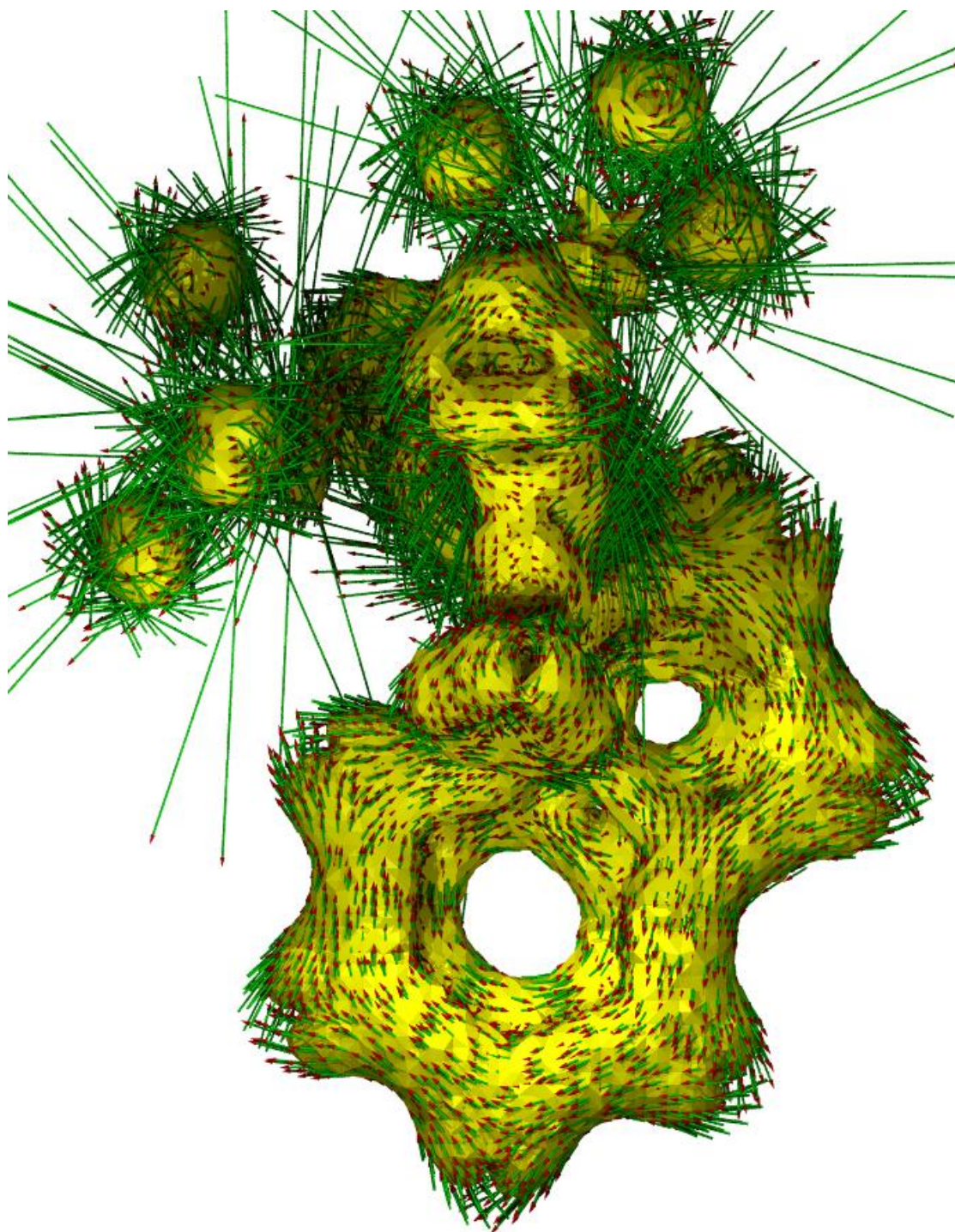


Fig. S12 The ACID graph of indolium *5-cis*. The magnetic field vectors are perpendicular to the ring and point forward. The iso-surface value of the current is 0.003 a.u..

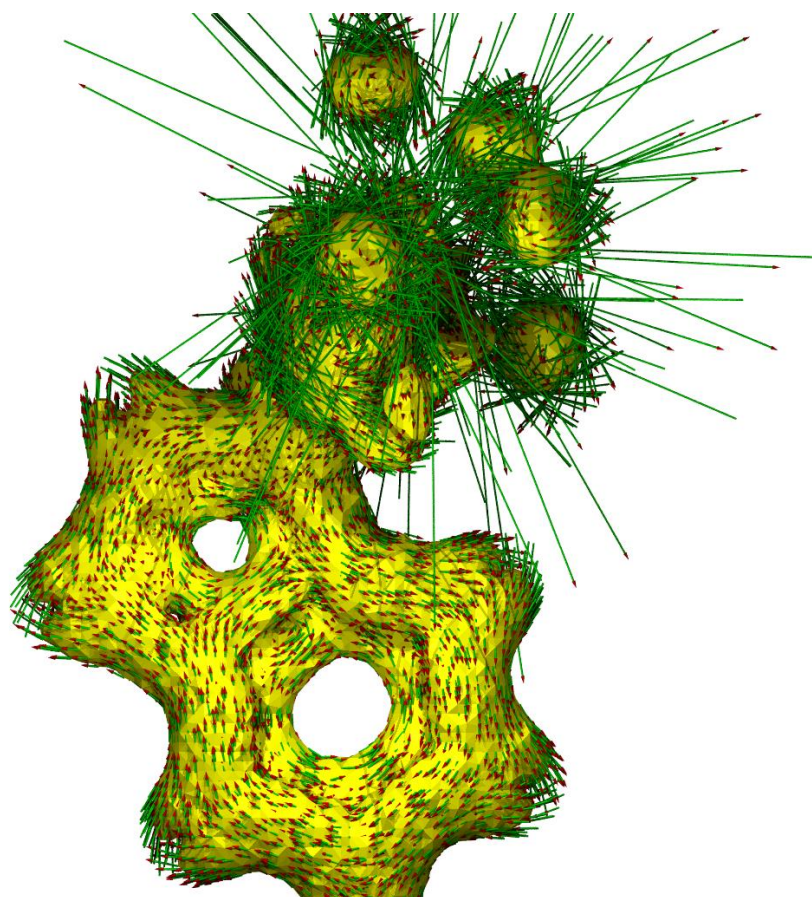


Fig. S13 The ACID graph of indolium **6-trans**. The magnetic field vectors are perpendicular to the ring and point forward. The iso-surface value of the current is 0.003 a.u..

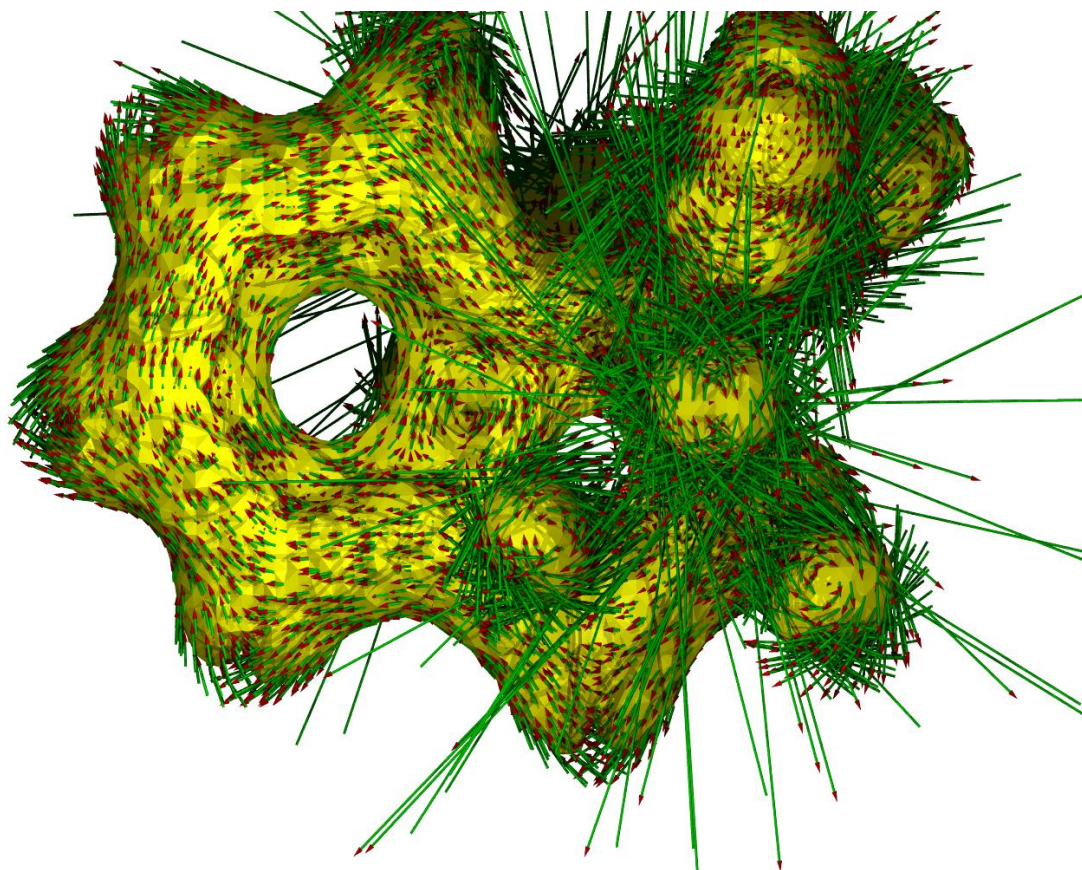


Fig. S14 The ACID graph of indolium **6-cis**. The magnetic field vectors are perpendicular to the ring and point forward. The iso-surface value of the current is 0.003 a.u..

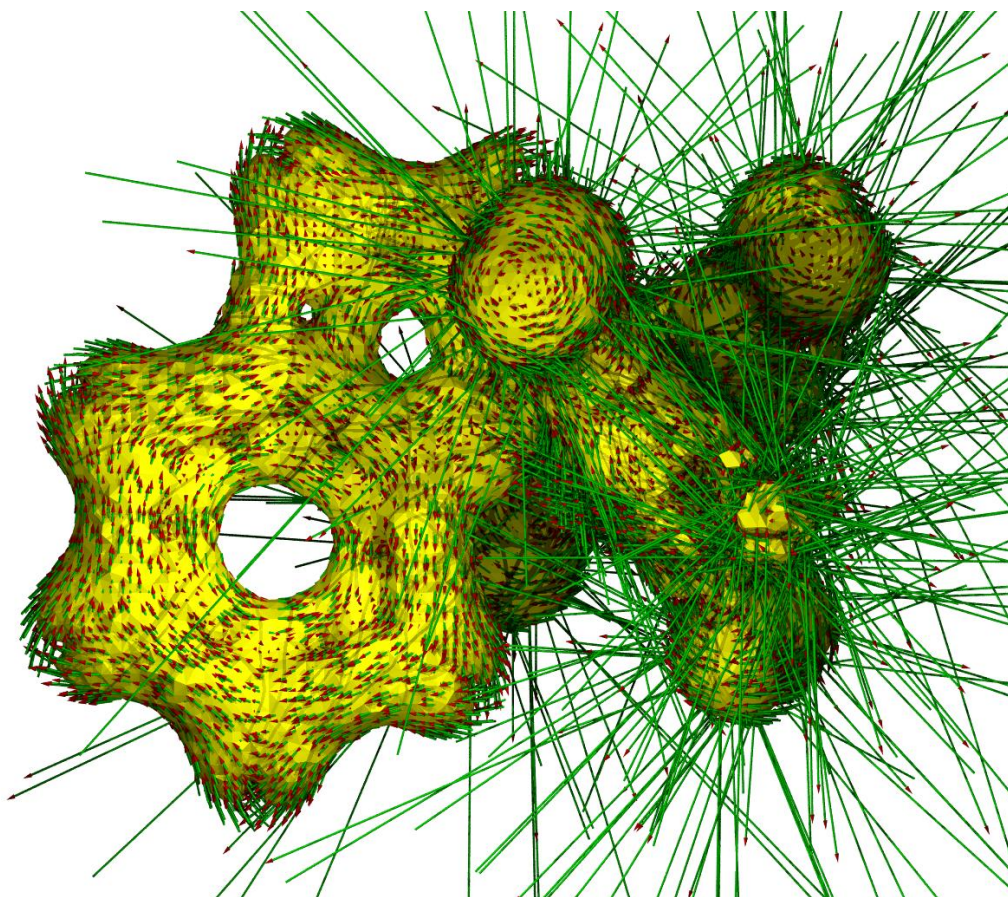


Fig. S15 The ACID graph of indolium **7-trans**. The magnetic field vectors are perpendicular to the ring and point forward. The iso-surface value of the current is 0.003 a.u..

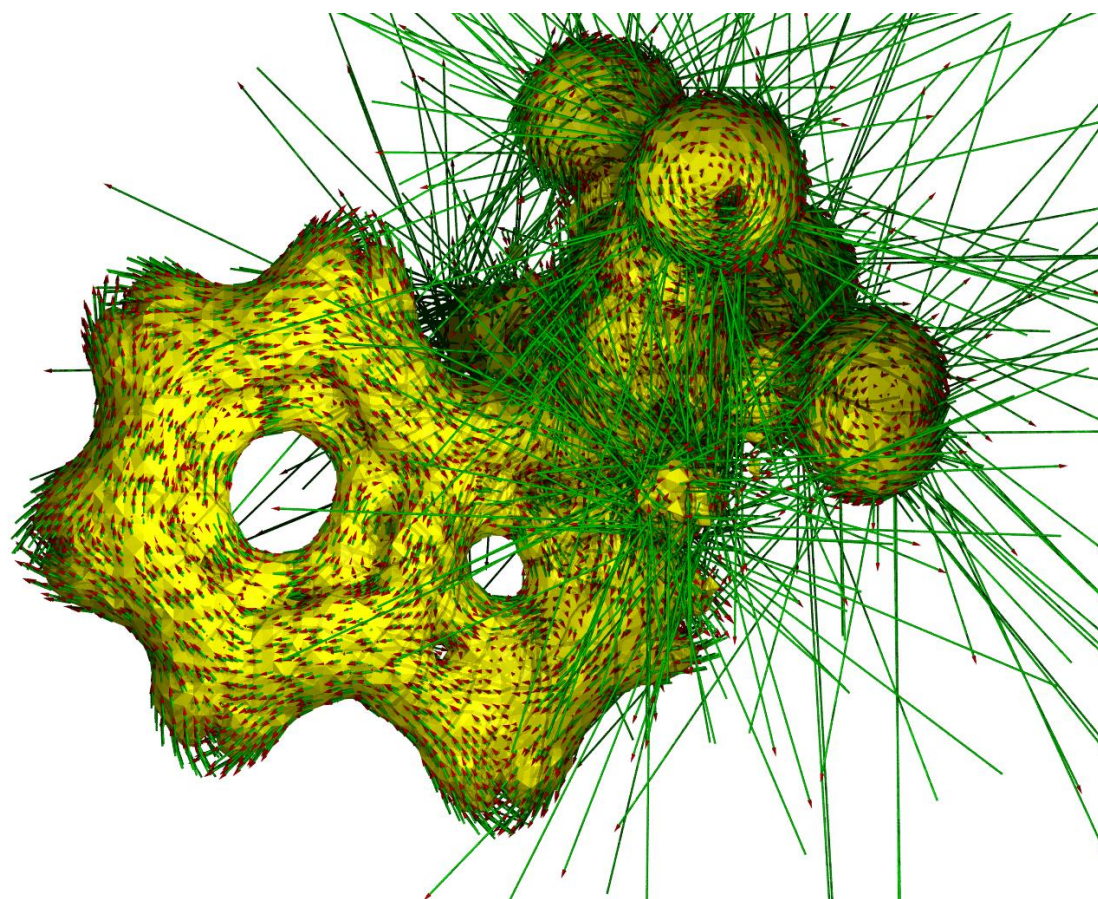


Fig. S16 The ACID graph of indolium **7-cis**. The magnetic field vectors are perpendicular to the ring and point forward. The iso-surface value of the current is 0.003 a.u..

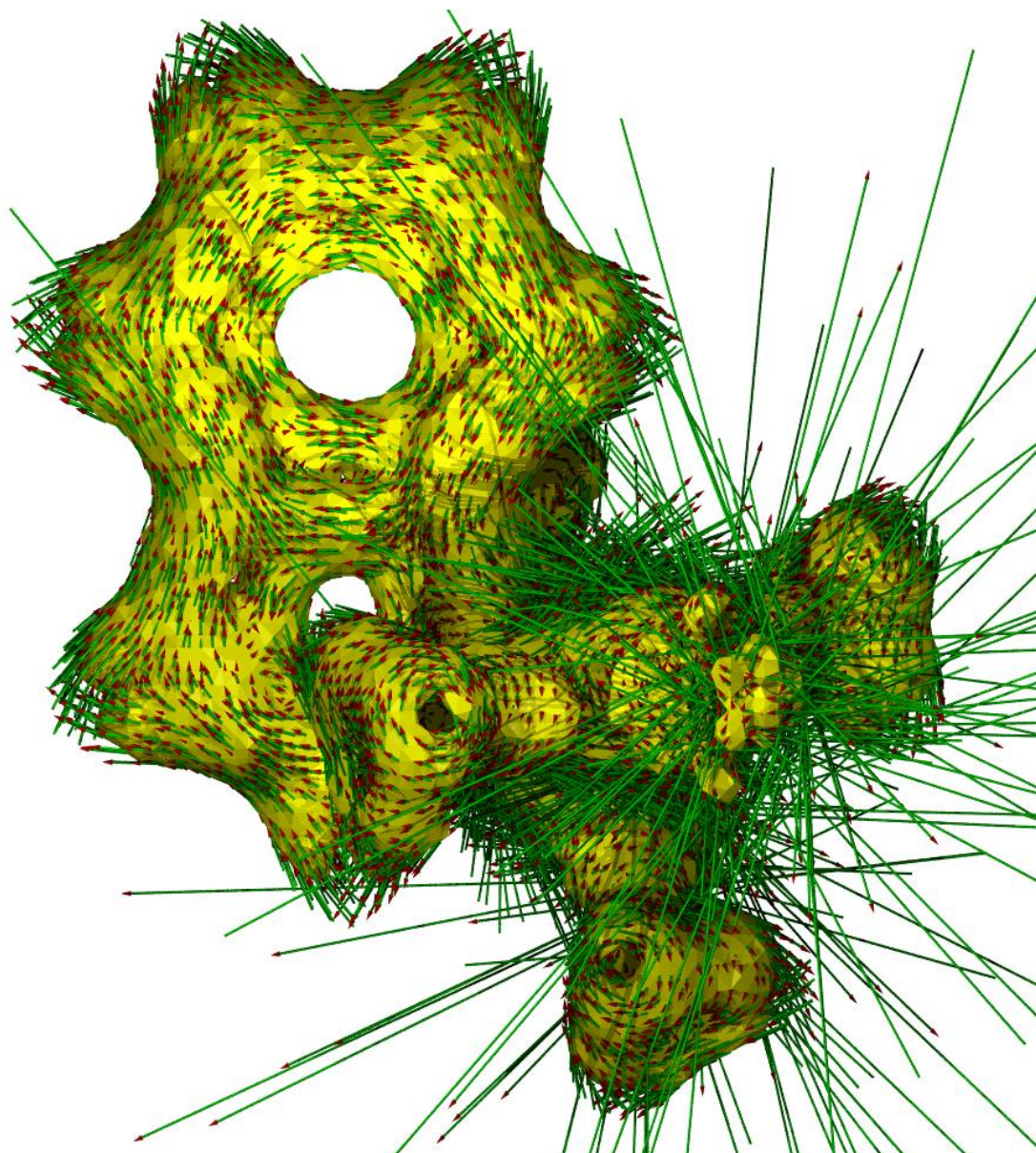


Fig. S17 The ACID graph of indolium **8-trans**. The magnetic field vectors are perpendicular to the ring and point forward. The iso-surface value of the current is 0.003 a.u..

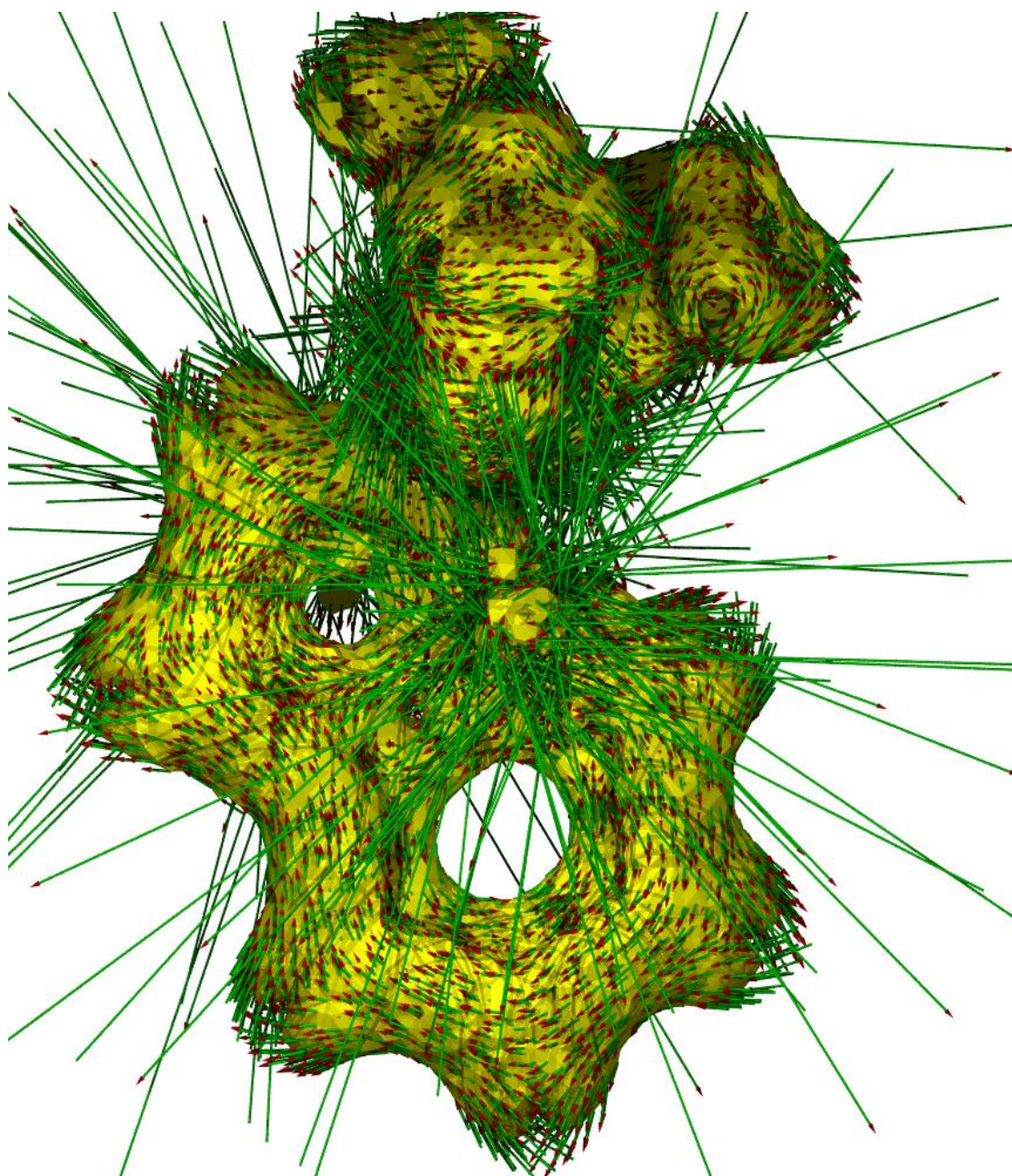


Fig. S18 The ACID graph of indolium **8-cis**. The magnetic field vectors are perpendicular to the ring and point forward. The iso-surface value of the current is 0.003 a.u..

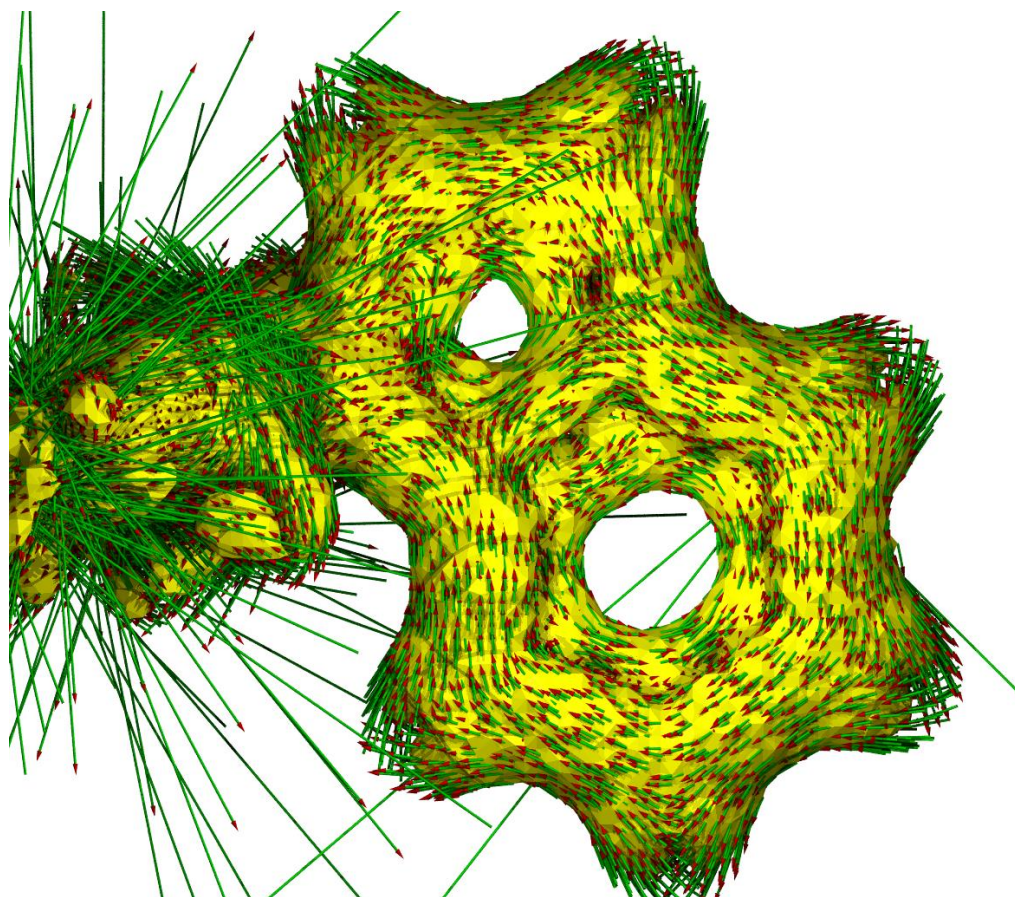


Fig. S19 The ACID graph of indolium **9-trans**. The magnetic field vectors are perpendicular to the ring and point forward. The iso-surface value of the current is 0.003 a.u..

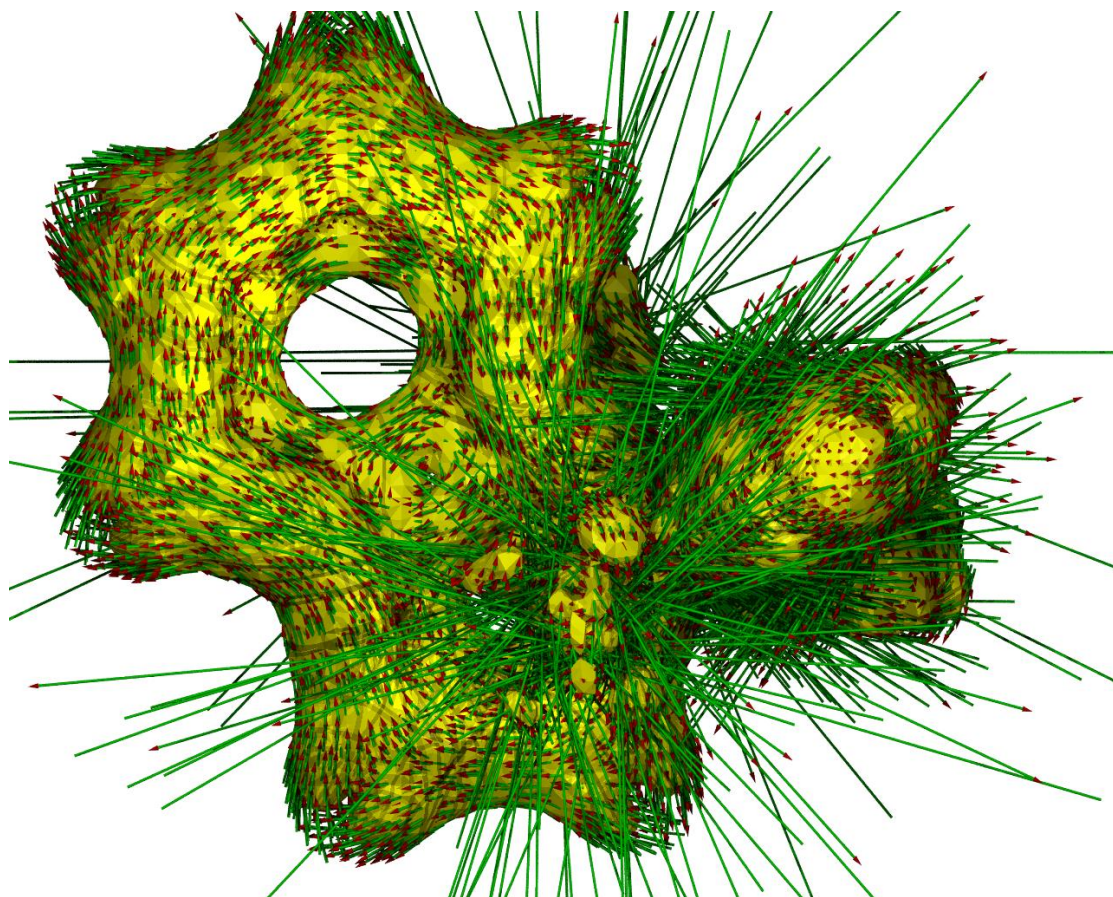


Fig. S20 The ACID graph of indolium *9-cis*. The magnetic field vectors are perpendicular to the ring and point forward. The iso-surface value of the current is 0.003 a.u..

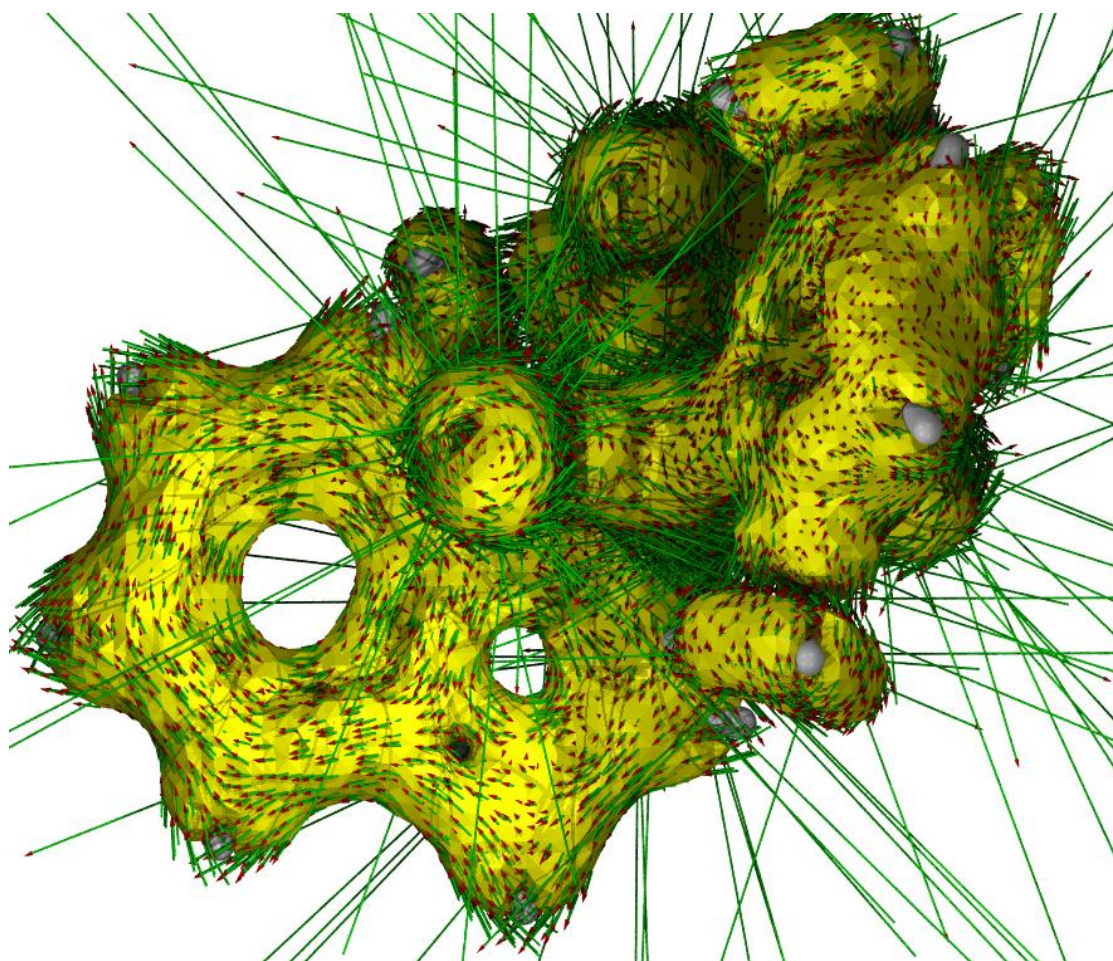


Fig. S21 The ACID graph of indolium **10-trans**. The magnetic field vectors are perpendicular to the ring and point forward. The iso-surface value of the current is 0.003 a.u..

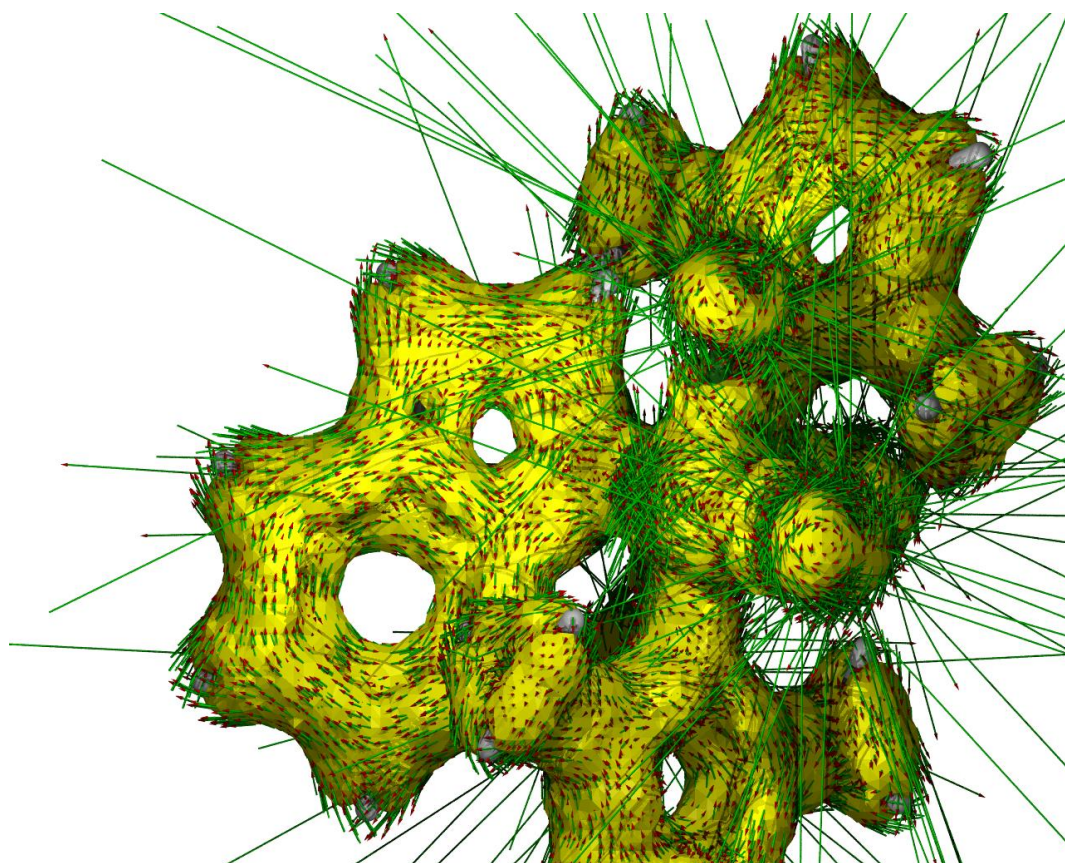


Fig. S22 The ACID graph of indolium **10-*cis***. The magnetic field vectors are perpendicular to the ring and point forward. The iso-surface value of the current is 0.003 a.u..

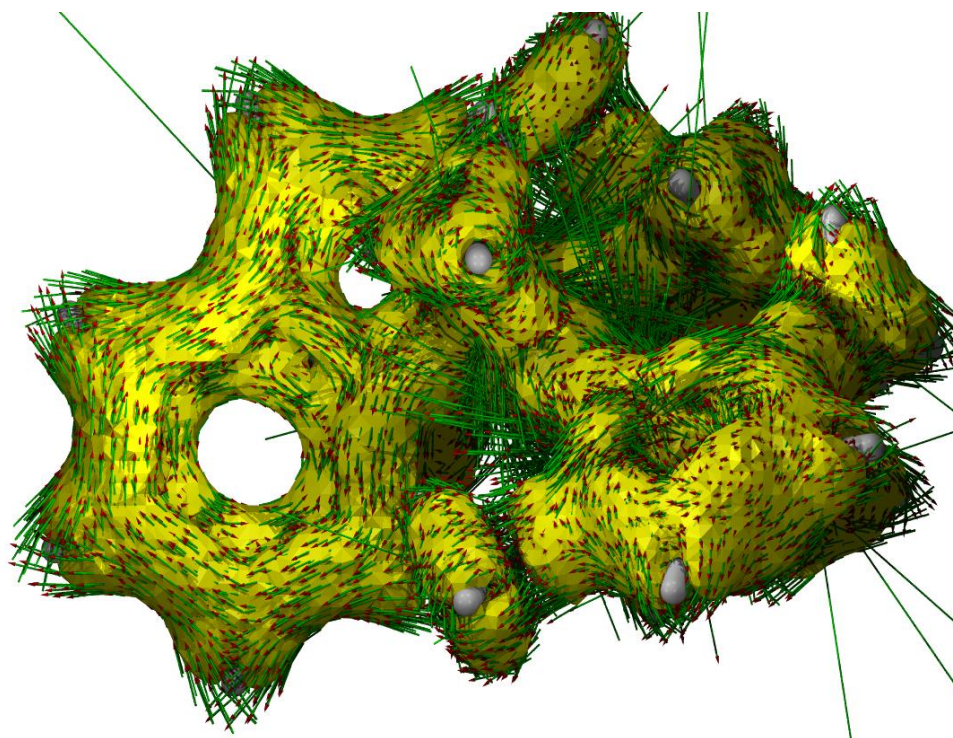


Fig. S23 The ACID graph of indolium **11-*trans***. The magnetic field vectors are perpendicular to the ring and point forward. The iso-surface value of the current is 0.003 a.u..

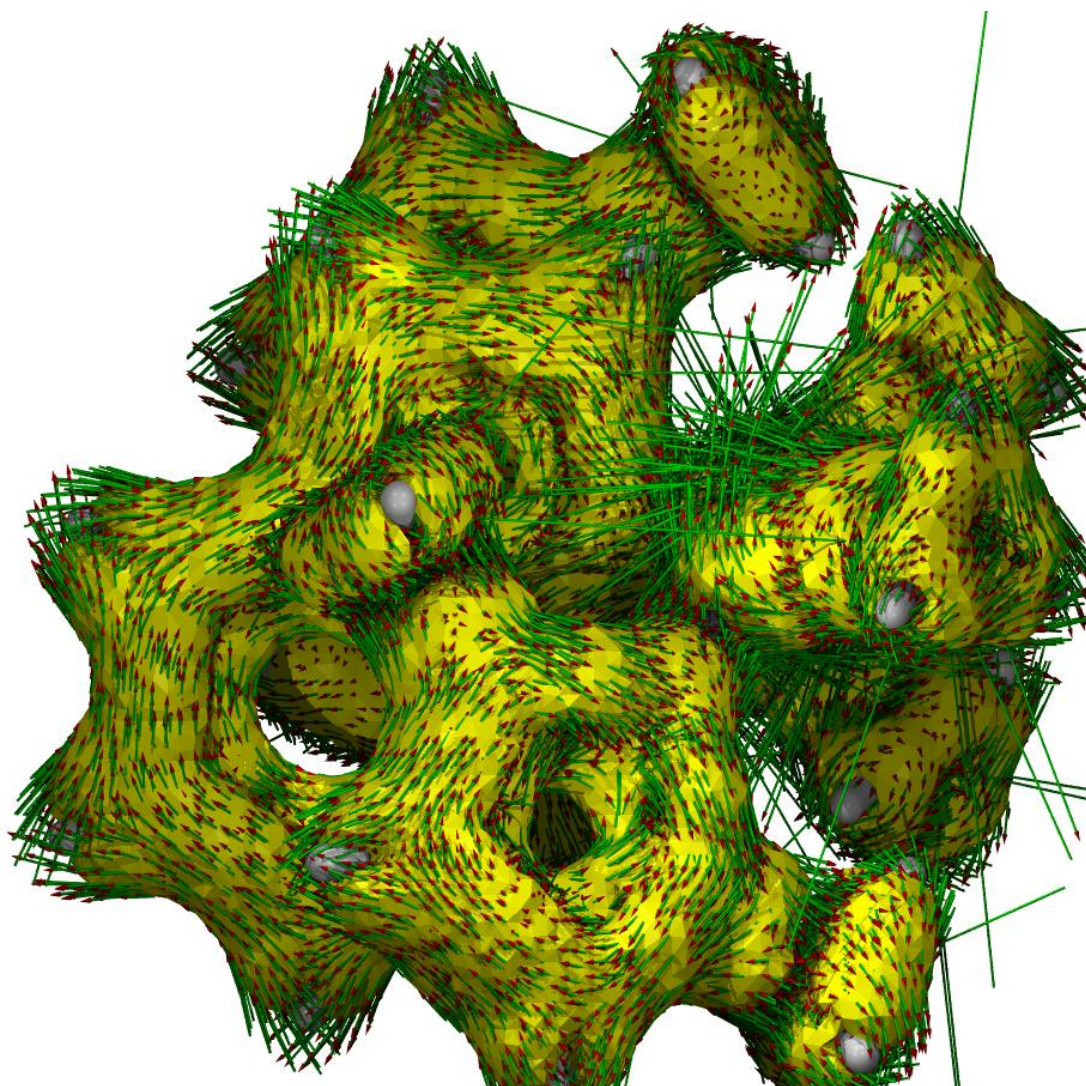


Fig. S24 The ACID graph of indolium **11-*cis***. The magnetic field vectors are perpendicular to the ring and point forward. The iso-surface value of the current is 0.003 a.u..

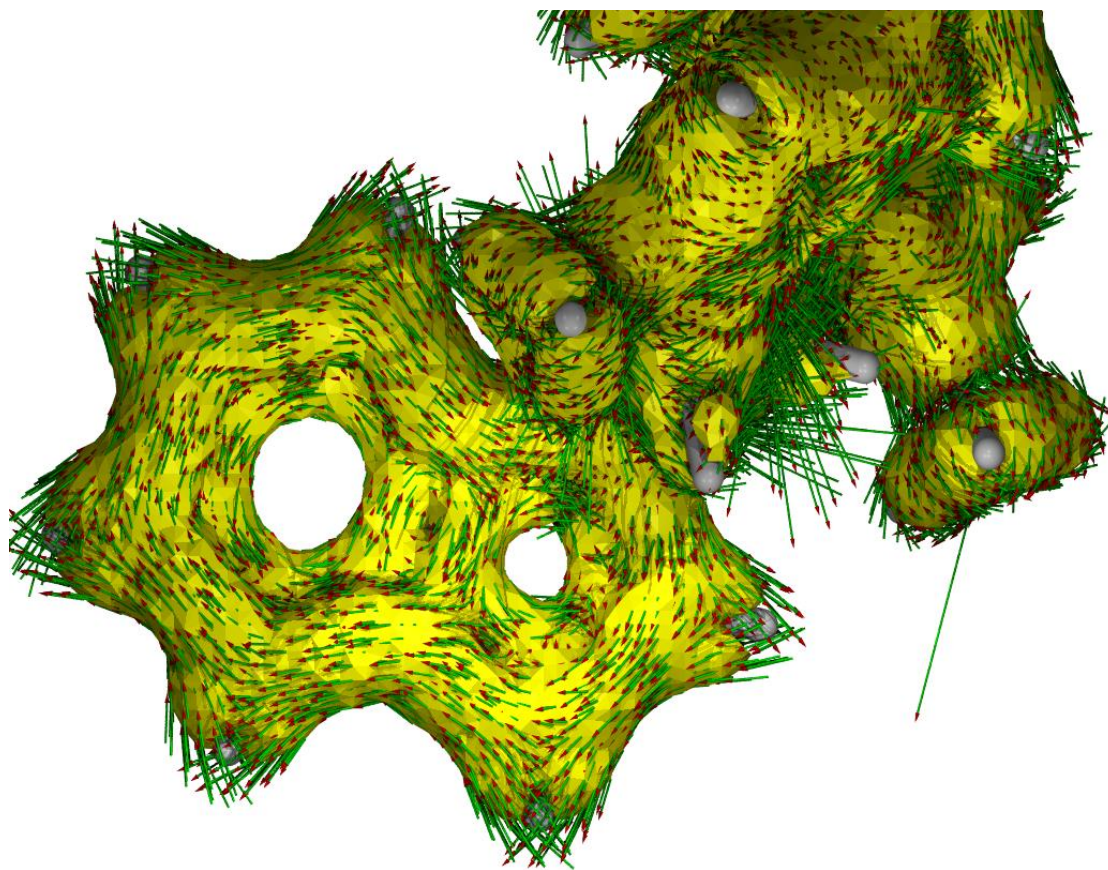


Fig. S25 The ACID graph of indolium **12-trans**. The magnetic field vectors are perpendicular to the ring and point forward. The iso-surface value of the current is 0.003 a.u..

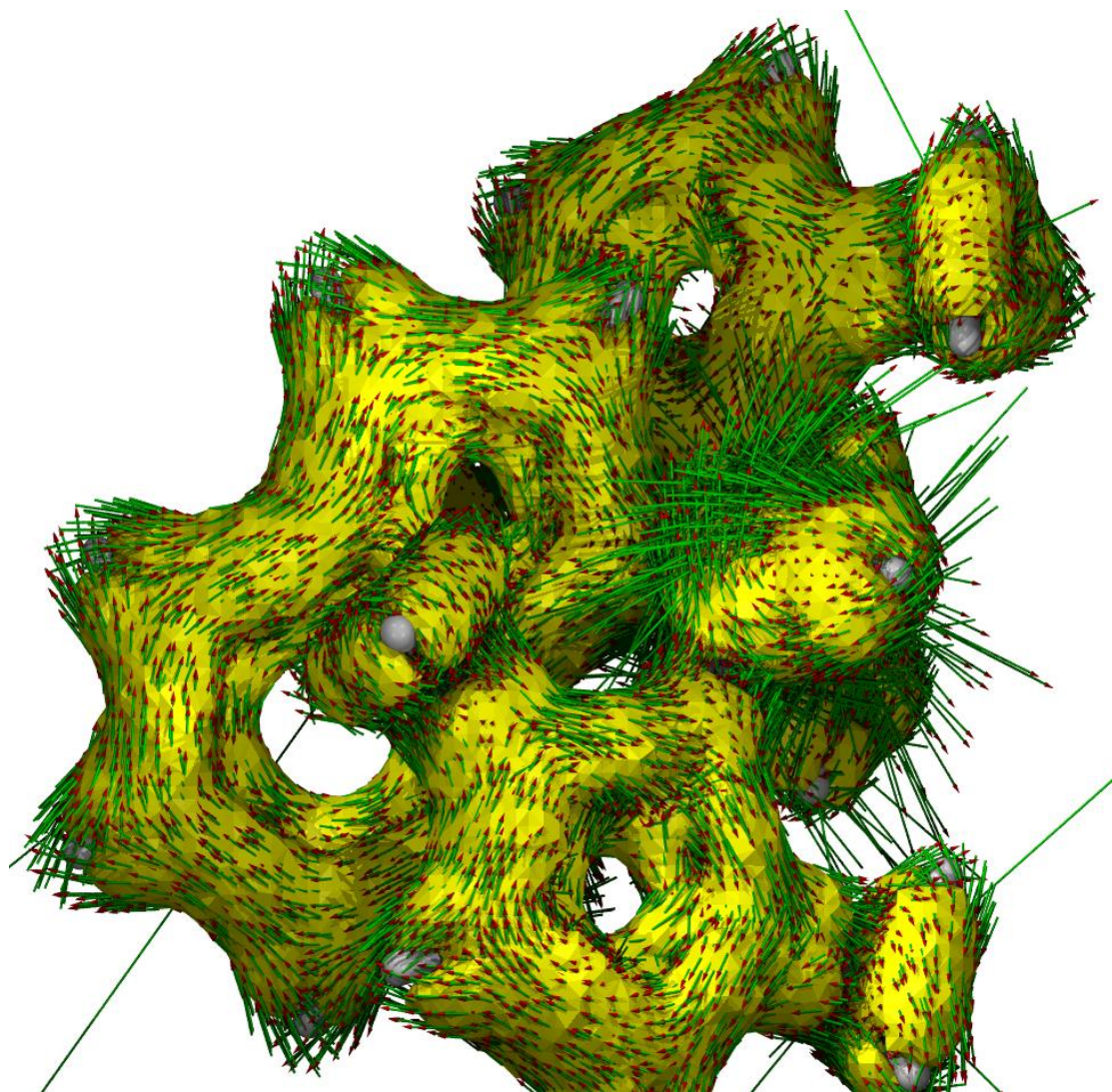


Fig. S26 The ACID graph of indolium **12-cis**. The magnetic field vectors are perpendicular to the ring and point forward. The iso-surface value of the current is 0.003 a.u..

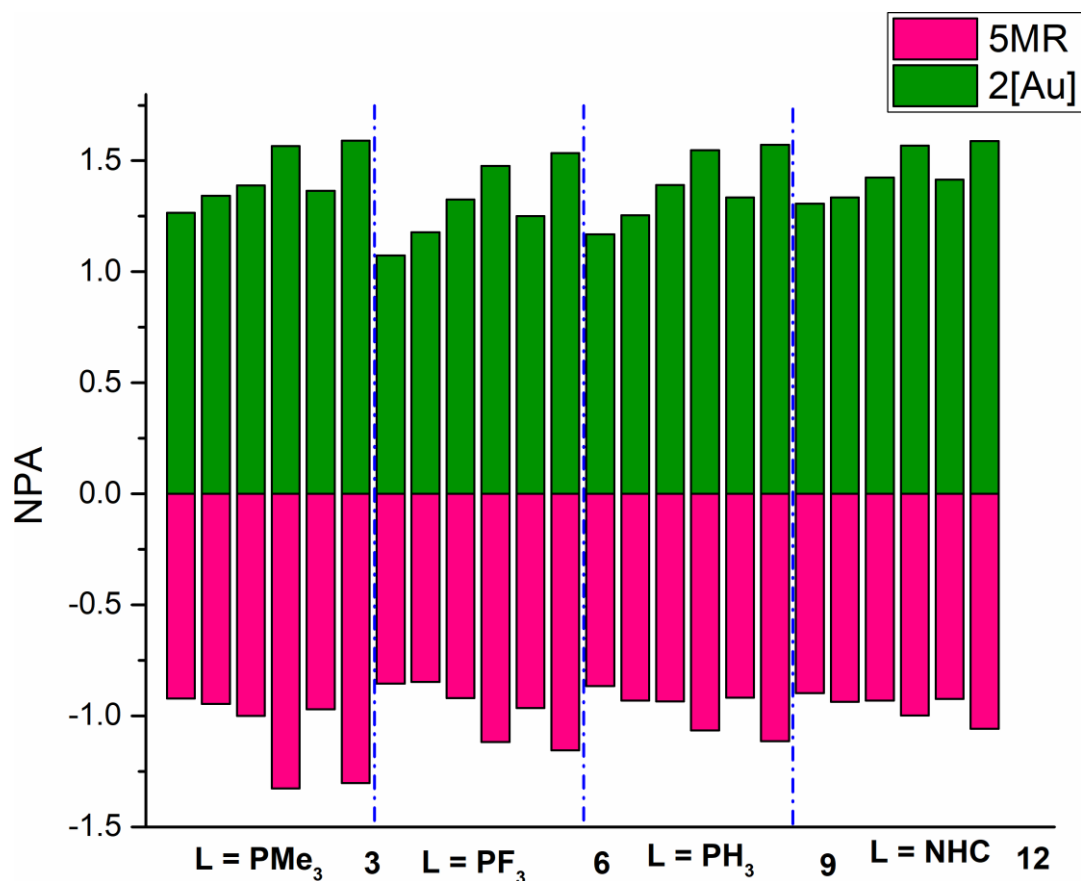


Fig. S27 The comparison of NPA analysis for Au(III)-substituents and the 5MRs' skeleton without H among indoliums **1-12**.

Table S1 The NPA charge of Au(III)-substituents and the 5MRs' skeleton without H in indoliums **1-12**.

	2[Au]	5MR		2[Au]	5MR
1-trans	1.265	-0.921	7-trans	1.166	-0.862
1-cis	1.342	-0.947	7-cis	1.255	-0.931
2-trans	1.409	-1.014	8-trans	1.391	-0.934
2-cis	1.566	-1.327	8-cis	1.547	-1.066
3-trans	1.406	-0.978	9-trans	1.334	-0.918
3-cis	1.59	-1.303	9-cis	1.572	-1.114
4-trans	1.073	-0.854	10-trans	1.306	-0.9
4-cis	1.178	-0.847	10-cis	1.244	-0.872
5-trans	1.326	-0.92	11-trans	1.425	-0.931
5-cis	1.496	-1.141	11-cis	1.568	-0.999
6-trans	1.289	-0.845	12-trans	1.409	-0.922
6-cis	1.535	-1.155	12-cis	1.591	-1.056

Cartesian coordinates

Indole

SCF = -363.888824 a.u.

0 1

C 0.49757600 0.62338900 0.00000000
C 0.00000000 -0.71798600 0.00000000
C -1.37147400 -1.01591600 0.00000000
C -2.26079000 0.06052800 0.00000000
C -1.79454300 1.39722300 0.00000000
C -0.43015300 1.68734200 0.00000000
C 1.93383100 0.53868500 0.00000000
C 2.26278500 -0.79863200 0.00000000
H -1.72931400 -2.04516500 0.00000000
H -3.33278400 -0.13241200 0.00000000
H -2.51821000 2.21147500 0.00000000
H -0.08206200 2.71986900 0.00000000
H 2.63492500 1.36510200 0.00000000
N 1.10113000 -1.55881800 0.00000000
H 1.06485800 -2.57053300 0.00000000
H 3.23128000 -1.28441400 0.00000000

1H-indolium

SCF = -364.225560 a.u.

1 1

C -0.18912000 0.76351700 0.00000600
C -0.18341100 -0.63980500 -0.00004200
C 0.95272800 -1.43096200 -0.00003400
C 2.17614100 -0.73185600 -0.00003900
C 2.21346300 0.67326900 0.00001800
C 1.03764300 1.44047000 0.00007600
C -1.57970600 1.22175900 -0.00008700
C -2.41962900 0.17163700 0.00000600
H 0.92157200 -2.51831900 -0.00007000
H 3.10546200 -1.29629500 -0.00007300
H 3.17717600 1.17723700 0.00001600
H 1.07741000 2.52699300 0.00010300
H -1.89876600 2.25892300 -0.00016300
H -3.49775000 0.07653600 -0.00010300
H -1.82623300 -1.67592000 -0.83040600
H -1.82603900 -1.67561400 0.83080700
N -1.61163900 -1.09738800 0.00006700

A

SCF = -2707.628613 a.u.

1 1

Au 1.49708400 1.03337100 -0.49323100
Au -1.39071500 0.98355900 -0.42120500
N 0.02494700 2.50876700 -0.88354500
C -0.03535300 3.04829100 -2.20839000
C -0.08624500 4.41290100 -2.17900800
C -0.05914800 4.82455600 -0.79262600
C -0.08671800 6.07395700 -0.14046000
H -0.13977700 6.99700400 -0.71535200
C -0.04386700 6.10375500 1.25522600
H -0.06365300 7.06146700 1.77236100
C 0.02558900 4.91287900 2.01420000
H 0.06000800 4.97039300 3.10069400
C 0.05327700 3.66253500 1.38847400
H 0.10935400 2.73536100 1.96041500
C 0.01047900 3.64275900 -0.01118000
P 2.89619200 -0.66363500 0.03617200
C 4.47241000 -0.15688400 0.79946100
C 5.04616800 1.07142300 0.41407900
H 4.52681200 1.71431600 -0.29671300
C 6.27716100 1.46473900 0.95148300
H 6.71753700 2.41488400 0.65489400
C 6.93412300 0.63991600 1.87629100
H 7.88847400 0.95027100 2.29806700
C 6.36132800 -0.57944800 2.26709000
H 6.86877400 -1.21487000 2.99076300
C 5.13111100 -0.98216400 1.73287000
H 4.68117500 -1.92361100 2.04510200
C 3.29273400 -1.72531500 -1.39912500
C 2.24368200 -2.05538800 -2.28229500
H 1.24723100 -1.64360500 -2.12202800
C 2.48180900 -2.91960400 -3.35583900
H 1.66777600 -3.17675900 -4.03154500
C 3.76697300 -3.44521200 -3.56157800
H 3.95335100 -4.11113600 -4.40236600
C 4.81314900 -3.10872000 -2.69131400
H 5.81113200 -3.51160400 -2.85466900
C 4.58099600 -2.25142100 -1.60646000
H 5.39433100 -1.99158500 -0.93084400
C 2.04350700 -1.77396100 1.22225600
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H 2.88075500 -3.61253600 0.43069700
C 1.49639300 -3.99493300 2.04929800

H 1.62373900 -5.07505100 1.99986200
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H 0.04687100 -4.07375100 3.65266600
C 0.45198700 -2.03940300 3.04617800
H -0.24374300 -1.60108900 3.75828000
C 1.16275700 -1.21181800 2.17055200
H 1.01855900 -0.13196400 2.20593800
P -2.84103800 -0.68269500 0.06712000
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C -4.80440400 0.54767900 -1.49826900
H -3.96788200 1.04550200 -1.98899800
C -6.11569000 0.78799800 -1.92536600
H -6.29800200 1.47222800 -2.75202900
C -7.18960400 0.15671800 -1.28154500
H -8.20920000 0.35051900 -1.60994800
C -6.95460100 -0.71721100 -0.20958300
H -7.78916900 -1.20165400 0.29414000
C -5.64606600 -0.96613100 0.22110300
H -5.46656700 -1.63887600 1.05822600
C -2.35586700 -2.23793000 -0.77002000
C -3.23789000 -2.94165600 -1.61005300
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C -2.80698400 -4.11917600 -2.23818200
H -3.49024700 -4.66130600 -2.88961700
C -1.50623900 -4.59683400 -2.02814300
H -1.17795000 -5.51230100 -2.51770100
C -0.62744400 -3.89704800 -1.18648100
H 0.38476700 -4.25979900 -1.01927400
C -1.04554400 -2.71746500 -0.56244800
H -0.36276100 -2.17496500 0.08997100
C -2.87268100 -1.07535000 1.85553900
C -2.75924500 -0.02361000 2.78700500
H -2.61997800 0.99979400 2.43748000
C -2.82740600 -0.29454600 4.15908200
H -2.74197900 0.52020000 4.87601400
C -3.00553800 -1.61318400 4.60722900
H -3.05933700 -1.82149400 5.67442000
C -3.11082000 -2.66207100 3.68199300
H -3.24623300 -3.68536100 4.02836900
C -3.04233100 -2.39832200 2.30741500
H -3.10992700 -3.21516600 1.59064700
H -0.03095000 2.36219300 -3.04738300
H -0.13544200 5.06489500 -3.04439400

B

SCF = -4548.496136 a.u.

1 1

Au 1.70354000 0.62995300 -0.20975300
Au -1.76140300 0.71032000 -0.21927500
N 0.00926200 1.97970900 -0.58868900
C -0.15239100 2.39293100 -1.95727500
C -0.09790900 3.74809000 -2.07375900
C 0.14000500 4.30017600 -0.75328000
C 0.31443500 5.60624400 -0.27358400
H 0.27511600 6.45719100 -0.95128100
C 0.54109800 5.79055000 1.09875600
H 0.67779200 6.79745600 1.48911500
C 0.58758700 4.69473000 1.97965800
H 0.75165400 4.86427000 3.04211300
C 0.41202600 3.38113300 1.51567900
H 0.42234700 2.53409700 2.19497900
C 0.19864800 3.20820000 0.14716400
H -0.26111600 1.62550800 -2.71219700
H -0.20558300 4.30899600 -2.99602800
P 3.54178100 -0.79718100 0.09316000
P -3.60681300 -0.72769600 0.05252800
Cl -0.79296100 -0.87951400 -1.66017900
Cl -2.73605600 2.34537300 1.07268000
Cl 0.67835600 -0.09093200 1.76444700
Cl 2.81963100 1.45321100 -2.06293600
C -4.64120800 -0.37481900 1.50406700
C -5.53228100 0.72047900 1.45655400
C -4.55191500 -1.16272500 2.66864600
C -6.33616300 1.00789300 2.56207300
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C -5.35614400 -0.85877900 3.77352800
H -3.87287100 -2.01139200 2.70973600
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C -4.19946800 -0.18906700 -2.64863800
C -6.04477600 -1.02260300 -1.27952900
C -5.04862800 -0.15797700 -3.76065000
H -3.16000900 0.11504000 -2.74917100
C -6.88160000 -0.99434500 -2.40061100

H -6.43549600 -1.34644200 -0.31660300
C -6.38613900 -0.56027400 -3.63891100
H -4.66479900 0.18400200 -4.71991600
H -7.92021400 -1.30503000 -2.30365800
H -7.04323300 -0.53176500 -4.50627100
C -2.99317800 -2.43415700 0.22777700
C -1.90173000 -2.68055500 1.08570800
C -3.60900900 -3.49451500 -0.46165800
C -1.44552900 -3.98979500 1.26524100
H -1.39815800 -1.85607100 1.58679600
C -3.13828200 -4.80127100 -0.27855000
H -4.43916500 -3.30323400 -1.13858500
C -2.06232800 -5.05051400 0.58450400
H -0.60541400 -4.17621600 1.93211400
H -3.61249300 -5.62212500 -0.81340600
H -1.70163500 -6.06857700 0.72130300
C 3.48738100 -1.76047100 1.63591400
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C 4.32121700 -1.45747000 2.72808100
C 2.52335800 -3.61366100 2.87414700
H 1.92330200 -3.06200800 0.87304400
C 4.25237200 -2.23820200 3.88912600
H 5.02773200 -0.63239600 2.66890700
C 3.35768800 -3.31386000 3.96318300
H 1.83254600 -4.45339500 2.93153600
H 4.90410900 -2.00876500 4.73001700
H 3.31158300 -3.92082500 4.86565800
C 3.63255300 -2.05074300 -1.22416400
C 2.85186000 -1.97829500 -2.39359400
C 4.51354800 -3.13904200 -1.02641100
C 2.96530000 -2.98280400 -3.36300400
H 2.16424000 -1.15159200 -2.54729100
C 4.63021400 -4.12579600 -2.01018200
H 5.09803600 -3.21305700 -0.11050700
C 3.85542700 -4.04892100 -3.17762800
H 2.35552300 -2.92796300 -4.26277100
H 5.31809000 -4.95599300 -1.86087100
H 3.94201200 -4.82337900 -3.93778300
C 5.03842500 0.23236900 0.12273300
C 5.03384200 1.39261900 0.92572100
C 6.17253900 -0.10190300 -0.63908500
C 6.17347100 2.20063400 0.97968000
H 4.14221300 1.66602500 1.49056500
C 7.30600400 0.71841100 -0.58126300

H 6.16616500 -0.98166200 -1.27915200
C 7.30886700 1.86374600 0.22667900
H 6.17039300 3.09707100 1.59680800
H 8.18292200 0.46456500 -1.17383400
H 8.19128600 2.49995800 0.26293600

A'

SCF = -1556.937930 a.u.

1 1

Au 1.58652100 -0.19912200 -0.20991200
Au -1.58910400 -0.19096600 -0.20709400
N 0.00150900 1.13105300 -0.64270400
C 0.00185400 1.62673700 -1.99383000
C 0.00751700 2.99122700 -2.01642200
C 0.01105500 3.45736700 -0.64695500
C 0.01718900 4.73358500 -0.04818700
H 0.02035000 5.63266800 -0.66187800
C 0.01911000 4.82002900 1.34569500
H 0.02389800 5.79849400 1.82248900
C 0.01488100 3.66037500 2.15416100
H 0.01635700 3.76175100 3.23783500
C 0.00875600 2.38436800 1.58148300
H 0.00528800 1.48137800 2.19264200
C 0.00712100 2.30816600 0.18299900
H -0.00201900 0.91067800 -2.80735200
H 0.00907300 3.61018400 -2.90712000
P 3.33406700 -1.54691000 0.28213200
P -3.34151800 -1.53302600 0.28197800
C -4.35510300 -0.90679400 1.68682400
H -4.73732000 0.09129400 1.44331500
H -5.19694500 -1.58406700 1.88129400
H -3.73103200 -0.83237100 2.58501600
C -2.88471000 -3.25296900 0.76121700
H -2.23631200 -3.22632200 1.64476800
H -3.78584200 -3.83755100 0.98842900
H -2.34025700 -3.72948000 -0.06232600
C -4.53360400 -1.73555900 -1.10758200
H -5.36675600 -2.38141900 -0.80125000
H -4.92173000 -0.75355500 -1.40189800
H -4.02244500 -2.18283100 -1.96805200
C 2.86973000 -3.13410200 1.09517900
H 3.76628900 -3.72464700 1.32467200
H 2.32696200 -2.92217300 2.02376600
H 2.21678000 -3.70893500 0.42809900

C 4.53822500 -0.76277300 1.43443500
H 5.36686800 -1.45098600 1.64638500
H 4.93131200 0.15483200 0.98166200
H 4.03157300 -0.50089300 2.37059900
C 4.33393600 -2.03999300 -1.18417700
H 4.71241800 -1.14120200 -1.68475200
H 5.17871400 -2.66929800 -0.87531400
H 3.70427300 -2.59496700 -1.88936000

1-trans

SCF = -3397.82081092

1 1

Au -1.68874200 -0.25509700 0.02444300
Au 1.81442800 -0.05581200 0.18770000
N -0.02813700 1.06829100 0.55067400
C 0.06045400 1.43274900 1.94313100
C -0.06964300 2.77750800 2.10738100
C -0.28666700 3.37171700 0.80066700
C -0.51056800 4.68515800 0.36428100
H -0.54302800 5.50961100 1.07394400
C -0.69149200 4.91182200 -1.00928200
H -0.86638100 5.92501500 -1.36592600
C -0.64307400 3.85303300 -1.93385900
H -0.77293400 4.05760300 -2.99457900
C -0.41637200 2.53201200 -1.51317600
H -0.35148200 1.71277200 -2.22412300
C -0.25175400 2.31843800 -0.14392200
H 0.18461300 0.64261300 2.67215700
H -0.02460300 3.30503900 3.05414200
P -3.54097600 -1.58364100 -0.48087300
P 3.69277400 -1.39408500 -0.13727300
C 5.04748600 -0.65449200 -1.12062100
H 5.41259600 0.25076800 -0.62500200
H 5.85754100 -1.39171400 -1.20444700
H 4.67977300 -0.38415400 -2.11536200
C 3.14950600 -2.90198900 -1.02601500
H 2.71115000 -2.61033000 -1.98755500
H 4.00832200 -3.56463900 -1.19537800
H 2.38770100 -3.41088600 -0.42618600
C 4.42711500 -1.90666100 1.46147800
H 5.24826800 -2.61140500 1.27514000
H 4.81495800 -1.02327000 1.98199000
H 3.65558700 -2.37979400 2.07732000
C -3.88414100 -2.72702000 0.90914100

H -4.76550200 -3.33757200 0.67226500
H -3.01620600 -3.37891900 1.06287500
H -4.06052300 -2.14206700 1.81744200
C -3.36048800 -2.62483300 -1.97723100
H -4.28544500 -3.20151100 -2.11332800
H -3.18189700 -1.99201700 -2.85249500
H -2.51058900 -3.30405300 -1.85616900
C -5.02560400 -0.54329300 -0.74581100
H -4.86104200 0.10828500 -1.61189100
H -5.89474000 -1.18804600 -0.93154700
H -5.19362200 0.07319700 0.14306500
Cl 0.92282300 -1.79759000 1.48856200
Cl 2.75677600 1.66296600 -1.01955500
Cl -0.51574700 -1.02040400 -1.84884600
Cl -2.92328300 0.50445300 1.82894800

1-cis

SCF = -3397.79355423

1 1

Au 1.57066700 -0.78567100 -0.44167900
Au -1.62167200 -0.37614900 0.54950200
N -0.05713000 0.69487700 -0.51947300
C -0.12167400 0.91687600 -1.94832600
C 0.02728400 2.23662600 -2.24977900
C 0.13635500 2.97124000 -1.00187000
C 0.26579400 4.33710500 -0.70077700
H 0.31549400 5.07907700 -1.49545100
C 0.32698900 4.72097100 0.64548600
H 0.42754800 5.77424500 0.89943600
C 0.24468400 3.76450100 1.67834000
H 0.27631800 4.08977400 2.71612400
C 0.11316300 2.39582300 1.39621600
H 0.03670400 1.65932900 2.19140200
C 0.07955400 2.01851900 0.04877100
H -0.21000900 0.05012100 -2.59004500
H 0.06209300 2.65621400 -3.24995600
P -3.36388800 0.22054400 -0.89613300
P 3.32067200 0.57392000 0.33922500
C -5.05002700 -0.18708600 -0.30557900
H -5.76274800 0.21710000 -1.03775100
H -5.16854400 -1.27157800 -0.22512500
H -5.22610700 0.26063100 0.67723700
C -3.39133700 2.03566600 -1.15942700

H -2.43650600 2.37832700 -1.56790100 H -0.17032800 3.22719100 -2.95953800
H -4.19982900 2.28526400 -1.85913000 P 3.65037200 -1.50967000 0.29029600
H -3.57322400 2.53179200 -0.19913600 P -3.80726000 -1.24890900 0.23887500
C -3.22555000 -0.60085500 -2.53056000 C -5.27061900 -0.34268800 0.88169200
H -2.34321300 -0.24273100 -3.06640400 H -5.58620800 0.42045000 0.16144200
H -3.13705300 -1.68269700 -2.38119000 H -6.09112900 -1.05513500 1.03917300
H -4.12677600 -0.37909700 -3.11743100 H -5.02252300 0.14390400 1.83084600
C 4.98434200 0.01998400 -0.20659500 C -3.45933900 -2.52461500 1.51733700
H 5.00448800 -0.08150700 -1.29707500 H -3.14648100 -2.03113500 2.44487600
H 5.71255700 0.77869700 0.11011400 H -4.35908000 -3.12438000 1.70652700
H 5.22842400 -0.94563300 0.24198900 H -2.64797100 -3.17446200 1.17303600
C 3.26294300 2.33393100 -0.19471000 C -4.44834800 -2.16129400 -1.22201400
H 4.26264100 2.76103800 -0.04107900 H -5.37001700 -2.69137500 -0.94949700
H 3.00452900 2.39788800 -1.25730200 H -4.66144100 -1.45333700 -2.03136100
H 2.53527700 2.89912700 0.39282700 H -3.69908300 -2.88055900 -1.56688700
C 3.33760200 0.55093100 2.16967400 C 4.23393200 -2.38446200 -1.21648100
H 2.39942400 0.96720800 2.55028900 H 5.16992600 -2.91594700 -1.00162500
H 3.42630500 -0.48832400 2.50589300 H 3.46975300 -3.10560500 -1.52980900
H 4.18855300 1.13913700 2.53747600 H 4.39337900 -1.66501800 -2.02532800
Cl -3.15814300 -1.49415000 1.84313200 C 3.53584500 -2.83089000 1.56213400
Cl 0.02631100 -0.93897700 2.16652400 H 4.50073000 -3.34949200 1.63502200
Cl -0.04383400 -2.27589000 -1.35174100 H 3.28146000 -2.39622600 2.53462000
Cl 3.08393100 -2.52134300 -0.41150800 H 2.75639900 -3.54856000 1.28326400

2-trans

SCF = -1716.52095493

1 1

Au 1.75632600 -0.30791000 -0.09246100 H -2.20526800 2.54360400 0.29544200
Au -1.90085600 -0.06828400 -0.16489200 H -3.72573700 1.77813900 0.80369000
N 0.01189700 0.92022400 -0.51384900 H -2.28923300 1.69928800 1.86268300
C -0.16518200 1.32540400 -1.88798800 C -1.15017400 -1.77482700 -1.26336400
C -0.05897200 2.67603800 -2.03180900 H -1.66380500 -1.87201600 -2.23062900
C 0.24215500 3.23640200 -0.72857100 H -0.07873000 -1.61558400 -1.45862200
C 0.48278900 4.54333500 -0.26463600 H -1.24300500 -2.72588500 -0.71967200
H 0.45888700 5.38910100 -0.94946100 C 2.78062800 0.66728500 -1.71373300
C 0.75025200 4.72985000 1.09496500 H 2.43543200 0.24620600 -2.66750800
H 0.93823600 5.73338600 1.47217300 H 2.50188400 1.72693600 -1.66742600
C 0.77665000 3.63981800 1.99142300 H 3.87638800 0.60123500 -1.68370800
H 0.98058600 3.81759100 3.04569100 C 0.72762300 -1.23447600 1.55274400
C 0.53811000 2.33328600 1.54806700 H -0.25073400 -0.74788100 1.68401100
H 0.54430600 1.49000200 2.23534900 H 0.55084000 -2.30033200 1.35182000
C 0.27935000 2.15337400 0.18504200 H 1.28074200 -1.14170700 2.49821500
H -0.33180900 0.55516300 -2.63131500

2-cis

SCF = -1716.55077198

1 1

Au 1.74720500 -1.00515200 -0.43928300
Au -1.75004800 -0.65149200 0.65856200
N -0.05514200 0.36034200 -0.44332700
C -0.16865800 0.59735300 -1.84682400
C -0.11319100 1.93125100 -2.15495900
C 0.00773700 2.65042700 -0.90699200
C 0.06942700 4.01816600 -0.57157800
H 0.04027800 4.78166700 -1.34733000
C 0.17048000 4.37369800 0.77647500
H 0.21989300 5.42505600 1.05367000
C 0.20303100 3.38886200 1.79069900
H 0.27277900 3.69547000 2.83279900
C 0.13712000 2.02526700 1.47832000
H 0.14460400 1.26988700 2.26120300
C 0.04837900 1.66768300 0.12397700
H -0.25564300 -0.25460300 -2.51180500
H -0.15262100 2.36140600 -3.15043800
P -3.46856800 0.28044100 -0.79650900
P 3.39567700 0.64523000 0.26610500
C -5.19022700 -0.21898300 -0.35625500
H -5.90177100 0.31708500 -0.99757700
H -5.32179500 -1.29731300 -0.50322000
H -5.40102200 0.02234600 0.69134700
C -3.52192200 2.11916000 -0.68969700
H -2.56644400 2.53339600 -1.02772700
H -4.33810200 2.51583600 -1.30751700
H -3.67830400 2.41436100 0.35472200
C -3.40465500 -0.08781800 -2.60448800
H -2.53101800 0.40055700 -3.04619700
H -3.33008600 -1.17065500 -2.76129000
H -4.31463400 0.28544800 -3.09228900
C 5.10159400 0.20067700 -0.28671900
H 5.13727700 0.17332500 -1.38254600
H 5.81332900 0.95302500 0.07667200
H 5.39314700 -0.78129100 0.09942300
C 3.25752800 2.39946900 -0.28807700
H 4.21919000 2.90357900 -0.12516700
H 3.00151100 2.43590300 -1.35268100
H 2.47877200 2.91628500 0.28021900
C 3.55065600 0.75347800 2.10098400
H 2.63242800 1.18517000 2.51429100

H 3.69094100 -0.25137400 2.51719700
H 4.40359900 1.38549500 2.38029900
C -3.20041600 -1.59840900 1.80810000
H -3.79527300 -0.82400700 2.30699700
H -3.83484000 -2.19640300 1.14538200
H -2.73464800 -2.24429400 2.55585100
C -0.41670300 -1.41677100 2.08273300
H -0.40204100 -2.51043000 2.01210100
H 0.59269800 -1.02926300 1.89207100
H -0.74325900 -1.11892300 3.08648100
C 0.49851400 -2.55721500 -1.09406900
H 0.45641800 -3.33617300 -0.32469200
H -0.51343700 -2.16551700 -1.26543700
H 0.89761100 -2.97933800 -2.02387000
C 3.24164900 -2.45499700 -0.47392600
H 3.92687900 -2.22615100 -1.29775800
H 3.77267800 -2.42496900 0.48508100
H 2.80280400 -3.44499300 -0.61817200

3-trans

SCF = -1559.22687138

1 1

Au 1.57127600 -0.34089900 -0.22181500
Au -1.70314400 -0.05024900 -0.12607700
N 0.02593400 1.10266300 -0.59633400
C -0.03387100 1.56712400 -1.96235200
C 0.17636700 2.90870400 -2.03209700
C 0.40369200 3.39727200 -0.68505500
C 0.66797900 4.67005900 -0.14620600
H 0.74797800 5.54066600 -0.79465600
C 0.82057100 4.79115000 1.23837500
H 1.02538100 5.76822500 1.67213700
C 0.70900000 3.66915100 2.08798800
H 0.82568500 3.79599800 3.16267700
C 0.44596200 2.39508600 1.57061900
H 0.34773400 1.52285000 2.21391900
C 0.30235700 2.28564900 0.18497900
H -0.21537100 0.83370000 -2.73749400
H 0.18696300 3.50203900 -2.94007900
P 3.28025200 -1.76580600 0.24805600
P -3.56912800 -1.27859100 0.28569600
C -4.57636900 -0.68128900 1.69798000
H -4.88749200 0.35088100 1.50173500

H -5.46023400 -1.31802500 1.83469900 H 0.37913400 1.14248800 2.17145300
H -3.96547900 -0.69337100 2.60770400 C 0.13743700 1.54041500 0.04871800
C -3.19103800 -3.04050700 0.64168100 H -0.53704900 -0.40518800 -2.50758400
H -2.54972600 -3.10505400 1.52832400 H -0.33538600 2.20116600 -3.20474600
H -4.12058000 -3.59580900 0.82280600 P -3.53100300 0.14585000 -0.36223400
H -2.66017100 -3.47165100 -0.21412500 P 3.40536900 0.17572400 0.21542000
C -4.68619200 -1.27913600 -1.17137500 C -5.09195400 -0.31283100 0.49895300
H -5.58546200 -1.87066200 -0.95562900 H -5.95349100 0.17246900 0.02265800
H -4.97617800 -0.24908800 -1.40898200 H -5.22056900 -1.40117500 0.46462800
H -4.15722200 -1.70616000 -2.03055800 H -5.03241400 -0.00180200 1.54860400
C 2.73635500 -3.33349400 1.03372900 C -3.50244200 1.98575500 -0.35128000
H 3.60304700 -3.97269100 1.24683800 H -2.63594700 2.33717600 -0.92203700
H 2.20618400 -3.09993900 1.96338600 H -4.42480000 2.38338800 -0.79425500
H 2.05213300 -3.86047800 0.35854900 H -3.40956700 2.34327500 0.68087300
C 4.44206200 -0.97264400 1.42822700 C -3.81540900 -0.32431700 -2.12069500
H 5.27022600 -1.65651300 1.65522500 H -2.99781000 0.06626000 -2.73607300
H 4.83742300 -0.05183000 0.98450300 H -3.84489400 -1.41639100 -2.21310000
H 3.90648000 -0.72128100 2.35056400 H -4.76696700 0.09559200 -2.47195000
C 4.28098200 -2.25058600 -1.21165000 C 4.97397800 -0.63057700 -0.32035800
H 4.70254100 -1.34842600 -1.66841700 H 4.95134200 -0.79306100 -1.40450700
H 5.08849800 -2.93106200 -0.91144600 H 5.83601500 -0.00135700 -0.06380900
H 3.63597600 -2.74609400 -1.94636100 H 5.07147300 -1.60344700 0.17545500
H -1.28884400 -1.13849200 -1.31113900 C 3.48748500 1.85976700 -0.52719400
H -2.14383000 1.01511600 1.03327300 H 4.48398500 2.28591600 -0.35130400
H 0.83122200 -0.79316200 1.19577300 H 3.30299600 1.79850900 -1.60578700
H 2.32513100 0.08905100 -1.61079900 H 2.72943800 2.50659200 -0.07404000
C 3.62873700 0.44129200 2.02426200
H 2.81013100 1.06253800 2.40242900
H 3.61964500 -0.52351700 2.54464900
H 4.58441900 0.94758700 2.21267700
H -2.55217200 -1.58234100 1.71084000
H -0.46717400 -1.47088800 1.64394000
H 2.56290400 -2.42795100 -0.44860700
H 0.52026600 -2.35904500 -0.91371900

3-cis

SCF = -1559.25338030

1 1

Au 1.55288600 -1.23024000 -0.41725000
Au -1.61106300 -0.80156700 0.72959100
N -0.09413400 0.23943300 -0.48780100
C -0.33611100 0.45594400 -1.88005400
C -0.22456100 1.77957500 -2.21121800
C 0.07389000 2.50476500 -0.99446700
C 0.28741200 3.86468500 -0.69035000
H 0.25020500 4.62130000 -1.47223000
C 0.54706100 4.22209200 0.63644000
H 0.71408400 5.26778700 0.88754800
C 0.58356400 3.25155800 1.66455500
H 0.76928900 3.56439500 2.69038800
C 0.37297000 1.89568200 1.38426500

4-trans

SCF = -3757.41144522

1 1

Au -1.69990200 -0.22950000 0.00304500
Au 1.75495900 -0.17855100 0.21346600
N -0.02122100 0.99740500 0.55887000
C 0.04570600 1.33961900 1.96264900
C -0.01648300 2.68905600 2.12975600

C -0.15713800 3.30865700 0.82375500
C -0.28835100 4.63701100 0.40336300
H -0.29620900 5.45176000 1.12419400
C -0.40869700 4.89348600 -0.97613100
H -0.51045700 5.92015500 -1.32081500
C -0.39303800 3.84915700 -1.91341700
H -0.47649200 4.07312800 -2.97425600
C -0.26002600 2.50745500 -1.50613100
H -0.22534200 1.69781800 -2.22970300
C -0.15543400 2.27099300 -0.13631300
H 0.10842200 0.53646000 2.68479200
H 0.03356100 3.20400800 3.08330700
P -3.57580000 -1.42810100 -0.49153900
P 3.69364000 -1.31908000 -0.12739600
Cl 0.76939300 -1.87924900 1.47280900
Cl 2.83240600 1.47783500 -1.00283500
Cl -0.52956400 -1.00884900 -1.86250300
Cl -2.97795300 0.54557100 1.77842900
F -4.84487900 -0.56404400 -0.79201200
F -3.50640900 -2.37115200 -1.73833300
F -4.04123900 -2.40053800 0.64112000
F 4.02439300 -1.58611500 -1.63233300
F 3.78517400 -2.75046300 0.49753900
F 4.98250900 -0.62705200 0.42564400

4-cis

SCF = -3757.39479935

1 1

Au -1.58613700 -0.86259300 0.39987600
Au 1.66223800 -0.27559600 -0.52106400
N 0.00032000 0.63126100 0.51778200
C 0.15593200 0.84803200 1.94406300
C -0.03092600 2.15780100 2.25569800
C -0.29150400 2.89010200 1.02799900
C -0.55540300 4.23898100 0.75766000
H -0.59003900 4.97123700 1.56153700
C -0.77421400 4.62241200 -0.57659400
H -0.98021300 5.66556900 -0.80612300
C -0.72463800 3.68225500 -1.62090700
H -0.88695000 4.00566800 -2.64651200
C -0.46205500 2.32445500 -1.36857900
H -0.41792700 1.60032100 -2.17723300
C -0.26079900 1.95544000 -0.03566400

H 0.36525800 -0.00997900 2.57027800
H 0.00448500 2.57536000 3.25654400
P 3.38436000 0.27133100 0.86475700
P -3.24225500 0.54785200 -0.29795700
F 4.50537800 1.14334600 0.21068400
F 3.06392100 1.11080400 2.15682300
F 4.14664600 -0.95238000 1.46782500
F -4.71642900 0.12792000 -0.00380600
F -3.21315500 1.99510200 0.31689300
F -3.26277800 0.82044200 -1.84201500
Cl 3.45203600 -1.19317700 -1.67946700
Cl 0.17921100 -0.96294700 -2.16819900
Cl -3.17343500 -2.54033200 0.31021100
Cl -0.02787600 -2.36953500 1.22152400

5-trans

SCF = -2076.15367674

1 1

Au 1.76831400 -0.29099300 -0.05255300
Au -1.84546900 -0.20339500 -0.16542900
N 0.00405500 0.83176400 -0.50499100
C -0.18119000 1.19714300 -1.90139900
C -0.14362800 2.54649700 -2.06566300
C 0.11585600 3.15321500 -0.77291200
C 0.28465500 4.48320700 -0.34838200
H 0.22259400 5.30510200 -1.05860900
C 0.53317800 4.72193500 1.00743100
H 0.66754200 5.74374900 1.35600200
C 0.60935400 3.66213100 1.93495000
H 0.79876400 3.87927500 2.98396400
C 0.44133000 2.33091500 1.53074600
H 0.48988700 1.51480300 2.24801500
C 0.20381100 2.10245600 0.17178700
H -0.29603100 0.40367400 -2.62943900
H -0.27748400 3.07094600 -3.00581600
P 3.65983400 -1.36007800 0.28212600
P -3.77994100 -1.16842000 0.22741100
F 4.90661200 -0.46015700 0.60955100
F 3.73454700 -2.41770800 1.44430200
F 4.16247300 -2.21629000 -0.93659700
F -4.17754600 -1.26195300 1.74572600
F -3.98246600 -2.66036600 -0.22952600
F -5.03813300 -0.47874000 -0.41541700

C	-2.70014100	1.52715900	0.82996500	F	-1.82601400	-1.55514900	-2.77574000
H	-2.24096000	1.60023200	1.82171800	F	0.45443300	-0.72818900	-2.58765100
H	-2.40435800	2.38262800	0.21179500	C	3.53021700	1.32563500	-1.02634700
H	-3.79108200	1.52713500	0.93260600	H	3.99895100	2.16215500	-0.49818900
C	-1.04147500	-1.92105000	-1.19731100	H	4.13213400	0.42002400	-0.90776500
H	-0.02150800	-1.69225600	-1.53776300	H	3.40301900	1.56319300	-2.08602300
H	-1.00225200	-2.78613100	-0.52527700	C	1.18469800	2.87598600	-1.05773300
H	-1.65759200	-2.17379300	-2.06925500	H	0.60081000	2.67318700	-1.96105200
C	0.79291000	-1.21434800	1.63619600	H	0.57635600	3.40305100	-0.31436300
H	-0.16854100	-0.71269600	1.81533000	H	2.09397100	3.43258100	-1.29353900
H	0.60681500	-2.27316100	1.41909000	C	-2.15718100	-0.99144400	2.34459400
H	1.40189600	-1.13818700	2.54557100	H	-3.01782800	-1.65691700	2.44157000
C	2.79657900	0.65523100	-1.71808900	H	-1.39292400	-1.23459500	3.09055700
H	3.89074000	0.64152000	-1.65928700	H	-2.45460700	0.05991900	2.41497300
H	2.47848100	0.16317000	-2.64399300	C	-2.11807600	-3.13396800	0.51673600
H	2.45473300	1.69572900	-1.69844100	H	-3.19285500	-3.03341600	0.33181700
				H	-1.65362800	-3.76938800	-0.24324800
				H	-1.93785900	-3.55260300	1.51043100

5-cis

SCF = -2076.19808285

1 1

Au	-1.28898400	-1.20113700	0.46782800
Au	1.62602300	1.03845500	-0.19297600
N	-0.45835800	0.86843400	0.62257300
C	-0.27289700	1.36702400	1.96008700
C	-1.04649000	2.46449400	2.20287200
C	-1.81771700	2.72865300	1.00564600
C	-2.77393200	3.70474500	0.66435400
H	-3.07283500	4.46306100	1.38537500
C	-3.32449400	3.68045800	-0.61938700
H	-4.06550000	4.42550600	-0.90147000
C	-2.93099000	2.70786900	-1.56424900
H	-3.36889900	2.71770900	-2.56015300
C	-1.98225200	1.73108500	-1.24159100
H	-1.67360700	1.00020200	-1.98701700
C	-1.44217800	1.74760400	0.05046900
H	0.39254900	0.83380400	2.62908700
H	-1.07754300	3.02911500	3.12854500
P	2.26338500	-1.00270800	0.84977500
P	-0.59771700	-1.61030200	-1.77886500
F	3.80650000	-1.18270000	1.13382400
F	1.66479600	-1.36701700	2.27655200
F	1.95964900	-2.35497600	0.06214000
F	-0.03542300	-3.05835500	-2.07882100

6-trans

SCF = -1918.84591335

1 1

Au	1.65376300	-0.10022600	-0.18048100
Au	-1.56908100	-0.30523300	-0.22346800
N	-0.02464200	1.09422700	-0.60346800
C	0.02425400	1.58101000	-1.97601000
C	-0.15610100	2.92456500	-2.00781300
C	-0.34896500	3.39818900	-0.64726300
C	-0.57033600	4.66986400	-0.09159300
H	-0.64026700	5.54892000	-0.72874900
C	-0.69300900	4.77687600	1.29839000
H	-0.86511500	5.75308500	1.74676800
C	-0.59322100	3.64441900	2.13349700
H	-0.68687000	3.76085800	3.21093100
C	-0.37234200	2.36847100	1.59832200
H	-0.28588900	1.48956000	2.23444500
C	-0.25982200	2.27923800	0.21026800
H	0.17460600	0.85486900	-2.76420700
H	-0.16751700	3.53494000	-2.90440600
P	3.45003200	-1.29497400	0.30576600
P	-3.17485100	-1.75066700	0.26629200
H	-2.33537900	0.17562500	-1.58509700
H	-0.78938800	-0.78846500	1.16555200

H 2.16964300 0.92866100 0.99094800
H 1.14815400 -1.12289200 -1.37806000
F 4.80930700 -0.55402800 0.06231900
F 3.55610600 -1.75088400 1.80287300
F 3.67720000 -2.64630300 -0.45737500
F -2.69285900 -3.22079700 0.52603100
F -4.31856400 -1.97006100 -0.78223400
F -3.98117100 -1.40622100 1.56621200

6-cis

SCF = -1918.88451014

1 1

Au 1.68746100 -1.27849500 -0.29080700
Au -1.74489800 -0.86394600 0.69382400
N -0.05342800 0.02868400 -0.38111700
C -0.37843100 0.30106000 -1.76074900
C -0.37224700 1.64406100 -2.01319500
C -0.03610100 2.32736900 -0.78133000
C 0.14534500 3.67907800 -0.43174000
H 0.01046700 4.46694500 -1.17000000
C 0.51111100 3.98461200 0.88242300
H 0.65855600 5.02379600 1.16874700
C 0.69227600 2.97334500 1.85229400
H 0.97175500 3.24693800 2.86738000
C 0.51256700 1.62259300 1.52964400
H 0.63885300 0.83698500 2.27468200
C 0.15351100 1.32632600 0.20596600
H -0.57221600 -0.53627700 -2.42214200
H -0.58599600 2.10927600 -2.96961500
P -3.38251400 0.35929600 -0.50291100
P 3.29677400 0.43420000 -0.00584700
F -4.83573600 0.21235700 0.08527200
F -3.24575600 1.92646300 -0.58931300
F -3.61706200 -0.04487200 -2.00902100
F 4.71923100 0.02924000 -0.54816500
F 3.09492000 1.82988700 -0.70792000
F 3.63331600 0.84262100 1.47852100
H -2.83591100 -1.57634500 1.57775400
H -0.82366800 -1.77830700 1.60423900
H 2.81979900 -2.37367200 -0.25407200
H 0.80758900 -2.58166100 -0.50033900

7-trans

SCF = -3161.771462 a.u.

1 1

Au -1.71723800 -0.45057600 -0.11164100
Au 1.75160300 -0.44805100 0.17763300
N -0.03150800 0.72242400 0.54623600
C 0.02625600 0.99200300 1.96624700
C 0.00180000 2.33090300 2.20441400
C -0.10406900 3.02039300 0.92980400
C -0.18510700 4.37191300 0.57245800
H -0.17580700 5.15085000 1.33201600
C -0.27689300 4.69822900 -0.79230200
H -0.33956300 5.74329100 -1.08830400
C -0.28246300 3.69980400 -1.78053500
H -0.34292700 3.97921800 -2.82995600
C -0.19944200 2.33816500 -1.43776800
H -0.17911500 1.56217500 -2.19824400
C -0.12183900 2.03093000 -0.08000100
H 0.05194200 0.15070500 2.64612900
H 0.05045600 2.79523500 3.18356500
P -3.49845100 -1.68821500 -0.90643200
P 3.70903500 -1.62105700 -0.16621000
Cl 0.75553000 -2.23296300 1.30196100
Cl 2.89057800 1.24269400 -0.92319900
Cl -0.57817700 -1.18101700 -2.02836600
Cl -2.99033400 0.23111000 1.68768700
H 4.03646800 -1.76873000 -1.52016600
H 4.83921300 -1.01389700 0.39632900
H 3.71621500 -2.92758200 0.34481200
H -3.90338500 -1.31801000 -2.19635600
H -3.20779500 -3.05435500 -1.02423200
H -4.66732800 -1.63631700 -0.13432300

7-cis

SCF = -3161.754420 a.u.

1 1

Au -1.68549300 -0.54530900 0.21486200
Au 1.68395100 -0.38972100 -0.21803100
N 0.03081800 0.73559900 0.56424700
C 0.00910700 0.94311900 2.00138000
C -0.05169300 2.26765600 2.30125100
C -0.03974600 3.01851000 1.05650700
C -0.06909300 4.39146100 0.76609100
H -0.12127400 5.12722100 1.56605500
C -0.02303200 4.79121900 -0.57749700

H -0.04221600 5.85103600 -0.82236900
C 0.06012700 3.84318200 -1.61470100
H 0.11077900 4.17827100 -2.64838900
C 0.09114300 2.46428200 -1.34268200
H 0.16986200 1.73195000 -2.14223600
C 0.02647500 2.07819600 -0.00062400
H -0.00367500 0.06758300 2.63868700
H -0.11543000 2.68384800 3.30148300
P 3.18552800 -0.01855600 1.49219500
H 4.40002700 0.52857200 1.06099800
H 2.75949400 0.84281900 2.51966000
H 3.54775200 -1.19645300 2.15753800
P -3.05970700 0.91664600 -0.92418600
H -4.30136600 1.12004100 -0.30909300
H -2.55966200 2.21143900 -1.15429700
H -3.37992700 0.44405900 -2.20274900
Cl 3.51195100 -1.54026600 -1.04398100
Cl 0.39140000 -0.89430800 -2.09913200
Cl -3.54638900 -1.88809000 -0.06915200
Cl -0.50198000 -2.21435400 1.34619800

8-trans

SCF = -1480.491033 a.u.

1 1

Au -1.87623500 -0.39589100 0.06612800
Au 1.74286900 -0.61200600 -0.02370800
N 0.01160100 0.55169600 0.47733400
C -0.16106900 0.84556900 1.88732800
C -0.07042200 2.18056500 2.13131300
C 0.20965900 2.84826500 0.87361100
C 0.42683700 4.19223900 0.52004100
H 0.39594800 4.97671500 1.27366000
C 0.68220800 4.49551800 -0.82128000
H 0.85298800 5.52945700 -1.11447100
C 0.71941000 3.48477800 -1.80462500
H 0.91510400 3.75118100 -2.84132900
C 0.50384700 2.14129800 -1.47078000
H 0.52219000 1.36126600 -2.22854500
C 0.25720800 1.84717900 -0.12634000
H -0.31385100 0.01694600 2.56760600
H -0.18174400 2.65558900 3.10023600
P -3.89906700 -1.30629600 -0.32499900
P 3.63652500 -1.74239600 -0.48335000
H -4.08565000 -2.66254200 -0.00432400

H -4.33192800 -1.25068300 -1.65957500
H -4.96147400 -0.68929000 0.35515600
H 3.62259700 -2.63605800 -1.56866100
H 4.74489700 -0.93171800 -0.77710600
H 4.12477800 -2.54344200 0.56120300
C 0.77707400 -1.40938800 -1.77553400
H 1.39275900 -1.27235000 -2.67604500
H 0.58544000 -2.48234300 -1.63913400
H -0.18540000 -0.90301400 -1.93878300
C 2.78506700 0.17865600 1.69566000
H 2.40776300 -0.31483300 2.59977700
H 3.87767200 0.06321200 1.66559500
H 2.55089800 1.24925300 1.73302700
C -1.15832300 -2.20775600 0.98458000
H -1.80893800 -2.52128500 1.81306000
H -1.11642900 -3.01613700 0.24250400
H -0.14446900 -2.05210300 1.38205800
C -2.66294400 1.40022800 -0.83574900
H -2.38486800 2.23190100 -0.17671400
H -2.18329400 1.53330600 -1.81266700
H -3.75344800 1.41647700 -0.97319900

8-cis

SCF = -1480.538390 a.u.

1 1

Au -1.92328300 -0.72505600 0.15867900
Au 1.88672300 -0.66575500 -0.24543500
N 0.01888700 0.35769400 0.43182000
C 0.00662400 0.61758500 1.84079300
C 0.00503900 1.96078100 2.11654500
C 0.04287700 2.65930900 0.84989200
C 0.05123900 4.02079400 0.48159100
H 0.03516200 4.80168300 1.23993300
C 0.07757400 4.34559500 -0.87742500
H 0.08460700 5.39108400 -1.17938900
C 0.10067200 3.34075400 -1.87183000
H 0.13002900 3.62703200 -2.92141100
C 0.09269400 1.98342200 -1.52923200
H 0.11523000 1.20535700 -2.29111100
C 0.05801500 1.65947000 -0.16308200
H -0.01878200 -0.22615300 2.52255200
H -0.02291000 2.41026800 3.10382100
P 3.14827600 0.61951500 1.39704100
H 4.53403100 0.68532500 1.15508100

H 2.83019400 1.98422800 1.50832300
H 3.15304700 0.23535100 2.75035700
P -3.03877300 1.30992400 -0.56648900
H -4.44189700 1.30098500 -0.44525900
H -2.71478300 2.50518500 0.09945500
H -2.90315400 1.71547200 -1.90550600
C 3.62535700 -1.60013800 -0.90700900
H 4.23425600 -0.84095800 -1.41261400
H 4.15459800 -1.98940600 -0.02920800
H 3.39078700 -2.41565300 -1.59499500
C 0.92595000 -1.70514700 -1.76496900
H 0.95090400 -2.77640100 -1.53934800
H -0.11249000 -1.35585800 -1.81228600
H 1.43969800 -1.50962400 -2.71220900
C -3.70380500 -1.79261800 -0.02208100
H -4.40553800 -1.39180100 0.71905800
H -4.08965600 -1.63551400 -1.03638600
H -3.53762000 -2.85770600 0.15424500
C -1.09132400 -2.49712800 0.85834200
H -1.65396100 -2.83332000 1.73586000
H -1.13851400 -3.25573600 0.07037200
H -0.04520700 -2.30127300 1.12417700

9-trans

SCF = -1323.189722 a.u.

1 1

Au -1.42691700 -0.90337900 0.06016200
Au 1.75018800 -0.19978100 0.05229900
N -0.10078900 0.67925400 0.56171500
C -0.11242400 1.04196400 1.96793900
C -0.47814900 2.33905000 2.12607300
C -0.74497600 2.90161500 0.81347000
C -1.14994400 4.17368300 0.37229900
H -1.33754800 4.97395500 1.08537700
C -1.30205000 4.38550900 -1.00214100
H -1.61611300 5.36326000 -1.36198100
C -1.05247500 3.35613700 -1.93407400
H -1.17421300 3.55265900 -2.99723400
C -0.64725100 2.08284900 -1.51342900
H -0.44482600 1.28320700 -2.22309800
C -0.50670600 1.88501200 -0.13893700
H 0.14501300 0.27651100 2.68818700
H -0.56792200 2.85722200 3.07473500
P -2.92848200 -2.53353000 -0.41654300

P 3.76596300 -1.06581900 -0.50891100
H -3.01612700 -3.54621700 0.55108700
H -2.78381500 -3.26130500 -1.60786600
H -4.25188800 -2.07415300 -0.49855800
H 3.95663500 -1.27305500 -1.88392000
H 4.84618100 -0.23502000 -0.17440100
H 4.14899600 -2.29951800 0.04012300
H 1.41102300 -1.40938800 1.13078100
H 2.11534700 1.00088400 -1.00620800
H -0.60477700 -1.10614200 -1.36409300
H -2.25722500 -0.71271500 1.46518200

9-cis

SCF = -1323.230532 a.u.

1 1

Au 1.80148800 1.04113600 0.15010100
Au -1.78780400 0.86945500 -0.40151000
N -0.02556500 -0.14061400 0.44799700
C -0.15571800 -0.35582400 1.86194100
C -0.15905300 -1.69010200 2.16896800
C -0.04149800 -2.42453900 0.92582000
C 0.02206800 -3.79476000 0.59630300
H -0.02486600 -4.55580100 1.37307800
C 0.15154600 -4.15345800 -0.74843200
H 0.20207000 -5.20614900 -1.01925100
C 0.21410700 -3.17666500 -1.76880100
H 0.30586000 -3.49104700 -2.80647100
C 0.15240100 -1.81094100 -1.46570200
H 0.19326300 -1.04991100 -2.24489500
C 0.02807800 -1.45735000 -0.11302500
H -0.21541200 0.50971500 2.51304500
H -0.23162400 -2.11345300 3.16535800
H -0.93463200 1.87738600 -1.28067500
H 1.06306800 2.40747600 0.47953600
H -2.95595700 1.65621200 -1.09559300
H 3.01882800 2.01982300 -0.00641100
P -3.31645800 -0.57040900 0.79858100
H -4.52718800 -0.84833900 0.14211300
H -2.86216000 -1.86186500 1.11739100
H -3.78721900 -0.12138900 2.04445400
P 3.17934200 -0.88565600 -0.33366700
H 4.54524600 -0.75243400 -0.03027000
H 2.85414900 -2.08304800 0.32670200
H 3.23962600 -1.31673700 -1.66891100

10-trans

SCF = -3085.348084 a.u.

1 1

Au -1.72334800 -0.11369700 0.15682800
Au 1.78479600 -0.00154700 0.12348500
N -0.00956000 1.13749300 0.50047800
C 0.17463800 1.57608400 1.86840600
C 0.12061200 2.93120500 1.96036500
C -0.14359300 3.46417900 0.63575500
C -0.32658100 4.76325000 0.13781400
H -0.27445700 5.62535400 0.80008500
C -0.57882800 4.92412700 -1.23202000
H -0.72310000 5.92434200 -1.63618500
C -0.64171900 3.81473900 -2.09612200
H -0.82501400 3.96918600 -3.15761600
C -0.45627700 2.50894800 -1.61518900
H -0.47602400 1.64939300 -2.28026400
C -0.21767600 2.36245400 -0.24790800
H 0.29323800 0.81863100 2.63254400
H 0.23881800 3.50700800 2.87210500
C -5.41910200 -1.89535200 -0.77385300
C -4.76954700 -2.98357400 -0.26221100
H -6.41786200 -1.78419100 -1.17133500
H -5.09303300 -4.00511600 -0.12215300
C 5.60088400 -1.77330700 0.02362700
C 4.94883500 -2.60192600 -0.84555100
H 6.62324700 -1.77091400 0.37372300
H 5.29304700 -3.45898400 -1.40666700
C -3.35485400 -1.24527700 -0.18789000
C 3.47772800 -1.06621400 -0.13143100
N -4.52885100 -0.82959800 -0.71926900
N -3.49277600 -2.56305800 0.09152800
N 3.63659800 -2.15140100 -0.92643700
N 4.67666800 -0.82878400 0.45296000
C -2.45017700 -3.39375900 0.72058800
H -1.49416000 -3.19221300 0.22914700
H -2.38059800 -3.14824100 1.78517300
H -2.72468900 -4.44358500 0.59213400
C -4.80375300 0.55381700 -1.14956800
H -4.70927700 1.21963500 -0.28649200
H -4.08774100 0.83915700 -1.92653700
H -5.81993600 0.59268400 -1.54851800
C 2.57610100 -2.72787200 -1.77198500
H 1.67179500 -2.85080500 -1.16968200

H 2.37452200 -2.05678100 -2.61280300
H 2.92064700 -3.69816300 -2.13760300
C 4.93863000 0.26190300 1.40949500
H 4.59586600 1.20381500 0.97130800
H 4.40775800 0.06045500 2.34551100
H 6.01481200 0.30494200 1.59256700
Cl -0.74333000 -1.07229400 -1.74192000
Cl -2.85395300 0.78093900 1.96078100
Cl 2.74300500 1.62246400 -1.20716400
Cl 0.95493700 -1.70724900 1.49819400

10-cis

SCF = -3085.318810 a.u.

1 1

Au -0.84742400 1.30917400 -0.46311300
Au 1.30018800 -0.97721200 0.65553300
N -0.22043400 -0.73066200 -0.91651400
C 0.45119100 -0.81286300 -2.20110400
C -0.15068700 -1.70245300 -3.02534700
C -1.28539900 -2.26987500 -2.32397200
C -2.25225400 -3.20667000 -2.71354200
H -2.22561600 -3.64415100 -3.70951900
C -3.24535700 -3.56725900 -1.79267000
H -4.00367200 -4.29556400 -2.07280500
C -3.25842300 -3.00875900 -0.50363600
H -4.01719200 -3.31753700 0.21254100
C -2.29263900 -2.07174300 -0.10112600
H -2.30405700 -1.69278300 0.91192000
C -1.32009700 -1.69228300 -1.03020200
H 1.27871700 -0.14668400 -2.38398600
H 0.16329900 -1.93779000 -4.03671600
C 4.08438700 1.93523100 -0.67878200
C 4.44392900 0.88240600 -1.46959700
H 4.48529300 2.93552300 -0.59927000
H 5.23569400 0.77404600 -2.19716800
C 2.66361800 0.24943000 -0.24545600
N 3.00323000 1.52050700 0.08541300
N 3.56379700 -0.15434000 -1.18361100
C 2.32933700 2.36101500 1.08537400
H 1.99268500 1.71753500 1.90223700
H 3.05869600 3.07556600 1.47606700
H 1.49195400 2.89414200 0.62311700
C 3.72562600 -1.53826500 -1.66413100
H 4.22024400 -1.51058000 -2.63874500

H	4.33073500	-2.10219200	-0.94647700	H	6.51127300	-1.58769600	1.11472300
H	2.74134000	-2.00312200	-1.76926100	H	5.37942800	-3.83583000	-0.08587000
Cl	0.03720400	-2.52203800	1.84072900	C	-5.71653600	-1.62398700	0.01339800
Cl	2.90758900	-1.08452900	2.31016600	C	-5.15560300	-2.37354900	1.00502800
Cl	0.61853200	2.24819100	-2.02565600	H	-6.71581200	-1.61990100	-0.39819800
Cl	-1.47367000	3.44247500	0.17515600	H	-5.57285700	-3.14166700	1.64060200
C	-3.45575000	0.27065100	2.70936000	C	3.43227300	-1.20416800	0.05977800
C	-4.32893200	0.28702700	1.65806300	C	-3.55813900	-0.98619000	0.21283600
H	-3.61000500	0.07948700	3.76183000	N	4.57201500	-0.74271000	0.64285000
H	-5.39470100	0.11267100	1.61564000	N	3.68239600	-2.49981100	-0.27156900
C	-2.28426200	0.75786000	0.85681100	N	-3.82554800	-1.97342800	1.11080500
N	-2.19977900	0.58008300	2.19893000	N	-4.72252600	-0.77191700	-0.45890200
N	-3.59290900	0.60602100	0.52590700	C	2.74886900	-3.37626600	-0.99284300
C	-0.98464800	0.72306100	3.01895900	H	1.73582300	-2.98869400	-0.85791700
H	-1.23978500	1.28778200	3.92023800	H	2.99981300	-3.39074700	-2.05926000
H	-0.58882900	-0.26499400	3.27194700	H	2.81785500	-4.38609200	-0.57735000
H	-0.24990300	1.28612800	2.43965700	C	4.72248500	0.61005800	1.20099800
C	-4.12946000	0.74081800	-0.84012900	H	4.25720500	1.32679200	0.51818800
H	-5.21906700	0.68543300	-0.78559400	H	4.23678700	0.66512700	2.18129800
H	-3.82963700	1.71216400	-1.24515300	H	5.78907100	0.82914200	1.29828300
H	-3.74709800	-0.07503900	-1.46249700	C	-2.87394700	-2.47443000	2.11271300

11-trans

SCF = -1404.048406 a.u.

1 1

Au	1.75926700	-0.16337300	-0.22032900	H	-2.94738500	-1.87770100	3.02865700
Au	-1.83768900	-0.02934000	-0.08593100	H	-3.11034100	-3.52050100	2.32757600
N	-0.00722900	1.02752500	-0.49435100	C	-4.87598800	0.18622100	-1.56356500
C	-0.25664000	1.47972000	-1.84319300	H	-4.28609300	1.07848000	-1.33554600
C	-0.20384700	2.83661100	-1.93961400	H	-4.52458100	-0.26252900	-2.49912100
C	0.12760400	3.35913500	-0.62857500	H	-5.93283200	0.45284700	-1.64948100
C	0.33653500	4.65785000	-0.12747700	C	2.67404300	0.78188500	-1.91108300
H	0.25225100	5.52475200	-0.78059900	H	2.22382100	0.39829900	-2.83632600
C	0.65321600	4.80900300	1.22571800	H	2.48369100	1.86094400	-1.84410400
H	0.81708400	5.80569300	1.63156900	H	3.75710200	0.60599200	-1.95419900
C	0.76013800	3.68952200	2.07840600	C	-1.11497600	-1.72460700	-1.20638500
H	0.99994100	3.83731700	3.12997400	H	-0.22621500	-1.44961000	-1.79488200
C	0.55475000	2.39046300	1.59688300	H	-0.83151300	-2.53391100	-0.51843700
H	0.62456400	1.52653900	2.25379800	H	-1.87880200	-2.11239100	-1.89480600
C	0.24242300	2.24634900	0.24091900	C	0.95011600	-1.13179800	1.52704700
H	-0.42849100	0.73329300	-2.60901000	H	0.78365200	-2.20056800	1.32796400
H	-0.36646300	3.41701300	-2.84171100	H	1.64308200	-1.04880200	2.37664400
C	5.53434500	-1.74783300	0.68101700	H	-0.00977700	-0.67990800	1.81799600
C	4.97853900	-2.84958100	0.10032200	C	-2.63415000	1.63267300	1.00537400
				H	-2.13492100	1.69523700	1.98063100
				H	-2.41779600	2.55034900	0.44257600
				H	-3.71730000	1.55305700	1.16765100

11-cis

SCF = -1404.085599 a.u.

1 1

Au 1.77224400 -1.07647200 -0.65790200
Au -1.61785900 -0.82107100 0.86319400
N -0.08652400 0.15490500 -0.49133100
C -0.57254700 0.31447000 -1.82321200
C -0.75371600 1.62992100 -2.15813400
C -0.38009000 2.41523300 -1.00376400
C -0.32948900 3.79911000 -0.73364500
H -0.62926000 4.52365500 -1.48993900
C 0.11618200 4.22237500 0.52304300
H 0.16350300 5.28689800 0.74678400
C 0.50486000 3.28944800 1.51296800
H 0.84405800 3.64803700 2.48317900
C 0.46163000 1.91393300 1.26331400
H 0.75990300 1.19124100 2.02061000
C 0.02515600 1.48931200 -0.00046300
H -0.74708200 -0.57427600 -2.41787700
H -1.10867000 2.00648500 -3.11175600
C -4.72102100 0.74927500 -1.72276000
C -4.55987200 1.82115300 -0.89418700
H -5.37511800 0.59555800 -2.56979500
H -5.04791700 2.78561100 -0.87535500
C -3.13184300 0.20270700 -0.19566100
N -3.84622700 -0.23407400 -1.27365300
N -3.59134400 1.46464700 0.03758300
C -3.68481500 -1.54841600 -1.90583000
H -4.66726400 -2.01403800 -2.03523200
H -3.19540500 -1.43812400 -2.88020100
H -3.06845700 -2.17179000 -1.25286800
C -3.13746000 2.34080700 1.12744900
H -2.58505700 3.19048000 0.71460700
H -4.00681600 2.68634300 1.69673200
H -2.47338300 1.76536400 1.77541400
C 4.32736900 1.72808300 1.43014700
C 4.11192200 2.44483000 0.28983600
H 4.89988600 1.95645800 2.31832900
H 4.46334600 3.42059700 -0.01478600
C 2.98934700 0.48287200 0.07949700
N 3.64249300 0.52671500 1.27892900
N 3.29957300 1.66517900 -0.52399200
C 3.59076900 -0.52319900 2.30392600
H 4.59182700 -0.66468400 2.72319400

H 2.89268000 -0.23924800 3.10011100
H 3.25538500 -1.45129300 1.83581200
C 2.85364400 2.06627300 -1.86460600
H 2.38328200 3.05199500 -1.80593000
H 3.71143200 2.09092400 -2.54598200
H 2.11906500 1.33807200 -2.21739500
C 3.41239200 -2.32220900 -0.90322800
H 3.38274300 -2.74420200 -1.91305000
H 4.33864700 -1.75871100 -0.75412800
H 3.33597500 -3.13164400 -0.16722700
C 0.65644300 -2.67470100 -1.40152600
H 0.78028500 -2.73385900 -2.49167700
H 0.98660800 -3.62252600 -0.96016800
H -0.40658300 -2.52772200 -1.16209300
C -2.99843300 -1.70355200 2.13201900
H -2.91543600 -1.21281000 3.10854300
H -4.00563400 -1.57126200 1.72573200
H -2.75691100 -2.76679400 2.22843100
C -0.17088400 -1.81583300 1.98525100
H -0.50986700 -2.01406500 3.00923200
H 0.07390300 -2.76948000 1.49936200
H 0.73686400 -1.19826700 2.02601400

12-trans

SCF = -1246.750099 a.u.

1 1

Au 1.66046800 0.15510500 -0.16149500
Au -1.58119400 -0.21097600 -0.26009500
N -0.08906300 1.27493700 -0.56565100
C -0.04217400 1.80256900 -1.90993500
C -0.26282100 3.14381100 -1.91989400
C -0.48793500 3.56994500 -0.55151000
C -0.76309100 4.81511400 0.04396500
H -0.85054400 5.71342100 -0.56467200
C -0.91771600 4.87260000 1.43223900
H -1.13052800 5.82750800 1.90954800
C -0.80034200 3.71360300 2.22980100
H -0.92283800 3.78990800 3.30872300
C -0.52606500 2.46653100 1.65529800
H -0.42908000 1.56509500 2.25725900
C -0.37558600 2.42131100 0.26689900
H 0.13967300 1.10578100 -2.71801900
H -0.28254800 3.77677200 -2.80059800
C 5.30268900 -1.94799400 -0.05351000

C 4.95893700 -2.03456800 1.26421900 H 0.63354500 4.85759600 -1.27846800
H 6.16985000 -2.30887800 -0.58808300 C 1.57550100 4.18987500 0.55526800
H 5.45921200 -2.50044800 2.10123400 H 2.00484800 5.16475300 0.77966400
C -5.01420100 -2.55555100 0.38088900 C 1.79518600 3.11564200 1.44805200
C -4.07617500 -3.54575000 0.34466200 H 2.38684400 3.27762600 2.34718700
H -6.08397400 -2.59355000 0.52971200 C 1.25219300 1.84988200 1.20184200
H -4.16925700 -4.61854200 0.43696000 H 1.40328900 1.02292100 1.89289400
C 3.32385400 -0.89162500 0.20566400 C 0.50264000 1.67936900 0.03054800
C -3.00785400 -1.58002100 0.04184900 H -1.31232800 0.15030000 -2.23690000
N 4.28490800 -1.24839600 -0.69161900 H -0.90674500 2.75862400 -2.81712800
N 3.74381400 -1.37469900 1.40870100 C -5.04399900 0.01812800 -1.03234500
N -2.84623000 -2.92863400 0.14253000 C -4.84764500 1.29507000 -0.59168800
N -4.34241200 -1.35390000 0.18599000 H -5.84053400 -0.41804800 -1.61880600
C 2.99898100 -1.24495100 2.66949400 H -5.43393200 2.19292800 -0.72857200
H 2.58220900 -0.23504600 2.72522100 C -3.11100100 0.04454400 0.14864100
H 2.18850500 -1.98110800 2.70333600 N -3.96846500 -0.73301400 -0.57035500
H 3.69122300 -1.41295700 3.49868800 N -3.66179700 1.29029400 0.13372500
C 4.27333900 -0.88967800 -2.11812100 C -3.81024900 -2.18165000 -0.77284900
H 3.26098100 -1.03527200 -2.50618500 H -4.34821600 -2.72974200 0.00837500
H 4.56983700 0.15742700 -2.24083000 H -4.20861400 -2.44620100 -1.75665300
H 4.97628400 -1.54133200 -2.64362600 H -2.74565600 -2.42793400 -0.73187600
C -1.56472300 -3.63114400 -0.01043700 C -3.04439100 2.48790900 0.72334700
H -1.38362000 -3.85337200 -1.06774000 H -2.57207800 3.08312600 -0.06447800
H -0.77028800 -2.98399300 0.37303900 H -3.81444300 3.07130500 1.23700300
H -1.60528700 -4.55955600 0.56626600 H -2.28344200 2.17160700 1.44139300
C -4.97297200 -0.02435700 0.18927300 C 4.63942700 -0.16837100 1.25409600
H -4.89278500 0.42465800 1.18508500 C 4.69170600 0.76084000 0.25563100
H -4.46091800 0.60463900 -0.54471500 H 5.29113300 -0.34504600 2.09823800
H -6.02464200 -0.13971400 -0.08623100 H 5.39844700 1.55414600 0.05731800
H -0.79395100 -0.71863200 1.11422500 C 2.86784000 -0.52989800 -0.11248200
H -2.36824000 0.28307400 -1.61015900 N 3.52128500 -0.95643400 1.00685800
H 1.23446200 -0.89318400 -1.37917300 N 3.60489700 0.51834100 -0.57381300
H 2.09958900 1.19686000 1.02161100 C 3.06346800 -2.04898900 1.87783000

12-cis

SCF = -1246.786337 a.u.

11

Au 1.08236700 -1.31244600 -0.88475200 H 3.05731800 2.35919500 -1.42381700
Au -1.31788900 -0.53920500 1.06627800 H 4.11393300 1.32306800 -2.44956900
N -0.11658900 0.49339900 -0.46667900 H 2.38704600 0.91304600 -2.22857600
C -0.76110900 0.89545000 -1.67618600 H 1.79053600 -2.65816500 -1.25945100
C -0.54515800 2.21780700 -1.94886800 H -0.21258700 -2.03428200 -1.50403500
C 0.26124700 2.75211200 -0.87233100 H -2.06816900 -1.28573300 2.22210500
C 0.80563800 4.02355000 -0.59980300 H -0.01206300 -1.02926700 1.86176600