Supporting Information

Modular and Versatile Hybrid Coordination Motifs on α-Helical Protein Surfaces

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Section S1. Experimental Figures

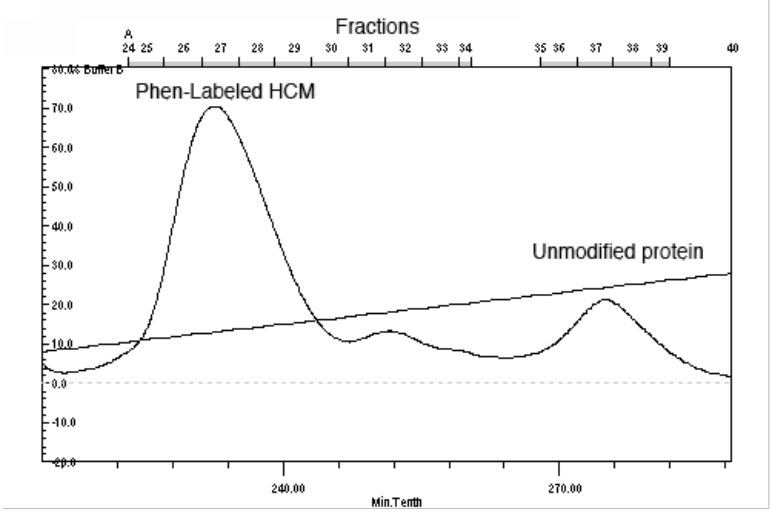

Figure S1.1 A representative FPLC trace (anion-exchange with a 5 mL Bio-Rad Uno-Q cartridge) for the purification of a HPhen2. Protein was prepared in 10 mM sodium phosphate buffer (pH 8) and eluted with a linear gradient of buffer B (0-50% 0.5 M NaCl in 10 mM sodium phosphate (pH 8)). Labeled protein generally elutes between 17.5 and 22% of buffer B. The trace shows three peaks with fractions 25-29 representing pure labeled protein, fractions 31-33 representing labeled protein as the major product along with a small unlabeled impurity, and fractions 36-39 corresponding to unlabeled protein.

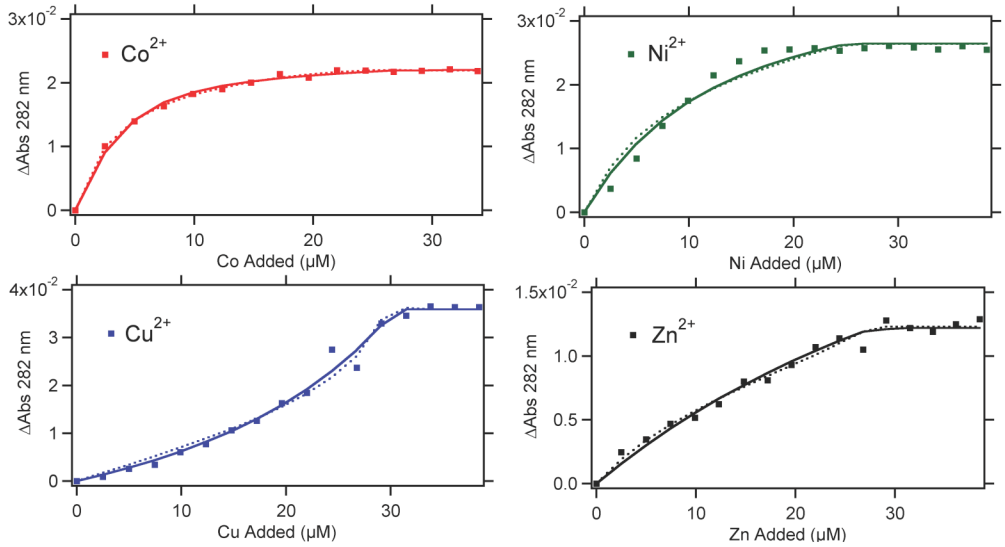

Figure S1.2 Titrations of HPhen2 with late first row transition metals as monitored by UV-vis spectroscopy. See Experimental Section for details. The data were fit to two different models. The first model assumes a simple 1:1 binding (solid line) and the second model uses a 1:1 and 1:2 mechanism (dotted line) the latter of which accounts for protein dimerization. In every case, the data were satisfactorily described by the 1:1 model. Corresponding K_d's can be found in Tables 1 and S2.1.

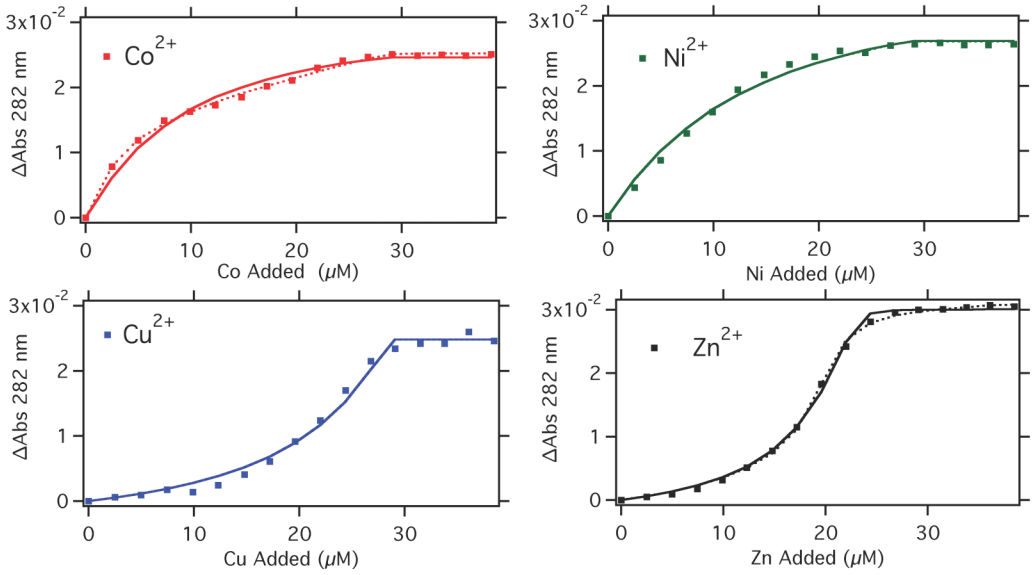

Figure S1.3. Titrations of HPhen3 with late first row transition metals as monitored by UV-vis spectroscopy. See Experimental Section for details. The data were fit to two different models. The first model assumes a simple 1:1 binding (solid line) and the second model uses a 1:1 and 1:2 mechanism (dotted line) the latter of which accounts for protein dimerization. In every case, the data were satisfactorily described by the 1:1 model. Corresponding K_d's can be found in Tables 1 and S2.1.

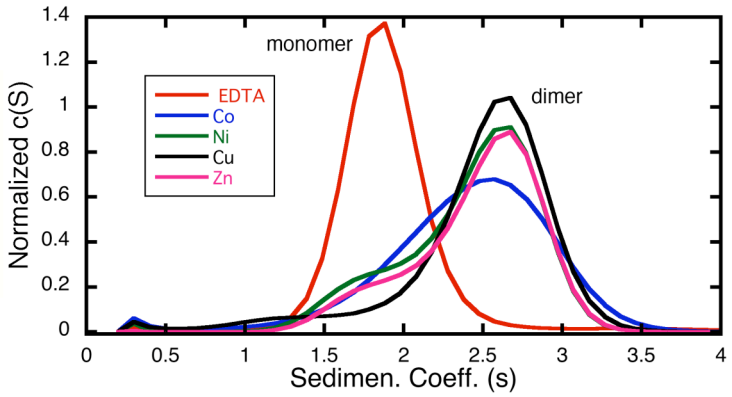

Figure S1.4. Sedimentation velocity profiles for HTerpy1 performed under similar conditions as metal binding titrations (5 µM HTerpy1 and 2.5 µM of M^{2+}). With every metal tested (Co^{2+}(blue), Ni^{2+} (green), Cu^{2+} (black), Zn^{2+}(pink) Metal free/EDTA(Red)), a dimeric species (2.6 S) is the major species present.

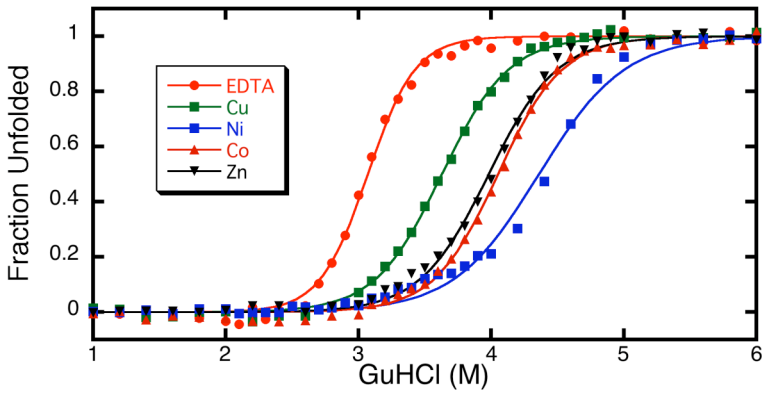

Figure S1.5. Chemical unfolding titrations for HPhen1 in the presence and absence (EDTA) of late first-row transition metals as monitored by CD spectroscopy. Titration data were fit assuming a two-state unfolding model. Fitting parameters are given in Table S2.2.

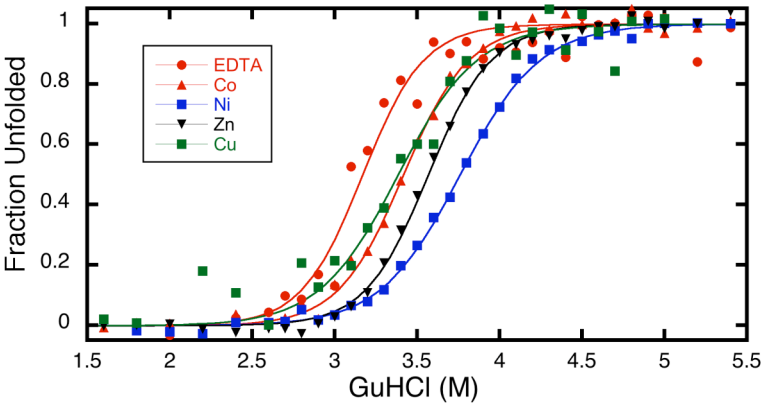

Figure S1.6. Chemical unfolding titrations for HPhen2 in the presence and absence (EDTA) of late first-row transition metals as monitored by CD spectroscopy. Titration data were fit assuming a two-state unfolding model. Fitting parameters are given in Table S2.3.

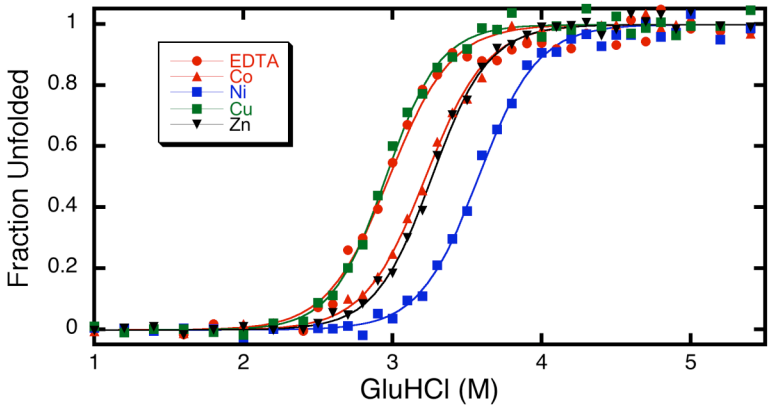

Figure S1.7. Chemical unfolding titrations for HPhen3 in the presence and absence (EDTA) of late first-row transition metals as monitored by CD spectroscopy. Titration data were fit assuming a two-state unfolding model. Fitting parameters are given in Table S2.4.

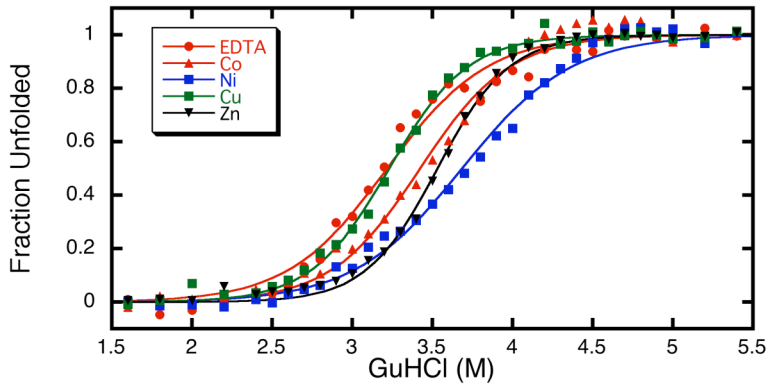

Figure S1.8. Chemical unfolding titrations of HTerpy1 in the presence and absence (EDTA) of late first-row transition metals, as monitored by circular dichroism (CD) spectroscopy. Titration data were fit assuming a two-state unfolding model. Fitting parameters are given in Table S2.5.

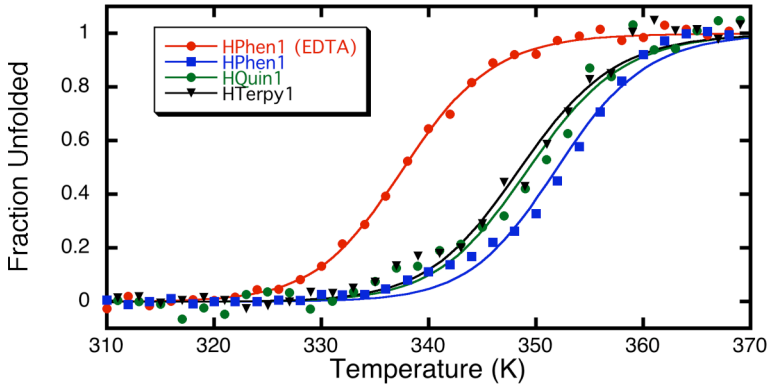

Figure S1.9. Thermal unfolding of 5 μM HPhen1, HQuin1 and HTerpy1 in the presence and absence (EDTA) of 1 mM Ni^{2+} as monitored by CD spectroscopy. Titrations were performed in 100 mM Tris buffer (pH 7.5) with 1.5 M GuHCl and fit to a two-state unfolding model. Fitting parameters are given in Table S2.6.

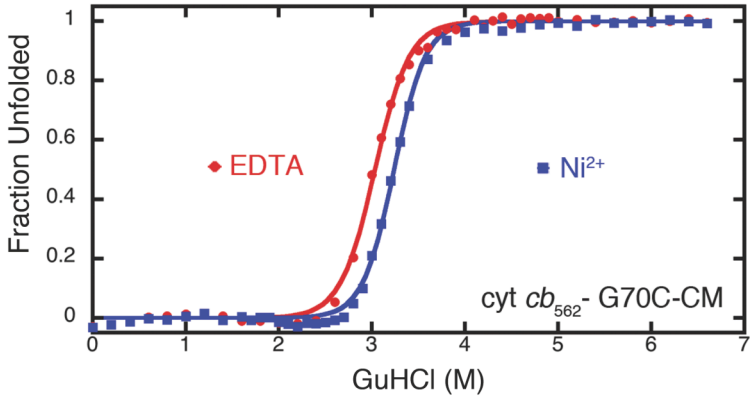

Figure S1.10. Chemical unfolding titration of G70C-CM cyt cb_{562} in the presence and absence (EDTA) of Ni^{2+} as monitored by CD spectroscopy.

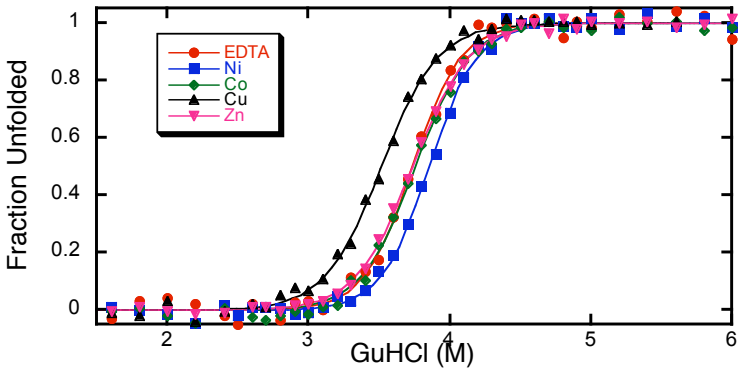

Figure S1.11. Chemical unfolding titration of APhen1 in the presence and absence (EDTA) of M^{2+} as monitored by CD spectroscopy.

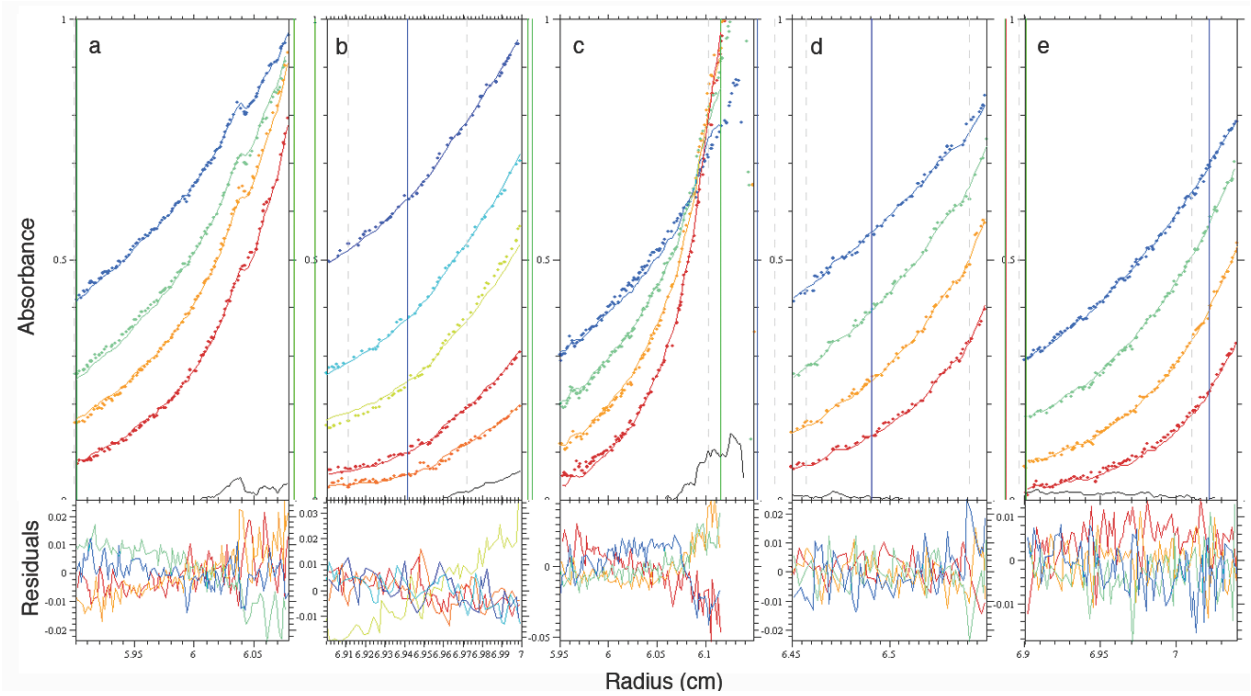

Figure S1.12. Sedimentation equilibrium profiles for HPhen1 in the presence of Ni^{2+}. (a) 10 µM (b) 20 µM (c) 40 µM (d) 60 µM and (e) 100 µM. Scans of each sample were taken after the samples were equilibrated at the following speeds for 14 hrs: 20,000 rpm (blue), 25,000 rpm (green), 30,000 rpm (yellow), 35,000 rpm (red) and 41,000 rpm (orange) rpm. All samples were in 20 mM TRIS buffer (pH 7) with a half equivalent of $NiSO_4$. Scans shown in a), b) and c) were globally fit to a monomer-dimer model yielding a minimized fit with a log $K_{d(2mer\text{-}1mer)}$ = 5.05 ± 0.02 M^{-1} or $K_{d(2mer\text{-}1mer)}$ = 8.9(1) µM. Experiments were conducted at 25°C.

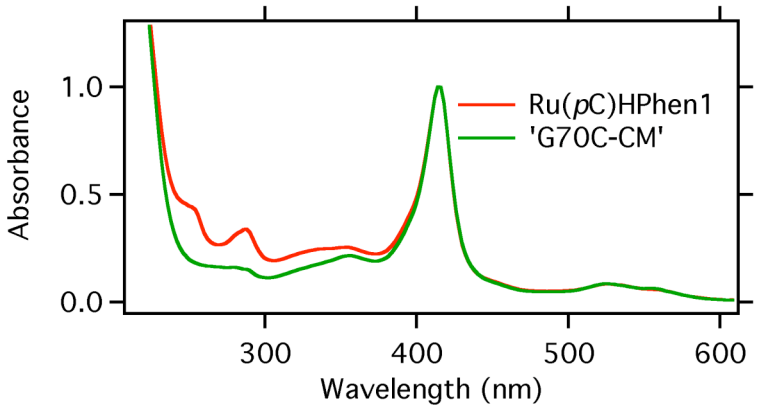

Figure S1.13. UV-visible spectra of Ru(*p*-cymene)-HPhen1 complex and G70C-CM cyt cb_{562}.

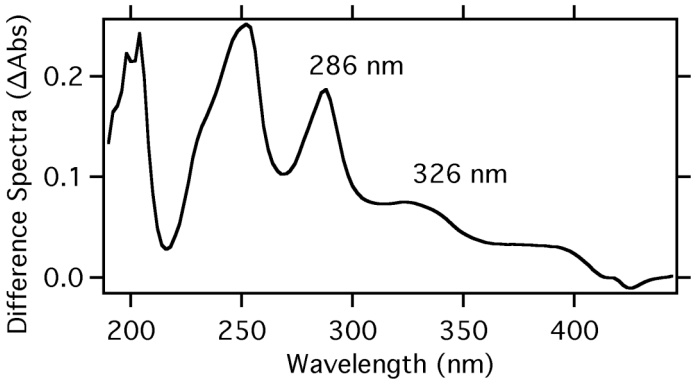

Figure S1.14. Difference spectrum (from Fig. S1.13) highlighting the changes in absorbance upon the formation of the Ru(*p*-cymene)-HPhen1 complex.

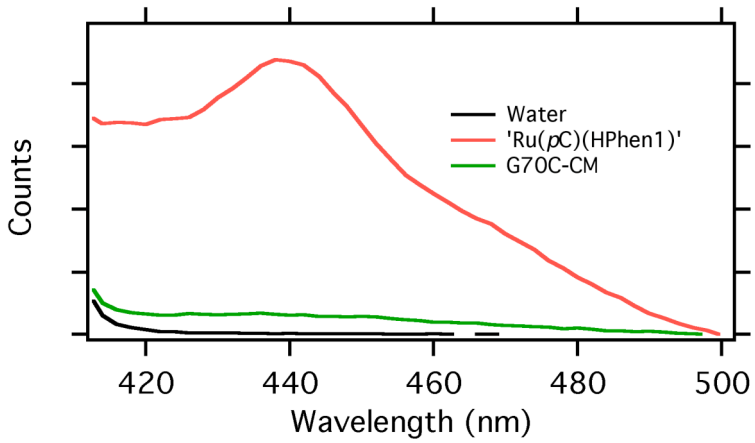

Figure S1.15. Fluorescence spectrum of 5 μM Ru(*p*-cymene)-HPhen1 as compared with that of 5 μM G70C-CM cyt cb_{562}. Spectra were taken in water and prepared anaerobically. (λ_{ex} = 326 nm; λ_{em} = 442 nm)

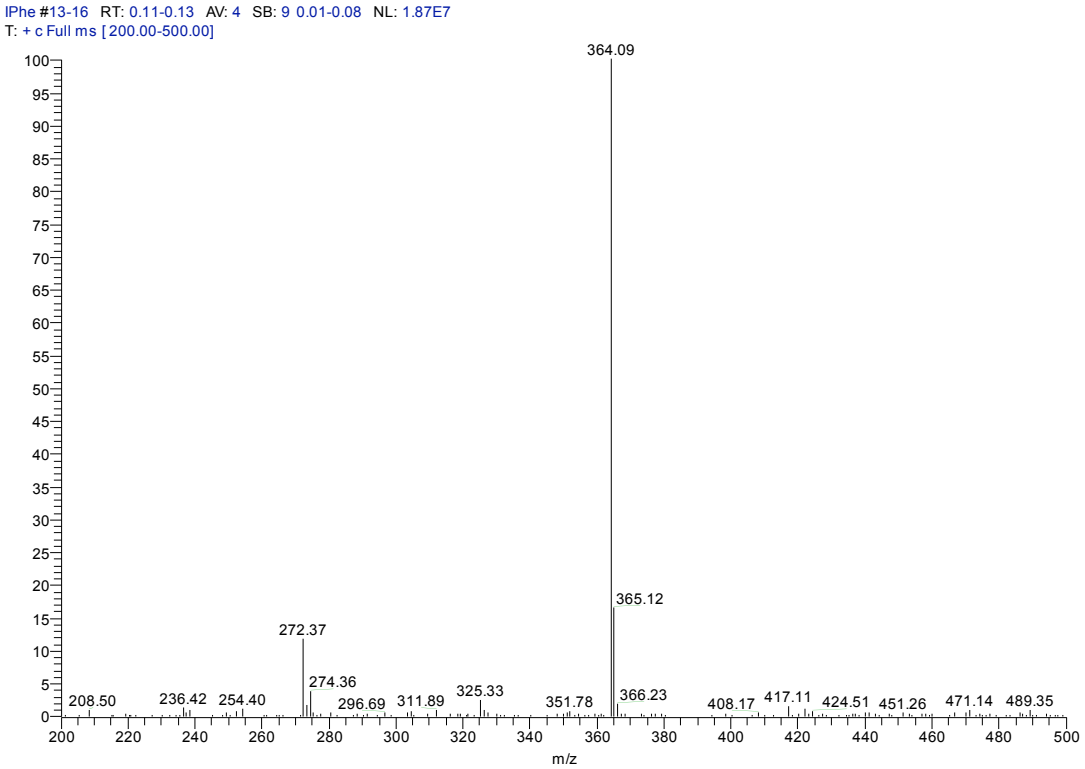

Figure S1.16. ESI-MS (positive mode) of 5-iodoacetamido-1,10-phenanthroline (IA-Phen). Measured MW = 364.09 m/z (exp.: 363.99) ($M + H^+$)

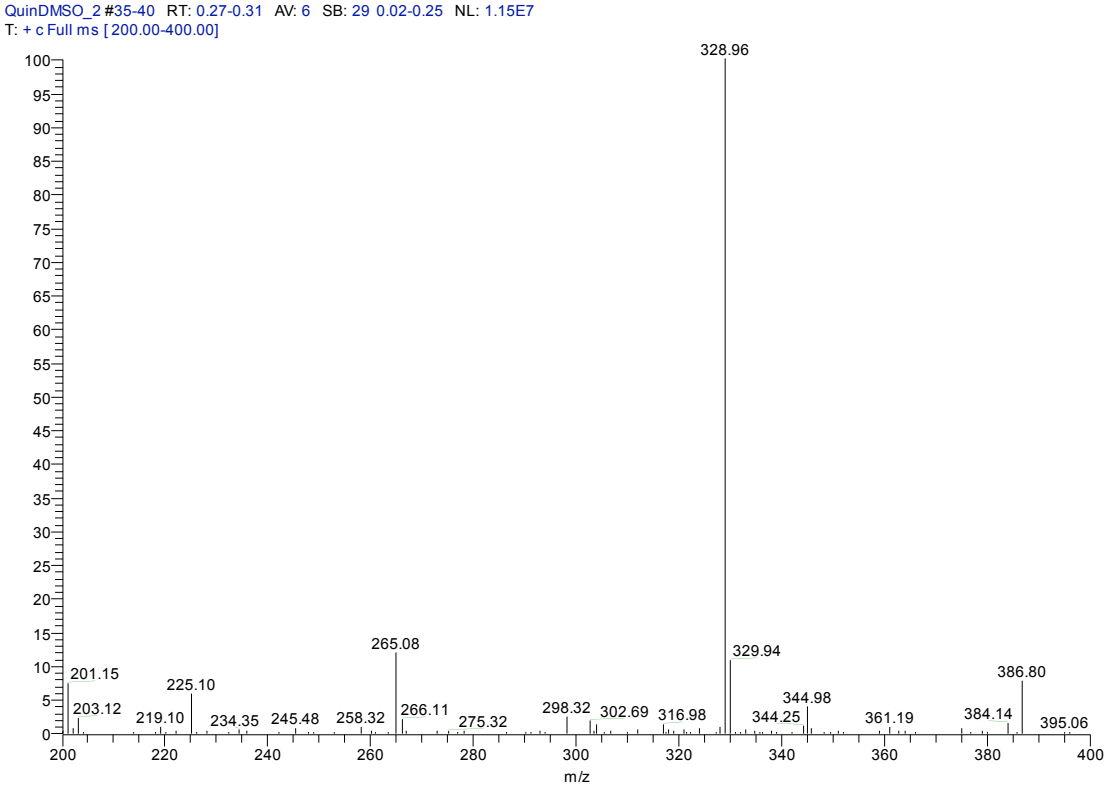

Figure S1.17. ESI-MS (positive mode) of 5-iodoacetamido-8-hydroxyquinoline (IA-Quin). Measured MW = 328.96 m/z (exp.: 363.99) ($M + H^+$)

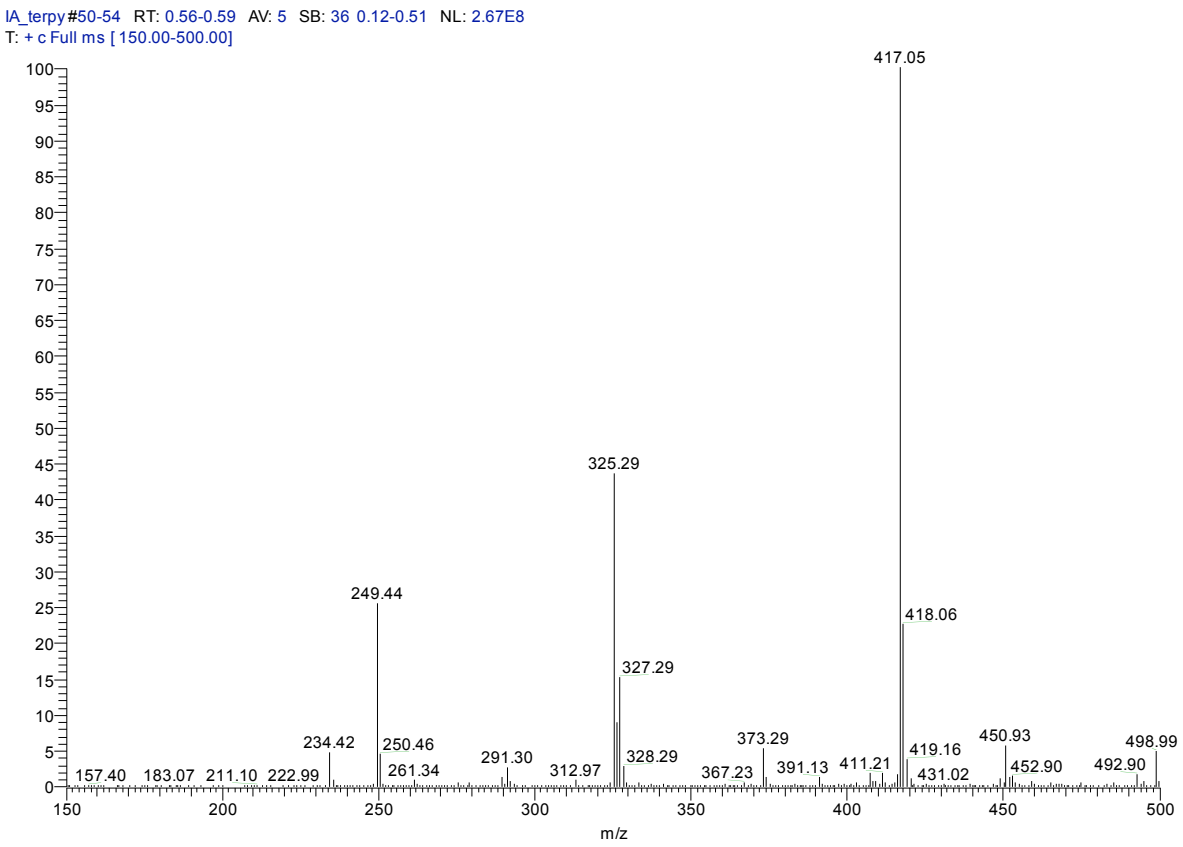

Figure S1.18. ESI-MS (positive mode) of 4-iodoacetamido-2,2':6',2"-terpyridine (ITerpy). Measured MW = 417.05 m/z (exp.: 417.22) ($M + H^+$). Observed peaks at 325.29 and 249.44 m/z correspond to 4-chloroacetamido-2,2':6',2"-terpyridine (ClA-Terpy) and 4-amino-2,2':6',2"-terpyridine (NH_2-Terpy) respectively.

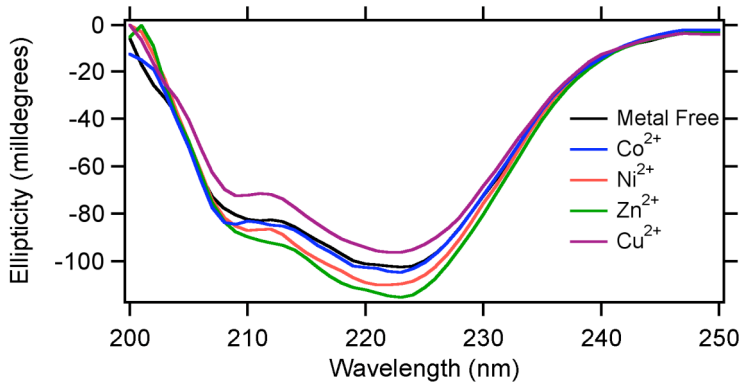

Figure S1.19. Wavelength scan of 6 µM HPhen1 in 20 mM sodium borate buffer (pH 7) at 25 °C and 200 µM of either EDTA (no metal) or M^{2+} as monitored by CD spectroscopy. Data shown are averages of 3 scans and was smoothed with a binomial function.

Section S2. Experimental Tables.

	Dissociation Constants (K_d)		
	HPhen1 (M)	**HPhen2 (M)**	**HPhen3 (M)**
Co^{2+}	4 (4) × 10^{-10}	5 (2) × 10^{-9}	2 (6) × 10^{-10}
Ni^{2+}	2 (80) × 10^{-9}	6 (24) × 10^{-11}	2 (15) × 10^{-10}
Cu^{2+}	6 (4) × 10^{-13}	1 (15) × 10^{-11}	2 (11) × 10^{-11}
Zn^{2+}	3 (3) × 10^{-8}	5 (3) × 10^{-8}	2 (2) × 10^{-7}

Table S2.1. Dissociation constants for metal binding titrations for the HPhen series with M^{2+}. Data were fit using a 1:1/1:2 model, which accounts for both metal binding and protein dimerization. In all cases EGTA was used as competing ligand. EGTA:metal dissociation constants were determined using Maxchelator (http://maxchelator.stanford.edu) (25° C and a ionic strength of 0.05 M) and were held fixed during regression analysis.

Cyt cb_{562} variant	Condition	Slope, m_1 (kcal/mol•M)	$[GuHCl]_m$, m_2 (M)
HPhen1	EDTA	3.2(1)	3.07 (1)
HPhen1	Co	2.42 (5)	4.05 (1)
HPhen1	Ni	1.82 (7)	4.36 (1)
HPhen1	Cu	2.33 (7)	3.63 (1)
HPhen1	Zn	2.26 (6)	3.98 (1)
G70C-CM	EDTA	2.9(1)	3.06(1)
G70C-CM	Ni	3.6(1)	3.24(1)
APhen1	EDTA	3.4 (1)	3.73 (1)
APhen1	Co	3.1 (1)	3.75 (1)
APhen1	Ni	3.4 (1)	3.85 (1)
APhen1	Cu	2.9 (1)	3.51 (1)
APhen1	Zn	2.9 (1)	3.73 (1)
HPhen1	EDTA (pH 5.5)	3.4 (1)	4.51 (1)
HPhen1	Ni (pH 5.5)	2.8 (1)	4.83 (1)

Table S2.2. Fitting parameters for chemical unfolding titrations of cyt cb_{562} variants: HPhen1, APhen1, G70C-CM cyt cb_{562}.

Cyt cb_{562} variant	Condition	Slope, m_1 (kcal/mol•M)	$[GuHCl]_m$, m_2 (M)
HPhen2	EDTA	3.1 (3)	3.16 (2)
HPhen2	Co	2.96 (1)	3.41 (1)
HPhen2	Ni	2.42 (1)	3.76 (1)
HPhen2	Cu	2.4 (2)	3.38 (2)
HPhen2	Zn	3.08 (1)	3.56 (1)

Table S2.3. Fitting parameters for chemical unfolding titrations for HPhen2 with M^{2+}.

Cyt cb_{562} variant	Condition	Slope, m_1 (kcal/mol•M)	$[GuHCl]_m$, m_2 (M)
HPhen3	EDTA	2.83 (2)	2.97 (1)
HPhen3	Co	2.86 (2)	3.21 (1)
HPhen3	Ni	2.96 (1)	3.57 (1)
HPhen3	Cu	3.22 (1)	2.95 (1)
HPhen3	Zn	3.07 (1)	3.26 (1)

Table S2.4. Fitting parameters for chemical unfolding titrations for HPhen3 with M^{2+}.

Cyt cb_{562} variant	Condition	Slope, m_1 (kcal/mol•M)	$[GuHCl]_m$, m_2 (M)
HTerpy1	EDTA	1.89 (1)	3.21 (1)
HTerpy1	Co	2.41 (1)	3.42 (1)
HTerpy1	Ni	1.73 (1)	3.68 (1)
HTerpy1	Cu	2.40 (1)	3.22 (1)
HTerpy1	Zn	2.66 (1)	3.53 (1)
HTerpy1	EDTA (pH 5)	2.67 (1)	4.46 (1)
HTerpy1	Ni (pH 5)	2.54 (1)	4.58 (1)
ATerpy1	EDTA	2.72 (1)	3.56 (1)
ATerpy1	Ni	3.2 4(1)	3.59 (1)

Table S2.5. Fitting parameters for chemical unfolding titrations for HTerpy1 and ATerpy1.

HCM variant	Condition	T_m (K)	slope (kJ/mol)
HPhen1	EDTA	337 (1)	54 (1)
HPhen1	Ni	352 (1)	59 (2)
HQuin1	Ni	349 (1)	55 (4)
HTerpy1	Ni	348 (1)	54 (3)

Table S2.6. Fitting parameters for thermal unfolding titrations of HCM variants: HPhen1, HQuin1 and HTerpy1

Model	Total Bonding Energy (kcal mol^{-1})	ΔE (kcal mol^{-1})
***cis*-HPhen$_2$:Ni BP86**	**-10804.01**	5.35
trans-HPhen$_2$:Ni	-10798.66	
***cis*- Phen$_2$:Ni OLYP**	**-10517.02**	5.01
trans-HPhen$_2$:Ni OLYP	-10512.01	

Table S2.7. Total bonding energies for geometry optimized models. Lowest energy isomer and corresponding total bonding energy are in bold. $\Delta E = \left|\right.$ *trans* isomer – *cis* isomer $\left|\right.$.

Section S3. Input Files For Density Functional Calculations

S3.1. Input file for inner-coordination sphere of the *cis*-HPhen1_2:Ni^{2+} complex (BP86).

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#$ -cwd

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#$ -m beas
#$ -N phentransu
#$ -q adf.q
#$ -pe mpi 8

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export temp_dir="/state/partition1/`whoami`.$JOB_ID"
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cd $temp_dir
echo With temp dir $temp_dir


# ADF enviroment variables, change as you need

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export ADFBIN=/share/apps/adf2007.01/bin
export ADFRESOURCES=/share/apps/adf2007.01/atomicdata
export SCMLICENSE=/share/apps/adf2007.01/license
export SCM_TMPDIR=$temp_dir
export SCM_USETMPDIR=yes
export NSCM=8
export SCM_IOBUFFERSIZE=512


 #Put main code here ***************************************

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TITLE Nicis geo opt

MAXMEMORYUSAGE 7000

RELATIVISTIC ZORA
CHARGE 2 3
UNRESTRICTED

SCF
 ITERATIONS 200
DIIS
END

XC
 LDA VWN
 GGA Becke Perdew
END

SYMMETRY NOSYM
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END

GEOMETRY
 GO
 ITERATIONS 100
 FREQUENCIES
END

BASIS
 type TZ2P
 core none
END

END INPUT
"
# end main code ******************************************

cp * $cur_dir/

# Optional, have to manually clean up otherwise
rm -rf $temp_dir
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S3.2. Input file for inner-coordination sphere of the *trans*-HPhen1_2:Ni^{2+} complex (BP86).

```
#$ -S /bin/bash
#$ -cwd

#$ -o output
#$ -e $JOB_ID.err
#$ -j y
#$ -M rradford@ucsd.edu
#$ -m beas
#$ -N phentransu
#$ -q adf.q
#$ -pe mpi 8

export cur_dir="`pwd`"
echo Running as user `whoami` on `hostname` at `date` in dir `pwd`
export temp_dir="/state/partition1/`whoami`.$JOB_ID"
mkdir $temp_dir
```

```
cd $temp_dir
echo With temp dir $temp_dir


# ADF enviroment variables, change as you need

export ADFHOME=/share/apps/adf2007.01/
export ADFBIN=/share/apps/adf2007.01/bin
export ADFRESOURCES=/share/apps/adf2007.01/atomicdata
export SCMLICENSE=/share/apps/adf2007.01/license
export SCM_TMPDIR=$temp_dir
export SCM_USETMPDIR=yes
export NSCM=8
export SCM_IOBUFFERSIZE=512


 #Put main code here ************************************

$ADFBIN/adf -n8 \
 <<< "
TITLE Nicis geo opt

MAXMEMORYUSAGE 7000

RELATIVISTIC ZORA
CHARGE 2 2
UNRESTRICTED

SCF
 ITERATIONS 200
DIIS
END

XC
 LDA VWN
 GGA Becke Perdew
END

SYMMETRY NOSYM
ATOMS
 C                  0.00000000    0.00000000    0.00000000
 C                  1.49256122    0.00000000    0.00000000
 C                  2.42693295    1.01015667    0.00000000
 N                  2.24529015   -1.16582375    0.02218498
 C                  3.56299355   -0.83228914    0.02976203
 N                  3.70228499    0.48144472    0.01702533
 C                 10.99154846    3.29300696   -0.91732029
 C                  9.76649252    2.57572479   -0.45595145
 C                  8.42465811    2.76330770   -0.70507607
 N                  9.80690694    1.49498046    0.41145927
 C                  8.53483249    1.07600525    0.64896160
 N                  7.67565567    1.83081541   -0.01410612
 Ni                 5.65295941    1.28472803   -0.00859172
 H                 10.74625400    3.95654088   -1.75289337
 H                 11.43520195    3.90761729   -0.11919016
 H                 11.76432279    2.59203105   -1.26701389
 H                 10.64217050    1.07372238    0.79822072
 H                  8.25741807    0.24781706    1.28724959
```

```
 H                  7.96193740    3.50267040   -1.34772477
 H                 -0.40717928   -0.69538441   -0.74906712
 H                 -0.41369760   -0.28481885    0.98041905
 H                 -0.37511359    1.00135511   -0.24127110
 H                  2.25463114    2.07933432   -0.00449593
 H                  4.38130839   -1.54009742    0.02399485
 H                  1.87848777   -2.10952611    0.01533945
 C                  4.69855903    3.62551319   -3.91832339
 C                  6.95525440   -2.59797330   -1.71575989
 C                  4.82493173    3.30322448   -2.55556408
 C                  6.59448059   -1.57173263   -0.83928322
 C                  5.03901876    2.65560725   -4.87776834
 C                  6.86023116   -2.36135354   -3.10540865
 C                  5.83549531    0.42080423   -5.40286890
 C                  6.29574577   -0.85678871   -5.02648906
 C                  5.49251641    1.39752677   -4.46428509
 C                  6.41742319   -1.13716794   -3.63288255
 C                  5.60236718    1.12009014   -3.07825958
 C                  6.06831524   -0.14251271   -2.65864971
 H                  6.37948554   -1.10621310   -7.06050337
 C                  4.55281559    5.02059536    2.00871462
 C                  6.83501076   -1.40804771    3.46938692
 C                  4.92317427    4.10133629    1.01120462
 C                  6.70708636   -0.93097127    2.16266644
 C                  4.64776446    4.63038406    3.35614212
 C                  6.48435915   -0.55161228    4.53602595
 C                  5.20505617    2.94175924    5.01201474
 C                  5.65999496    1.65871079    5.37622809
 C                  5.10422279    3.34686458    3.67888899
 C                  6.01551740    0.75629719    4.33136710
 C                  5.46545152    2.45734126    2.63553763
 C                  5.91620355    1.16093150    2.95677486
 H                  5.77972003    2.51833853    7.10855185
 H                  4.34972070    4.59109841   -4.21974834
 H                  7.29571029   -3.54148639   -1.34323765
 H                  4.57110116    4.02864600   -1.81109536
 H                  6.65641476   -1.72140320    0.21838538
 H                  4.95171578    2.87852403   -5.92064240
 H                  7.13584618   -3.14383389   -3.78117552
 H                  4.20540236    5.99829608    1.74736174
 H                  7.19049349   -2.39954196    3.65772485
 H                  4.85717991    4.37992148   -0.01978279
 H                  6.96446737   -1.55718134    1.33410385
 H                  4.37187037    5.31264037    4.13287167
 H                  6.57952556   -0.91303750    5.53863014
 N                  6.53384187   -1.54391308   -6.17473091
 N                  6.17197396   -0.40312850   -1.32792989
 N                  5.26394220    2.08581038   -2.18284070
 N                  5.36006422    2.87344891    1.34557680
 N                  6.26208552    0.31021958    1.95269374
 N                  5.63233111    1.60284057    6.73419909
 H                  6.35379620    0.99043632    7.05738502
 H                  6.86337833   -2.48716750   -6.13378188
 H                  5.74549280    0.65106919   -6.44391529
 H                  4.92724985    3.62946358    5.78323869
END

GEOMETRY
```

```
 GO
 ITERATIONS 100
 FREQUENCIES
END

BASIS
 type TZ2P
 core none
END

END INPUT
"
# end main code ******************************************

cp * $cur_dir/

# Optional, have to manually clean up otherwise
rm -rf $temp_dir
```

S3.3. Input file for the inner-coordination sphere of the *cis*-HPhen1_2:Ni^{2+} complex (OLYP).

```
#$ -S /bin/bash
#$ -cwd

#$ -o output
#$ -e $JOB_ID.err
#$ -j y
#$ -M rradford@ucsd.edu
#$ -m beas
#$ -N phencisu
#$ -q adf.q
#$ -pe mpi 8

export cur_dir="`pwd`"
echo Running as user `whoami` on `hostname` at `date` in dir `pwd`
export temp_dir="/state/partition1/`whoami`.$JOB_ID"
mkdir $temp_dir
cd $temp_dir
echo With temp dir $temp_dir


# ADF enviroment variables, change as you need

export ADFHOME=/share/apps/adf2007.01/
export ADFBIN=/share/apps/adf2007.01/bin
export ADFRESOURCES=/share/apps/adf2007.01/atomicdata
export SCMLICENSE=/share/apps/adf2007.01/license
export SCM_TMPDIR=$temp_dir
export SCM_USETMPDIR=yes
export NSCM=8
export SCM_IOBUFFERSIZE=512


 #Put main code here ***************************************
```

```
$ADFBIN/adf -n8 \
 <<< "
TITLE phencisu geo opt

MAXMEMORYUSAGE 7000

RELATIVISTIC ZORA
CHARGE 2 2
UNRESTRICTED

SCF
 ITERATIONS 200
DIIS
END

XC
 GGA OLYP
END

SYMMETRY NOSYM
ATOMS
   C         3.646596   -2.316668    4.277425
   C         2.833686   -1.391510    3.436131
   C         2.013071   -1.604722    2.352389
   N         2.746520   -0.034432    3.665771
   C         1.903356    0.513799    2.756207
   N         1.422419   -0.417429    1.942404
   C        -2.649755    2.580494    4.907523
   C        -2.308750    1.713671    3.742030
   C        -1.224684    1.686317    2.896374
   N        -3.137450    0.719682    3.258844
   C        -2.554965    0.144277    2.178770
   N        -1.382143    0.711045    1.920150
   Ni       -0.028201   -0.006653    0.424470
   H         4.670080   -1.941386    4.422577
   H         3.195299   -2.455701    5.271509
   H         3.714716   -3.299681    3.799774
   H         1.836712   -2.553224    1.866928
   H         3.247190    0.476222    4.383491
   H         1.694169    1.573972    2.712869
   H        -3.068163    1.996252    5.739281
   H        -1.752834    3.090709    5.275590
   H        -3.386792    3.350546    4.633735
   H        -0.353676    2.322632    2.952374
   H        -4.029160    0.445007    3.658921
   H        -3.008061   -0.669231    1.631719
   C         2.677497   -2.057177   -2.413996
   C        -1.592429   -4.106877    1.117160
   C         1.141254    4.244071   -0.034398
   C        -2.503340    1.345639   -3.033613
   C         1.654838   -1.806142   -1.479809
   C        -0.871760   -2.905274    1.240705
   C         0.489202    3.073904    0.374242
   C        -1.619907    1.326428   -1.945192
   C         3.464594   -1.015916   -2.859041
   C        -2.509793   -4.248525    0.097677
   C         2.221732    4.144150   -0.893671
   C        -3.245735    0.214422   -3.314965
```

```
   C         3.994734    1.422573   -2.768319
   C        -3.660573   -3.227535   -1.861728
   C        -3.868044   -2.157243   -2.715900
   C         3.735283    2.691459   -2.287016
   C        -2.723287   -3.173113   -0.801541
   C         3.233851    0.293062   -2.366919
   C        -3.109502   -0.933299   -2.507489
   C         2.635513    2.879400   -1.356579
   C        -1.953744   -1.994606   -0.588017
   C         2.186588    0.443244   -1.419586
   C        -2.170293   -0.865679   -1.441780
   C         1.895661    1.748291   -0.909867
   H         2.828423   -3.070699   -2.779410
   H        -1.413910   -4.910208    1.829379
   H         0.786443    5.210882    0.315460
   H        -2.591967    2.242985   -3.642007
   H         1.015973   -2.611876   -1.125248
   H        -0.142818   -2.777550    2.032455
   H        -0.370588    3.117726    1.037222
   H        -1.030623    2.207235   -1.699882
   H         4.256382   -1.187146   -3.587089
   H        -3.075666   -5.171376   -0.020914
   H         2.719557    5.051142   -1.230210
   H        -3.922647    0.228220   -4.167317
   N        -1.032116   -1.876233    0.406975
   N        -1.448888    0.256478   -1.172045
   N         0.857259    1.856834   -0.033405
   N         1.413365   -0.589434   -0.994559
   N         4.436660    3.791143   -2.719318
   N        -4.750490   -2.237688   -3.751645
   H        -5.038287   -1.424927   -4.275334
   H        -5.319812   -3.065768   -3.862516
   H         5.227603    3.628933   -3.330166
   H         4.555621    4.580847   -2.097873
   H         4.809494    1.272918   -3.476648
   H        -4.233844   -4.143327   -1.999235
END

GEOMETRY
 GO
 ITERATIONS 100
 FREQUENCIES
END

BASIS
 type TZ2P
 core none
END

END INPUT
"
# end main code ********************************************

cp * $cur_dir/

# Optional, have to manually clean up otherwise
rm -rf $temp_dir
```

S3.4. Input file for inner-coordination sphere of the *trans*-HPhen1_2:Ni^{2+} complex (OLYP).

```
#$ -S /bin/bash
#$ -cwd

#$ -o output
#$ -e $JOB_ID.err
#$ -j y
#$ -M rradford@ucsd.edu
#$ -m beas
#$ -N phentransu
#$ -q adf.q
#$ -pe mpi 8

export cur_dir="`pwd`"
echo Running as user `whoami` on `hostname` at `date` in dir `pwd`
export temp_dir="/state/partition1/`whoami`.$JOB_ID"
mkdir $temp_dir
cd $temp_dir
echo With temp dir $temp_dir


# ADF enviroment variables, change as you need

export ADFHOME=/share/apps/adf2007.01/
export ADFBIN=/share/apps/adf2007.01/bin
export ADFRESOURCES=/share/apps/adf2007.01/atomicdata
export SCMLICENSE=/share/apps/adf2007.01/license
export SCM_TMPDIR=$temp_dir
export SCM_USETMPDIR=yes
export NSCM=8
export SCM_IOBUFFERSIZE=512


 #Put main code here ***************************************

$ADFBIN/adf -n8 \
 <<< "
TITLE phentransu geo opt

MAXMEMORYUSAGE 7000

RELATIVISTIC ZORA
CHARGE 2 2
UNRESTRICTED

SCF
 ITERATIONS 200
DIIS
END

XC
 GGA OLYP
END

SYMMETRY NOSYM
```

```
ATOMS
  C        -0.346320   -0.738165   -5.586200
   C        -0.225678   -0.176541   -4.209579
   C        -0.291713   -0.757351   -2.964659
   N         0.021772    1.161285   -3.956126
   C         0.096019    1.359410   -2.620295
   N        -0.085666    0.203620   -1.987482
   C        -0.459579   -1.582978    5.244033
   C        -0.185467   -0.866345    3.965354
   C        -0.326274   -1.221924    2.643056
   N         0.320230    0.420290    3.927617
   C         0.459001    0.810902    2.641828
   N         0.075946   -0.171756    1.831264
   Ni        0.005717   -0.037581   -0.084331
   H        -1.109517   -2.443260    5.068453
   H         0.465910   -1.945290    5.712392
   H        -0.962548   -0.924731    5.962669
   H         0.539070    0.993274    4.735904
   H         0.809418    1.788051    2.346498
   H        -0.679654   -2.158784    2.235337
   H        -1.120195   -0.218666   -6.168294
   H         0.601940   -0.656343   -6.136656
   H        -0.614800   -1.798301   -5.539212
   H        -0.457102   -1.795527   -2.718850
   H         0.254118    2.321523   -2.157662
   H         0.131708    1.885394   -4.658142
   C        -3.667215   -1.808998   -0.024867
   C         1.372982   -4.798541   -1.116702
   C        -1.470899    4.772514    0.879471
   C         3.716954    1.662150    0.146046
   C        -2.316492   -1.457624   -0.122741
   C         0.512624   -3.708703   -0.888785
   C        -0.627902    3.742759    0.440954
   C         2.360206    1.363205    0.043886
   C        -4.586869   -0.822324    0.248284
   C         2.731068   -4.593394   -1.027383
   C        -2.805933    4.476470    1.069416
   C         4.624213    0.626383    0.030811
   C        -5.083844    1.535971    0.743896
   C         4.617092   -3.040369   -0.656645
   C         5.112044   -1.779425   -0.406621
   C        -4.691558    2.838845    0.965628
   C         3.226241   -3.299476   -0.729788
   C        -4.158220    0.515396    0.423302
   C         4.178053   -0.685124   -0.220705
   C        -3.286309    3.173541    0.825214
   C         2.267267   -2.259641   -0.534326
   C        -2.766414    0.807059    0.274022
   C         2.766525   -0.923727   -0.290586
   C        -2.332139    2.179803    0.440134
   H        -3.963640   -2.847615   -0.148170
   H         0.961689   -5.776431   -1.359660
   H        -1.079214    5.771146    1.059921
   H         4.037321    2.686166    0.321973
   H        -1.540853   -2.198145   -0.291687
   H        -0.567106   -3.860646   -0.959516
   H         0.426374    3.959220    0.251335
   H         1.601208    2.136761    0.126080
```

```
   H        -5.645246   -1.058569    0.345307
   H         3.433727   -5.409357   -1.191583
   H        -3.475379    5.258726    1.421736
   H         5.684443    0.841191    0.144729
   N        -1.025593    2.490400    0.238543
   N        -1.882405   -0.199374    0.011860
   N         0.930944   -2.480418   -0.598479
   N         1.897898    0.121220   -0.139467
   N         6.461982   -1.546591   -0.283679
   N        -5.585278    3.798834    1.357908
   H        -5.389017    4.776922    1.198641
   H        -6.570461    3.562865    1.368737
   H         6.828704   -0.635127   -0.508371
   H         7.082638   -2.304932   -0.543188
   H        -6.136003    1.265597    0.828404
   H         5.307210   -3.867899   -0.819032
END

GEOMETRY
 GO
 ITERATIONS 100
 FREQUENCIES
END

BASIS
 type TZ2P
 core none
END

END INPUT
"
# end main code ********************************************

cp * $cur_dir/

# Optional, have to manually clean up otherwise
rm -rf $temp_dir
```

Section S4. Results From DFT Calculations

S4.1. Optimized cartesian coordinates and molecular structure for the inner-coordination sphere of the *cis*-HPhen1$_2$:Ni^{2+} complex (BP86).

<Feb24-2010> <20:18:19> Geometry Converged
Coordinates in Geometry Cycle 59

Atom	X	Y	Z (Angstrom)
1.C	3.646596	-2.316668	4.277425
2.C	2.833686	-1.391510	3.436131
3.C	2.013071	-1.604722	2.352389
4.N	2.746520	-0.034432	3.665771
5.C	1.903356	0.513799	2.756207
6.N	1.422419	-0.417429	1.942404
7.C	-2.649755	2.580494	4.907523
8.C	-2.308750	1.713671	3.742030
9.C	-1.224684	1.686317	2.896374
10.N	-3.137450	0.719682	3.258844
11.C	-2.554965	0.144277	2.178770
12.N	-1.382143	0.711045	1.920150
13.Ni	-0.028201	-0.006653	0.424470
14.H	4.670080	-1.941386	4.422577
15.H	3.195299	-2.455701	5.271509
16.H	3.714716	-3.299681	3.799774
17.H	1.836712	-2.553224	1.866928
18.H	3.247190	0.476222	4.383491
19.H	1.694169	1.573972	2.712869
20.H	-3.068163	1.996252	5.739281
21.H	-1.752834	3.090709	5.275590
22.H	-3.386792	3.350546	4.633735
23.H	-0.353676	2.322632	2.952374
24.H	-4.029160	0.445007	3.658921
25.H	-3.008061	-0.669231	1.631719
26.C	2.677497	-2.057177	-2.413996
27.C	-1.592429	-4.106877	1.117160
28.C	1.141254	4.244071	-0.034398
29.C	-2.503340	1.345639	-3.033613
30.C	1.654838	-1.806142	-1.479809
31.C	-0.871760	-2.905274	1.240705
32.C	0.489202	3.073904	0.374242
33.C	-1.619907	1.326428	-1.945192
34.C	3.464594	-1.015916	-2.859041
35.C	-2.509793	-4.248525	0.097677
36.C	2.221732	4.144150	-0.893671
37.C	-3.245735	0.214422	-3.314965
38.C	3.994734	1.422573	-2.768319
39.C	-3.660573	-3.227535	-1.861728
40.C	-3.868044	-2.157243	-2.715900
41.C	3.735283	2.691459	-2.287016
42.C	-2.723287	-3.173113	-0.801541
43.C	3.233851	0.293062	-2.366919
44.C	-3.109502	-0.933299	-2.507489
45.C	2.635513	2.879400	-1.356579
46.C	-1.953744	-1.994606	-0.588017
47.C	2.186588	0.443244	-1.419586
48.C	-2.170293	-0.865679	-1.441780

49.C	1.895661	1.748291	-0.909867
50.H	2.828423	-3.070699	-2.779410
51.H	-1.413910	-4.910208	1.829379
52.H	0.786443	5.210882	0.315460
53.H	-2.591967	2.242985	-3.642007
54.H	1.015973	-2.611876	-1.125248
55.H	-0.142818	-2.777550	2.032455
56.H	-0.370588	3.117726	1.037222
57.H	-1.030623	2.207235	-1.699882
58.H	4.256382	-1.187146	-3.587089
59.H	-3.075666	-5.171376	-0.020914
60.H	2.719557	5.051142	-1.230210
61.H	-3.922647	0.228220	-4.167317
62.N	-1.032116	-1.876233	0.406975
63.N	-1.448888	0.256478	-1.172045
64.N	0.857259	1.856834	-0.033405
65.N	1.413365	-0.589434	-0.994559
66.N	4.436660	3.791143	-2.719318
67.N	-4.750490	-2.237688	-3.751645
68.H	-5.038287	-1.424927	-4.275334
69.H	-5.319812	-3.065768	-3.862516
70.H	5.227603	3.628933	-3.330166
71.H	4.555621	4.580847	-2.097873
72.H	4.809494	1.272918	-3.476648
73.H	-4.233844	-4.143327	-1.999235

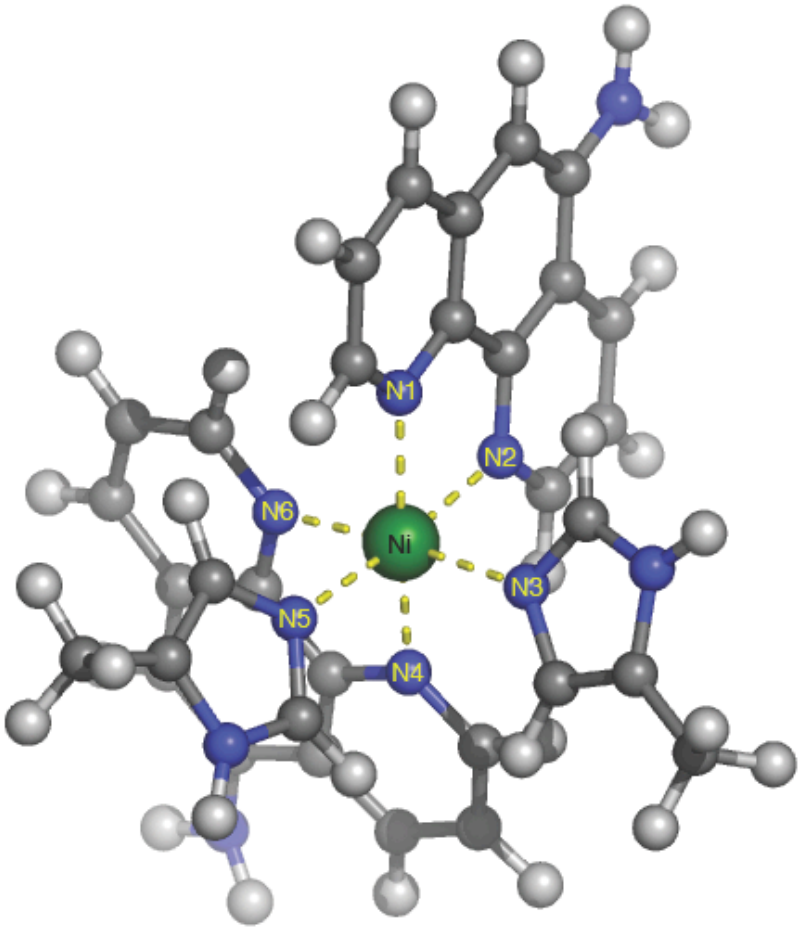

Figure S4.2. Computationally optimized geometry for the inner-sphere of the model *cis*-HPhen1$_2$:Ni^{2+} complex (BP86).

Table S4.3. Calculated bond distances for the computationally minimized inner-coordination sphere of *cis*-HPhen1_2:Ni^{2+} complex.

Bond (Å)	*Cis*-HPhen1_2:Ni^{2+} Model
Ni-N1	2.12
Ni-N2	2.15
Ni-N3	2.14
Ni-N4	2.11
Ni-N5	2.14
Ni-N6	2.10

Table S4.4. Calculated bond angles the inner-coordination sphere of the computationally minimized *cis*-HPhen1_2:Ni^{2+} complex (BP86).

Angle (°)	*Cis*-HPhen1_2:Ni^{2+} Model
N1-Ni-N2	77.8
N1-Ni-N3	90.1
N1-Ni-N4	166.7
N1-Ni-N5	99.0
N1-Ni-N6	94.3
N2-Ni-N3	93.4
N2-Ni-N4	90.4
N2-Ni-N5	175.5
N2-Ni-N6	89.2
N3-Ni-N4	96.8
N3-Ni-N5	89.8
N3-Ni-N6	175.3

S4.5. Optimized cartesian coordinates and molecular structure for the inner-coordination sphere of the *trans*-HPhen1$_2$:Ni^{2+} complex.

<Feb25-2010> <21:17:12> Geometry Converged
  Coordinates in Geometry Cycle 26

Atom	X	Y	Z (Angstrom)
1.C	0.065415	0.502308	0.026248
2.C	1.538608	0.274729	0.063979
3.C	2.619108	1.124516	-0.009279
4.N	2.100447	-0.983148	0.192705
5.C	3.449462	-0.867699	0.187827
6.N	3.801323	0.406944	0.067866
7.C	10.761681	3.644221	-1.145690
8.C	9.674188	2.765409	-0.627640
9.C	8.313574	2.733377	-0.837653
10.N	9.908357	1.732628	0.262025
11.C	8.732863	1.129878	0.560269
12.N	7.736940	1.714418	-0.095784
13.Ni	5.748174	1.111962	-0.029650
14.H	10.364085	4.344997	-1.886160
15.H	11.221799	4.231618	-0.338292
16.H	11.556113	3.057582	-1.627718
17.H	10.812639	1.471646	0.639743
18.H	8.650923	0.299739	1.246552
19.H	7.726311	3.377660	-1.478770
20.H	-0.410788	-0.088967	-0.768204
21.H	-0.410095	0.229276	0.978936
22.H	-0.149425	1.557599	-0.167191
23.H	2.608414	2.201708	-0.111290
24.H	4.116481	-1.714970	0.260784
25.H	1.586983	-1.854751	0.266162
26.C	4.602335	3.542898	-3.650128
27.C	7.086733	-2.711133	-2.020289
28.C	4.765395	3.097498	-2.328030
29.C	6.761954	-1.736063	-1.074192
30.C	4.990623	2.726897	-4.687452
31.C	6.945095	-2.405659	-3.358750
32.C	5.867591	0.530127	-5.415866
33.C	6.339681	-0.738507	-5.132009
34.C	5.515620	1.443521	-4.395251
35.C	6.491645	-1.128452	-3.741182
36.C	5.664111	1.095919	-3.021578
37.C	6.168549	-0.207783	-2.698417
38.H	6.544714	-1.348098	-7.094767
39.C	4.610770	4.984522	1.904002
40.C	6.579978	-1.412344	3.708425
41.C	4.990698	4.002458	0.972856
42.C	6.442552	-0.987706	2.381731
43.C	4.608350	4.667815	3.244171
44.C	6.309324	-0.510445	4.718710
45.C	5.146553	3.025875	5.015518
46.C	5.605309	1.789312	5.412660
47.C	5.019220	3.377609	3.646906
48.C	5.905216	0.796455	4.394951
49.C	5.350467	2.439305	2.625921
50.C	5.778903	1.131503	3.010477
51.H	5.616521	2.198872	7.418898
52.H	4.168265	4.523643	-3.833763

53.H	7.446194	-3.685401	-1.695523
54.H	4.416262	3.721672	-1.515641
55.H	6.889193	-1.958353	-0.022354
56.H	4.878881	3.041467	-5.723575
57.H	7.191974	-3.164027	-4.099185
58.H	4.335450	5.976367	1.554624
59.H	6.884643	-2.433542	3.923655
60.H	5.053669	4.267213	-0.075362
61.H	6.650957	-1.694879	1.586046
62.H	4.322470	5.403923	3.994217
63.H	6.389897	-0.832573	5.755382
64.N	6.647464	-1.616858	-6.126208
65.N	6.299557	-0.522743	-1.382094
66.N	5.315593	1.925927	-2.001498
67.N	5.309467	2.753708	1.298257
68.N	6.065443	0.236030	2.020178
69.N	5.731526	1.457417	6.738334
70.H	6.397917	0.749342	7.015132
71.H	7.014368	-2.537382	-5.948192
72.H	5.742397	0.838611	-6.452824
73.H	4.905059	3.779652	5.764288

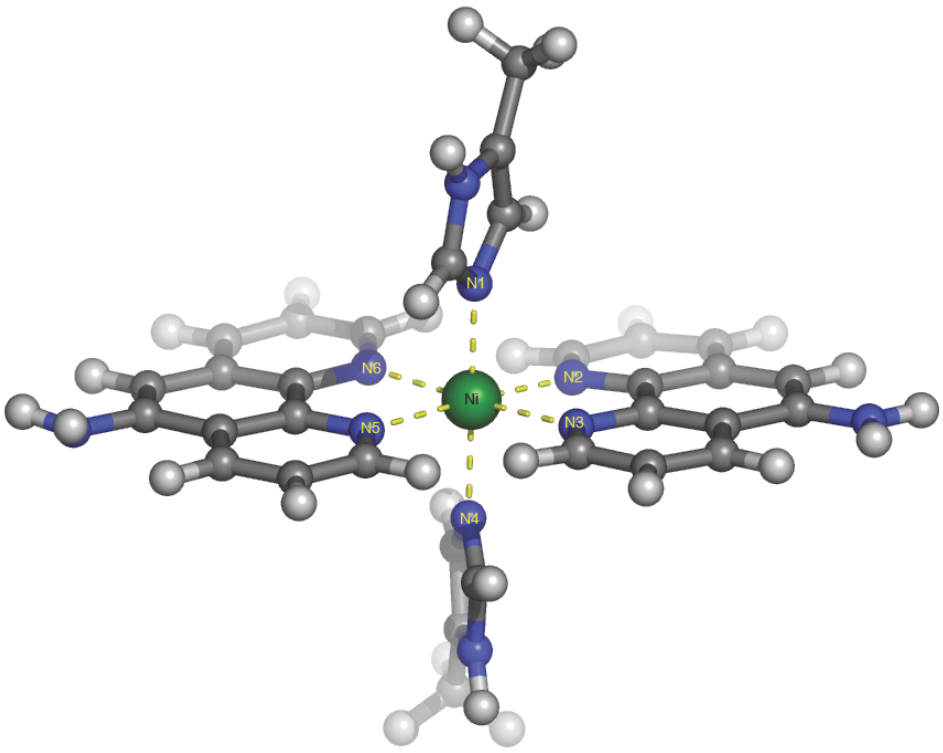

Figure S4.6. Optimized geometry of the inner-coordination sphere of the *trans*-HPhen1_2:Ni^{2+} complex (BP86).

Table S4.7. Calculated bond distances for the computational minimized inner-coordination sphere of the *trans*-HPhen1_2:Ni^{2+} complex (BP86).

Bond (Å)	*trans*-HPhen1_2:Ni^{2+} Model
Ni-N1	2.08
Ni-N2	2.18
Ni-N3	2.19
Ni-N4	2.25
Ni-N5	2.16
Ni-N6	2.07

Table S4.8 Calculated bond angles for the computationally minimized inner-coordination sphere of the HPhen1_2:Ni^{2+} complex (BP86).

Angle (°)	Model
N1-Ni-N2	93.0
N1-Ni-N3	87.4
N1-Ni-N4	90.4
N1-Ni-N5	89.6
N1-Ni-N6	176.8
N2-Ni-N3	76.7
N2-Ni-N4	176.6
N2-Ni-N5	103.4
N2-Ni-N6	89.0
N3-Ni-N4	103.6
N3-Ni-N5	177.0
N3-Ni-N6	90.6

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S4.9 Optimized cartesian coordinates for the inner-coordination sphere of the *cis*-HPhen1$_2$:Ni^{2+} complex (OLYP).

<Feb27-2010> <07:11:25> Geometry Converged
  Coordinates in Geometry Cycle 13

Atom	X	Y	Z (Angstrom)
1.C	3.713803	-2.392940	4.257187
2.C	2.896331	-1.451127	3.440179
3.C	2.081145	-1.619910	2.346650
4.N	2.803770	-0.105677	3.721713
5.C	1.967507	0.472253	2.833562
6.N	1.490425	-0.421308	1.981880
7.C	-2.716451	2.614526	4.972299
8.C	-2.371958	1.764641	3.796451
9.C	-1.262008	1.700191	2.990533
10.N	-3.220818	0.816594	3.269257
11.C	-2.627312	0.236173	2.203865
12.N	-1.422789	0.747912	1.995832
13.Ni	-0.031127	-0.003427	0.429434
14.H	4.751508	-2.054229	4.347301
15.H	3.307549	-2.493390	5.270728
16.H	3.723395	-3.384484	3.801801
17.H	1.915609	-2.532706	1.798518
18.H	3.287325	0.375940	4.466211
19.H	1.760717	1.527576	2.841783
20.H	-3.001167	2.008995	5.839607
21.H	-1.860154	3.227312	5.260596
22.H	-3.550549	3.289514	4.748782
23.H	-0.366970	2.289442	3.090818
24.H	-4.136423	0.579033	3.624756
25.H	-3.101715	-0.541999	1.630498
26.C	2.703242	-2.029957	-2.422951
27.C	-1.656310	-4.126880	1.122740
28.C	1.175843	4.276247	-0.068911
29.C	-2.555512	1.322035	-3.024046
30.C	1.688392	-1.776001	-1.485937
31.C	-0.957732	-2.917399	1.269678
32.C	0.523200	3.111178	0.343274
33.C	-1.673185	1.302255	-1.939374
34.C	3.480315	-0.988263	-2.876155
35.C	-2.526658	-4.281161	0.068030
36.C	2.255043	4.169924	-0.924041
37.C	-3.276674	0.184755	-3.319009
38.C	4.008859	1.442241	-2.793994
39.C	-3.647744	-3.269100	-1.906241
40.C	-3.865236	-2.199774	-2.752213
41.C	3.764517	2.711391	-2.315571
42.C	-2.728531	-3.208198	-0.832873
43.C	3.247893	0.318245	-2.386570
44.C	-3.125101	-0.969652	-2.526835
45.C	2.667328	2.904911	-1.384195
46.C	-1.976154	-2.025429	-0.600407
47.C	2.207108	0.470635	-1.434986
48.C	-2.191393	-0.896494	-1.455953
49.C	1.923177	1.779218	-0.930121
50.H	2.855910	-3.042910	-2.781057

51.H	-1.500637	-4.923780	1.842979
52.H	0.822342	5.243079	0.273968
53.H	-2.658160	2.223268	-3.618983
54.H	1.060908	-2.582621	-1.127127
55.H	-0.284864	-2.772206	2.103493
56.H	-0.337114	3.167551	0.997728
57.H	-1.099298	2.185053	-1.692237
58.H	4.266931	-1.158423	-3.605769
59.H	-3.072191	-5.210556	-0.070791
60.H	2.749618	5.074807	-1.259615
61.H	-3.947819	0.201225	-4.170843
62.N	-1.088137	-1.899402	0.421176
63.N	-1.486175	0.230433	-1.177310
64.N	0.888426	1.895507	-0.055899
65.N	1.442788	-0.562921	-1.003362
66.N	4.480483	3.798913	-2.762165
67.N	-4.728298	-2.296529	-3.807449
68.H	-5.101777	-1.473540	-4.246055
69.H	-5.322769	-3.107583	-3.869982
70.H	5.303879	3.599058	-3.310092
71.H	4.613284	4.577822	-2.137835
72.H	4.815076	1.285258	-3.504867
73.H	-4.204924	-4.189548	-2.053730

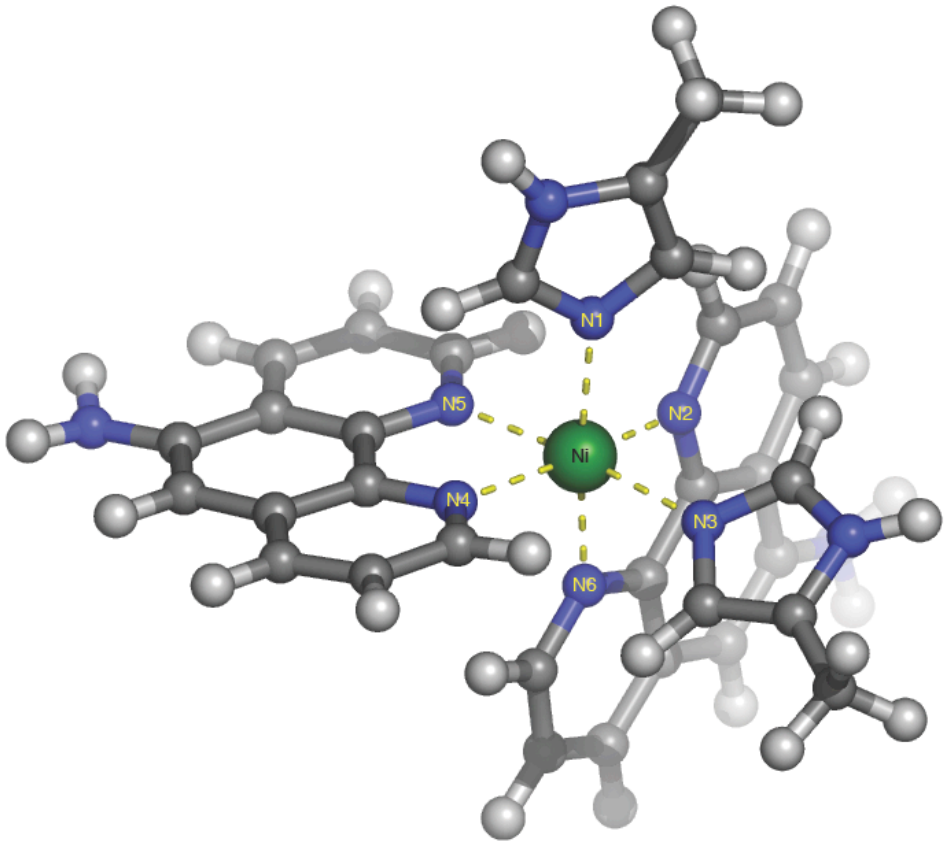

Figure S4.10. Optimized geometry of the inner-coordination sphere for the HPhen1$_2$:Ni^{2+} complex (OLYP).

Bond (Å)	Model
Ni-N1	2.23
Ni-N2	2.16
Ni-N3	2.21
Ni-N4	2.17
Ni-N5	2.18
Ni-N6	2.13

Table S4.11. Calculated bond distances for the computationally minimized inner-coordination sphere of the $HPhen1_2:Ni^{2+}$ complex (OLYP).

Angle (°)	Model
N1-Ni-N2	97.3
N1-Ni-N3	89.9
N1-Ni-N4	89.6
N1-Ni-N5	93.7
N1-Ni-N6	173.9
N2-Ni-N3	91.7
N2-Ni-N4	166.4
N2-Ni-N5	91.4
N2-Ni-N6	77.6
N3-Ni-N4	99.9
N3-Ni-N5	174.77
N3-Ni-N6	86.9

Table S4.12. Calculated bond angles for the computationally minimized inner-coordination sphere for the $HPhen1_2:Ni^{2+}$ complex (OLYP).

S4.13 Optimized cartesian coordinates for inner-coordination sphere of the *trans*-HPhen1$_2$:Ni^{2+} complex (OLYP).

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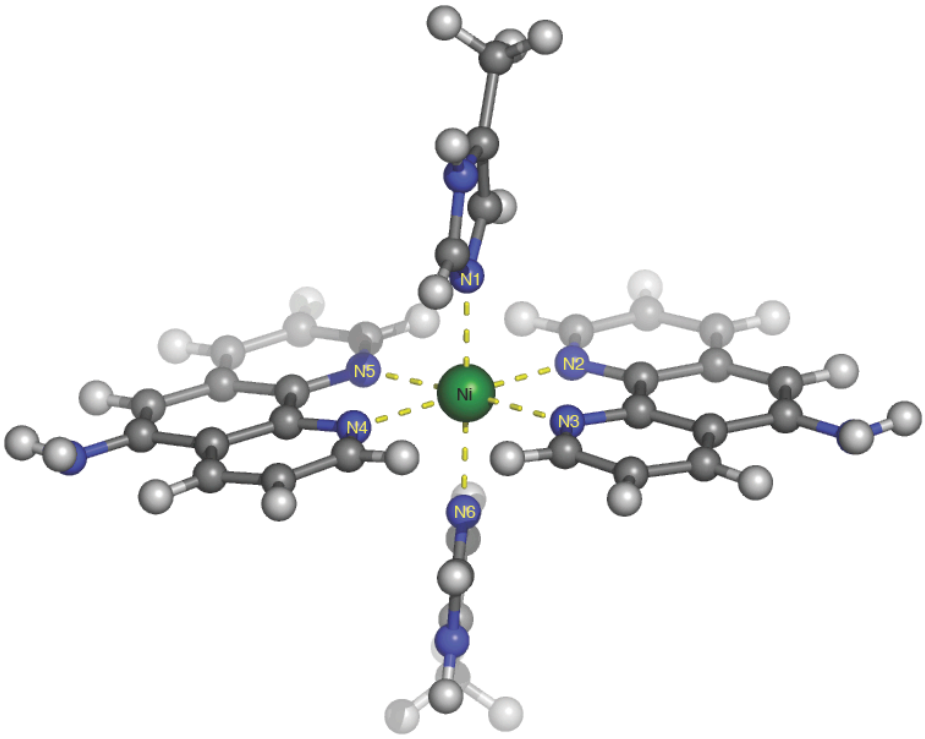
<Feb27-2010> <10:39:01>  Geometry Converged
  Coordinates in Geometry Cycle 17
    Atom         X           Y           Z   (Angstrom)
    1.C       -0.378602   -0.741591   -5.837344
    2.C       -0.229027   -0.168909   -4.469181
    3.C       -0.307592   -0.721247   -3.214199
    4.N        0.054664    1.159724   -4.234325
    5.C        0.133734    1.365555   -2.901788
    6.N       -0.079810    0.236484   -2.243113
    7.C       -0.527704   -1.757903    5.379347
    8.C       -0.229236   -1.001967    4.129398
    9.C       -0.374093   -1.297311    2.795375
   10.N        0.319648    0.262845    4.138104
   11.C        0.481092    0.681448    2.865477
   12.N        0.067513   -0.245462    2.014534
   13.Ni      -0.006733   -0.044517   -0.122052
   14.H       -1.085650   -2.667195    5.150417
   15.H        0.390813   -2.048931    5.901143
   16.H       -1.130335   -1.160807    6.072516
   17.H        0.551011    0.799250    4.961693
   18.H        0.889996    1.646975    2.620557
   19.H       -0.765535   -2.204433    2.364435
   20.H       -1.179313   -0.246482   -6.397915
   21.H        0.545662   -0.641967   -6.417704
   22.H       -0.620723   -1.804085   -5.778470
   23.H       -0.512041   -1.749996   -2.968731
   24.H        0.333620    2.333772   -2.474468
   25.H        0.172949    1.871274   -4.941635
   26.C       -4.050286   -1.839631   -0.039377
   27.C        1.188421   -4.453450   -0.861949
   28.C       -1.274739    4.462314    0.755860
   29.C        4.052239    1.773969    0.097208
   30.C       -2.685858   -1.576292   -0.207221
   31.C        0.442512   -3.288670   -0.631410
   32.C       -0.538406    3.334844    0.383518
   33.C        2.676488    1.556365    0.028591
   34.C       -4.880948   -0.810739    0.329920
   35.C        2.559550   -4.376736   -0.861394
   36.C       -2.626663    4.318086    0.981258
   37.C        4.895555    0.691122   -0.029420
   38.C       -5.162442    1.586295    0.835925
   39.C        4.583750   -2.981532   -0.628216
   40.C        5.196463   -1.763468   -0.435821
   41.C       -4.659426    2.857988    0.983647
   42.C        3.177400   -3.125882   -0.637850
   43.C       -4.340007    0.481732    0.512627
   44.C        4.362164   -0.591798   -0.244728
   45.C       -3.232803    3.059629    0.815279
   46.C        2.329500   -1.998286   -0.445537
   47.C       -2.939435    0.647192    0.319831
   48.C        2.940817   -0.714344   -0.268027
   49.C       -2.383634    1.962403    0.469449
```

50.H	-4.425637	-2.844044	-0.204101
51.H	0.673787	-5.393868	-1.031793
52.H	-0.782833	5.423257	0.867869
53.H	4.436432	2.775893	0.253859
54.H	-2.031560	-2.377978	-0.503633
55.H	-0.633803	-3.367705	-0.617764
56.H	0.520231	3.452180	0.189053
57.H	2.002962	2.394558	0.117857
58.H	-5.945653	-0.974594	0.468231
59.H	3.169670	-5.259334	-1.030955
60.H	-3.203934	5.180911	1.294970
61.H	5.965214	0.849458	0.048589
62.N	-1.049595	2.114191	0.258564
63.N	-2.125157	-0.386292	-0.024207
64.N	0.974384	-2.085140	-0.434002
65.N	2.120385	0.360954	-0.128353
66.N	6.563553	-1.657262	-0.368438
67.N	-5.471103	3.909545	1.338297
68.H	-5.231645	4.838762	1.034076
69.H	-6.464936	3.737826	1.313441
70.H	7.006986	-0.795827	-0.636422
71.H	7.096068	-2.472285	-0.632700
72.H	-6.228364	1.412843	0.947778
73.H	5.190052	-3.868274	-0.787588

Figure S4.14. Optimized geometry for the computationally minimized inner-coordination sphere of the HPhen1_2:Ni^{2+} complex (OLYP).



Bond (Å)	Model
Ni-N1	2.14
Ni-N2	2.29
Ni-N3	2.17
Ni-N4	2.43
Ni-N5	2.15
Ni-N6	2.15

Table S4.15. Calculated bond distances for computationally minimized inner-coordination sphere of the *trans*-HPhen1_2:Ni^{2+} complex (OLYP).

Angle (°)	Model
N1-Ni-N2	89.8
N1-Ni-N3	90.3
N1-Ni-N4	91.3
N1-Ni-N5	91.8
N1-Ni-N6	177.8
N2-Ni-N3	75.2
N2-Ni-N4	178.8
N2-Ni-N5	106.7
N2-Ni-N6	92.1
N3-Ni-N4	104.8
N3-Ni-N5	177.0
N3-Ni-N6	89.2

Table S4.16. Calculated bond angles for the computationally minimized inner-coordination sphere of the HPhen1_2:Ni^{2+} complex (OLYP).