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### Supporting Information for

## Efficient electro/photocatalytic water reduction using a $[\text{Ni}^{\text{II}}(\text{N}_2\text{Py}_3)]$ complex

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## Materials and Methods

### Materials

All the reagents and solvents were used as received from commercial sources.

### General methods

<sup>1</sup>H-NMR spectra were recorded in a Mercury FT-NMR 400 MHz instrument using CDCl<sub>3</sub> as the solvent. Infrared spectra were obtained as KBr pellets on a Bruker Tensor 27 FTIR spectrometer scanning from 4000 to 650 cm<sup>-1</sup>. ESI-(+) mass spectrometry was measured in a triple quadrupole Micromass Quattro LC equipment. The elemental analysis (C, H, N) was performed using an Exeter analytical CHN analyzer by Midwest Microlab, Indianapolis, IN, USA. Single crystal X-ray diffraction was performed in a Bruker X8 APEX-II kappa geometry diffractometer with Mo radiation and a graphite monochromator. Various programs and softwares such as APEX-II, SHELX, COSMO, APEX II, SAINT, and SADABS were used to solve and refine the structure. UV-visible spectra were recorded in acetonitrile or pH 7 phosphate buffer solutions and obtained in a Varian Cary 50 spectrophotometer in the range of 200 to 1650 nm with quartz cells at room temperature. Values of  $\epsilon$  are given in M<sup>-1</sup> cm<sup>-1</sup>.

### Electrochemistry and bulk electrolysis

The electrochemical behavior of the complex was investigated with a BAS 50W potentiostat/galvanostat. Cyclic voltammograms (CV) were obtained at room temperature in acetonitrile containing 0.1 M of *n*-Bu<sub>4</sub>NPF<sub>6</sub> as the supporting electrolyte under argon atmosphere. The electrochemical cell employed three electrodes: glassy-carbon (working), platinum wire (auxiliary) and Ag/AgCl (reference). The ferrocene/ferrocenium redox couple Fc/Fc<sup>+</sup> ( $E^{\circ} = 401 \text{ mV}_{\text{NHE}}$ ) was used as the internal standard. Peak to peak potential separations ( $\Delta E_p = |E_{pc} - E_{pa}|$ ) and  $|i_{pa} / i_{pc}|$  values were measured to evaluate the reversibility of the redox processes.

Bulk electrolysis (BE) was performed in a custom-made air-tight H-type cell under inert conditions. The cell was comprised of two compartments separated by a frit. On one side of the frit the working (vitreous carbon) and reference electrodes (Ag/AgCl) were placed, while the auxiliary electrode (coiled 12 inch Pt wire) was placed on the other side. BE experiments were performed in acetonitrile (20 mL) with *n*-Bu<sub>4</sub>NPF<sub>6</sub> as the supporting electrolyte until the calculated final charges were reached. All potentials were measured versus the Ag/AgCl reference electrode. During BE, potentials were controlled by a BAS 50W potentiostat/galvanostat, and the UV-visible spectra were collected after BE with a Varian Cary 50 apparatus at room temperature.

### Electrocatalysis

Electrocatalysis was performed in the above-described custom-made air-tight H-type cell under inert conditions, where one side of the frit the working (mercury pool) and reference electrodes (Ag/AgCl) were placed, while the auxiliary electrode (coiled 12 inch Pt wire) was placed on the other side. During electrocatalysis the cell was purged with N<sub>2</sub> gas for 10-15 min. followed by sampling of the head space gas (100  $\mu$ L) to ensure an O<sub>2</sub> free environment in the gas-chromatograph. For water reduction (phosphate buffer medium) 0.14  $\mu$ mol (0.1 mg) of **1** was used; for proton reduction (acetonitrile medium) 5.0  $\mu$ mol (3.5 mg) of **1** was used. The volume of the phosphate buffer/acetonitrile that is used for electrocatalysis was 20 ml. The amount of hydrogen generated was determined in a Gow-Mac 400 gas chromatograph (GC) equipped with a thermal conductivity detector, and a 8 ft x 1/8 in., 5 Å molecular sieve column operating at a temperature of 60°C. Nitrogen was used as a carrier gas at a flow rate of 30 mL.min<sup>-1</sup>. The amount of H<sub>2</sub> produced was quantified using a calibration curve of moles of hydrogen versus peak area. Turnover numbers and the Faradaic efficiency of the metal complex were calculated from the amount of H<sub>2</sub> released and the charge consumed as shown below:

**Turnover number (TON):** The number of moles of hydrogen generated per mole of catalyst used.

**TON** = number of moles of hydrogen / number of moles of catalyst

**Faradaic efficiency (FE):** The ratio of the number of moles of hydrogen generated ( $n_{\text{H}_2}$ ) to half of the moles of the number of electrons passed during the BE experiment ( $n_e/2$ ).

**FE** =  $n_{\text{H}_2} / (n_e/2)$

### X-ray structural determination

A pink colored hexagonal-shaped crystal of dimensions 0.26 x 0.41 x 0.56 mm was mounted on a mitogen loop using paratone oil. Diffraction data were collected on a Bruker APEX-II Kappa geometry diffractometer with Mo radiation and a graphite monochromator using a Bruker charge-coupled device (CCD) detector equipped with an Oxford Cryostream low-temperature apparatus. Data was measured at a temperature of 100 K with omega and phi scans of 0.5° per frame for 10 s. The crystal structure was solved by direct methods using the SHELXS-97 program which is part of APEX II suite and refined by least squares method on SHELXL-97, which was incorporated in OLEX2.<sup>1,2</sup> The structure was solved in the space group P2<sub>1</sub>/C to a resolution of 0.82 Å with a completeness of 98.7%. Hydrogen atoms were placed in calculated positions. The structure consisted of one molecule in the asymmetric unit, and two perchlorate counterions. The perchlorate ions and hydrogen atoms were omitted for clarity.

### Computational methods

Electronic structure calculations were carried out with the Gaussian 09 software package<sup>3</sup> using B3LYP density functional.<sup>4,5</sup> The SDD basis set and effective core potential<sup>6</sup> were used for Ni atom and the 6-31G(d,p) basis set<sup>7,8</sup> was used for the other atoms. Solvation effects in water were incorporated by using the implicit SMD solvation model<sup>9</sup> and were included during structure optimization. All of the optimized structures were confirmed as minima by harmonic vibrational frequency calculations and the converged wave functions were tested for the SCF stability. The spin density plots (isovalue = 0.004 au) and canonical orbitals (isovalue = 0.05 au) of the calculated structures were visualized using GaussView.<sup>10</sup> The zero-point energy and thermal corrections were included for the calculation of the free energies. The standard states of 1 M concentration were considered for all the reactants and products for calculating the free energies of reactions. The literature value of -270.3 kcal/mol is used for the free energy of proton in water.<sup>11</sup> The calculation of the reduction potentials of the complexes included zero-point energy and thermal corrections and standard thermodynamic equation  $\Delta G = -nFE$  was used. The calculated potentials were referenced to a value of  $E_{1/2} = 4.01$  V for the ferrocene/ferrocenium couple calculated under our level of theory.

### Photocatalysis

Samples for photocatalysis were prepared in 15 ml vials with gas tight screw caps and septa. All the samples were protected from light before use. The amounts of Ni catalyst and fluorescein were varied depending on the condition used. The pH of the solutions was adjusted using NaOH and HCl as measured with a pH meter. The total volume of the samples was 5.0 mL. During the photocatalytic process the cell was purged with N<sub>2</sub> gas for 5 min followed by sampling of the head space gas (100µL) to ensure an O<sub>2</sub> free environment in the gas-chromatograph. The amount of hydrogen generated was determined by a Gow-Mac 400 gas chromatograph. Nitrogen was used as the carrier gas at a flow rate of 30 mL.min<sup>-1</sup>. The amount of H<sub>2</sub> produced was quantified using a calibration curve of moles of hydrogen versus peak area. All the photocatalytic samples were placed in a water jacketed cell at 20°C for irradiation with green light (green light emitting diode at 520 nm).

### Synthesis and characterization

Synthesis of the ligand was carried out as described previously.<sup>12</sup> For the complexation reaction, the ligand was treated with nickel(II) perchlorate in a 1:1 mole ratio in methanol. After 10 min. a pink precipitate appeared. The reaction continued for 2h when the solid was collected by vacuum filtration (**Figure 1**) and recrystallized in a mixture of methanol and acetonitrile (1:1) to yield pink colored X-ray quality crystals. Yield: 90%. IR (KBr, cm<sup>-1</sup>) 3050 (w); 3030 (w) (Aromatic-CH); 3000 (w), 2970 (w), 2940 (w) (aliphatic CH); 1608 (s) (C=N); 1449 (s) (C=C); 2360 (m) (nitrile); 1096 (s) (ClO<sub>4</sub>). ESI position in MeOH: m/z = 488.115 for [Ni<sup>II</sup>(L)(Cl)]<sup>+</sup>. Anal.Calc. for C<sub>27</sub>H<sub>28</sub>Cl<sub>2</sub>N<sub>6</sub>NiO<sub>8</sub>: C: 46.62; H: 4.07; N: 12.11; Found: C: 46.43; H: 3.94; N: 11.95.

**Table ST1.** Selected bond lengths (Å) of **1**.

Ni1–N1	2.115(3)	N5–C21	1.332(4)
Ni1–N2	2.092(3)	N6–C25	1.108(6)
Ni1–N3	2.054(3)	C27–C2	1.399(5)
Ni1–N4	2.082(3)	C27–C18	1.385(5)
Ni1–N5	2.113(3)	C2–C15	1.387(5)
Ni1–N6	2.028(3)	C3–C4	1.508(4)
Cl1–O2	1.433(3)	C4–C8	1.383(5)
Cl1–O3	1.425(3)	C5–C6	1.375(5)

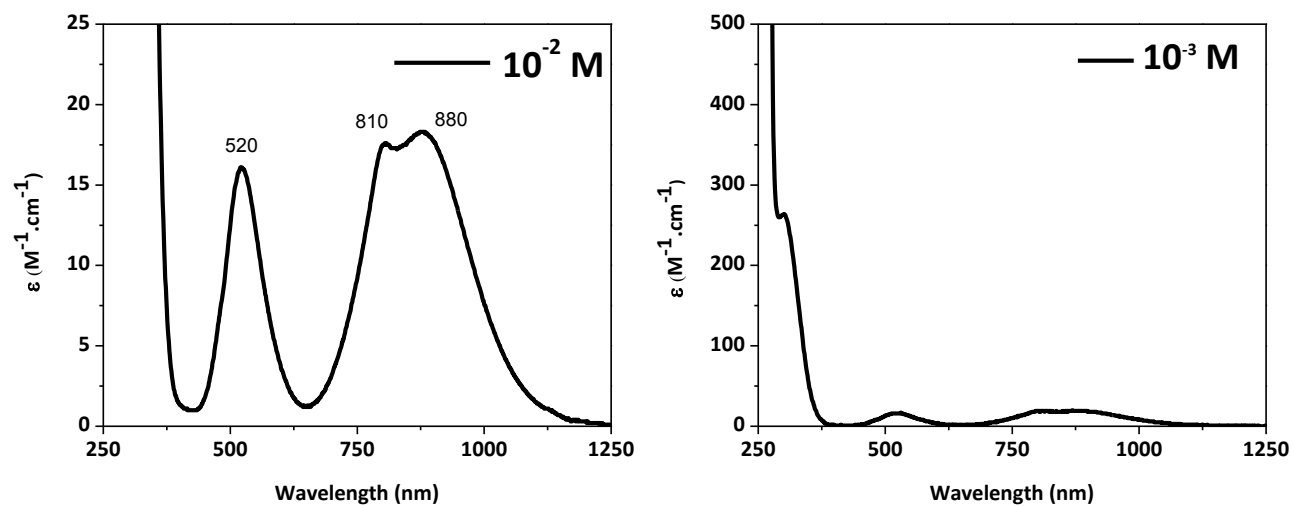
**Table ST2.** Important crystallographic parameters of **1**.

Crystal Data	<b>1</b>
Empirical formula	C <sub>27</sub> H <sub>28</sub> Cl <sub>2</sub> N <sub>6</sub> NiO <sub>8</sub>
Formula weight	694.16
Temperature (K)	100.1
Wavelength (Å)	0.71073
Crystal system, space group	Monoclinic, P2 <sub>1</sub> /c
a (Å)	9.5286(8)
b (Å)	17.0040(14)
c (Å)	17.9431(15)
α (°)	90
β (°)	96.744(3)
γ (°)	90
Volume (Å <sup>3</sup> )	2887.1(4)
Z	4
Calculated density (g/cm <sup>3</sup> )	1.5969
Absorption coefficient (mm <sup>-1</sup> )	0.919
F (000)	1435.2
R(F) (%)	4.85

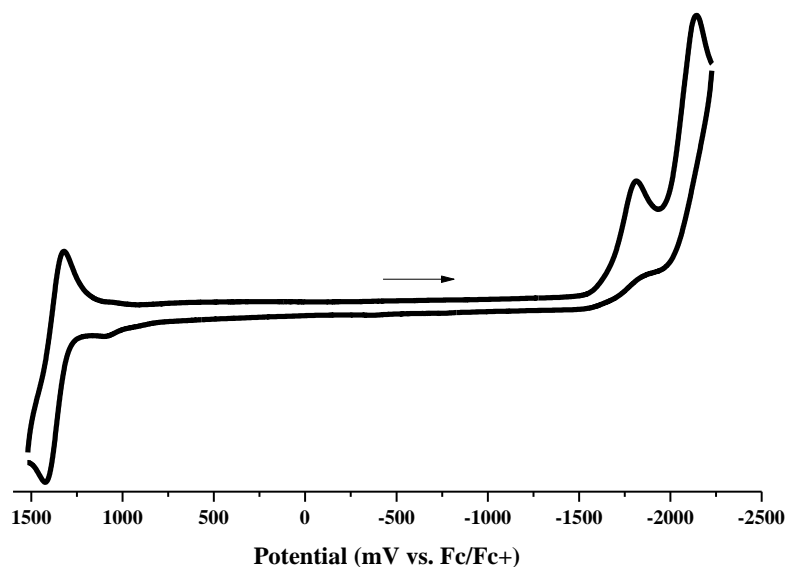
**Table ST3.** Bond angles (°) of **1**.

N2	Ni1	N1	84.06(11)	C10	N4	Ni1	114.2(2)
N3	Ni1	N1	162.60(11)	C11	N4	Ni1	127.3(2)
N3	Ni1	N2	81.72(10)	C11	N4	C10	118.6(3)
N4	Ni1	N1	96.14(11)	C20	N5	Ni1	112.2(2)
N4	Ni1	N2	82.39(11)	C21	N5	Ni1	129.0(2)
N4	Ni1	N3	91.89(11)	C21	N5	C20	118.5(3)
N5	Ni1	N1	78.84(11)	C25	N6	Ni1	168.6(4)
N5	Ni1	N2	97.08(11)	C15	C2	C0AA	119.9(3)
N5	Ni1	N3	92.97(11)	C4	C3	N2	109.5(3)
N5	Ni1	N4	174.98(11)	C3	C4	N3	114.9(3)
N6	Ni1	N1	98.31(12)	C8	C4	N3	121.3(3)
N6	Ni1	N2	175.37(12)	C8	C4	C3	123.8(3)
N6	Ni1	N3	96.59(12)	C6	C5	N3	121.9(3)
N6	Ni1	N4	93.38(12)	C7	C6	C5	118.8(3)
N6	Ni1	N5	87.30(12)	C8	C7	C6	120.2(3)
O3	Cl1	O2	112.2(2)	C7	C8	C4	118.5(3)
O4	Cl1	O2	107.80(19)	C10	C9	N2	114.0(3)
O4	Cl1	O3	109.21(19)	C9	C10	N4	118.3(3)
O5	Cl1	O2	109.13(18)	C14	C10	N4	121.7(3)
O5	Cl1	O3	109.19(18)	C14	C10	C9	120.0(3)
O5	Cl1	O4	109.2(2)	C12	C11	N4	122.2(3)
O7	Cl2	O6	109.47(18)	C13	C12	C11	119.2(3)
O8	Cl2	O6	109.37(17)	C14	C13	C12	118.8(3)
O8	Cl2	O7	108.95(16)	C13	C14	C10	119.6(3)
O9	Cl2	O6	110.60(19)	C16	C15	C2	120.3(3)
O9	Cl2	O7	108.87(19)	C17	C16	C15	119.6(3)
O9	Cl2	O8	109.55(18)	C18	C17	C16	120.1(4)
C1	N1	Ni1	116.2(2)	C24	C20	N5	121.7(3)
C19	N1	Ni1	104.1(2)	C24	C20	C19	122.3(3)
C19	N1	C1	108.6(3)	C22	C21	N5	123.0(3)
C2	N2	Ni1	106.99(19)	C23	C22	C21	118.9(3)
C3	N2	Ni1	103.73(18)	C24	C23	C22	118.6(3)
C3	N2	C2	113.8(3)	C23	C24	C20	119.3(3)
C9	N2	Ni1	110.5(2)	C26	C25	N6	177.0(6)

**Figure S1.** UV-visible absorption spectra of **1** in MeCN.



**Figure S2.** Cyclic voltammogram of **1** in dry acetonitrile.



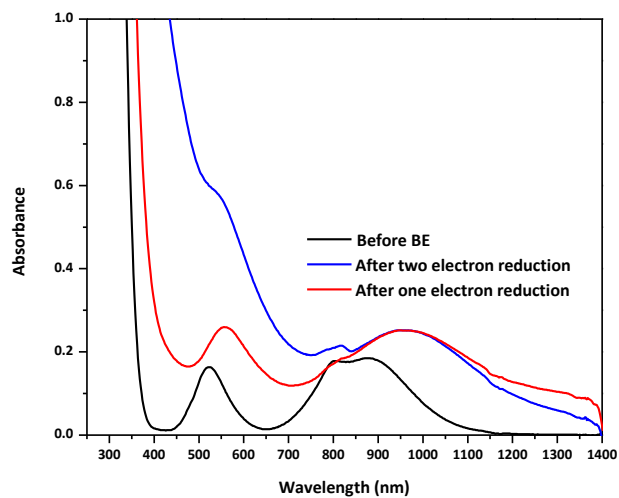
**Table ST4.** Electrochemical properties of **1**.

	Ni(II)/Ni(III) $E_{1/2}$ , [ $E_{pc}$ ; $E_{pa}$ ], mV ( $\Delta E$ , mV) $ i_{pc}/i_{pa} $	Ni(II)/Ni(I) $E_{1/2}$ , [ $E_{pc}$ ; $E_{pa}$ ], mV ( $\Delta E$ , mV) $ i_{pc}/i_{pa} $	L/L <sup>-</sup> $E_{1/2}$ , [ $E_{pc}$ ; $E_{pa}$ ], mV ( $\Delta E$ , mV) $ i_{pc}/i_{pa} $
In ACN	+1390,[+1345,+1429](84)  0.227	wave at $E_{pc}$ = -1830	wave at $E_{pc}$ = -2140

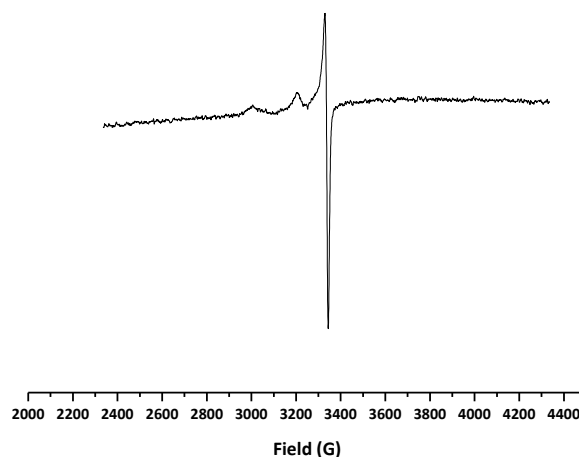
**Table S15.** Comparison of experimentally-measured and DFT-calculated potentials

	Experimentally-measured reduction potential (vs. Fc/Fc+) in MeCN solvent	DFT-calculated reduction potential (vs. Fc/Fc+) in MeCN solvent
$E_{\text{Ni(II)}/\text{Ni(I)}}$	-1.83 V	-1.50 V
$E_{\text{Ni(I)L}/\text{Ni(I)L}\bullet}$	-2.14 V	-2.30 V

**Figure S3.** UV Visible absorption spectra of the Ni complex ( $\text{Ni}^{\text{II}}\text{L}$ ), one electron reduced species ( $\text{Ni}^{\text{I}}\text{L}$ ) and two electron reduced species ( $\text{Ni}^{\text{I}}\text{L}\bullet$ )

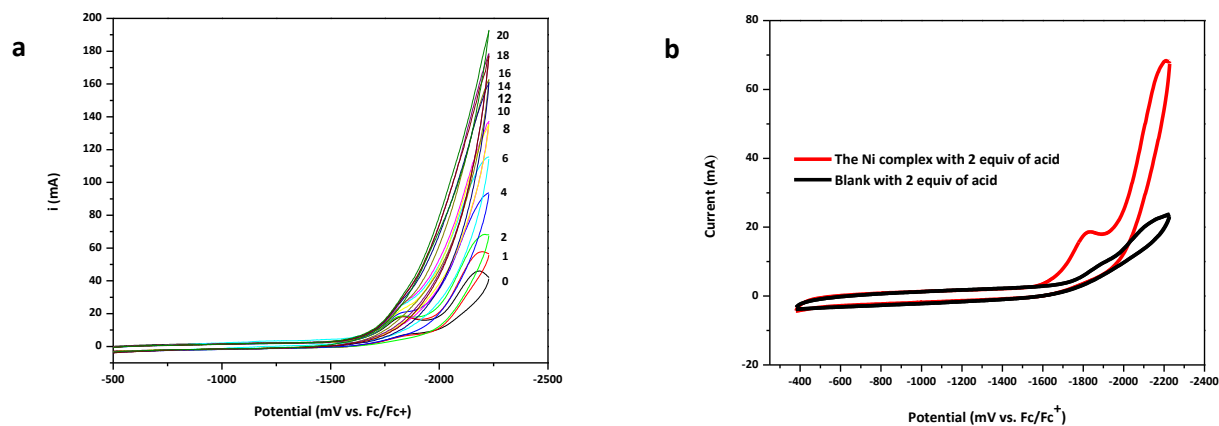


**Figure S4.** EPR of the one electron reduced species ( $\text{Ni}^{\text{I}}\text{L}$ )

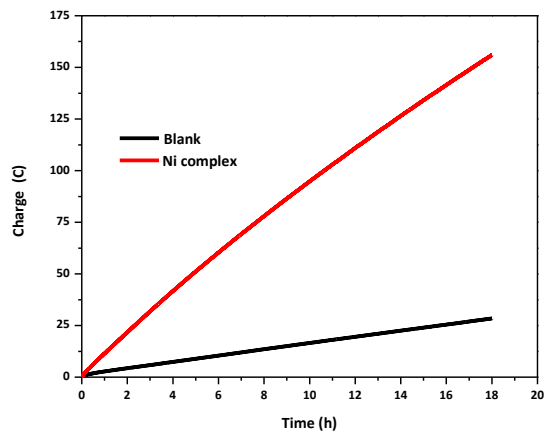




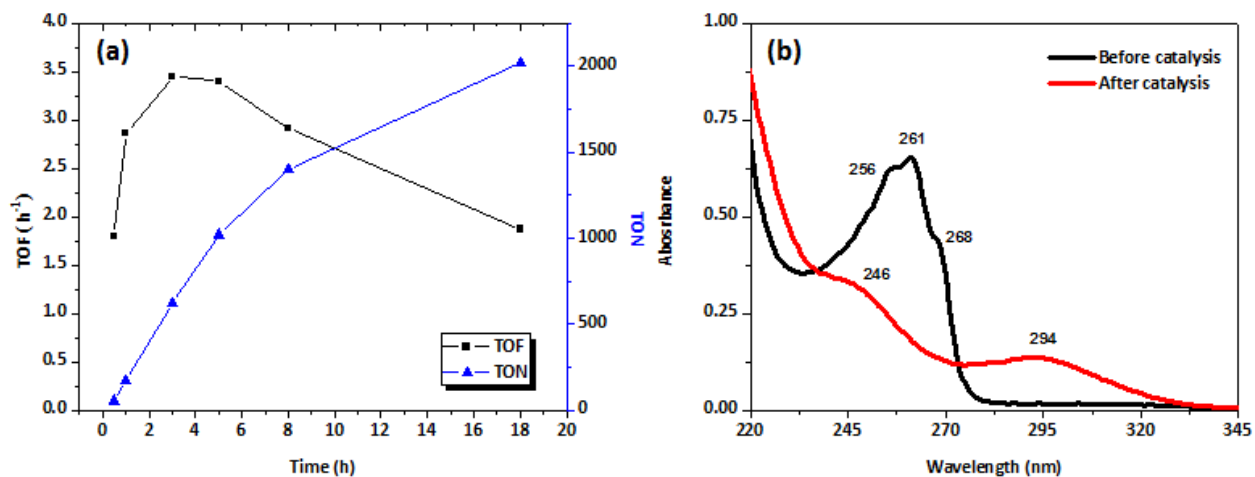
**Figure S5.** Electrocatalysis of **1** in MeCN with acetic acid as the proton donor. **(a)** Acid titration with the Ni complex up to 20 equivalents of acid. **(b)** With and without the Ni complex upon addition of two equivalent of acid.



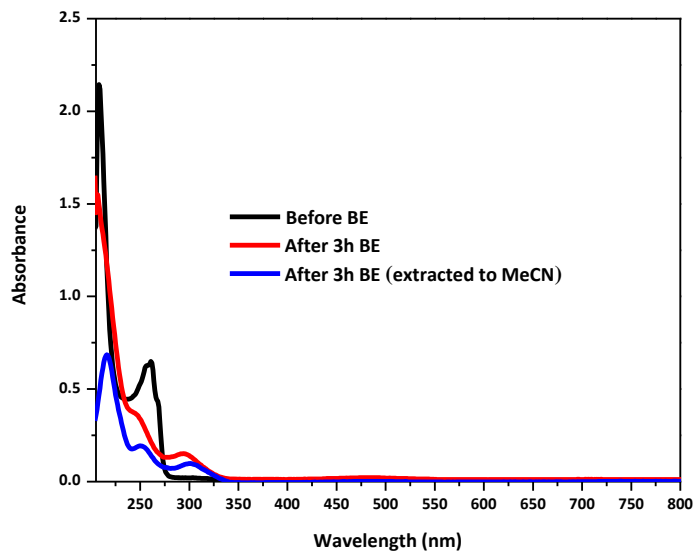
**Figure S6.** Charge versus time plot for 18 h during the BE of **1** (0.1  $\mu\text{mol}$ ). Applied potential  $-1700 \text{ V}_{\text{Ag}/\text{AgCl}}$ .



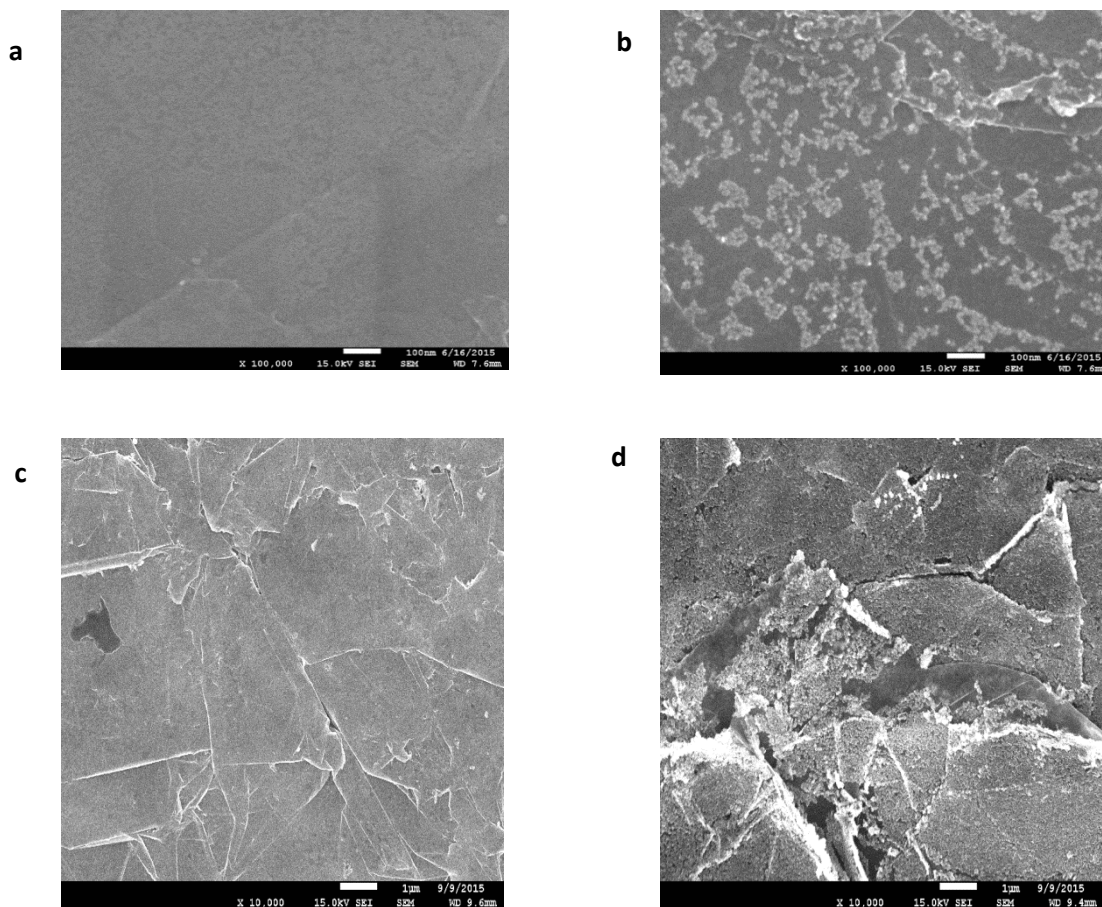
**Figure 7 (a)** Plots of TON vs. time (blue) and TOF vs. time (black) for **1** (0.1  $\mu\text{mol}$ ) at an applied potential of  $-1700 \text{ mV}_{\text{Ag}/\text{AgCl}}$ . **(b)** Absorption spectra of **1** (60  $\mu\text{M}$ ) before (black) and after catalysis (red). Both graphs in aqueous phosphate buffer (1M, pH 7).



**Figure S8.** UV-visible absorption spectra of **1** before and after catalysis in phosphate buffer and acetonitrile.



**Figure S9.** SEM images of the grafoil electrodes after catalysis. **(a)** Blank grafoil electrode after 3 h BE. **(b)** Grafoil electrode with complex **1** after 3 h BE. **(c)** Blank grafoil electrode after 8 h BE. **(d)** Grafoil electrode with complex **1** after 8 h BE.



**Table ST6.** EDS analysis of the grafoil electrode after 3 h BE with 1.

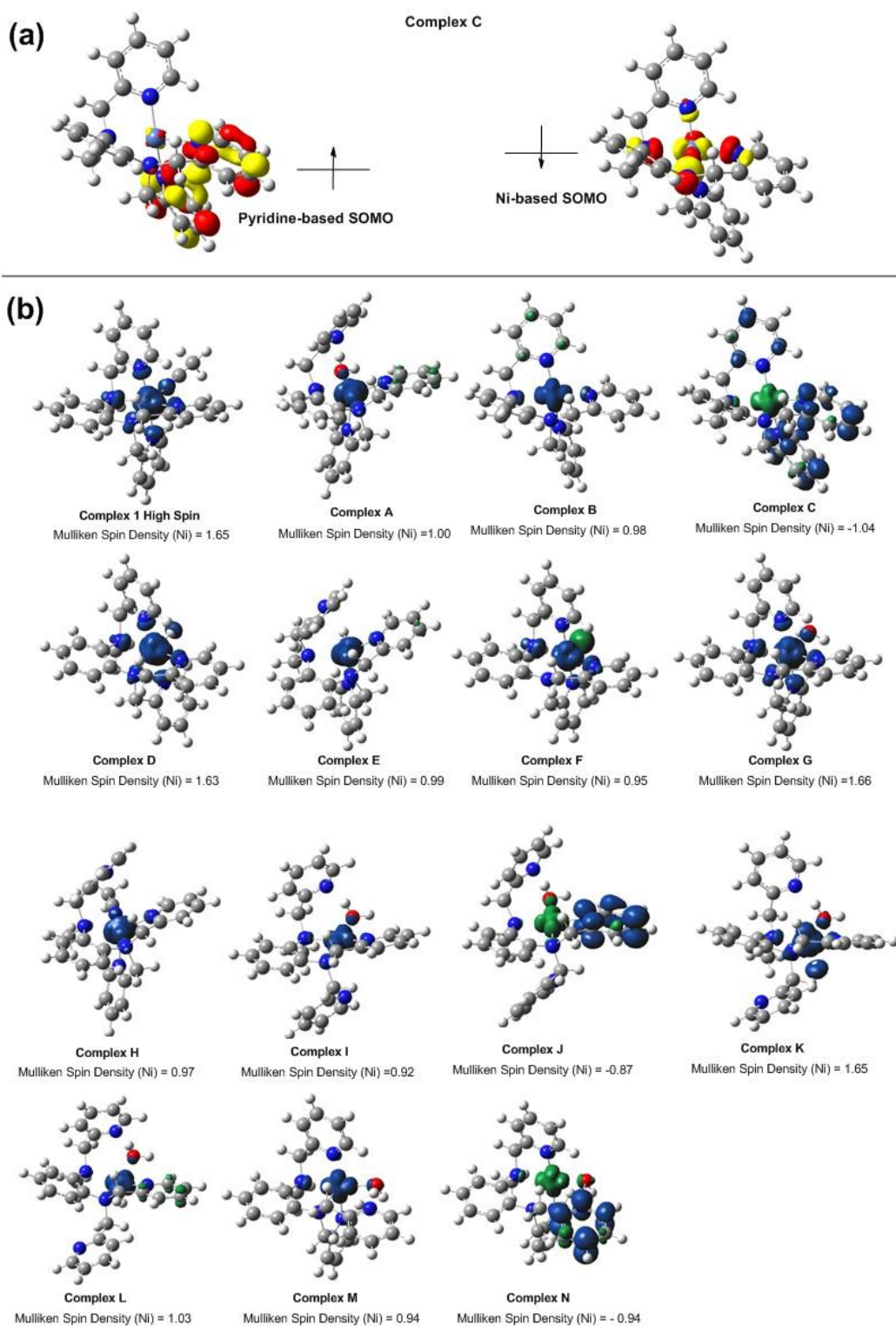
<b>Element</b>	<b>Wt %</b>	<b>At %</b>
<b>C K</b>	<b>86.38</b>	<b>91.24</b>
<b>O K</b>	<b>06.60</b>	<b>05.24</b>
<b>Ni L</b>	<b>00.22</b>	<b>00.05*</b>
<b>Na K</b>	<b>04.83</b>	<b>02.67</b>
<b>P K</b>	<b>01.97</b>	<b>00.81</b>
<b>Total</b>	<b>100.00</b>	<b>100.00</b>

\* Detection limit is 1% for Pegasus Apex 2 EDS detecting unit on JSM-7600F SEM.

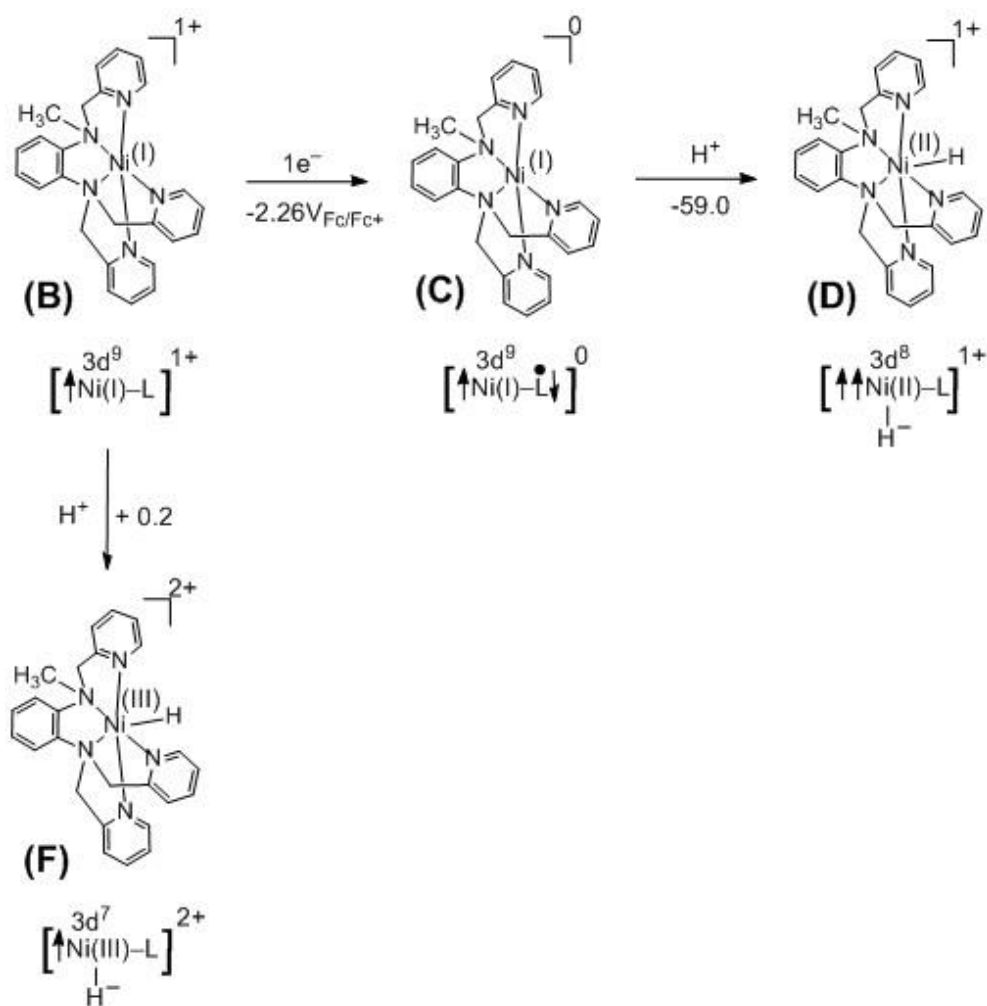
**Table ST7.** EDS analysis of the grafoil electrode after 8 h BE with 1.

<b>Element</b>	<b>Wt %</b>	<b>At %</b>
<b>C K</b>	<b>99.58</b>	<b>99.84</b>
<b>P K</b>	<b>0.42</b>	<b>0.16</b>
<b>Ni K</b>	<b>0.00</b>	<b>0.00</b>
<b>Total</b>	<b>100.00</b>	<b>100.00</b>

**Figure S10.** (a) Unrestricted canonical orbitals (isovalue=0.05 au) containing the unpaired electrons on nickel and L<sup>N2Py3</sup> ligand framework in complex C. (b) Spin density plots (isovalue=0.004 au) with Mulliken spin density values on Ni centers of the calculated structures.

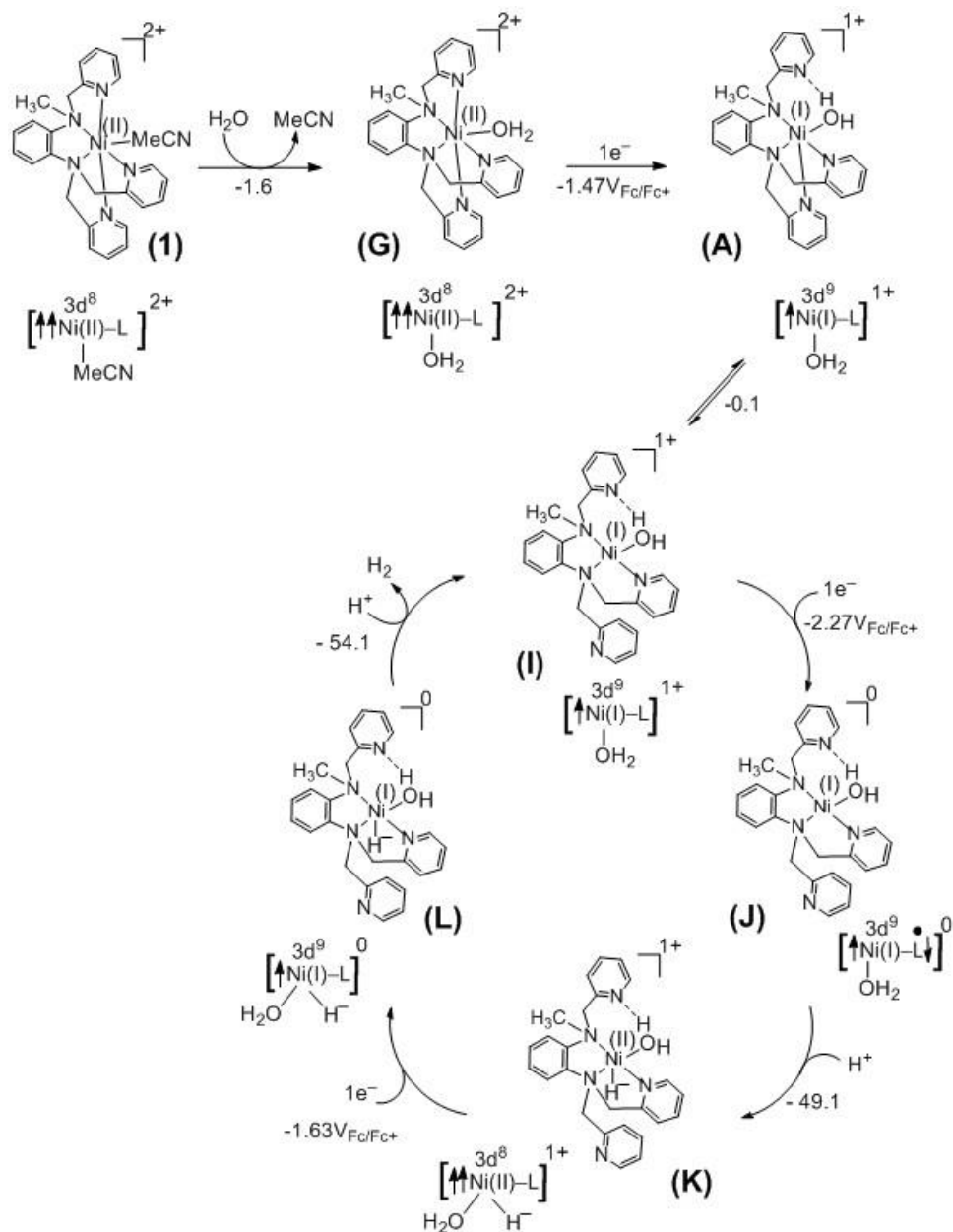


**Figure S11.** Energies for formation of  $\text{Ni}^{\text{I}}\bullet$  species vs. trivalent  $\text{Ni}^{\text{III}}-\text{H}^-$  complex in water solvent. The free energies (kcal/mol) and potentials (volt) have been calculated at B3LYP/SDD/6-31G(d,p) level of theory.



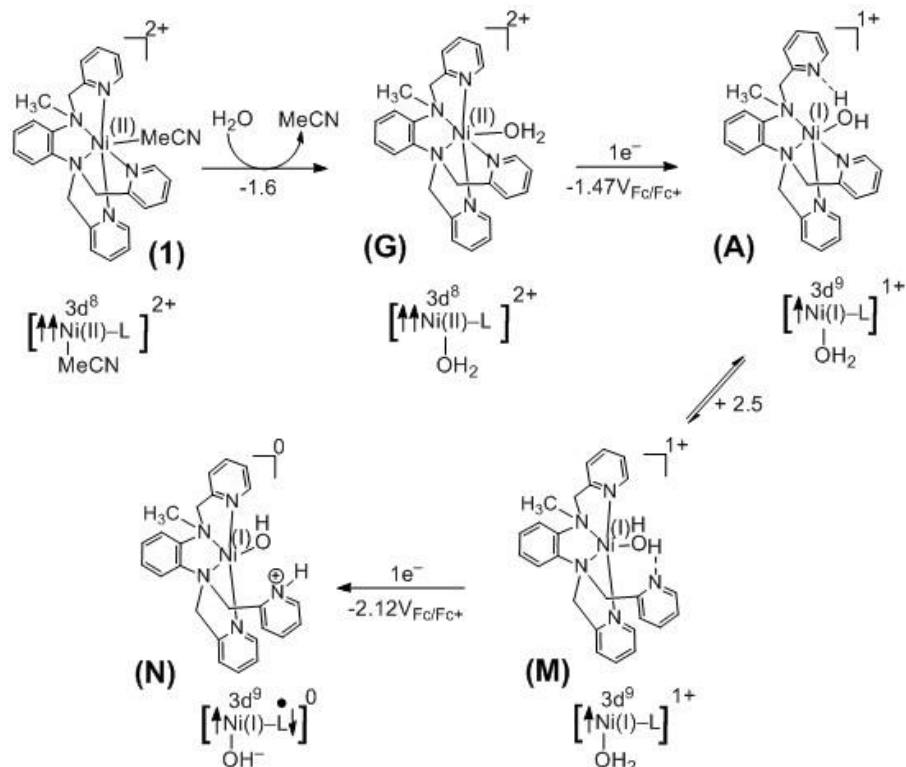
The formation of the  $\text{Ni}^{\text{II}}-\text{H}^-$  intermediate **D** from the ligand-reduced species **C** is favorable by 59 kcal/mol at pH = 0 but the formation of the trivalent  $\text{Ni}^{\text{III}}-\text{H}^-$  intermediate **F** from the metal-reduced complex **B** is only isoenergetic at + 0.2 kcal/mol at pH = 0. Changing from a standard state of pH = 0 to pH = 7 would increase the free energies of the addition of a proton by approximately 9.5 kcal/mol. These results support the involvement of **D** as a mechanistically relevant intermediate for water reduction by catalyst **1**.

**Figure S12.** The catalytic pathway involving a water-bound four-coordinate Ni<sup>I</sup> species (**I**) in water solvent. The free energies (kcal/mol) and potentials (volt) have been calculated at B3LYP/SDD/6-31G(d,p) level of theory.



The substitution of the MeCN ligand by a solvent water molecule on the parent complex **1** is slightly favorable by 1.6 kcal/mol and it gives rise to species **G**. Reduction of the latter complex can lead to the five-coordinate Ni<sup>I</sup> intermediate **A** where the pendant pyridine moiety is hydrogen-bonded to the water molecule coordinated to the nickel center. The five-coordinate square-pyramidal Ni<sup>I</sup> complex **A** can lose coordination of the axial pyridine unit to converge to its four-coordinate analogue **I**. The latter complex can get reduced at -2270 mV<sub>Fc/Fc+</sub> to give rise to the ligand-reduced intermediate **J**. Protonation of **J** leads to the Ni<sup>II</sup>-H<sup>-</sup> intermediate **K** which can further get reduced to the Ni<sup>I</sup>-H<sup>-</sup> complex **L**. Uptake of another proton by the latter species and release of dihydrogen complete the catalytic cycle and this event is found to be favorable by 54 kcal/mol.

**Figure S13.** Energies for formation of a Ni<sup>I</sup>(OH) intermediate (**N**) that can potentially initiate catalyst decomposition in water solvent. The free energies (kcal/mol) and potentials (volt) have been calculated at B3LYP/SDD/6-31G(d,p) level of theory.

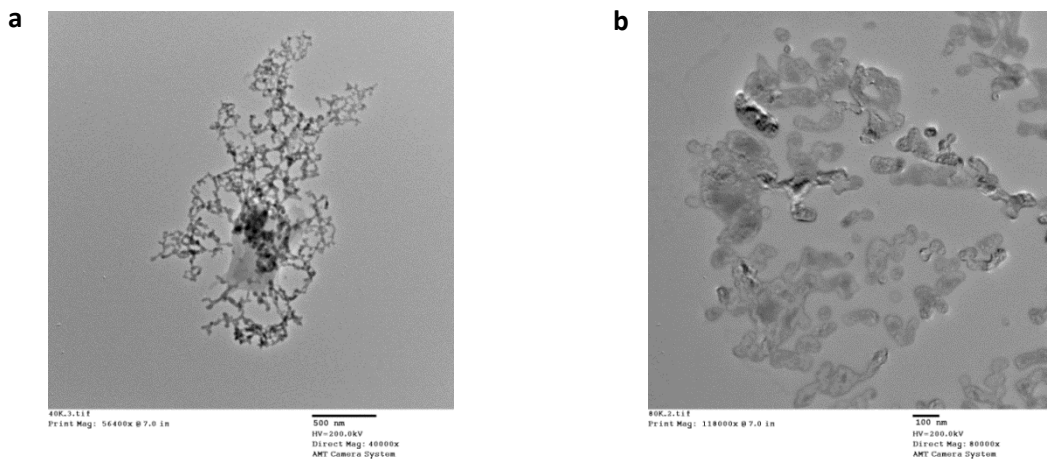


The substitution of the MeCN ligand by a solvent water molecule on the parent complex **1** is slightly favorable by 1.6 kcal/mol and it gives rise to species **G**. Reduction of the latter complex can lead to the five-coordinate Ni<sup>I</sup> intermediate **A** where the pendant axial pyridine moiety is hydrogen-bonded to the water molecule coordinated to the nickel center. Complex **A** can potentially isomerize to intermediate **M** where the equatorial pyridine is found to be pendant instead of the axial pyridine and this equatorial pyridine is hydrogen-bonded to the water molecule. The water molecule being coordinated to the nickel center becomes more acidic than a free water molecule in solvent and, as a result, reduction of intermediate **M** leads to the transfer of a proton from the coordinated water molecule to the equatorial pyridine unit. The resulting complex **N** being a Ni<sup>I</sup>(OH) species loses its catalytic efficiency for water reduction to dihydrogen.

**Table ST8.** Hg test for nanoparticle formation. (Ni complex (5 μM), FI (1 mM), TEA (5 % v/v), Hg (1 mL) in EtOH/water (1:1)).

	TON (Without Hg)	TON (With Hg)
Run 1	3660	3540
Run 2	3420	3420
Run 3	3570	3520
Average	3550	3493.333
STD	121.2436	64.29101

**Figure S14.** TEM images of the photocatalytic system. **(a)** Blank photocatalytic system (buffer/water) without complex **1**. **(b)** Photocatalytic system with complex **1**.



**Table ST9.** EDS analysis of the photocatalytic systems with complex **1**. Presence of nickel is below detection limits.

Element	Wt %	At %
O K	53.6	65.5
Na K	26.9	22.9
Si L	6.7	4.7
Cl K	12.7	7.0
Total	100.0	100.0





**Table ST11.** XYZ coordinates of the DFT-calculated Structures.

=====  
Complex 1 High Spin

C	-3.325657000	2.854023000	-3.438254000
C	-2.019735000	2.487753000	-3.122647000
C	0.223811000	0.440481000	-2.870664000
C	-4.393211000	2.327339000	-2.708070000
C	-1.759070000	1.596463000	-2.073317000
C	-0.922058000	-3.966137000	-2.407816000
C	-4.145843000	1.431585000	-1.671560000
C	-2.012751000	-3.188605000	-2.027450000
C	0.349034000	-3.620473000	-1.947011000
C	0.469781000	2.392806000	-1.454034000
C	-2.834431000	1.062415000	-1.346607000
C	-1.803590000	-2.090615000	-1.192003000
C	0.479245000	-2.500719000	-1.135233000
C	-2.962336000	-1.285152000	-0.661266000
C	0.084532000	3.040229000	-0.150365000
C	0.255327000	4.406882000	0.069327000
C	2.660375000	-0.078780000	0.867536000
C	-3.243083000	0.477788000	1.015303000
C	-0.043566000	4.932684000	1.323990000
C	4.064728000	-0.166811000	1.217342000
C	-0.665327000	2.727741000	2.021681000
C	-2.567222000	-0.236496000	2.167052000
C	-0.509137000	4.076024000	2.321575000
C	-0.576895000	-1.066428000	3.039547000
C	-3.258515000	-0.585954000	3.326112000
C	-1.196147000	-1.433343000	4.228984000
C	-2.562190000	-1.188277000	4.372569000
H	-3.507364000	3.547458000	-4.253311000
H	0.373958000	1.077730000	-3.749687000
H	-1.195750000	2.897345000	-3.697713000
H	-0.432237000	-0.386455000	-3.141800000
H	-5.414239000	2.607918000	-2.946525000
H	1.189835000	0.046823000	-2.548654000
H	-1.060819000	-4.825724000	-3.055758000
H	0.447443000	3.124013000	-2.268132000
H	-3.016938000	-3.423208000	-2.364274000
H	1.226986000	-4.196177000	-2.217507000
H	-3.783049000	-1.271625000	-1.383337000
H	1.500879000	2.029989000	-1.376555000
H	-4.973419000	1.009871000	-1.110052000
H	0.617848000	5.038189000	-0.734825000
H	1.449668000	-2.182862000	-0.771061000
H	-3.336462000	-1.797019000	0.231743000
H	-4.312224000	0.243322000	1.004138000
H	4.639033000	0.523481000	0.593372000
H	4.417863000	-1.188389000	1.052442000
H	-3.142588000	1.558550000	1.149927000
H	0.082176000	5.992949000	1.519132000
H	4.195036000	0.098881000	2.269978000
H	-1.027231000	2.031462000	2.769875000
H	0.481965000	-1.240389000	2.876287000
H	-0.753589000	4.439334000	3.313368000
H	-4.322261000	-0.386605000	3.399133000
H	-0.618499000	-1.903288000	5.016836000
H	-3.080332000	-1.467842000	5.284368000
N	-0.381981000	1.208664000	-1.748596000

N	-0.574286000	-1.750909000	-0.760731000
N	-2.582900000	0.110507000	-0.270272000
N	1.539868000	-0.009633000	0.586807000
N	-0.378315000	2.216030000	0.810638000
N	-1.246638000	-0.481559000	2.031433000
Ni	-0.499006000	0.154903000	0.164091000

=====  
Complex 1 Low Spin

C	-3.326239000	2.877353000	-3.435433000
C	-2.022971000	2.499654000	-3.121951000
C	0.204275000	0.429967000	-2.874450000
C	-4.397574000	2.357257000	-2.706134000
C	-1.769032000	1.602936000	-2.075687000
C	-0.915551000	-3.980346000	-2.363274000
C	-4.156667000	1.455477000	-1.673276000
C	-2.010584000	-3.200175000	-2.002251000
C	0.351767000	-3.622338000	-1.901281000
C	0.467982000	2.383685000	-1.461652000
C	-2.848178000	1.073884000	-1.350712000
C	-1.810844000	-2.086706000	-1.184862000
C	0.473485000	-2.488594000	-1.108138000
C	-2.978080000	-1.276819000	-0.679031000
C	0.089192000	3.030720000	-0.156653000
C	0.266061000	4.395616000	0.067831000
C	2.674199000	-0.062261000	0.872294000
C	-3.253550000	0.477138000	1.009161000
C	-0.029292000	4.917960000	1.324824000
C	4.076239000	-0.138570000	1.235544000
C	-0.659893000	2.713103000	2.015785000
C	-2.568815000	-0.242486000	2.152377000
C	-0.497587000	4.059766000	2.319749000
C	-0.569879000	-1.070609000	3.009205000
C	-3.252390000	-0.604858000	3.312055000
C	-1.182129000	-1.450435000	4.198275000
C	-2.548486000	-1.212680000	4.350236000
H	-3.502636000	3.574955000	-4.248090000
H	0.355905000	1.065119000	-3.754697000
H	-1.196438000	2.904797000	-3.696460000
H	-0.458409000	-0.392730000	-3.142102000
H	-5.416385000	2.647287000	-2.942780000
H	1.168521000	0.030796000	-2.554186000
H	-1.047925000	-4.851449000	-2.997008000
H	0.447402000	3.114909000	-2.275622000
H	-3.012133000	-3.444009000	-2.340486000
H	1.233397000	-4.199307000	-2.156692000
H	-3.782119000	-1.262588000	-1.419967000
H	1.496757000	2.014033000	-1.387422000
H	-4.986779000	1.038001000	-1.112240000
H	0.630401000	5.028165000	-0.734485000
H	1.440253000	-2.161092000	-0.743333000
H	-3.374231000	-1.788389000	0.204685000
H	-4.323253000	0.243552000	1.006731000
H	4.650568000	0.558983000	0.619742000
H	4.440550000	-1.156219000	1.070641000
H	-3.151237000	1.557166000	1.148848000
H	0.101249000	5.976916000	1.523737000
H	4.194399000	0.124487000	2.290266000
H	-1.023652000	2.015710000	2.761837000
H	0.488973000	-1.237808000	2.839415000
H	-0.739435000	4.420486000	3.313109000

H	-4.316706000	-0.411055000	3.391523000
H	-0.598572000	-1.924350000	4.979376000
H	-3.061129000	-1.502113000	5.262048000
N	-0.393336000	1.205244000	-1.752959000
N	-0.585029000	-1.736064000	-0.752965000
N	-2.603578000	0.115777000	-0.281030000
N	1.555586000	-0.003773000	0.580184000
N	-0.375993000	2.205405000	0.802473000
N	-1.247462000	-0.480282000	2.009777000
Ni	-0.504481000	0.163962000	0.155078000

=====  
Complex H

C	-2.810750000	2.613064000	-3.588157000
C	-1.549219000	2.375242000	-3.048967000
C	0.847347000	0.710820000	-2.413813000
C	-3.932859000	2.004656000	-3.021218000
C	-1.377436000	1.528204000	-1.942441000
C	-1.493121000	-3.839585000	-3.049412000
C	-3.775332000	1.155332000	-1.929848000
C	-2.418543000	-3.058860000	-2.355973000
C	-0.138583000	-3.708669000	-2.743182000
C	0.596620000	2.558762000	-0.895915000
C	-2.506743000	0.899867000	-1.389117000
C	-1.961725000	-2.177577000	-1.376489000
C	0.235138000	-2.798029000	-1.758375000
C	-2.908281000	-1.358079000	-0.532464000
C	-0.102718000	3.260159000	0.247970000
C	-1.185117000	4.120989000	0.022749000
C	2.754713000	-0.805181000	0.827990000
C	-2.971192000	0.569260000	0.982463000
C	-1.778930000	4.769637000	1.104231000
C	4.161319000	-1.052125000	1.094633000
C	-0.170956000	3.698099000	2.512402000
C	-2.371688000	-0.051855000	2.224207000
C	-1.264472000	4.551773000	2.381467000
C	-0.463487000	-0.872052000	3.254638000
C	-3.109539000	-0.204182000	3.396502000
C	-1.127279000	-1.034186000	4.465449000
C	-2.479915000	-0.697999000	4.539223000
H	-2.916335000	3.272642000	-4.444177000
H	1.077082000	1.424729000	-3.216788000
H	-0.683437000	2.859004000	-3.489753000
H	0.378054000	-0.169897000	-2.852985000
H	-4.923448000	2.188619000	-3.425628000
H	1.784792000	0.414420000	-1.937778000
H	-1.824033000	-4.532639000	-3.816554000
H	0.710846000	3.262258000	-1.733128000
H	-3.480899000	-3.127842000	-2.566780000
H	0.618110000	-4.291165000	-3.257740000
H	-3.900536000	-1.319629000	-0.994080000
H	1.598043000	2.278648000	-0.563263000
H	-4.646815000	0.682991000	-1.487383000
H	-1.548460000	4.283987000	-0.985764000
H	1.280124000	-2.657442000	-1.495936000
H	-3.026475000	-1.862565000	0.433041000
H	-4.063082000	0.461775000	0.990967000
H	4.755118000	-0.188578000	0.781961000
H	4.492928000	-1.936201000	0.542704000
H	-2.748285000	1.641573000	0.989356000
H	-2.618860000	5.440210000	0.949606000

H	4.309632000	-1.221277000	2.164949000
H	0.269347000	3.520523000	3.490831000
H	0.585876000	-1.131590000	3.151987000
H	-1.686940000	5.038268000	3.254358000
H	-4.160243000	0.067501000	3.407635000
H	-0.592897000	-1.422872000	5.325660000
H	-3.034145000	-0.820965000	5.464228000
N	-0.049829000	1.295195000	-1.383831000
N	-0.651335000	-2.046791000	-1.081938000
N	-2.367255000	0.000101000	-0.251640000
N	1.629791000	-0.610508000	0.618796000
N	0.406622000	3.062592000	1.480254000
N	-1.063338000	-0.390581000	2.146546000
Ni	-0.298470000	-0.329823000	0.223215000

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Complex B

C	-3.624418000	3.475258000	-3.052528000
C	-2.318783000	3.002346000	-2.919776000
C	-0.286347000	0.590685000	-3.157986000
C	-4.664216000	2.836044000	-2.377762000
C	-2.025034000	1.901343000	-2.105758000
C	-0.768323000	-4.344412000	-1.103852000
C	-4.390469000	1.724047000	-1.582589000
C	-1.861458000	-3.501175000	-1.281766000
C	0.447229000	-3.793254000	-0.694690000
C	0.357835000	2.464411000	-1.767420000
C	-3.081637000	1.246089000	-1.431949000
C	-1.714396000	-2.130146000	-1.051814000
C	0.512256000	-2.421330000	-0.480158000
C	-2.878769000	-1.189967000	-1.315296000
C	0.288131000	3.054223000	-0.383961000
C	0.534503000	4.402978000	-0.142320000
C	-3.527516000	0.089003000	0.691631000
C	0.550944000	4.874938000	1.170527000
C	0.055048000	2.639792000	1.888930000
C	-2.752890000	-0.603668000	1.797513000
C	0.309837000	3.967889000	2.204583000
C	-0.713532000	-0.927681000	2.852154000
C	-3.407097000	-1.366965000	2.765826000
C	-1.294988000	-1.688101000	3.862966000
C	-2.670165000	-1.914276000	3.815415000
H	-3.824025000	4.336495000	-3.682820000
H	-0.229932000	1.206923000	-4.066027000
H	-1.518363000	3.502306000	-3.455044000
H	-1.026093000	-0.193665000	-3.318775000
H	-5.685342000	3.192339000	-2.474577000
H	0.687265000	0.126052000	-2.985524000
H	-0.863518000	-5.411993000	-1.276314000
H	0.317318000	3.254599000	-2.525340000
H	-2.824708000	-3.892059000	-1.594203000
H	1.326795000	-4.408397000	-0.539481000
H	-2.901747000	-0.983832000	-2.390065000
H	1.332230000	1.972296000	-1.877315000
H	-5.201224000	1.217346000	-1.068847000
H	0.714647000	5.068815000	-0.980189000
H	1.435940000	-1.950874000	-0.157912000
H	-3.819074000	-1.707678000	-1.084660000
H	-4.519876000	-0.372672000	0.604812000
H	-3.677799000	1.129768000	0.996835000
H	0.744096000	5.922044000	1.380022000

H	-0.145703000	1.911128000	2.666767000
H	0.355574000	-0.736400000	2.842396000
H	0.312159000	4.280006000	3.243478000
H	-4.477963000	-1.525686000	2.691298000
H	-0.679702000	-2.094936000	4.657993000
H	-3.160842000	-2.510007000	4.578807000
N	-0.657805000	1.402636000	-1.973060000
N	-0.541209000	-1.598804000	-0.655329000
N	-2.805006000	0.101332000	-0.595480000
N	0.041376000	2.170802000	0.618611000
N	-1.420521000	-0.392147000	1.841565000
Ni	-0.637908000	0.393259000	0.028781000

Complex C

C	-3.256880000	3.613643000	-3.114401000
C	-1.988468000	3.086204000	-2.867505000
C	0.008254000	0.655896000	-2.989275000
C	-4.380884000	2.994487000	-2.568223000
C	-1.819127000	1.949784000	-2.068415000
C	-1.434861000	-4.428600000	-0.068060000
C	-4.229802000	1.847683000	-1.788754000
C	-2.296364000	-3.490987000	-0.652070000
C	-0.166622000	-3.971310000	0.359680000
C	0.519839000	2.413793000	-1.417005000
C	-2.961274000	1.312418000	-1.525894000
C	-1.897694000	-2.167530000	-0.796857000
C	0.168414000	-2.642831000	0.177346000
C	-2.768772000	-1.138051000	-1.467631000
C	0.272177000	2.959835000	-0.038889000
C	0.486775000	4.296649000	0.279726000
C	-3.700650000	0.055392000	0.473988000
C	0.336490000	4.728426000	1.599588000
C	-0.254984000	2.470293000	2.173295000
C	-3.086042000	-0.786433000	1.565752000
C	-0.038852000	3.783276000	2.561477000
C	-1.222928000	-1.173221000	2.916030000
C	-3.805538000	-1.769226000	2.236829000
C	-1.876755000	-2.164946000	3.622942000
C	-3.212460000	-2.483547000	3.285662000
H	-3.361234000	4.502157000	-3.729745000
H	0.195138000	1.326351000	-3.840156000
H	-1.118700000	3.571851000	-3.297854000
H	-0.721405000	-0.093565000	-3.296520000
H	-5.373673000	3.394190000	-2.752610000
H	0.941798000	0.150647000	-2.729147000
H	-1.731796000	-5.464978000	0.053355000
H	0.615820000	3.228393000	-2.145001000
H	-3.286087000	-3.782779000	-0.994086000
H	0.551514000	-4.646357000	0.815687000
H	-2.373470000	-0.907512000	-2.462069000
H	1.481268000	1.883081000	-1.407182000
H	-5.106567000	1.359349000	-1.375899000
H	0.773904000	4.987993000	-0.506593000
H	1.144775000	-2.275272000	0.483248000
H	-3.786495000	-1.527807000	-1.608261000
H	-4.687272000	-0.346124000	0.204757000
H	-3.843101000	1.079807000	0.838359000
H	0.502630000	5.766484000	1.868101000
H	-0.563029000	1.716674000	2.889508000
H	-0.198395000	-0.903866000	3.162929000

H	-0.169359000	4.059168000	3.602918000
H	-4.828511000	-1.975269000	1.932299000
H	-1.361425000	-2.679556000	4.428451000
H	-3.759022000	-3.255332000	3.817422000
N	-0.490419000	1.399505000	-1.807867000
N	-0.656260000	-1.718877000	-0.397910000
N	-2.800294000	0.141507000	-0.702515000
N	-0.105842000	2.036362000	0.892554000
N	-1.791611000	-0.462081000	1.902102000
Ni	-0.764226000	0.311375000	0.193436000

Complex D

C	-3.061068000	3.355491000	-3.239464000
C	-1.803921000	2.836990000	-2.934047000
C	0.243536000	0.504893000	-2.790244000
C	-4.197698000	2.833631000	-2.619580000
C	-1.663307000	1.796510000	-2.007485000
C	-1.380534000	-4.583692000	-1.055007000
C	-4.071076000	1.785645000	-1.709770000
C	-2.344853000	-3.592038000	-1.212990000
C	-0.093653000	-4.219824000	-0.653284000
C	0.579243000	2.346863000	-1.229090000
C	-2.810815000	1.260780000	-1.398876000
C	-1.993940000	-2.261535000	-0.971309000
C	0.170335000	-2.875984000	-0.417049000
C	-2.977040000	-1.143527000	-1.227871000
C	0.101750000	2.970056000	0.058568000
C	0.336578000	4.309825000	0.367493000
C	-3.468302000	0.261329000	0.748565000
C	-0.090952000	4.804519000	1.598155000
C	-0.952048000	2.625811000	2.095250000
C	-2.893272000	-0.558033000	1.884047000
C	-0.749527000	3.947153000	2.480120000
C	-0.982172000	-1.318955000	2.961274000
C	-3.709795000	-1.124239000	2.863688000
C	-1.727406000	-1.899739000	3.982309000
C	-3.118073000	-1.800375000	3.929324000
H	-3.149909000	4.164768000	-3.957618000
H	0.450683000	1.150894000	-3.653013000
H	-0.923945000	3.249052000	-3.417195000
H	-0.450204000	-0.280059000	-3.095747000
H	-5.180995000	3.232423000	-2.849018000
H	1.177046000	0.046051000	-2.456400000
H	-1.629588000	-5.624511000	-1.236874000
H	0.717394000	3.114222000	-1.999040000
H	-3.356966000	-3.835402000	-1.519593000
H	0.687815000	-4.958800000	-0.515368000
H	-2.952221000	-0.930052000	-2.300830000
H	1.555020000	1.877545000	-1.058264000
H	-4.956168000	1.365775000	-1.242988000
H	0.842628000	4.947369000	-0.349874000
H	1.147509000	-2.540042000	-0.084305000
H	-3.995476000	-1.476848000	-0.999762000
H	-4.517212000	-0.013635000	0.590863000
H	-3.444296000	1.315558000	1.042443000
H	0.080574000	5.843571000	1.861267000
H	-1.459650000	1.923787000	2.748972000
H	0.102130000	-1.376040000	2.948085000
H	-1.105957000	4.290590000	3.444927000
H	-4.787993000	-1.032423000	2.785482000

H	-1.226404000	-2.420212000	4.790833000
H	-3.733738000	-2.248429000	4.702943000
N	-0.343837000	1.268159000	-1.663424000
N	-0.757041000	-1.915471000	-0.578734000
N	-2.670198000	0.126326000	-0.499061000
N	-0.533152000	2.143330000	0.912851000
N	-1.550701000	-0.659532000	1.938939000
Ni	-0.568357000	0.083536000	0.194694000
H	1.016488000	-0.117172000	0.594304000

Complex E

C	-2.818317000	2.581604000	-3.587464000
C	-1.549116000	2.369876000	-3.056383000
C	0.891583000	0.762115000	-2.417319000
C	-3.922954000	1.958982000	-3.002595000
C	-1.347180000	1.534810000	-1.944137000
C	-1.576562000	-3.834321000	-3.072024000
C	-3.737495000	1.121486000	-1.906579000
C	-2.469763000	-3.050083000	-2.341351000
C	-0.210336000	-3.709033000	-2.817631000
C	0.600442000	2.618332000	-0.919935000
C	-2.459399000	0.887074000	-1.375059000
C	-1.971847000	-2.172607000	-1.378782000
C	0.206017000	-2.801894000	-1.847535000
C	-2.877530000	-1.353504000	-0.492965000
C	-0.122353000	3.298260000	0.222375000
C	-1.190223000	4.173966000	-0.014315000
C	-2.891397000	0.593363000	0.997138000
C	-1.813480000	4.799863000	1.063787000
C	-0.263691000	3.672780000	2.493847000
C	-2.335675000	-0.048695000	2.246874000
C	-1.343674000	4.541789000	2.350852000
C	-0.474243000	-0.916460000	3.318318000
C	-3.103126000	-0.181042000	3.402808000
C	-1.167986000	-1.061068000	4.514169000
C	-2.513526000	-0.690960000	4.559749000
H	-2.943923000	3.232104000	-4.447869000
H	1.122717000	1.466945000	-3.230220000
H	-0.695327000	2.865739000	-3.507532000
H	0.436059000	-0.129132000	-2.850485000
H	-4.921706000	2.122737000	-3.395781000
H	1.829291000	0.475372000	-1.933926000
H	-1.940501000	-4.525393000	-3.825902000
H	0.700122000	3.329617000	-1.754055000
H	-3.540019000	-3.113993000	-2.509915000
H	0.523275000	-4.293916000	-3.362151000
H	-3.888623000	-1.309892000	-0.912640000
H	1.608609000	2.365920000	-0.583711000
H	-4.599259000	0.643500000	-1.451402000
H	-1.520180000	4.363465000	-1.029810000
H	1.260503000	-2.665660000	-1.624575000
H	-2.959293000	-1.860752000	0.475281000
H	-3.988107000	0.540688000	0.998297000
H	-2.616079000	1.653525000	1.001531000
H	-2.642170000	5.482271000	0.900147000
H	0.141367000	3.463395000	3.481203000
H	0.571237000	-1.199742000	3.238999000
H	-1.790586000	5.008164000	3.222580000
H	-4.145691000	0.120854000	3.390314000
H	-0.661050000	-1.459942000	5.386420000

H	-3.090534000	-0.797850000	5.472772000
N	-0.013201000	1.344146000	-1.401395000
N	-0.649028000	-2.045636000	-1.134358000
N	-2.308006000	-0.004785000	-0.230978000
N	0.344323000	3.061677000	1.464389000
N	-1.035301000	-0.424258000	2.193644000
Ni	-0.219986000	-0.500226000	0.285014000
H	1.405622000	-0.732067000	0.600432000

Complex F

C	-3.629245000	3.117886000	-3.625991000
C	-2.342149000	2.694015000	-3.303619000
C	-0.210834000	0.506336000	-3.030483000
C	-4.725316000	2.625842000	-2.914222000
C	-2.135353000	1.780220000	-2.263752000
C	-1.150853000	-3.913845000	-2.177744000
C	-4.530591000	1.706484000	-1.886257000
C	-2.283763000	-3.131650000	-1.976560000
C	0.075613000	-3.478391000	-1.672454000
C	0.126010000	2.438089000	-1.591790000
C	-3.238154000	1.284307000	-1.556216000
C	-2.166662000	-1.934466000	-1.270376000
C	0.127119000	-2.269942000	-0.993795000
C	-3.373926000	-1.094060000	-0.954143000
C	-0.227624000	3.039273000	-0.260443000
C	0.000505000	4.381559000	0.033699000
C	-3.749029000	0.625053000	0.772817000
C	-0.266902000	4.850798000	1.317127000
C	-0.976884000	2.640223000	1.908549000
C	-3.135738000	-0.144828000	1.919553000
C	-0.759488000	3.962362000	2.272517000
C	-1.176442000	-1.028762000	2.817562000
C	-3.869428000	-0.544733000	3.034340000
C	-1.840272000	-1.446224000	3.965783000
C	-3.209486000	-1.199293000	4.073571000
H	-3.774228000	3.829271000	-4.432730000
H	-0.030810000	1.127850000	-3.914796000
H	-1.493725000	3.073062000	-3.863617000
H	-0.903258000	-0.293280000	-3.294109000
H	-5.730928000	2.951300000	-3.160419000
H	0.734786000	0.074587000	-2.698553000
H	-1.222411000	-4.848986000	-2.723444000
H	0.139743000	3.205731000	-2.371760000
H	-3.253852000	-3.435455000	-2.354545000
H	0.982607000	-4.056233000	-1.807268000
H	-4.040317000	-1.043077000	-1.817973000
H	1.136627000	2.019080000	-1.526226000
H	-5.383163000	1.311566000	-1.343842000
H	0.386243000	5.037066000	-0.739305000
H	1.056231000	-1.880856000	-0.596872000
H	-3.932953000	-1.590864000	-0.154915000
H	-4.815978000	0.400483000	0.689224000
H	-3.644676000	1.698975000	0.954234000
H	-0.093476000	5.892283000	1.567574000
H	-1.356755000	1.920434000	2.621829000
H	-0.114125000	-1.201569000	2.679855000
H	-0.978059000	4.279792000	3.285551000
H	-4.934409000	-0.344693000	3.079843000
H	-1.293252000	-1.955645000	4.750854000
H	-3.758844000	-1.518400000	4.953440000

N	-0.787046000	1.315016000	-1.922275000
N	-0.975044000	-1.515586000	-0.794524000
N	-3.020417000	0.300356000	-0.494620000
N	-0.725448000	2.190416000	0.663504000
N	-1.811836000	-0.390304000	1.820308000
Ni	-1.026654000	0.299111000	-0.005899000
H	0.362602000	0.186097000	0.315039000

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Complex G

C	-3.328131000	2.834307000	-3.456370000
C	-2.020902000	2.478545000	-3.134236000
C	0.245414000	0.453789000	-2.848813000
C	-4.394352000	2.308817000	-2.723342000
C	-1.757614000	1.598849000	-2.075764000
C	-0.902845000	-3.962189000	-2.383692000
C	-4.144448000	1.423517000	-1.678465000
C	-1.993942000	-3.182915000	-2.008585000
C	0.366581000	-3.616028000	-1.918965000
C	0.459374000	2.420809000	-1.449220000
C	-2.831798000	1.064241000	-1.347231000
C	-1.787171000	-2.082486000	-1.175533000
C	0.494191000	-2.493688000	-1.110437000
C	-2.949978000	-1.279226000	-0.649906000
C	0.077075000	3.061510000	-0.140938000
C	0.243630000	4.428237000	0.082027000
C	-3.239141000	0.490131000	1.018915000
C	-0.049025000	4.948906000	1.340294000
C	-0.657389000	2.739317000	2.034647000
C	-2.565182000	-0.222918000	2.173174000
C	-0.504250000	4.087145000	2.338190000
C	-0.578940000	-1.054812000	3.052251000
C	-3.261201000	-0.574616000	3.328787000
C	-1.202887000	-1.423713000	4.238699000
C	-2.569355000	-1.178413000	4.377320000
H	-3.511957000	3.518934000	-4.278372000
H	0.403322000	1.083709000	-3.731867000
H	-1.197828000	2.887790000	-3.710909000
H	-0.400264000	-0.380955000	-3.120836000
H	-5.416341000	2.581817000	-2.966433000
H	1.210208000	0.070965000	-2.507995000
H	-1.039925000	-4.823391000	-3.029829000
H	0.423705000	3.153607000	-2.261436000
H	-2.997321000	-3.418062000	-2.347463000
H	1.245354000	-4.193120000	-2.183733000
H	-3.769766000	-1.273558000	-1.373166000
H	1.495485000	2.070214000	-1.380866000
H	-4.971012000	1.001755000	-1.115481000
H	0.598807000	5.063561000	-0.722246000
H	1.465330000	-2.179887000	-0.745224000
H	-3.322900000	-1.788981000	0.244859000
H	-4.308466000	0.256221000	1.007717000
H	-3.137690000	1.571164000	1.150919000
H	0.073996000	6.009005000	1.538069000
H	-1.011362000	2.039158000	2.783018000
H	0.480227000	-1.232445000	2.894899000
H	-0.742678000	4.446015000	3.333067000
H	-4.325427000	-0.376222000	3.397359000
H	-0.628527000	-1.895710000	5.027716000
H	-3.091298000	-1.459668000	5.286423000
H	1.817617000	-0.757874000	1.031555000

H	2.083671000	0.072798000	-0.234582000
N	-0.379256000	1.226782000	-1.740994000
N	-0.559113000	-1.740073000	-0.741872000
N	-2.577992000	0.119581000	-0.265050000
N	-0.376826000	2.232535000	0.820010000
N	-1.243750000	-0.467222000	2.042360000
O	1.593481000	0.083119000	0.603235000
Ni	-0.497003000	0.177540000	0.174782000

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Complex A

C	-3.272762000	2.598263000	-3.475639000
C	-1.969871000	2.358882000	-3.045944000
C	0.357859000	0.460733000	-2.677978000
C	-4.340556000	1.948493000	-2.852855000
C	-1.703232000	1.478610000	-1.985095000
C	-1.158772000	-3.812800000	-2.969869000
C	-4.089141000	1.066516000	-1.806172000
C	-2.185285000	-3.093703000	-2.353948000
C	0.146261000	-3.646110000	-2.509637000
C	0.473531000	2.428979000	-1.298198000
C	-2.780712000	0.822374000	-1.364628000
C	-1.875905000	-2.236099000	-1.299790000
C	0.372220000	-2.760311000	-1.458233000
C	-2.950003000	-1.485401000	-0.544177000
C	0.118956000	3.138238000	-0.012217000
C	-0.842721000	4.151446000	0.028784000
C	-3.204230000	0.420427000	0.996134000
C	-1.106307000	4.791662000	1.239951000
C	0.558038000	3.397308000	2.247020000
C	-2.541920000	-0.145326000	2.230579000
C	-0.390914000	4.409834000	2.373648000
C	-0.554488000	-0.738073000	3.266168000
C	-3.264430000	-0.426746000	3.386705000
C	-1.204738000	-1.023427000	4.461042000
C	-2.590320000	-0.869799000	4.526440000
H	-3.451249000	3.285329000	-4.297182000
H	0.524019000	1.106073000	-3.551432000
H	-1.148294000	2.859736000	-3.547136000
H	-0.249524000	-0.390044000	-2.985709000
H	-5.360695000	2.127048000	-3.178527000
H	1.324767000	0.098407000	-2.322149000
H	-1.376172000	-4.486049000	-3.793143000
H	0.405422000	3.133548000	-2.135507000
H	-3.214656000	-3.194805000	-2.682479000
H	0.977435000	-4.182131000	-2.955212000
H	-3.901426000	-1.531854000	-1.084639000
H	1.513946000	2.105384000	-1.235269000
H	-4.915853000	0.560730000	-1.316446000
H	-1.367707000	4.433851000	-0.877448000
H	1.376661000	-2.597563000	-1.077231000
H	-3.101007000	-1.988655000	0.417156000
H	-4.280947000	0.212498000	1.010077000
H	-3.075492000	1.508238000	1.003992000
H	-1.850067000	5.580821000	1.293329000
H	1.139965000	3.071825000	3.105361000
H	0.520844000	-0.858043000	3.181888000
H	-0.554881000	4.885679000	3.334454000
H	-4.341596000	-0.293834000	3.389236000
H	-0.631421000	-1.365225000	5.316209000
H	-3.134099000	-1.092546000	5.438821000

H	1.507874000	1.110428000	0.924756000
H	1.858437000	-0.299278000	1.500976000
N	-0.327745000	1.194130000	-1.577498000
N	-0.609663000	-2.064213000	-0.858841000
N	-2.553120000	-0.080719000	-0.246042000
N	0.811891000	2.771922000	1.087101000
N	-1.196131000	-0.305993000	2.157903000
O	1.611317000	0.149505000	0.679833000
Ni	-0.487427000	-0.149077000	0.236522000

Complex I

C	-3.214997000	2.450362000	-3.500568000
C	-1.928246000	2.209724000	-3.023999000
C	0.368206000	0.253406000	-2.386705000
C	-4.312469000	1.861907000	-2.869520000
C	-1.711687000	1.385726000	-1.909902000
C	-1.876705000	-2.980151000	-3.754457000
C	-4.108453000	1.024155000	-1.776093000
C	-2.652100000	-2.283451000	-2.827371000
C	-0.720857000	-3.620490000	-3.312318000
C	0.452287000	2.378895000	-1.241005000
C	-2.816929000	0.772256000	-1.293437000
C	-2.246830000	-2.246628000	-1.488985000
C	-0.397997000	-3.539419000	-1.957705000
C	-3.068851000	-1.523155000	-0.448829000
C	0.028311000	3.252318000	-0.080963000
C	-0.883565000	4.299168000	-0.239191000
C	-3.306732000	0.364651000	1.066896000
C	-1.212582000	5.089192000	0.862835000
C	0.296631000	3.764584000	2.163924000
C	-2.692669000	-0.257514000	2.301671000
C	-0.611267000	4.819056000	2.090761000
C	-0.752143000	-0.986384000	3.343427000
C	-3.451110000	-0.559528000	3.430399000
C	-1.439732000	-1.303447000	4.510023000
C	-2.816284000	-1.083789000	4.556164000
H	-3.357176000	3.095585000	-4.362036000
H	0.560488000	0.781863000	-3.330043000
H	-1.084489000	2.669777000	-3.526912000
H	-0.227788000	-0.633664000	-2.597223000
H	-5.319979000	2.048528000	-3.228155000
H	1.322326000	-0.049240000	-1.949736000
H	-2.173216000	-3.024410000	-4.798022000
H	0.451736000	2.968077000	-2.164233000
H	-3.562166000	-1.776507000	-3.130947000
H	-0.085272000	-4.177704000	-3.992488000
H	-4.123431000	-1.510315000	-0.748488000
H	1.479427000	2.052884000	-1.069800000
H	-4.959257000	0.557566000	-1.289581000
H	-1.321757000	4.491921000	-1.212325000
H	0.490563000	-4.037639000	-1.577221000
H	-2.997390000	-2.073347000	0.491211000
H	-4.383821000	0.158363000	1.037113000
H	-3.176307000	1.450702000	1.111271000
H	-1.919661000	5.906561000	0.759930000
H	0.793827000	3.522758000	3.099581000
H	0.317310000	-1.154851000	3.267471000
H	-0.831030000	5.410793000	2.972729000
H	-4.521840000	-0.384155000	3.419348000
H	-0.903121000	-1.718615000	5.356015000

H	-3.386913000	-1.324148000	5.447603000
N	-0.356675000	1.124663000	-1.415451000
N	-1.137417000	-2.877389000	-1.055212000
N	-2.612529000	-0.120783000	-0.161408000
N	0.614004000	2.998936000	1.109051000
N	-1.356072000	-0.465895000	2.256889000
Ni	-0.592954000	0.086152000	0.449920000
O	1.447807000	0.393256000	1.014546000
H	1.326346000	1.372916000	1.173254000
H	1.627066000	0.014441000	1.887004000

Complex J

C	-3.224706000	2.488176000	-3.476063000
C	-1.939936000	2.238150000	-2.998188000
C	0.326687000	0.230603000	-2.351712000
C	-4.325555000	1.900867000	-2.849899000
C	-1.728184000	1.407601000	-1.887661000
C	-1.888016000	-3.015943000	-3.712142000
C	-4.125518000	1.054266000	-1.762454000
C	-2.669003000	-2.304068000	-2.802422000
C	-0.736896000	-3.653293000	-3.248531000
C	0.464024000	2.377015000	-1.259248000
C	-2.836566000	0.789281000	-1.277381000
C	-2.278409000	-2.246571000	-1.459228000
C	-0.428212000	-3.552927000	-1.892907000
C	-3.106816000	-1.500332000	-0.444133000
C	0.073902000	3.294246000	-0.121018000
C	-0.834467000	4.342103000	-0.294647000
C	-3.326543000	0.372961000	1.103373000
C	-1.131347000	5.173645000	0.785699000
C	0.405001000	3.888971000	2.094484000
C	-2.731526000	-0.307953000	2.298458000
C	-0.500276000	4.944704000	2.006999000
C	-0.744813000	-0.842192000	3.447379000
C	-3.489487000	-0.878574000	3.299599000
C	-1.448549000	-1.404008000	4.483185000
C	-2.879075000	-1.445096000	4.444287000
H	-3.362033000	3.139229000	-4.334055000
H	0.513449000	0.731428000	-3.311777000
H	-1.094283000	2.696158000	-3.499747000
H	-0.284230000	-0.652718000	-2.531284000
H	-5.331977000	2.095196000	-3.208060000
H	1.282597000	-0.075160000	-1.920766000
H	-2.174002000	-3.073932000	-4.758056000
H	0.473361000	2.942258000	-2.197576000
H	-3.574069000	-1.797818000	-3.122439000
H	-0.096218000	-4.222670000	-3.913827000
H	-4.154994000	-1.478530000	-0.768764000
H	1.484507000	2.032123000	-1.085367000
H	-4.978869000	0.588153000	-1.279801000
H	-1.295336000	4.503744000	-1.262925000
H	0.455353000	-4.048340000	-1.496787000
H	-3.068640000	-2.034203000	0.508984000
H	-4.411131000	0.207728000	1.052457000
H	-3.146387000	1.455800000	1.139092000
H	-1.836291000	5.991302000	0.670771000
H	0.925717000	3.679488000	3.025222000
H	0.343007000	-0.810017000	3.479106000
H	-0.694475000	5.569195000	2.872248000
H	-4.573440000	-0.868968000	3.198027000

H	-0.901803000	-1.813892000	5.329169000
H	-3.462498000	-1.891218000	5.241841000
N	-0.373073000	1.136679000	-1.394626000
N	-1.173717000	-2.875670000	-1.005092000
N	-2.639408000	-0.107562000	-0.152948000
N	0.690376000	3.082178000	1.061594000
N	-1.326156000	-0.273337000	2.323692000
Ni	-0.613487000	0.169597000	0.504801000
O	1.498770000	0.448626000	1.050103000
H	1.378628000	1.430707000	1.174622000
H	1.588908000	0.091335000	1.945044000

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Complex K

C	0.072197000	0.419003000	-2.982092000
C	0.397505000	0.540563000	-1.633233000
C	0.728583000	-0.684297000	1.205783000
C	-1.200997000	-0.014574000	-3.352284000
C	-0.536728000	0.233449000	-0.634678000
C	-5.174518000	-3.931515000	-2.254711000
C	-2.125096000	-0.357642000	-2.368670000
C	-4.739878000	-3.153049000	-1.182907000
C	-4.220922000	-4.518758000	-3.084392000
C	0.484084000	1.710868000	1.068778000
C	-1.799138000	-0.259136000	-1.009039000
C	-3.365252000	-2.972730000	-0.981593000
C	-2.873733000	-4.304622000	-2.795471000
C	-2.844711000	-2.159515000	0.186207000
C	-0.271064000	2.960167000	0.665126000
C	0.081805000	3.689917000	-0.473443000
C	-4.080953000	-0.010359000	-0.169626000
C	-0.611045000	4.861795000	-0.776341000
C	-1.925187000	4.504293000	1.188997000
C	-4.871983000	-0.002367000	1.117253000
C	-1.638934000	5.278041000	0.067485000
C	-4.806962000	0.202008000	3.430353000
C	-6.263258000	-0.097182000	1.131695000
C	-6.191850000	0.127902000	3.524741000
C	-6.932663000	-0.024001000	2.352061000
H	0.809691000	0.670836000	-3.737770000
H	1.678208000	-0.615061000	0.660446000
H	1.386835000	0.887490000	-1.356857000
H	0.271547000	-1.654066000	1.009207000
H	-1.472391000	-0.097870000	-4.399966000
H	0.922176000	-0.591517000	2.276077000
H	-6.235117000	-4.083774000	-2.430686000
H	1.468189000	1.721192000	0.589849000
H	-5.452729000	-2.701001000	-0.500473000
H	-4.507418000	-5.137768000	-3.928135000
H	-3.481267000	-2.328971000	1.057138000
H	0.654396000	1.727310000	2.147439000
H	-3.108086000	-0.710663000	-2.658636000
H	0.891727000	3.346184000	-1.106396000
H	-2.104348000	-4.763216000	-3.412880000
H	-1.840333000	-2.503365000	0.432081000
H	-4.667109000	-0.478977000	-0.965171000
H	-3.893577000	1.025538000	-0.471551000
H	-0.347665000	5.440940000	-1.655893000
H	-2.708905000	4.794007000	1.883337000
H	-4.188641000	0.299091000	4.317652000
H	-2.202798000	6.183467000	-0.128161000

H	-6.803248000	-0.225591000	0.199756000
H	-6.671459000	0.180303000	4.495553000
H	-8.015163000	-0.093910000	2.388027000
N	-0.204808000	0.401679000	0.782212000
N	-2.440522000	-3.553995000	-1.771822000
N	-2.752325000	-0.659211000	0.017559000
N	-1.256660000	3.379588000	1.485054000
N	-4.160875000	0.146862000	2.252328000
Ni	-2.073144000	0.085642000	1.933807000
O	-1.629602000	1.551010000	3.388882000
H	-1.544758000	2.358401000	2.783188000
H	-2.410258000	1.713722000	3.938895000
H	-1.713428000	-1.213784000	2.795329000

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Complex L

C	0.306622000	0.222624000	-2.940955000
C	0.587205000	0.402022000	-1.589189000
C	0.980822000	-0.570500000	1.263880000
C	-0.954982000	-0.230831000	-3.328097000
C	-0.371869000	0.132311000	-0.599691000
C	-5.304406000	-3.672463000	-2.414303000
C	-1.904183000	-0.531557000	-2.355204000
C	-4.825171000	-2.953073000	-1.320680000
C	-4.395833000	-4.381422000	-3.198861000
C	0.453662000	1.767675000	1.035761000
C	-1.622738000	-0.382978000	-0.987185000
C	-3.449690000	-2.949671000	-1.051157000
C	-3.048833000	-4.344381000	-2.841768000
C	-2.882241000	-2.195682000	0.138271000
C	-0.511261000	2.878058000	0.684493000
C	-0.429530000	3.564728000	-0.530368000
C	-3.859541000	0.082356000	-0.181221000
C	-1.327688000	4.599194000	-0.793296000
C	-2.289671000	4.204283000	1.360507000
C	-4.680975000	0.157809000	1.079574000
C	-2.281010000	4.926397000	0.169699000
C	-4.682153000	0.512407000	3.368463000
C	-6.073093000	0.122678000	1.053123000
C	-6.069802000	0.515848000	3.417509000
C	-6.788855000	0.307411000	2.237483000
H	1.065517000	0.445983000	-3.684775000
H	1.934782000	-0.409896000	0.740412000
H	1.565585000	0.769201000	-1.297308000
H	0.645853000	-1.592689000	1.083946000
H	-1.198658000	-0.356308000	-4.378720000
H	1.142678000	-0.438147000	2.335824000
H	-6.366032000	-3.686608000	-2.642326000
H	1.391842000	1.925128000	0.488829000
H	-5.506001000	-2.410688000	-0.672429000
H	-4.718494000	-4.959965000	-4.058207000
H	-3.563545000	-2.308766000	0.985566000
H	0.689551000	1.830279000	2.100375000
H	-2.882565000	-0.885116000	-2.659142000
H	0.330106000	3.291835000	-1.254214000
H	-2.316182000	-4.902533000	-3.421044000
H	-1.931311000	-2.653391000	0.412744000
H	-4.475257000	-0.277613000	-1.013397000
H	-3.535358000	1.098218000	-0.435644000
H	-1.278348000	5.143073000	-1.731564000
H	-3.007053000	4.431732000	2.144539000



H	-4.100897000	0.640551000	4.276662000
H	-2.996587000	5.726022000	0.011787000
H	-6.583701000	-0.034467000	0.108167000
H	-6.572461000	0.667894000	4.366958000
H	-7.873894000	0.288391000	2.239246000
N	-0.066348000	0.380487000	0.806914000
N	-2.572248000	-3.652474000	-1.795917000
N	-2.624828000	-0.719664000	0.009958000
N	-1.428735000	3.207484000	1.616727000
N	-3.976093000	0.334260000	2.227151000
Ni	-1.960051000	-0.123259000	2.069528000
O	-1.325107000	1.404840000	3.662549000
H	-1.412789000	2.165468000	3.021019000
H	-2.070966000	1.498349000	4.271271000
H	-1.511754000	-1.482074000	2.937142000

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Complex M

C	-5.118384000	2.302630000	-1.420533000
C	-3.766068000	2.496017000	-1.681031000
C	-1.200975000	1.572971000	-2.938562000
C	-5.514135000	1.246548000	-0.597788000
C	-2.780748000	1.665838000	-1.119963000
C	-0.580167000	-2.772655000	-3.513152000
C	-4.548463000	0.417247000	-0.038063000
C	-1.519893000	-2.600617000	-2.499181000
C	0.611328000	-2.049851000	-3.454743000
C	-0.899464000	3.242708000	-1.204244000
C	-3.174482000	0.614890000	-0.267917000
C	-1.251575000	-1.711812000	-1.455076000
C	0.799764000	-1.170766000	-2.394033000
C	-2.206135000	-1.610273000	-0.279471000
C	-0.616339000	3.432488000	0.261451000
C	-0.918918000	4.610790000	0.938729000
C	-2.395564000	-0.284101000	1.849478000
C	-0.561095000	4.736837000	2.281698000
C	0.344021000	2.518992000	2.165330000
C	-1.734030000	-1.417440000	2.608682000
C	0.084899000	3.668678000	2.904155000
C	0.186299000	-2.448593000	3.398375000
C	-2.530284000	-2.351787000	3.280428000
C	-0.537989000	-3.408893000	4.099753000
C	-1.928500000	-3.357502000	4.035764000
H	-5.855883000	2.962474000	-1.867316000
H	-1.716700000	2.305749000	-3.573405000
H	-3.467068000	3.301046000	-2.344512000
H	-1.596544000	0.581062000	-3.160282000
H	-6.565752000	1.066370000	-0.396253000
H	-0.135180000	1.592212000	-3.176322000
H	-0.774069000	-3.458643000	-4.331856000
H	-1.583257000	4.017591000	-1.567987000
H	-2.455479000	-3.150567000	-2.505448000
H	1.377288000	-2.153127000	-4.215520000
H	-3.206561000	-1.927887000	-0.599358000
H	0.043699000	3.360825000	-1.750844000
H	-4.862930000	-0.410458000	0.589808000
H	-1.425829000	5.414306000	0.414526000
H	1.706364000	-0.578887000	-2.316966000
H	-1.872563000	-2.348454000	0.455917000
H	-3.456269000	-0.308980000	2.117982000
H	-1.994235000	0.667134000	2.215834000

H	-0.785192000	5.646902000	2.829090000
H	0.843829000	1.668221000	2.614061000
H	1.273217000	-2.452052000	3.414071000
H	0.382013000	3.715868000	3.946241000
H	-3.610584000	-2.285015000	3.208359000
H	-0.021768000	-4.170778000	4.673454000
H	-2.536814000	-4.086272000	4.562428000
H	0.788399000	-0.670986000	1.708776000
H	1.800265000	-0.986814000	0.564689000
N	-1.381538000	1.866726000	-1.493419000
N	-0.110145000	-0.991089000	-1.414690000
N	-2.214788000	-0.281375000	0.361749000
N	0.008492000	2.392713000	0.863851000
N	-0.388004000	-1.473566000	2.676232000
O	1.464261000	-0.251455000	1.097398000
Ni	-0.042535000	0.672425000	-0.180936000

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Complex N

C	-5.060292000	2.365860000	-1.445135000
C	-3.701261000	2.528331000	-1.692644000
C	-1.144826000	1.551698000	-2.929265000
C	-5.486666000	1.314810000	-0.631523000
C	-2.739547000	1.672471000	-1.128633000
C	-0.670426000	-2.742419000	-3.580016000
C	-4.544676000	0.459262000	-0.070290000
C	-1.598595000	-2.567147000	-2.555804000
C	0.547700000	-2.066451000	-3.505539000
C	-0.835231000	3.216431000	-1.198317000
C	-3.163322000	0.623042000	-0.287622000
C	-1.293038000	-1.720872000	-1.485394000
C	0.771619000	-1.228948000	-2.417431000
C	-2.234703000	-1.615589000	-0.303236000
C	-0.605775000	3.417919000	0.274439000
C	-0.951380000	4.591415000	0.939444000
C	-2.443814000	-0.334314000	1.837957000
C	-0.647491000	4.721159000	2.295844000
C	0.292356000	2.515507000	2.211422000
C	-1.735106000	-1.420284000	2.590104000
C	-0.011267000	3.660301000	2.941476000
C	0.323266000	-2.368634000	3.431332000
C	-2.431280000	-2.387141000	3.289846000
C	-0.356001000	-3.323838000	4.128776000
C	-1.785349000	-3.354859000	4.089126000
H	-5.778418000	3.045405000	-1.894183000
H	-1.642435000	2.293412000	-3.569242000
H	-3.378136000	3.330180000	-2.348897000
H	-1.554666000	0.567145000	-3.157270000
H	-6.543840000	1.158296000	-0.438551000
H	-0.076888000	1.553443000	-3.158711000
H	-0.893340000	-3.395205000	-4.418454000
H	-1.489180000	4.000141000	-1.597961000
H	-2.553798000	-3.082326000	-2.574254000
H	1.306556000	-2.174818000	-4.272908000
H	-3.239758000	-1.931942000	-0.613926000
H	0.130193000	3.307299000	-1.710664000
H	-4.885339000	-0.364187000	0.549074000
H	-1.449699000	5.388120000	0.396548000
H	1.700938000	-0.674784000	-2.325802000
H	-1.901928000	-2.346160000	0.444113000
H	-3.507265000	-0.440427000	2.077739000

H	-2.127098000	0.651525000	2.203625000
H	-0.905241000	5.627171000	2.835210000
H	0.783311000	1.668202000	2.676847000
H	1.405703000	-2.303819000	3.415768000
H	0.243817000	3.710076000	3.994723000
H	-3.515847000	-2.380306000	3.216558000
H	0.203846000	-4.055973000	4.702980000
H	-2.350853000	-4.104073000	4.630655000
H	0.268335000	-0.839203000	2.031213000
H	1.655650000	-1.047813000	0.565563000
N	-1.333421000	1.846690000	-1.486704000
N	-0.125413000	-1.044650000	-1.429089000
N	-2.231490000	-0.294052000	0.343936000
N	0.010039000	2.386150000	0.897779000
N	-0.332891000	-1.381560000	2.703086000
O	1.461374000	-0.221978000	1.029484000
Ni	0.023530000	0.629877000	-0.137765000

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## References

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