Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Spin-crossover in Ni-porphyrin: triggered by π-π interaction inducing trans-cis isomerization

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***trans*-sqp (M06-2X) xyz (in Ångstrom)**

E(M06-2X) = -5492.613511 a.u.
E([10,11]-CASSCF) = -5487.214787 a.u.
E([10,11]-CASPT2) = -5492.102181 a.u.

98

Ni	0.29928600	0.30009000	-0.05152000
N	2.10049600	0.75574600	0.65994000
N	0.49827400	-1.54815600	0.64730000
N	0.14282500	2.11347100	-0.85601200
N	-1.56323700	-0.10207600	-0.59977100
N	0.27861900	-1.37629100	-3.08047700
N	0.58233700	-2.55129300	-2.83394600
N	3.87167400	-1.89721200	-1.24603300
C	2.75489100	1.95010000	0.53420400
C	2.88696400	-0.00946500	1.47418800
C	3.97470400	1.94675100	1.30972900
C	4.04251900	0.73921600	1.91485000
C	1.56432600	-2.06932000	1.32278400
C	-0.37006200	-2.58897300	0.47027900
C	1.38700600	-3.48766600	1.53345600
C	0.18502900	-3.81162000	0.99968200
C	-0.89225000	2.59470500	-1.61360600
C	1.11678200	3.06744300	-0.91729100
C	-0.53956000	3.86404400	-2.20433100
C	0.70146500	4.16938400	-1.74981600
C	-2.44484000	0.74315500	-1.21411700
C	-2.22580800	-1.28844500	-0.47545700
C	-3.72260400	0.10133200	-1.39976100
C	-3.58380900	-1.16962700	-0.95193200
C	2.66553300	-1.34857100	1.79474700
C	2.34013900	3.02926600	-0.24149100
C	-2.12727300	1.97003300	-1.79986900
C	-1.66438800	-2.48915600	-0.03535100
C	-2.50780400	-3.71573700	-0.07211600
C	-2.22041600	-4.77740400	-0.93136700
C	-3.62055400	-3.84767800	0.76086700
C	-3.00860100	-5.92499000	-0.96966000
C	-4.42395500	-4.98468600	0.73927700
C	-4.11410100	-6.02725900	-0.12980600
C	3.62566200	-2.05249600	2.68863200
C	4.98067300	-2.20971200	2.38267600
C	3.18428400	-2.59698100	3.90047800
C	5.85257400	-2.89269200	3.22762700
C	4.03688500	-3.28573700	4.75781000

C	5.37901700	-3.43352200	4.41909900
C	3.24015200	4.21158100	-0.34685100
C	3.48008700	5.04098100	0.74987300
C	3.87288600	4.53322400	-1.54869700
C	4.32455800	6.14462300	0.66382800
C	4.71735100	5.63480600	-1.65996400
C	4.94347400	6.44130400	-0.54771700
C	-3.04872800	2.51652600	-2.84597600
C	-3.69454000	3.74164600	-2.65078700
C	-3.24780800	1.81048200	-4.06130800
C	-4.51874100	4.28739700	-3.63246900
C	-4.07816600	2.37752500	-5.03607800
C	-4.70438200	3.60479100	-4.83241900
C	-2.67958400	0.44486100	-4.26234200
C	-3.49631100	-0.59835200	-4.71352900
C	-1.38181600	0.12481400	-3.84515600
C	-3.05576200	-1.92650600	-4.67286900
C	-0.97791200	-1.20034800	-3.71724000
C	-1.81569200	-2.24562600	-4.13502100
C	1.82582000	-2.72679200	-2.18058700
C	2.18376700	-4.03554500	-1.86372400
C	2.70922700	-1.68397900	-1.84533100
C	3.41001400	-4.25820100	-1.24479500
C	4.21493700	-3.15684100	-0.96063700
H	4.68251000	2.76769200	1.37827000
H	4.81279800	0.37556900	2.58814800
H	2.10149400	-4.14582700	2.02037200
H	-0.29785300	-4.78460900	0.97848200
H	-1.17204600	4.44496900	-2.86849800
H	1.28895800	5.05824800	-1.96150300
H	-4.59228700	0.57224100	-1.85064000
H	-4.32328200	-1.96529000	-0.95580900
H	-3.54439300	4.26609700	-1.70491300
H	-5.01444300	5.24338000	-3.45851000
H	-4.22044500	1.84555500	-5.97878500
H	-5.33964500	4.02659100	-5.61251100
H	-4.51512200	-0.37934100	-5.04082900
H	-0.67661400	0.89146600	-3.52819500
H	-3.71821300	-2.72139400	-5.01927000
H	-1.48071400	-3.27569200	-4.01409100
H	1.49224600	-4.84255100	-2.11162100
H	2.44056800	-0.65085700	-2.08428400
H	3.74003200	-5.26457500	-0.98589000
H	5.18691000	-3.29236500	-0.47711800
F	-5.47091100	-5.08262000	1.53876800
F	-4.86862600	-7.10899200	-0.15904700

F	-2.71391900	-6.91277900	-1.79717400
F	-1.17302800	-4.71688800	-1.74022800
F	-3.94502700	-2.87259500	1.59318200
F	2.90775700	4.78115800	1.91415900
F	4.53662300	6.91237600	1.71790600
F	5.74331700	7.48570000	-0.64133400
F	5.30553100	5.91767200	-2.80864700
F	3.67033000	3.79016900	-2.62344400
F	1.91927300	-2.46849600	4.26531700
F	3.58331300	-3.79078900	5.89129600
F	6.19798200	-4.08106500	5.22415700
F	7.12576900	-3.03021100	2.90058800
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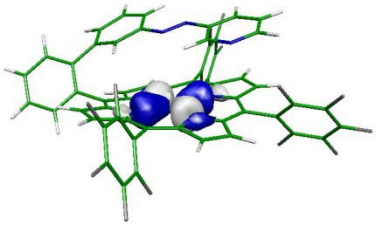
***trans*-sqp (M06-2X) [10,11]-CASSCF**



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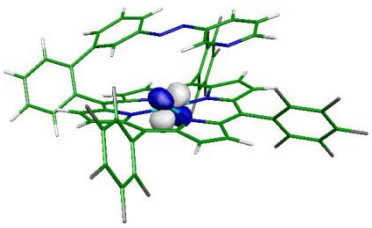
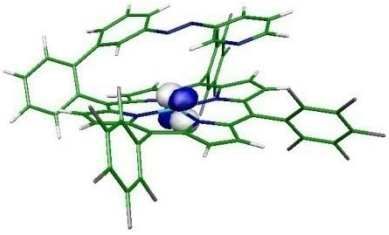


$3d_{xz}$



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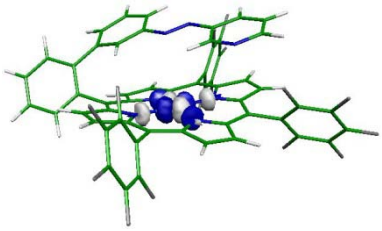

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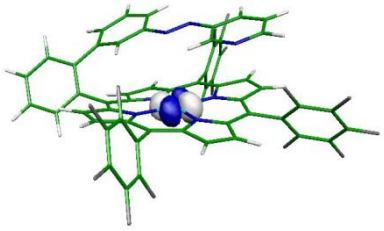
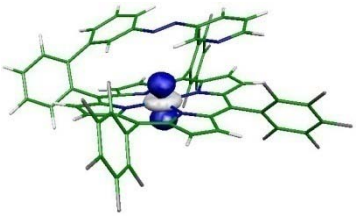
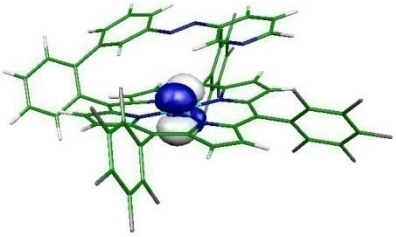


$3d_{x^2-y^2}$



$3d_{z^2}$



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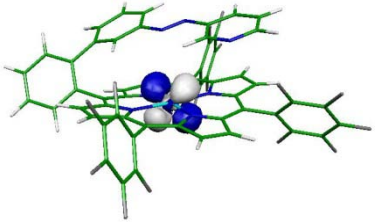

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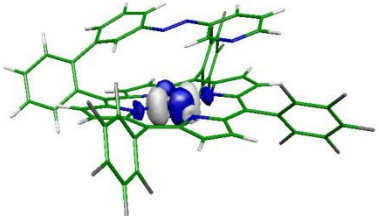
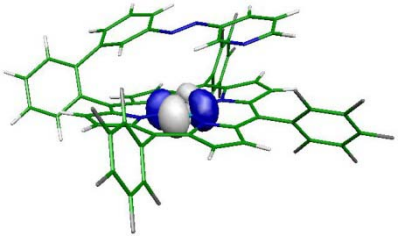
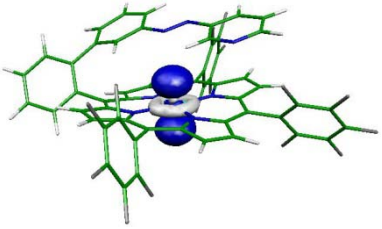


$4d_{xy}$

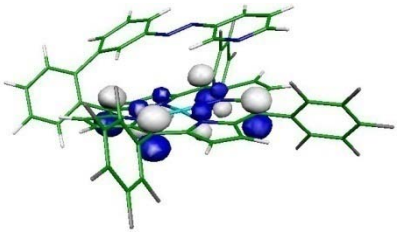


$4d_{x^2-y^2}$

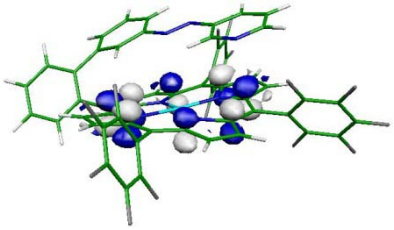


$4d_{z^2}$

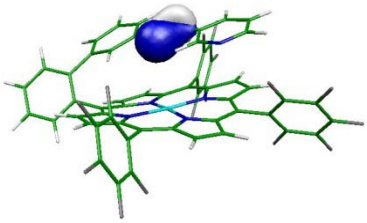
***trans*-sqp (M06-2X) [10,8]-CASSCF**



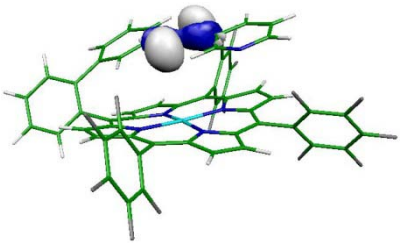
$\pi_{porp\ h}$



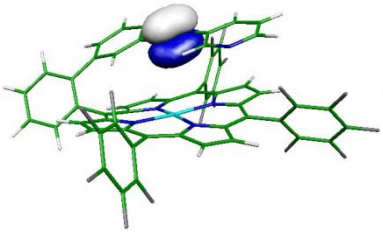
$\pi_{porp\ h}$



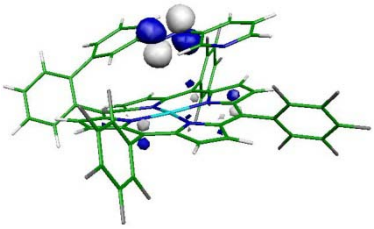
n_{azo}



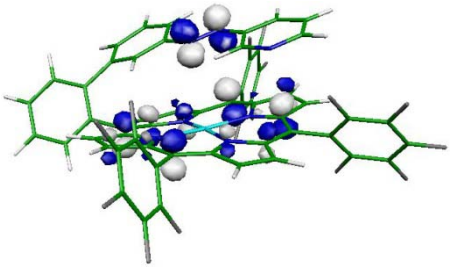
n_{azo}



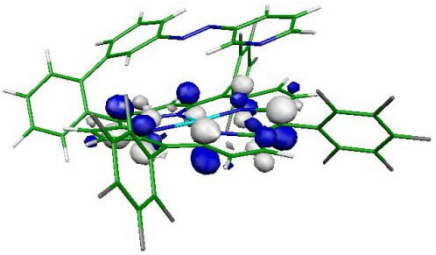
π_{azo}



π^*_{azo}



$\pi^*_{azo\ +porp\ h}$



$\pi^*_{porp\ h}$

***trans*-sqp (M06-2X) large basis set xyz (in Ångstrom)**

E(M06-2X) = -5496.941477 a.u.

98

Ni	0.33541600	0.18021300	0.00311500
N	2.12698500	0.54129400	0.78318900
N	0.53061600	-1.73874700	0.46785200
N	0.17696200	2.08142200	-0.55110800
N	-1.50587600	-0.15331800	-0.64464600
N	0.28731000	-1.05843700	-3.45587300
N	0.48137700	-2.25865100	-3.22665000
N	3.79344200	-1.89296000	-1.59626700
C	2.76888200	1.74685400	0.83894000
C	2.92117500	-0.32759400	1.47587400
C	3.98695200	1.63695800	1.60186800
C	4.07076700	0.35791300	2.01284200
C	1.59698300	-2.34265100	1.06880000
C	-0.35154900	-2.74476300	0.18748500
C	1.40114300	-3.76888200	1.12604000
C	0.19303900	-4.01784800	0.58218400
C	-0.84346500	2.65430400	-1.26491300
C	1.13807800	3.04374800	-0.44893500
C	-0.48879900	3.99487900	-1.65456300
C	0.72859400	4.24377500	-1.12712300
C	-2.37699400	0.75891400	-1.17273800
C	-2.17479200	-1.34249700	-0.65402900
C	-3.64329300	0.13983200	-1.45777900
C	-3.51575400	-1.16617900	-1.14634100
C	2.69779800	-1.68959100	1.61290000
C	2.34226800	2.91606900	0.23426400
C	-2.05980900	2.05406800	-1.56565100
C	-1.63480500	-2.57416100	-0.30612500
C	-2.51191500	-3.77214900	-0.41069100
C	-2.32428800	-4.74799600	-1.38062400
C	-3.56242400	-3.95828200	0.47995500
C	-3.14647300	-5.85934000	-1.47017400
C	-4.39816200	-5.05981600	0.41084600
C	-4.18790200	-6.01368500	-0.57100100
C	3.65861500	-2.49663200	2.41243800
C	4.99146400	-2.66189700	2.05128500
C	3.24729700	-3.12441500	3.58550000
C	5.86850200	-3.42759100	2.80271100
C	4.10495400	-3.89485700	4.35184100
C	5.42243300	-4.04911400	3.95571000
C	3.22279100	4.11319800	0.32344100
C	3.32484000	4.84953100	1.49633700
C	3.97397900	4.54099500	-0.76343000
C	4.14089500	5.96428700	1.59292600

C	4.79444200	5.65455300	-0.69347900
C	4.87713100	6.36697200	0.49127500
C	-2.98633500	2.76447200	-2.49971200
C	-3.61984900	3.93745500	-2.09559700
C	-3.20860000	2.27260100	-3.80407800
C	-4.44717400	4.64107900	-2.95852100
C	-4.03662200	2.99882500	-4.66030100
C	-4.64669600	4.17431300	-4.25012500
C	-2.66708100	0.95456800	-4.23433000
C	-3.51426100	0.01203500	-4.81330200
C	-1.36623600	0.56253200	-3.92061900
C	-3.09678200	-1.30336300	-5.00466500
C	-0.98731500	-0.76554900	-4.02001000
C	-1.84936700	-1.71550300	-4.57045400
C	1.73514400	-2.54840700	-2.62175500
C	2.06950000	-3.88793100	-2.50276000
C	2.62551800	-1.58273200	-2.13881500
C	3.29593000	-4.21542600	-1.94533200
C	4.12042100	-3.18624700	-1.51644800
H	4.67797200	2.44209700	1.79070400
H	4.84388900	-0.09411100	2.61155200
H	2.10735400	-4.47737700	1.52783700
H	-0.29710300	-4.96999700	0.45956400
H	-1.10387700	4.65129800	-2.24673400
H	1.30896000	5.14970400	-1.19334200
H	-4.49846500	0.65227200	-1.86773300
H	-4.25006600	-1.94839000	-1.24958800
H	-3.45664700	4.29442800	-1.08552400
H	-4.93084200	5.54962700	-2.62323100
H	-4.19046300	2.63380200	-5.66884000
H	-5.27856600	4.72288300	-4.93703500
H	-4.53092400	0.29241500	-5.06380600
H	-0.64960700	1.26218400	-3.51134000
H	-3.77566500	-2.01903800	-5.45119800
H	-1.53287500	-2.74759600	-4.63869500
H	1.37129400	-4.63704300	-2.85583900
H	2.36984600	-0.53107400	-2.20084900
H	3.61102900	-5.24551000	-1.84607900
H	5.09233500	-3.40122300	-1.08734400
F	-5.39042100	-5.21170400	1.27753800
F	-4.97862700	-7.07305800	-0.64707100
F	-2.94337100	-6.77452200	-2.40988600
F	-1.33120900	-4.63480700	-2.25674600
F	-3.78952100	-3.06278100	1.43458200
F	2.62866100	4.48897200	2.56954000
F	4.21828700	6.64892900	2.72653500
F	5.65866400	7.43292200	0.56976800
F	5.50010300	6.04207600	-1.74749100
F	3.91381000	3.87886300	-1.91348300
F	1.99562100	-2.98849900	4.01106000

F	3.67669100	-4.47842300	5.46336100
F	6.25285900	-4.78351200	4.67928100
F	7.13145500	-3.57080800	2.42121300
F	5.47189500	-2.07567100	0.96094100

***trans*-sqp (BP86) xyz (in Ångstrom)**

E(BP86) = -5494.417117 a.u.

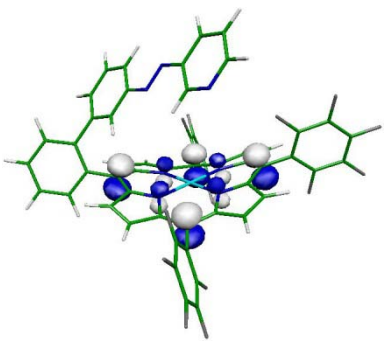
98

Ni	-0.09348800	0.15601500	0.33263100
N	1.69353200	0.52751600	0.97769500
N	-0.14128600	-1.45820300	1.40606800
N	-0.04628700	1.77286500	-0.73961600
N	-1.88167900	-0.21742200	-0.30998300
N	1.53747200	-1.18338200	-4.49157600
N	2.22974400	-2.22560600	-4.70873700
N	5.55042800	-0.85176900	-3.65889700
C	2.37578200	1.73328500	0.92306100
C	2.56548600	-0.35212300	1.59960500
C	3.67946300	1.61360700	1.54051100
C	3.81319100	0.30547100	1.92463700
C	0.93497600	-2.13661700	1.95973800
C	-1.25507000	-2.20757100	1.75017700
C	0.49250700	-3.34309500	2.62500600
C	-0.87449500	-3.36198000	2.53567600
C	-0.87608900	2.10624500	-1.80218200
C	0.83326400	2.83808200	-0.61973900
C	-0.49061600	3.38133300	-2.36967300
C	0.53609000	3.86054400	-1.59866200
C	-2.51638100	0.34365400	-1.40825800
C	-2.81756000	-1.07432900	0.24970300
C	-3.86246300	-0.17238700	-1.53955600
C	-4.06593400	-1.01659600	-0.47986400
C	2.25392300	-1.66096400	1.99739100
C	1.94898300	2.87598100	0.23154600
C	-2.01364600	1.38716300	-2.20204100
C	-2.55963900	-1.98524700	1.28520400
C	-3.66755800	-2.84028700	1.81280700
C	-4.18389100	-3.92807500	1.07762500
C	-4.22342000	-2.59240000	3.08566200
C	-5.21876100	-4.73789800	1.58035400
C	-5.25843100	-3.38878300	3.60999900
C	-5.75673800	-4.46439400	2.85177900
C	3.33294900	-2.51179200	2.58766300
C	4.29205700	-3.13002400	1.75756400
C	3.44571700	-2.71732300	3.97879300
C	5.32280400	-3.92929500	2.28552600
C	4.46689500	-3.51308900	4.52978800
C	5.40744200	-4.12051400	3.67708100
C	2.78533800	4.11392900	0.30449500

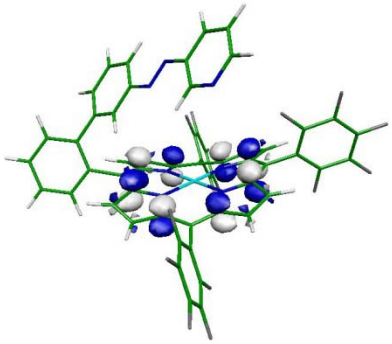
C	2.74221300	4.94282800	1.44535900
C	3.65769400	4.48670000	-0.73980100
C	3.52989300	6.10426000	1.54723600
C	4.45374800	5.64427200	-0.66154500
C	4.38721800	6.45422700	0.48762500
C	-2.81020900	1.83684200	-3.39246100
C	-3.61190500	2.99628400	-3.28475300
C	-2.83089100	1.08669900	-4.60532700
C	-4.42668300	3.42325000	-4.34485800
C	-3.66627100	1.52922600	-5.65945700
C	-4.45491300	2.68264600	-5.53839100
C	-2.00638700	-0.14322000	-4.80675000
C	-2.59788900	-1.32385200	-5.31563900
C	-0.61964900	-0.15535300	-4.54320300
C	-1.82784900	-2.48206500	-5.54455300
C	0.15589400	-1.31123000	-4.77887300
C	-0.45524900	-2.48771700	-5.27980900
C	3.60975400	-2.09602500	-4.42242400
C	4.41397800	-3.22940000	-4.66836000
C	4.23770200	-0.92712800	-3.91175300
C	5.78746500	-3.15304200	-4.40371700
C	6.30396000	-1.94409100	-3.90231200
H	4.40985400	2.42564700	1.62890300
H	4.66693000	-0.17434100	2.41631000
H	1.14881500	-4.06761100	3.11953000
H	-1.57063400	-4.11214700	2.92747900
H	-0.97504300	3.85694500	-3.22927700
H	1.07435700	4.80898700	-1.70232800
H	-4.56806100	0.12075100	-2.32465600
H	-4.97261300	-1.57559100	-0.22317000
H	-3.60395000	3.55679900	-2.33652000
H	-5.04333100	4.32910200	-4.23413900
H	-3.67002400	0.96185200	-6.60372300
H	-5.08705100	3.00651300	-6.38028100
H	-3.68098900	-1.34079300	-5.51661400
H	-0.09857400	0.73880800	-4.17143400
H	-2.31758200	-3.39056600	-5.93058800
H	0.17282700	-3.37436100	-5.44869800
H	3.93536300	-4.14014600	-5.06167400
H	3.62111200	-0.03468100	-3.70995400
H	6.45173700	-4.01333300	-4.58075800
H	7.38370200	-1.84980100	-3.68389100
F	-5.77259000	-3.12932000	4.81741900
F	-6.73980700	-5.22637100	3.33867400
F	-5.68995500	-5.76491300	0.86330800
F	-3.68430500	-4.21885200	-0.13139000

F	-3.76972400	-1.57457200	3.82807700
F	1.93424300	4.63283100	2.46781700
F	3.46721200	6.87686500	2.63775500
F	5.13855900	7.55537100	0.57243100
F	5.27378200	5.97683500	-1.66474500
F	3.74717800	3.73008100	-1.84158300
F	2.56982400	-2.14361500	4.81519000
F	4.55294500	-3.69172200	5.85308200
F	6.38105000	-4.87832200	4.18905300
F	6.21698000	-4.50997000	1.47725200
F	4.23302100	-2.96721200	0.43018500

***trans*-sqp (BP86) [10,8]-CASSCF**



$\pi_{porp\ h}$



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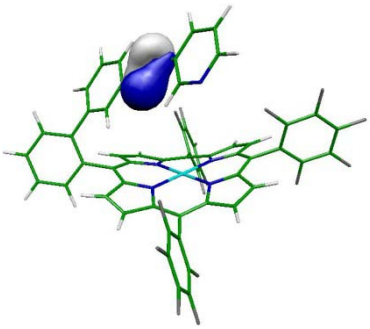

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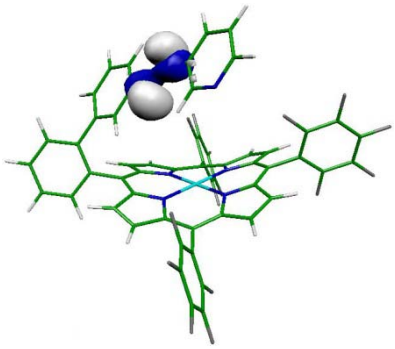
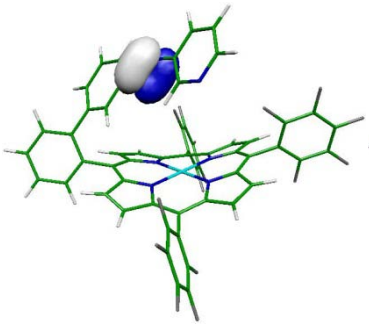


n_{azo}



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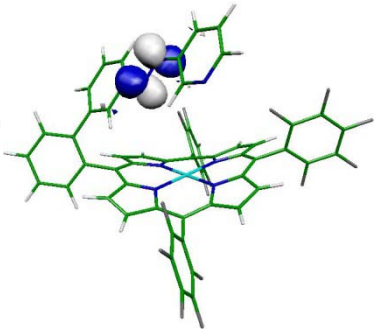

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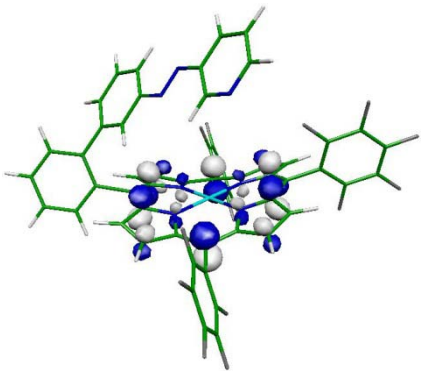
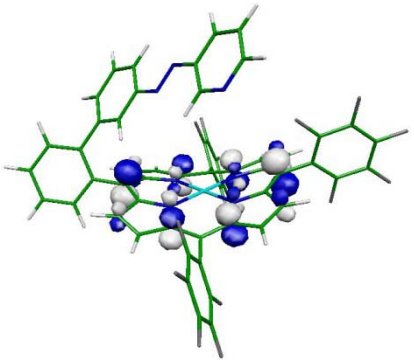


$\pi^*_{porp\ h}$



$\pi^*_{porp\ h}$

***trans*-sqp (B97D) xyz (in Ångstrom)**

E(BP86) = -5492.312958 a.u.

98

Ni	0.26758000	0.06592000	0.03512300
N	2.05217400	0.49714300	0.71340400
N	0.43298100	-1.72417900	0.79107900
N	0.12949700	1.83400100	-0.77677800
N	-1.54920500	-0.34146000	-0.54547300
N	0.39313100	-0.62297600	-3.45856200
N	0.76861100	-1.70591200	-2.92988100
N	4.06948300	-0.47094400	-1.69544800
C	2.85709000	1.54982100	0.32972600
C	2.76875400	-0.17443900	1.68662700
C	4.10324200	1.53161100	1.06105000
C	4.02172400	0.49739800	1.94918900
C	1.36657700	-2.17615200	1.69844900
C	-0.33431700	-2.82711200	0.47552100
C	1.19213600	-3.58773200	1.95033000
C	0.15875600	-4.00331300	1.15336600
C	-0.98787600	2.43537300	-1.32937600
C	1.17973500	2.68732000	-1.05199900
C	-0.62910900	3.68733200	-1.95829400
C	0.72192500	3.83398400	-1.80315100
C	-2.50448000	0.54190500	-1.01711700
C	-2.14638700	-1.58466600	-0.60336200
C	-3.74693600	-0.14903900	-1.27751900
C	-3.51092000	-1.47667200	-1.06406500
C	2.42090100	-1.41793300	2.22517500
C	2.49179100	2.54701300	-0.58067400
C	-2.26179400	1.85806900	-1.43202100
C	-1.53720600	-2.78997700	-0.23646400
C	-2.23380200	-4.07768900	-0.52316700
C	-1.75330400	-4.94427100	-1.52373900
C	-3.37700500	-4.47767400	0.19454000
C	-2.38967800	-6.16448300	-1.81295100
C	-4.03443100	-5.69052100	-0.07740900
C	-3.53615000	-6.53561700	-1.08630200
C	3.21770500	-2.01096100	3.33916900
C	4.54061500	-2.46838200	3.18902600
C	2.61977200	-2.17157300	4.60759300
C	5.25589800	-3.04488500	4.25361600
C	3.31069800	-2.74757800	5.68802900
C	4.63633600	-3.18353700	5.50883200
C	3.51449500	3.53735200	-1.02568400
C	4.03983100	4.51198900	-0.15575300
C	3.97652100	3.53347700	-2.35669800
C	5.01127300	5.43589300	-0.57938100

C	4.94471300	4.44819900	-2.80646900
C	5.46311900	5.40214000	-1.91139400
C	-3.29040000	2.53974000	-2.29146200
C	-3.96688500	3.68194900	-1.82249600
C	-3.58363600	2.03939200	-3.60264800
C	-4.93142600	4.32949000	-2.61266700
C	-4.56511500	2.69531100	-4.37432800
C	-5.23276200	3.83210100	-3.89116600
C	-2.90979900	0.80314000	-4.09704800
C	-3.64594300	-0.31484300	-4.54595900
C	-1.52032900	0.65384600	-3.93331700
C	-3.01937200	-1.56812600	-4.71366000
C	-0.92132600	-0.61694400	-3.96502300
C	-1.67498400	-1.74755700	-4.36543400
C	2.03394800	-1.63899000	-2.30263900
C	2.40246900	-2.74017800	-1.50422900
C	2.91632800	-0.52806200	-2.36764000
C	3.60609100	-2.67653600	-0.79442000
C	4.39693100	-1.51978400	-0.91790100
H	4.92053800	2.23924700	0.92010800
H	4.76217900	0.17553900	2.68265200
H	1.80763300	-4.17833100	2.63191000
H	-0.27371800	-5.00175100	1.06194000
H	-1.33505000	4.34774800	-2.46434000
H	1.36068500	4.65495500	-2.13425500
H	-4.65858500	0.33538800	-1.62973600
H	-4.19550500	-2.31599600	-1.19176500
H	-3.73454000	4.05572300	-0.81755100
H	-5.44917800	5.21680600	-2.22698100
H	-4.78780700	2.31182400	-5.37811900
H	-5.98421300	4.33172000	-4.51576100
H	-4.72868000	-0.22052600	-4.69903900
H	-0.89112900	1.50184500	-3.65490700
H	-3.61400900	-2.42563900	-5.05490900
H	-1.19690000	-2.73291700	-4.37297800
H	1.72218800	-3.59641500	-1.43679400
H	2.64266200	0.33674000	-2.98361000
H	3.92398400	-3.49358000	-0.13793100
H	5.33547900	-1.43415300	-0.35286600
F	-5.11917300	-6.04780500	0.61468100
F	-4.14996600	-7.68884200	-1.35258800
F	-1.91984800	-6.96749000	-2.77109100
F	-0.66587000	-4.61524400	-2.23196000
F	-3.86417700	-3.69422500	1.16313500
F	3.61554600	4.57612200	1.11247100
F	5.49782300	6.34870500	0.26601300
F	6.38119800	6.27573300	-2.32604200
F	5.37216600	4.42141800	-4.07079700
F	3.48698600	2.65139900	-3.23439200
F	1.36044200	-1.77053100	4.80545600

F	2.72254400	-2.88091100	6.87864600
F	5.30251900	-3.73006500	6.52543700
F	6.50962400	-3.47002700	4.07829900
F	5.15739600	-2.37889200	2.00126500

***trans*-sqp open (M06-2X) xyz (in Ångstrom)**

E(M06-2X) = -5492.602484 a.u.

98

Ni	-0.21130500	-0.71150000	0.00108400
N	1.73602000	-0.67077500	-0.41968500
N	0.07620200	-2.30369000	1.16795500
N	-0.49827900	0.87714700	-1.16697900
N	-2.15869000	-0.75030100	0.42644000
N	-2.89889700	1.53295300	-7.14719800
N	-2.46540100	0.81479000	-8.05835600
N	-1.94115300	3.48339800	-10.58333300
C	2.38548700	0.19856100	-1.25255300
C	2.70564500	-1.50101700	0.06596700
C	3.79999500	-0.09285400	-1.29406300
C	3.99836900	-1.15380800	-0.47789100
C	1.26393700	-2.90754600	1.46769200
C	-0.86923100	-2.98648100	1.88332500
C	1.06809300	-3.98810100	2.40653600
C	-0.25997700	-4.04004200	2.66150900
C	-1.67931900	1.52749600	-1.40710800
C	0.43928500	1.55034600	-1.89487400
C	-1.47624500	2.64409600	-2.29848300
C	-0.15941700	2.65021700	-2.61381400
C	-3.12611100	0.09625200	-0.04518000
C	-2.81980500	-1.66316600	1.19626800
C	-4.42971200	-0.30501200	0.42627400
C	-4.23841100	-1.40348300	1.19820900
C	2.51434500	-2.55077200	0.96355800
C	1.80120200	1.24567000	-1.95983800
C	-2.93050100	1.17992600	-0.90143600
C	-2.23483200	-2.71847100	1.90095600
C	-3.11533200	-3.59159800	2.72430200
C	-3.30271800	-4.93845700	2.40770400
C	-3.78084100	-3.09512800	3.84704200
C	-4.11849800	-5.76529500	3.17592400
C	-4.60427800	-3.90221500	4.62782600
C	-4.77096700	-5.24273200	4.28962500
C	3.70556900	-3.32201100	1.41337000
C	4.69685100	-2.72369300	2.19433600
C	3.87349000	-4.66739700	1.08021800
C	5.81409400	-3.43051400	2.63046800
C	4.98107900	-5.39513800	1.50758300
C	5.95396100	-4.77232800	2.28519500
C	2.67347400	2.09012200	-2.82176600

C	2.90033300	3.43589300	-2.52680300
C	3.29413900	1.56734800	-3.95792300
C	3.70606500	4.23815000	-3.33067500
C	4.10943000	2.34867900	-4.77282900
C	4.31281800	3.68967200	-4.45767100
C	-4.11643500	2.00006200	-1.30000100
C	-4.69867000	2.84770600	-0.34978200
C	-4.63439400	1.97068200	-2.61132400
C	-5.77655200	3.66536500	-0.67887200
C	-5.71450400	2.80602100	-2.92864300
C	-6.28529800	3.64488000	-1.97602700
C	-4.05807900	1.10112400	-3.67536700
C	-3.83931900	-0.26765500	-3.47367600
C	-3.73303500	1.65167000	-4.91922000
C	-3.30067200	-1.06043400	-4.48958800
C	-3.19480900	0.85840100	-5.93356700
C	-2.97182300	-0.50789200	-5.72113400
C	-2.16399600	1.49272300	-9.26590400
C	-1.76194000	0.70707800	-10.34535600
C	-2.23441100	2.88536500	-9.43674900
C	-1.45747700	1.33448500	-11.54852000
C	-1.56484600	2.72357700	-11.61382600
H	4.54021900	0.45429800	-1.87075900
H	4.93150300	-1.66518600	-0.25929800
H	1.85259200	-4.61537200	2.81996100
H	-0.78768900	-4.71682800	3.32754100
H	-2.25483800	3.32338800	-2.63412700
H	0.36728800	3.33469300	-3.27242200
H	-5.36266700	0.19418000	0.18012300
H	-4.98686900	-1.99557800	1.71742400
H	-4.28165600	2.86851600	0.65916600
H	-6.21251900	4.32167500	0.07544600
H	-6.12153000	2.77425300	-3.94121500
H	-7.13103000	4.27845200	-2.24682500
H	-4.10230600	-0.72054900	-2.51610300
H	-3.87653700	2.71528500	-5.12014300
H	-3.14006300	-2.12467600	-4.31148100
H	-2.54688300	-1.10556500	-6.52649400
H	-1.70053400	-0.37452600	-10.21422900
H	-2.53907100	3.51128000	-8.59486100
H	-1.14262400	0.76318000	-12.42190800
H	-1.33347700	3.25000100	-12.54474800
F	-5.21978600	-3.40758700	5.68693500
F	-5.54885200	-6.01681700	5.02102600
F	-4.27968900	-7.03612400	2.85325800
F	-2.69634800	-5.46345300	1.35591100

F	-3.64145200	-1.82611700	4.19296800
F	2.33750300	3.98524600	-1.46295900
F	3.89916600	5.50961100	-3.02854000
F	5.08112100	4.43794300	-5.22515400
F	4.68473800	1.82854100	-5.84254300
F	3.12344300	0.29643500	-4.28281800
F	2.96416500	-5.28855500	0.34761100
F	5.11668700	-6.66722800	1.17843000
F	7.00509600	-5.45373500	2.69644600
F	6.73375000	-2.84026200	3.37273000
F	4.59059800	-1.45076100	2.53718300

***cis*-sqp (M06-2X) xyz (in Ångstrom)**

E(M06-2X) = -5492.595590 a.u.

98

Ni	0.37416800	-0.09193200	0.32009600
N	2.09009600	0.48979100	1.16187000
N	0.24802200	-1.60310500	1.63020700
N	0.47771600	1.43898500	-0.96107900
N	-1.39822800	-0.61420200	-0.45740700
N	-0.92522900	-3.75842700	-4.39746300
N	-0.42685800	-4.37107400	-3.44788500
N	1.34995100	-2.07244900	-1.09276900
C	2.86762000	1.55112900	0.79560600
C	2.74071000	-0.10082100	2.20540100
C	4.03413300	1.64550300	1.64652700
C	3.96170300	0.61098200	2.51560300
C	1.15249400	-1.94072400	2.59014600
C	-0.69254700	-2.59256600	1.64547200
C	0.75633500	-3.15866100	3.26286000
C	-0.38938500	-3.56837400	2.66947200
C	-0.40762900	1.74250700	-1.95882100
C	1.48436500	2.34915300	-1.07708100
C	0.06004100	2.86924200	-2.73183700
C	1.24073200	3.24704800	-2.18318700
C	-2.05775700	-0.01000000	-1.49183300
C	-2.13348700	-1.71937200	-0.15122900
C	-3.26691000	-0.72924600	-1.81549700
C	-3.30462100	-1.80680900	-0.99313300
C	2.33105500	-1.25045700	2.88211900
C	2.61422300	2.43008600	-0.25538300
C	-1.60621800	1.08364500	-2.22971000
C	-1.80366500	-2.68102400	0.80948000
C	-2.66746000	-3.88814400	0.92189300
C	-2.17823200	-5.14552000	0.56101600
C	-3.98306800	-3.81495800	1.38140100
C	-2.96171600	-6.29208400	0.65808000
C	-4.78725600	-4.94718600	1.48078600
C	-4.27162900	-6.18905600	1.11952300
C	3.23526200	-1.81913400	3.91894000
C	3.46867200	-1.17354900	5.13362200
C	3.89174800	-3.03138400	3.69681200
C	4.31996800	-1.71163200	6.09607000
C	4.74198600	-3.59190400	4.64502900
C	4.95487800	-2.92640900	5.84994000
C	3.60465500	3.50870200	-0.52524900

C	3.27731200	4.85526700	-0.35318700
C	4.89650900	3.21303900	-0.96537100
C	4.19397500	5.87172200	-0.60914500
C	5.83104900	4.21241400	-1.22318000
C	5.47576000	5.54676600	-1.04512900
C	-2.41940700	1.53981800	-3.40163900
C	-3.37923300	2.54355000	-3.23674200
C	-2.21748100	0.97571700	-4.67663100
C	-4.13749300	2.98992400	-4.31742200
C	-2.98260600	1.43438500	-5.75419600
C	-3.93788800	2.43399800	-5.57946400
C	-1.19791100	-0.09861300	-4.88422600
C	0.09935600	0.21762900	-5.30486700
C	-1.52684600	-1.43383300	-4.63884900
C	1.05195400	-0.78880100	-5.46867600
C	-0.54635100	-2.42240800	-4.72822400
C	0.74108000	-2.11276700	-5.17114900
C	0.50066800	-3.80579400	-2.51240600
C	1.34524800	-4.72908200	-1.89192400
C	0.52970600	-2.47771400	-2.05348700
C	2.21496400	-4.29561600	-0.89763100
C	2.18191500	-2.95081800	-0.53293400
H	4.80380900	2.40932700	1.57965700
H	4.66459900	0.34738800	3.30069200
H	1.28697500	-3.62727200	4.08704000
H	-0.99179200	-4.44052800	2.90802100
H	-0.46566600	3.30452800	-3.57779900
H	1.89456600	4.05612000	-2.49615900
H	-3.97527300	-0.43758400	-2.58695400
H	-4.05416500	-2.59191700	-0.95367100
H	-3.52433000	2.97556700	-2.24447900
H	-4.88385300	3.77215200	-4.17237900
H	-2.82258300	0.99270500	-6.73977600
H	-4.52758600	2.77655000	-6.43101100
H	0.35955200	1.25857500	-5.50479800
H	-2.53276800	-1.71458200	-4.32368400
H	2.05551400	-0.53397500	-5.81204900
H	1.48900800	-2.90200900	-5.26155000
H	1.28197300	-5.77561300	-2.19464000
H	-0.15231300	-1.72192700	-2.44624400
H	2.88947400	-4.98532200	-0.39045500
H	2.83385600	-2.57018400	0.26001600
F	-6.03126700	-4.85117300	1.91614100
F	-5.02409100	-7.26760900	1.21479400
F	-2.47449900	-7.47162000	0.31749900
F	-0.93511200	-5.27249600	0.12319200

F	-4.50170500	-2.64759700	1.72579300
F	2.06711900	5.19699900	0.05706700
F	3.85669200	7.13783400	-0.43993900
F	6.35209600	6.50171800	-1.28928600
F	7.04635700	3.90355500	-1.64024000
F	5.26623000	1.95537700	-1.14292900
F	3.71093900	-3.68279500	2.55531100
F	5.35128100	-4.74030100	4.40841400
F	5.75754900	-3.44666700	6.75775600
F	4.52726000	-1.08147000	7.23852200
F	2.88203800	-0.01678900	5.39214300

***cis*-sqp open (M06-2X) xyz (in Ångstrom)**

E(M06-2X) = -5492.580401 a.u.

98

Ni	0.00568500	0.37774800	1.08948800
N	1.94566000	0.49914200	1.53143300
N	-0.11708000	-1.33071600	2.10854000
N	0.13510700	2.07418100	0.05077200
N	-1.94224900	0.27580400	0.68194000
N	-0.27841700	-0.64195800	-4.02345600
N	0.24635600	-1.15217900	-5.01678200
N	-1.63456100	-0.41176100	-8.12303600
C	2.81648200	1.48784100	1.16381000
C	2.66699800	-0.34164100	2.33000700
C	4.11122800	1.28049700	1.77079200
C	4.01757600	0.14410400	2.49878500
C	0.88912200	-1.97463600	2.77025600
C	-1.22158800	-2.12224800	2.26667300
C	0.41556400	-3.21429900	3.34219200
C	-0.89912400	-3.30263400	3.03463900
C	-0.86803300	2.69771400	-0.64179100
C	1.26074000	2.80079500	-0.20845200
C	-0.35453300	3.82876300	-1.37666100
C	0.97304000	3.89044700	-1.10910100
C	-2.68625600	1.17324800	-0.03580300
C	-2.82037200	-0.69328300	1.07046300
C	-4.07143400	0.77144500	-0.07732900
C	-4.15345700	-0.39760500	0.60224100
C	2.20059700	-1.52081400	2.91114300
C	2.53110200	2.56022500	0.32347100
C	-2.20585300	2.30732600	-0.68852900
C	-2.50233600	-1.84216500	1.79941200
C	-3.58933800	-2.81787100	2.08977800
C	-4.64612700	-2.49589100	2.94356500
C	-3.58921100	-4.09068200	1.51639600
C	-5.66869100	-3.40036400	3.21777600
C	-4.59934900	-5.01243300	1.77815200
C	-5.64263000	-4.66310000	2.63164900
C	3.14741000	-2.33182300	3.72446000
C	4.27088700	-2.93299300	3.15183500
C	2.94881600	-2.51560700	5.09488800
C	5.16837100	-3.68061500	3.90956800
C	3.82931500	-3.26443500	5.87095400
C	4.94451100	-3.84644400	5.27387300
C	3.63051800	3.50190800	-0.02267900

C	4.74634700	3.08132200	-0.75070600
C	3.58385300	4.84392000	0.36251600
C	5.77528800	3.95747800	-1.08707300
C	4.59702700	5.73896400	0.03064300
C	5.69654100	5.29179400	-0.69720000
C	-3.16169500	3.12296200	-1.50069300
C	-3.55387900	4.38203500	-1.03166400
C	-3.70089800	2.63716700	-2.71086900
C	-4.46949700	5.15942000	-1.73677000
C	-4.62809500	3.42691800	-3.40348600
C	-5.01053800	4.67763000	-2.92723500
C	-3.33226800	1.30328200	-3.26309800
C	-4.33500800	0.39357300	-3.62285500
C	-1.99466200	0.92721400	-3.42019400
C	-4.00592300	-0.87132500	-4.10863100
C	-1.67052500	-0.31781100	-3.95814300
C	-2.67518100	-1.23662400	-4.28102900
C	-0.43397400	-1.32310100	-6.25941200
C	-0.28258700	-2.53917600	-6.92477800
C	-1.10260300	-0.27814600	-6.91561100
C	-0.86828700	-2.68520200	-8.17719100
C	-1.53657300	-1.59248100	-8.73139200
H	4.97057400	1.93568000	1.65956200
H	4.78582500	-0.32518500	3.10653000
H	1.01895800	-3.92013800	3.90583700
H	-1.59721600	-4.08918100	3.30634700
H	-0.94615000	4.47578200	-2.01831100
H	1.70006700	4.60119600	-1.49203100
H	-4.86576000	1.32307100	-0.57274000
H	-5.03312900	-1.01108500	0.77387400
H	-3.13639200	4.74402200	-0.08978400
H	-4.76387600	6.13709600	-1.35288300
H	-5.03494900	3.05276500	-4.34516400
H	-5.72682400	5.27789700	-3.48984900
H	-5.38241800	0.66880700	-3.48366300
H	-1.18233000	1.60006900	-3.14116000
H	-4.79715300	-1.58195500	-4.35087800
H	-2.41170900	-2.22659300	-4.65457800
H	0.28234900	-3.34239500	-6.44846500
H	-1.18660900	0.70227000	-6.43587700
H	-0.79589900	-3.62391500	-8.72683800
H	-2.00248800	-1.67360300	-9.71791900
F	-4.57831000	-6.20986100	1.22030500
F	-6.60485800	-5.52841500	2.88558400
F	-6.65669000	-3.07123600	4.03106800
F	-4.69788300	-1.30258700	3.51099600

F	-2.60880100	-4.45382800	0.70588500
F	4.85270000	1.82142100	-1.13677400
F	6.81787600	3.53371600	-1.77844900
F	6.66146300	6.13120500	-1.01756400
F	4.52191100	7.00488700	0.40202600
F	2.55550700	5.30029800	1.05816500
F	1.89866400	-1.97455200	5.69080500
F	3.61918400	-3.41791800	7.16636100
F	5.79079700	-4.55142600	5.99899100
F	6.22646400	-4.23519100	3.34483600
F	4.51238900	-2.79417200	1.85916900

***trans*-spy (M06-2X) xyz (in Ångstrom)**

E(M06-2X) = -5492.618525 a.u.
E([10,11]-CASSCF) = -5487.236001 a.u.
E([10,11]-CASPT2) = -5492.100951 a.u.

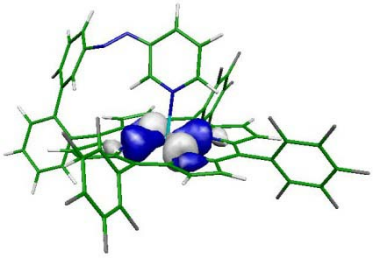
98

Ni	0.59053800	-0.12577100	0.00544500
N	2.24412200	0.56836800	0.99937200
N	0.53864400	-1.75919100	1.24789800
N	0.38992900	1.68627400	-0.97283800
N	-1.30129500	-0.61681000	-0.72590900
N	0.30817600	-0.74067700	-5.02154700
N	0.60720500	-1.92412800	-4.80550800
N	1.76447100	-1.22476900	-1.45159600
C	2.93376100	1.69731100	0.68760900
C	2.96108700	-0.10115200	1.93604400
C	4.15414300	1.75477900	1.47531500
C	4.16413800	0.64800500	2.25904100
C	1.48586300	-2.11107700	2.15379500
C	-0.34223900	-2.79084400	1.15913800
C	1.18854400	-3.42938000	2.68665300
C	0.05517100	-3.85059700	2.07022800
C	-0.65197400	2.12282000	-1.74140200
C	1.33156100	2.66533200	-0.98283700
C	-0.34420600	3.43294300	-2.27899800
C	0.88993400	3.76590200	-1.81556600
C	-2.11281500	0.12403600	-1.53915800
C	-1.93115100	-1.80068600	-0.51090900
C	-3.30670900	-0.63142700	-1.86066800
C	-3.18396200	-1.83501000	-1.24291400
C	2.61996100	-1.34846500	2.49137100
C	2.53453600	2.66791100	-0.24435200
C	-1.84733100	1.42291800	-2.00747100
C	-1.47694400	-2.83504900	0.33302400
C	-2.28855700	-4.08531100	0.37907900
C	-1.78624300	-5.28213600	-0.13554500
C	-3.56332000	-4.11423200	0.94609900
C	-2.51880200	-6.46537800	-0.09209300
C	-4.31550100	-5.28537800	0.99935900
C	-3.78869000	-6.46435300	0.47835100
C	3.56805700	-1.93896700	3.47638200
C	4.85122600	-2.33173700	3.09084400
C	3.21214100	-2.13247600	4.81229400

C	5.75505500	-2.88446900	3.99324300
C	4.09691900	-2.68872700	5.73299800
C	5.37340000	-3.06234500	5.32065100
C	3.45115500	3.82418100	-0.45633400
C	3.71240100	4.75145500	0.55459500
C	4.08599300	4.01806700	-1.68541000
C	4.57726600	5.82513700	0.35956300
C	4.95290100	5.08509700	-1.90371900
C	5.19901700	5.99061600	-0.87517400
C	-2.94479800	2.18316300	-2.71288800
C	-3.54110600	3.20518900	-1.95851700
C	-3.42849900	1.94559800	-4.02341100
C	-4.58066700	3.98209100	-2.45996000
C	-4.47917400	2.73667600	-4.51208200
C	-5.05318200	3.74660000	-3.74854900
C	-2.87501000	0.87799100	-4.89883100
C	-3.68966900	0.03961400	-5.67254800
C	-1.50174900	0.64463100	-4.92289500
C	-3.14406700	-1.02853500	-6.39498400
C	-0.97804200	-0.48515000	-5.55072800
C	-1.78866500	-1.33453500	-6.30707400
C	1.50450700	-2.00253300	-3.70767700
C	2.47580600	-2.97890200	-3.50670000
C	1.19290200	-1.14726400	-2.64150900
C	3.11685200	-3.01511900	-2.26700500
C	2.72772600	-2.13319700	-1.25847900
H	4.90292100	2.54123400	1.43286100
H	4.91525500	0.36064800	2.99028200
H	1.77173100	-3.96222200	3.43303700
H	-0.47128000	-4.78889200	2.22429300
H	-0.99546300	4.01559400	-2.92552200
H	1.44031300	4.68397400	-2.00361800
H	-4.12399700	-0.27780300	-2.48425500
H	-3.88534300	-2.66479500	-1.26504500
H	-3.17334200	3.38053300	-0.94569600
H	-5.01909400	4.76695700	-1.84231700
H	-4.83005300	2.56542600	-5.53149900
H	-5.86105900	4.35148900	-4.16232400
H	-4.77062500	0.19411900	-5.67991400
H	-0.81186700	1.27455800	-4.36191000
H	-3.80411300	-1.66661500	-6.98451300
H	-1.36644800	-2.22718500	-6.76912200
H	2.71798300	-3.68952000	-4.29824400
H	0.38923100	-0.41926600	-2.75889300

H	3.89882500	-3.74728100	-2.06751800
H	3.18094600	-2.16684800	-0.26324900
F	-5.51837000	-5.28747000	1.54628500
F	-4.49214200	-7.57978500	0.52520100
F	-2.01982700	-7.58316600	-0.59197900
F	-0.58018600	-5.31445400	-0.67908200
F	-4.09193400	-3.01191900	1.45173900
F	3.13717700	4.62384800	1.73947600
F	4.80700300	6.68864400	1.33374300
F	6.02145800	7.00348400	-1.07006300
F	5.54854000	5.24076000	-3.07346800
F	3.87399200	3.17441700	-2.68195200
F	2.00547800	-1.79246300	5.23324400
F	3.73639000	-2.85913500	6.99257700
F	6.21823200	-3.59007000	6.18574200
F	6.96339600	-3.24843700	3.59943500
F	5.23702900	-2.18750800	1.82993100

***trans*-spy (M06-2X) [10,11]-CASSCF**



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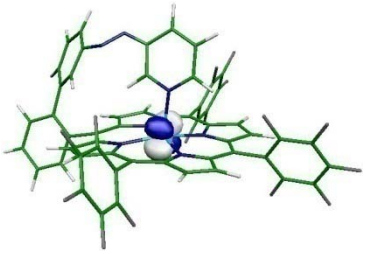

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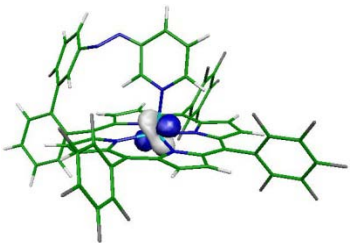

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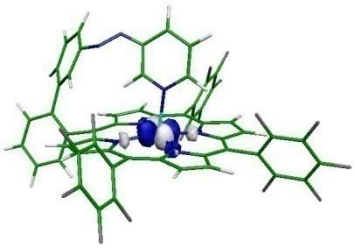

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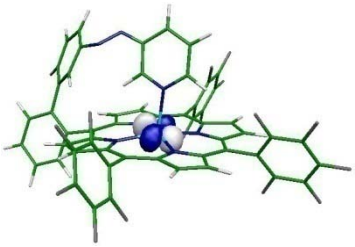
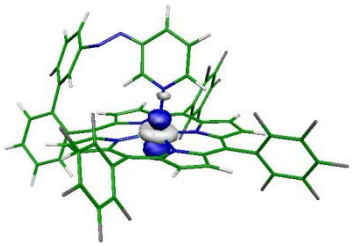
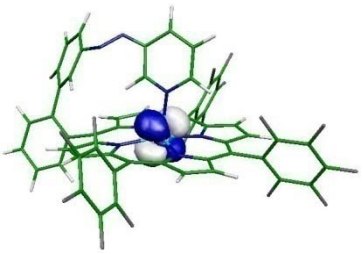


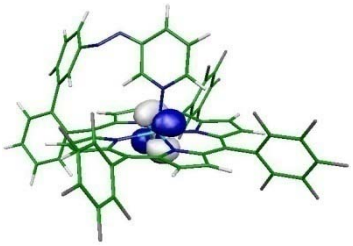
$3d_{x^2-y^2}$



$3d_{z^2}$



$4d_{xz}$



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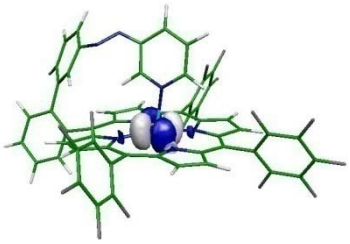
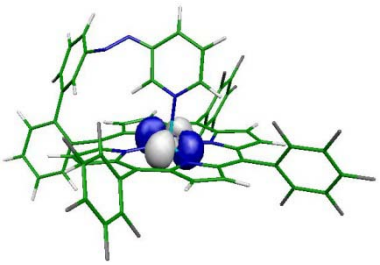
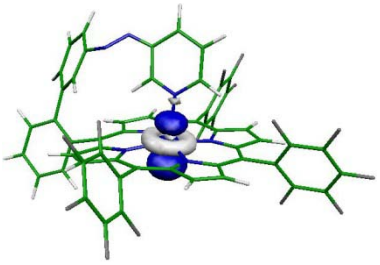


$4d_{xy}$

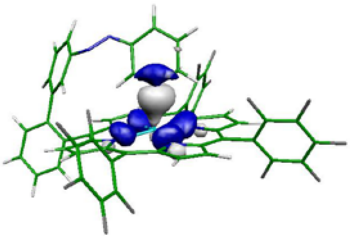


$4d_{x^2-y^2}$

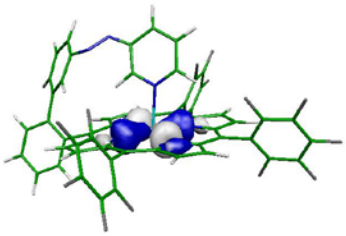


$4d_{z^2}$

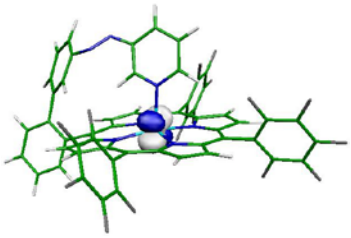
***trans*-spy (M06-2X) [12,12]-CASSCF**



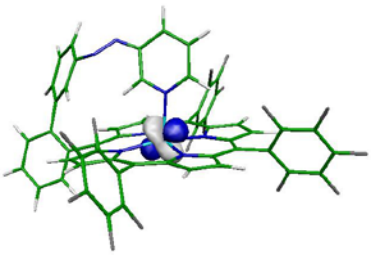
$\sigma_{ax.}$



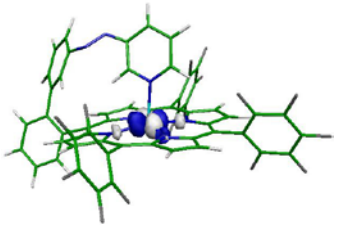
$\sigma_{eq.}$



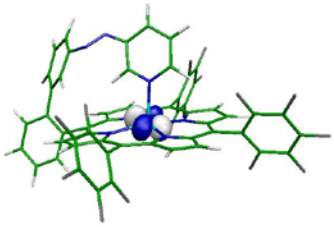
$3d_{xz}$



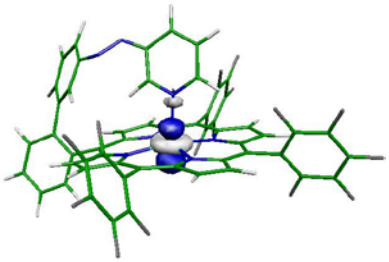
$3d_{yz}$



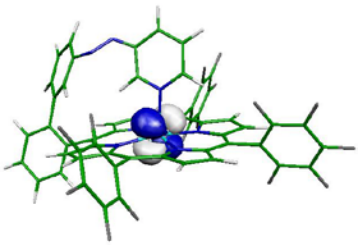
$3d_{xy}$



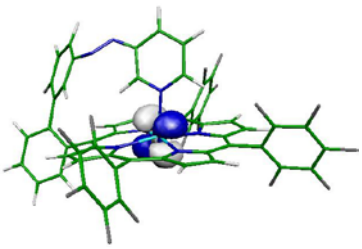
$3d_{x^2-y^2}$



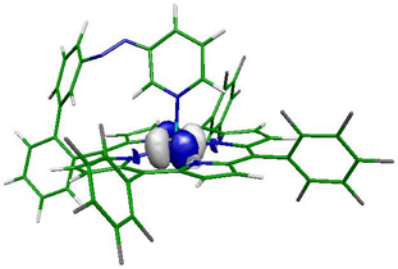
$3d_{z^2}$



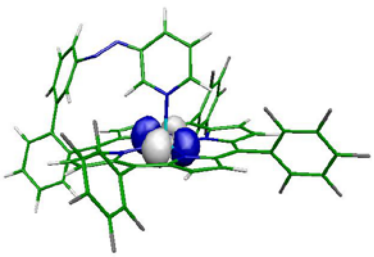
$4d_{xz}$



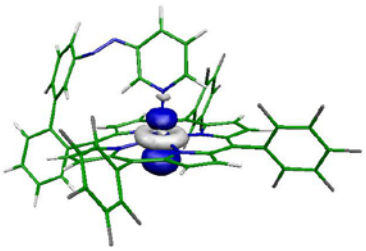
$4d_{yz}$



$4d_{xy}$



$4d_{x^2-y^2}$



$4d_{z^2}$

***cis*-spy (M06-2X) xyz (in Ångstrom)**

E(M06-2X) = -5492.628896 a.u.
E([10,11]-CASSCF) = -5487.249315 a.u.
E([10,11]-CASPT2) = -5492.111754 a.u.

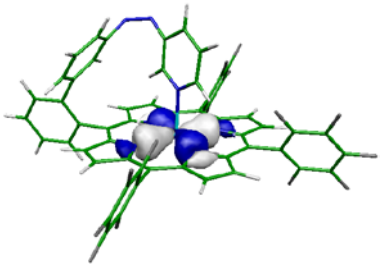
98

Ni	-0.11450600	0.30077800	0.39161300
N	1.89379900	0.51068900	0.80460000
N	-0.18033300	-1.34636800	1.63723500
N	-0.10646100	2.16247700	-0.50276900
N	-2.18248700	0.31172300	0.33216200
N	-2.64027000	-1.44830100	-4.58128100
N	-1.91548400	-2.31080800	-4.07946400
N	0.17043100	-0.90397800	-1.37843200
C	2.70852900	1.50795700	0.36291200
C	2.67031700	-0.37018200	1.48738900
C	4.07048400	1.25422200	0.79574600
C	4.04801100	0.08751100	1.48910500
C	0.88839600	-1.98505300	2.17762500
C	-1.28001600	-2.09766500	1.91438800
C	0.45174800	-3.20127200	2.84317800
C	-0.89365200	-3.26535600	2.68871700
C	-1.18111200	2.80065400	-1.04250700
C	0.98492300	2.92177800	-0.77296600
C	-0.75245900	4.02947000	-1.68270400
C	0.59424200	4.10119300	-1.52271600
C	-2.96372400	1.20295200	-0.34363200
C	-2.99921800	-0.67698800	0.77808900
C	-4.34218000	0.75649800	-0.32836900
C	-4.36395100	-0.41327800	0.36495200
C	2.22482900	-1.55495000	2.10133300
C	2.30702500	2.62559400	-0.38491500
C	-2.51569800	2.36168800	-0.99780200
C	-2.59349200	-1.81030100	1.51372100
C	-3.65163700	-2.79071700	1.88815900
C	-4.67948700	-2.45279700	2.77102000
C	-3.65719800	-4.08401600	1.36105500
C	-5.67675700	-3.36020200	3.11821000
C	-4.64237900	-5.00908400	1.69560100
C	-5.65637600	-4.64288600	2.57669200
C	3.26986600	-2.43926400	2.68785500
C	4.20329100	-3.07140800	1.86365700
C	3.36358900	-2.67064700	4.06099400

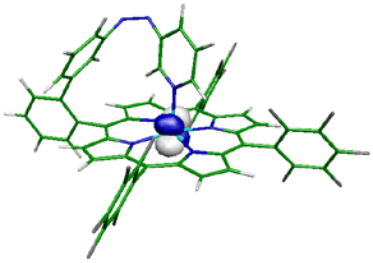
C	5.19964300	-3.89539700	2.37780700
C	4.35066700	-3.49297400	4.59912800
C	5.27046600	-4.10615100	3.75266600
C	3.37144000	3.58761000	-0.78807400
C	4.37578900	3.22086500	-1.68594100
C	3.41077700	4.88632000	-0.27626600
C	5.38238200	4.10560200	-2.06347300
C	4.40601400	5.78931400	-0.64114600
C	5.39592700	5.39459000	-1.53720400
C	-3.52860700	3.20246900	-1.71393900
C	-4.34289600	4.08342800	-0.99413700
C	-3.63511600	3.15709800	-3.11760600
C	-5.24563300	4.91850900	-1.64950400
C	-4.53482900	4.00903700	-3.76642400
C	-5.33737700	4.88612000	-3.03963700
C	-2.80188800	2.20436600	-3.90888300
C	-1.70529800	2.65520000	-4.65303100
C	-3.10757700	0.84095600	-3.89802400
C	-0.90092300	1.74866800	-5.34110300
C	-2.27846800	-0.06222800	-4.56168800
C	-1.17156200	0.38406200	-5.28739900
C	-0.76811500	-1.97323800	-3.29722900
C	0.43037800	-2.64789300	-3.52489600
C	-0.85957000	-1.11974500	-2.19298700
C	1.50816300	-2.39023000	-2.68499900
C	1.33808500	-1.50959200	-1.61986500
H	4.92624400	1.89755800	0.60811000
H	4.88171200	-0.40796600	1.98014200
H	1.09259800	-3.90677400	3.36521300
H	-1.56935200	-4.02807400	3.06677500
H	-1.40998000	4.74198900	-2.17486100
H	1.26385500	4.88244200	-1.87248300
H	-5.17603700	1.27849800	-0.79172000
H	-5.22465600	-1.04205200	0.57735100
H	-4.25082800	4.11576700	0.09337000
H	-5.87124400	5.60064000	-1.07208200
H	-4.60923200	3.96812800	-4.85491900
H	-6.03803300	5.54050200	-3.56010100
H	-1.47589500	3.72172700	-4.67701300
H	-3.97563100	0.47061000	-3.34775900
H	-0.04612600	2.10623300	-5.91673900
H	-0.54329100	-0.33535700	-5.81483100
H	0.49780100	-3.35878300	-4.35015000
H	-1.79913300	-0.61989300	-1.94537300

H	2.47041900	-2.87987000	-2.83197800
H	2.15464600	-1.29543500	-0.92640400
F	-4.62713100	-6.22433500	1.17675800
F	-6.59617000	-5.50986800	2.89951400
F	-6.63708000	-3.01568900	3.95822700
F	-4.72691100	-1.24137300	3.30034100
F	-2.70771400	-4.46266200	0.52061900
F	4.39144000	2.00268200	-2.20406100
F	6.32004200	3.73392200	-2.91782300
F	6.34540300	6.24013100	-1.88842700
F	4.42206500	7.01046800	-0.13628000
F	2.48526900	5.29110500	0.57761300
F	2.50281400	-2.10266000	4.88897600
F	4.42429100	-3.69136700	5.90332800
F	6.21057800	-4.88496200	4.25212400
F	6.06876900	-4.48497700	1.57563600
F	4.15666400	-2.89296400	0.55001500

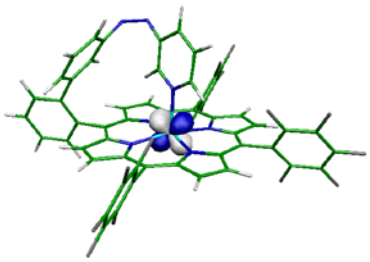
***cis*-spy (M06-2X) [10,11]-CASSCF**



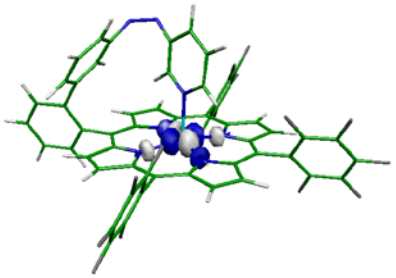
σ



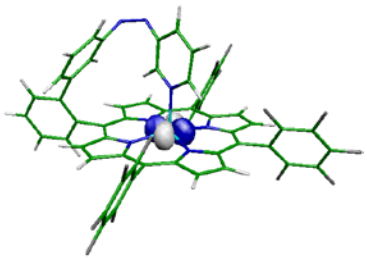
$3d_{xz}$



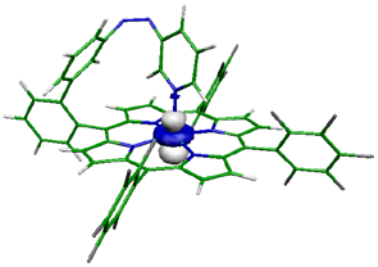
$3d_{yz}$



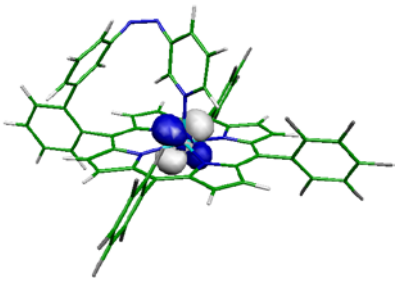
$3d_{xy}$



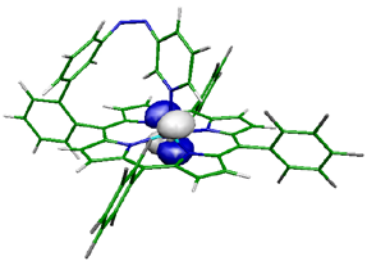
$3d_{x^2-y^2}$



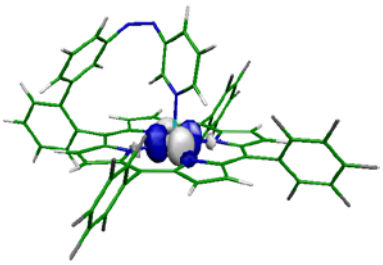
$3d_{z^2}$



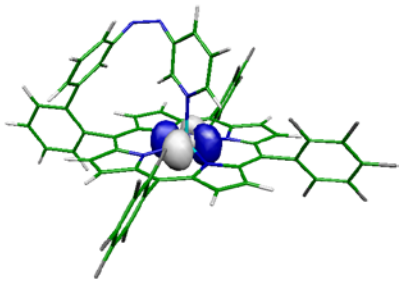
$4d_{xz}$



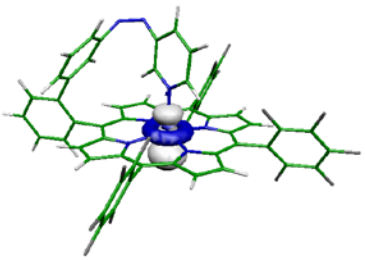
$4d_{yz}$



$4d_{xy}$

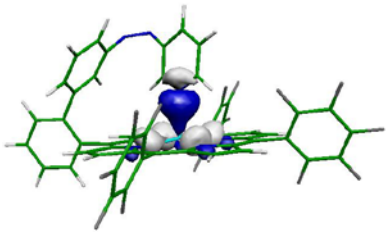


$4d_{x^2-y^2}$

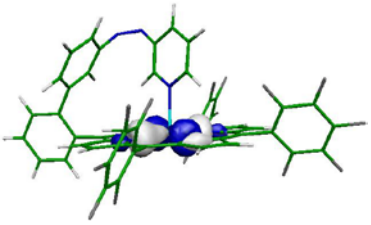


$4d_{z^2}$

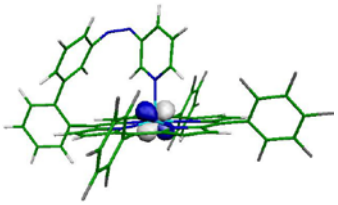
***cis*-spy (M06-2X) [12,12]-CASSCF**



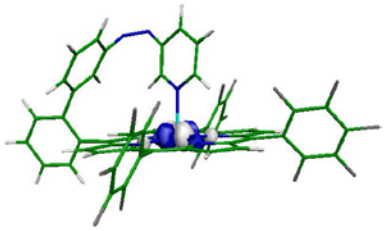
$\sigma_{ax.}$



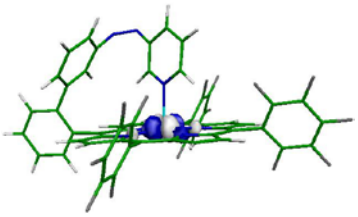
$\sigma_{eq.}$



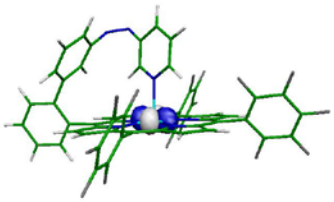
$3d_{xz}$



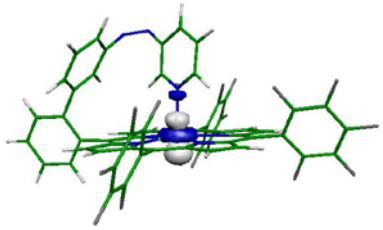
$3d_{yz}$



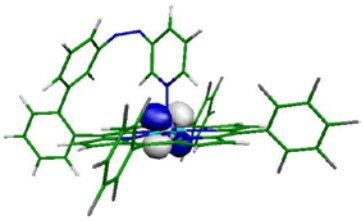
$3d_{xy}$



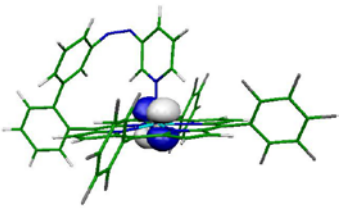
$3d_{x^2-y^2}$



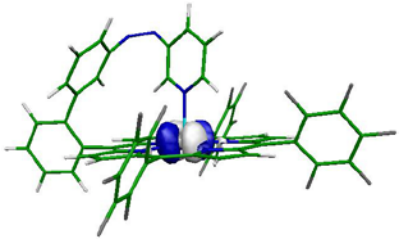
$3d_{z^2}$



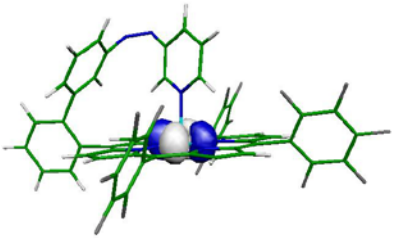
$4d_{xz}$



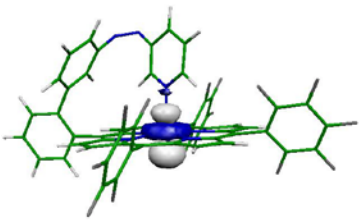
$4d_{yz}$



$4d_{xy}$



$4d_{x^2-y^2}$



$4d_{z^2}$

cis-spy (M06-2X) large basis set xyz (in Ångstrom)

E(M06-2X) = -5496.960881 a.u.

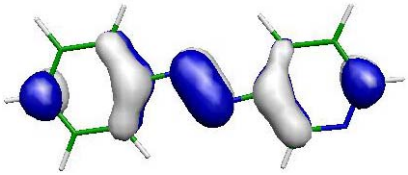
98

Ni	-0.11497300	0.31094900	0.40676600
N	1.88579000	0.52583500	0.83326800
N	-0.17996000	-1.31958500	1.66535700
N	-0.10959300	2.17211100	-0.47576200
N	-2.17697600	0.32994900	0.35690200
N	-2.66808700	-1.42390600	-4.54842800
N	-1.94857200	-2.29108600	-4.05038700
N	0.15531600	-0.88687300	-1.36481900
C	2.70360300	1.50827200	0.36606100
C	2.66267300	-0.34631600	1.52640100
C	4.06353700	1.25024700	0.79004500
C	4.03851500	0.10563000	1.50804900
C	0.88511300	-1.95173000	2.21889500
C	-1.27510200	-2.08625100	1.91538200
C	0.44721500	-3.17253400	2.86700600
C	-0.88761000	-3.25289600	2.68325700
C	-1.18450500	2.81868500	-1.00475800
C	0.98391800	2.92322400	-0.75712900
C	-0.75070600	4.04322000	-1.64078100
C	0.59214200	4.10492300	-1.49456400
C	-2.95949600	1.22286000	-0.31468600
C	-2.98871000	-0.67211200	0.77935300
C	-4.33001100	0.76403600	-0.31272200
C	-4.34777200	-0.41159500	0.35918600
C	2.21212000	-1.51303100	2.15475300
C	2.29978700	2.61075600	-0.38822000
C	-2.51245500	2.37973000	-0.95937700
C	-2.57536200	-1.80745100	1.49306300
C	-3.61941100	-2.82146800	1.81038600
C	-4.60330100	-2.59357000	2.76400700
C	-3.64840500	-4.04268400	1.14830800
C	-5.57667700	-3.53603800	3.05177900
C	-4.60894800	-5.00206700	1.41924500
C	-5.57718600	-4.74459400	2.37547000
C	3.24811800	-2.38039300	2.77999800
C	4.15089000	-3.08829900	1.99632400
C	3.35983900	-2.52223400	4.15717000
C	5.12814500	-3.89820800	2.54809800
C	4.32647100	-3.32903600	4.73484300
C	5.21376700	-4.01800800	3.92524100
C	3.37174700	3.54014400	-0.84358000
C	4.23900700	3.18205800	-1.86770500
C	3.55255700	4.79142500	-0.26846100
C	5.24528900	4.02564200	-2.30663800

C	4.55118300	5.65413200	-0.68975200
C	5.40005500	5.26725500	-1.71310800
C	-3.52414700	3.21899300	-1.67397300
C	-4.33380800	4.09575200	-0.95578500
C	-3.63020300	3.17233400	-3.07069800
C	-5.23383700	4.92667500	-1.60848100
C	-4.52706900	4.01949700	-3.71730900
C	-5.32601400	4.89331100	-2.99307200
C	-2.80115800	2.22024200	-3.86120500
C	-1.71158500	2.66736700	-4.60578200
C	-3.10984100	0.86328800	-3.85209100
C	-0.91593600	1.76379900	-5.29732400
C	-2.28888200	-0.03421700	-4.51775800
C	-1.19009600	0.40526300	-5.24610000
C	-0.78748400	-1.94683600	-3.27624100
C	0.40539900	-2.60915500	-3.52102700
C	-0.87963100	-1.11056900	-2.16926600
C	1.48791600	-2.34582700	-2.69760900
C	1.32393600	-1.47842600	-1.62920900
H	4.91597000	1.87532500	0.57616300
H	4.86676100	-0.38388200	1.99535600
H	1.08136700	-3.86845100	3.39233500
H	-1.55590300	-4.02222500	3.03574500
H	-1.40259400	4.75711300	-2.11892200
H	1.25871000	4.87936100	-1.83909200
H	-5.15844900	1.28280400	-0.76885700
H	-5.19875600	-1.04328900	0.55834700
H	-4.24098800	4.12828500	0.12340000
H	-5.85460000	5.60392700	-1.03580500
H	-4.60240700	3.97759100	-4.79744200
H	-6.02206700	5.54224100	-3.50921700
H	-1.48061700	3.72509900	-4.62748800
H	-3.97212000	0.49849800	-3.30502900
H	-0.06913200	2.11765000	-5.87141300
H	-0.57217100	-0.30904800	-5.77601500
H	0.47088200	-3.30875000	-4.34526900
H	-1.81249400	-0.62435500	-1.90944800
H	2.44515100	-2.82150700	-2.85994800
H	2.13841700	-1.25778600	-0.94987800
F	-4.61335000	-6.15890000	0.77001400
F	-6.50334900	-5.65284600	2.64208100
F	-6.50306200	-3.29346800	3.97011700
F	-4.62782400	-1.44462400	3.43162200
F	-2.73820000	-4.31513000	0.21842500
F	4.11483900	1.99806200	-2.46112400
F	6.05707000	3.65715900	-3.28985700
F	6.35832500	6.08385200	-2.12409600
F	4.70300600	6.84262300	-0.12017400
F	2.75655000	5.19055800	0.71759800
F	2.52678100	-1.87100100	4.96171500

F	4.41167500	-3.44419300	6.05351200
F	6.14186600	-4.79203800	4.46652400
F	5.97436000	-4.56394900	1.77249500
F	4.08845500	-3.00154500	0.66852300

***trans* 3-phenylazopyridine (3-PAPy) [12,9]-CASSCF**



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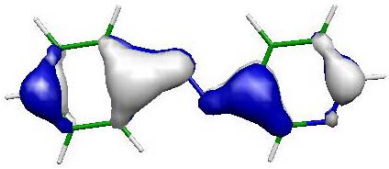

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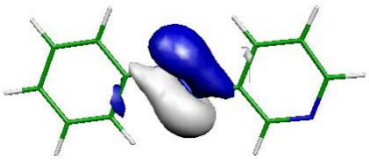

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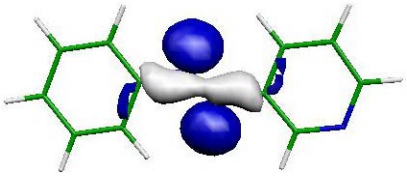

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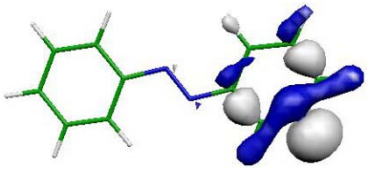

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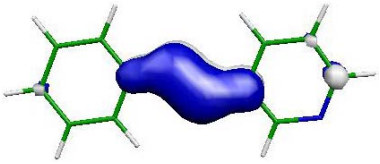

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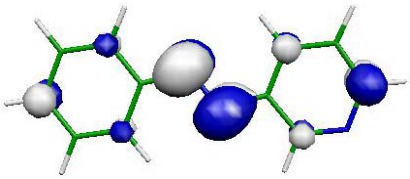

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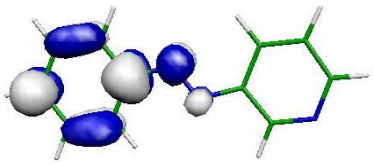

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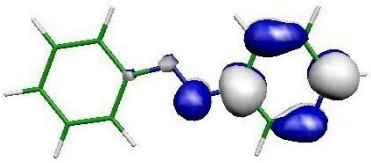

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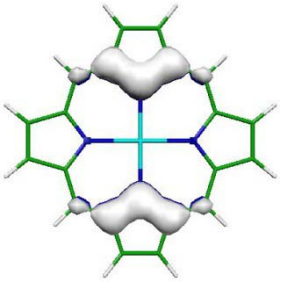
Ni-porphyrin (D_{2h} point group symmetry) [16,14]-CASSCF



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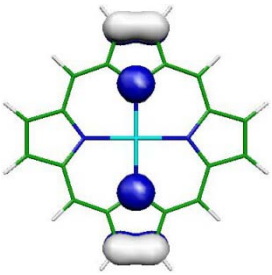

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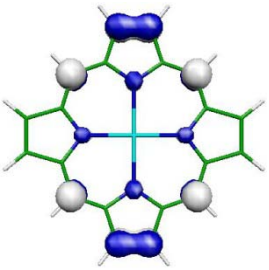

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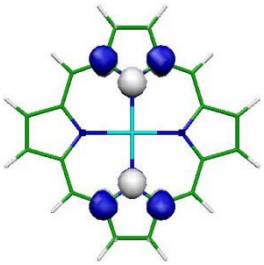

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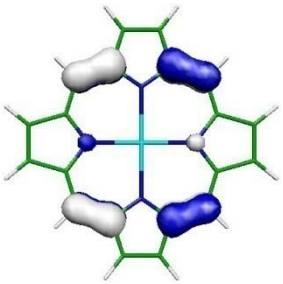

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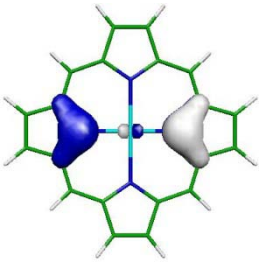

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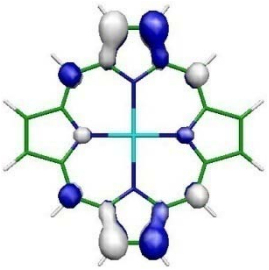

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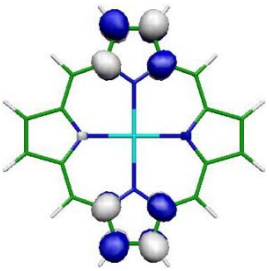

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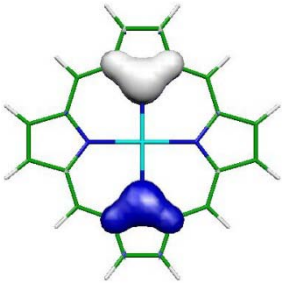

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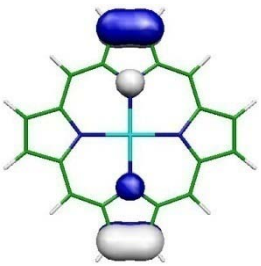

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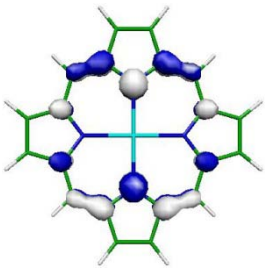

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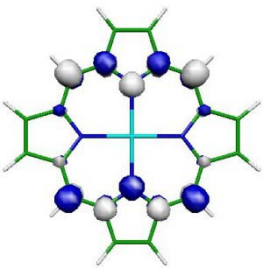

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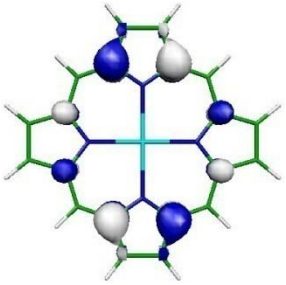

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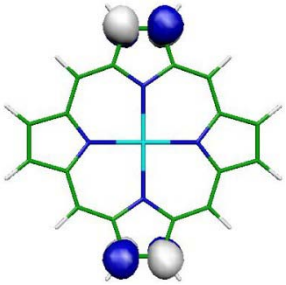

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