Electronic Supplementary Information

Alkynyl transmetalation triggered by a nucleophilic attack

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General methods

Unless otherwise stated, all reactions and manipulations were performed using standard Schlenk techniques. All solvents were purified by distillation using standard methods.

Commercially available reagents were used without further purification. NMR spectra were recorded by using a Bruker 400 MHz spectrometer. Chemical shifts are reported in ppm from tetramethylsilane with the solvent resonance as the internal standar (^{1}H NMR $CDCl_3$: 7.26 ppm; ^{13}C NMR $CDCl_3$: 77.0 ppm). Mass spectra were recorded on the HP-5989 instrument by EI/ESI methods. X-ray diffraction analysis was performed by using a Bruker Smart-1000X-ray diffractometer.

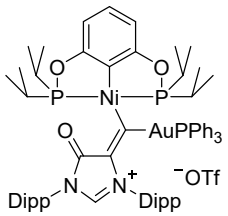
The group 10 metal acetylides **1a**~**1c** were synthesized by the procedures previously reported.[1]

Preparation and characterization

Cyclization of 1a in presence of PPh_3AuOTf at room temperature:

The mixture of **1a** (100 mg, 0.12 mmol) and PPh_3AuOTf (75 mg, 0.12 mmol) was stirred in the DCE (3 mL) at 25 °C. After stirring for 2 h, the volatiles were removed under vacuum, and the residue was dissolved in DCM and filtered. After the solvents in the filtrate were evaporated, the crude product was washed twice with diethyl ether to afford pure **2a** as a white solid (162 mg, 92%). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.57 (d, J = 2.0 Hz, 1H, N-C<u>H</u>=N), 7.55-7.47 (m, 2H, H_{Ar}), 7.45-7.40 (m, 3H, H_{Ar}), 7.31 (d, J = 7.8, 4H, H_{Ar}), 7.17-7.06 (m, 13H, H_{Ar}), 6.68 (d, J = 8.0 Hz, 2H, PO-C=C<u>H</u>), 2.84-2.75 (m, 2H, C<u>H</u>$(CH_3)_2$), 2.64-2.55 (m, 2H, C<u>H</u>$(CH_3)_2$), 2.41-2.26 (m, 4H, C<u>H</u>$(CH_3)_2$), 1.26-1.17 (m, 42H, CH_3), 1.15-1.10 (m, 6H, CH_3). Our characterization data for **2a** are in full agreement previously reported literature data.[1]

Synthesis of 3b



The mixture of **1b** (100 mg, 0.12 mmol) and PPh_3AuOTf (75 mg, 0.12 mmol) was stirred in the DCE (3 mL) at -20 °C. After stirring for 2 h, all the volatiles were removed under vacuum, and the residue was dissolved in DCM and filtered. After the solvents in the filtrate were evaporated, the crude product was washed twice with diethyl ether to afford pure **3b** as an orange solid (154 mg, 90%). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 9.42 (s, 1H, N-C<u>H</u>=N), 7.55-7.45 (m, 5H, H_{Ar}), 7.34-7.27 (m, 10H, H_{Ar}), 7.25-7.21 (m, 3H, H_{Ar}), 7.13-7.01 (m, 4H, H_{Ar}), 6.53 (d, J = 8.0 Hz, 2H, PO-C=C<u>H</u>), 2.76-2.64 (m, 2H, C<u>H</u>$(CH_3)_2$), 2.64-2.54 (m, 2H, C<u>H</u>$(CH_3)_2$), 2.52-2.40 (m, 2H, C<u>H</u>$(CH_3)_2$), 2.06-1.95 (m, 2H, C<u>H</u>$(CH_3)_2$), 1.32-1.22 (m, 20H, CH_3), 1.20-1.14 (m, 22H, CH_3), 0.83 (dd, J = 16.4, 7.6 Hz, 6H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$) δ = 165.6

(s, Ni-C-Au), 157.5 (d, $J_{P\text{-}C}$ = 10.0 Hz, C(Ni)=C-O), 145.7 (d, $J_{P\text{-}C}$ = 8.6 Hz, C=O), 143.9 (s, C_{Ar}), 134.6-133.7 (m, C_{Ar}), 132.8 (s, C_{Ar}), 131.5 (s, C_{Ar}), 131.1 (s, C_{Ar}), 130.9-128.3 (m, C_{Ar}), 126.8 (s, C_{Ar}), 124.3 (s, C_{Ar}), 104.3 (s, C_{Ar}), 31.8 (s, $CH(CH_3)_2$), 29.1 (s, $CH(CH_3)_2$), 28.7 (s, $CH(CH_3)_2$), 26.1 (s, $CH(CH_3)_2$), 23.8 (d, $J_{P\text{-}C}$ = 8.8 Hz, $PCH(CH_3)_2$), 22.4 (s, CH_3), 17.3 (s, CH_3), 17.0 (s, CH_3), 16.8 (s, CH_3), 16.5 (s, CH_3); ^{31}P NMR (162 MHz, $CDCl_3$) δ = 189.40, 40.59 (s, PPh_3); HRMS (MALDI): m/z [M-OTf]$^+$ calcd. for $C_{64}H_{81}AuN_2NiO_3P_3^+$: 1273.4479; found: 1273.4589; Anal. calcd. for $C_{65}H_{81}AuF_3N_2NiO_6P_3S$: C, 54.83; H, 5.73; N, 1.97; found: C, 54.57; H, 5.73; N, 1.90.

Cyclization of 1b in presence of PPh_3AuOTf at room temperature:

The mixture of **1b** (100 mg, 0.12 mmol) and PPh_3AuOTf (85 mg, 0.14 mmol) was stirred in the DCE (3 mL) at room temperature. After stirring for 2 h, all the volatiles were removed under vacuum, and the residue was dissolved in DCM and filtered. After the solvents in the filtrate were evaporated, the crude product was washed twice with diethyl ether to afford a mixture of **2b** and **3b** in the ratio of 13:87 as an orange solid (166 mg, 97%).

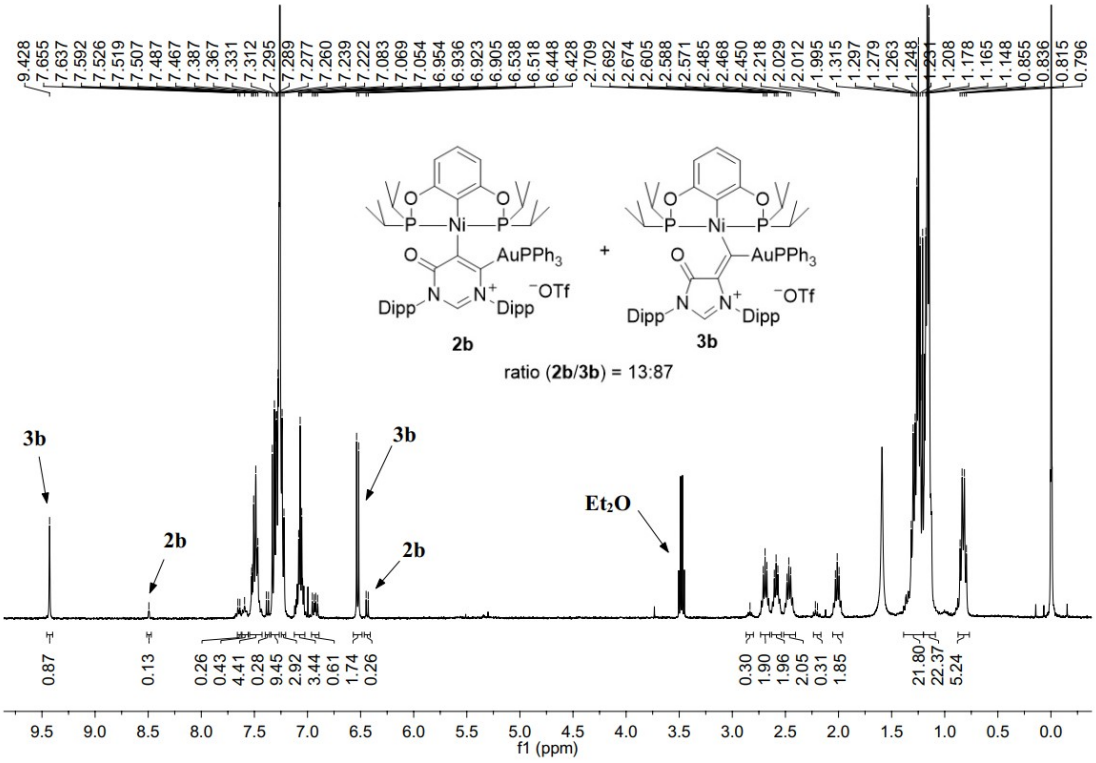


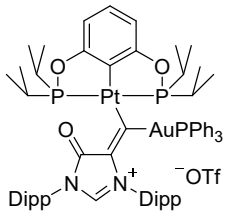
Figure S1. ^{1}H NMR spectra (400 MHz, $CDCl_3$) of the mixtures of **2b** and **3b**.

Synthesis of 2b from the isomerization of 3b at 50 °C:

In a nitrogen-filled round-bottom flask, was charged with **3b** (50 mg, 0.035 mmol) and stirred in the DCE (1 mL) at 50 °C. After stirring for 1 h, the volatiles were removed under vacuum to afford **2b** with a conversion of one hundred percent determinded by 1H NMR

analysis. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.44 (s, 1H, N-C<u>H</u>=N), 7.65 (t, J = 7.8 Hz, 1H, H_{Ar}), 7.52-7.41 (m, 4H, H_{Ar}), 7.37 (d, J = 7.8 Hz, 2H, H_{Ar}), 7.30 (d, J = 7.8 Hz, 2H, H_{Ar}), 7.28-7.26 (m, 2H, H_{Ar}), 7.25-7.21 (m, 4H, H_{Ar}), 6.99 (t, J = 7.8 Hz, 1H, PO-C=CH-C<u>H</u>), 6.92 (dd, J = 12.4, 7.8 Hz, 6H, H_{Ar}), 6.44 (d, J = 8.0 Hz, 2H, PO-C=C<u>H</u>), 2.90-2.77 (m, J = 2H, C<u>H</u>$(CH_3)_2$), 2.74-2.61 (m, 2H, C<u>H</u>$(CH_3)_2$), 2.61-2.50 (m, 2H, C<u>H</u>$(CH_3)_2$), 2.50-2.37 (m, 2H, C<u>H</u>$(CH_3)_2$), 1.35 (dd, J = 16.6, 7.8 Hz, 6H, CH_3), 1.26 (d, J = 6.8 Hz, 6H, CH_3), 1.24-1.14 (m, 36H, CH_3). Our characterization data for **2b** are in full agreement previously reported literature data.[1]

Synthesis of 3c



The mixture of **1c** (100 mg, 0.11 mmol) and PPh_3AuOTf (79 mg, 0.13 mmol) was stirred in the DCE (3 mL) at -20 °C. After stirring for 2 h, all the volatiles were removed under vacuum, and the residue was dissolved in DCM and filtered. After the solvents in the filtrate were evaporated, the crude product was washed twice with diethyl ether to afford pure **3c** as an orange solid (163 mg, 95%). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 9.55 (s, 1H, N-C<u>H</u>=N), 7.53-7.45 (m, 4H, H_{Ar}), 7.35-7.27 (m, 10H, H_{Ar}), 7.25-7.20 (m, 4H, H_{Ar}), 7.07-6.90 (m, 4H, H_{Ar}), 6.63 (d, J = 8.0Hz, 2H, PO-C=C<u>H</u>), 2.77-2.65 (m, 2H, C<u>H</u>$(CH_3)_2$), 2.65-2.53 (m, 2H, C<u>H</u>$(CH_3)_2$), 2.48-2.33 (m, 2H, C<u>H</u>$(CH_3)_2$), 2.20-2.05 (m, 2H, C<u>H</u>$(CH_3)_2$), 1.27-1.15 (m, 30H, CH_3), 1.09 (dd, J = 15.6, 7.6 Hz, 12H, CH_3), 0.83 (dd, J = 17.2, 7.6 Hz, 6H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$) δ = 163.2 (t, $J_{P\text{-}C}$ = 5.8 Hz, Pt-<u>C</u>-Au), 158.1 (d, $J_{P\text{-}C}$ = 11.4 Hz, <u>C</u>(Pt)=C-O), 145.8 (<u>s, C</u>=O), 145.3 (s, C_{Ar}), 144.4 (s, C_{Ar}), 143.9 (s, C_{Ar}), 134.5-133.5 (m, C_{Ar}), 132.8 (s, C_{Ar}), 131.5 (s, C_{Ar}), 131.1 (s, C_{Ar}), 129.9 (t, $J_{P\text{-}C}$ = 5.8 Hz, C_{Ar}), 129.5 (s, C_{Ar}), 129.4 (s, C_{Ar}), 129.0 (s, C_{Ar}), 128.7 (s, C_{Ar}), 128.6 (s, C_{Ar}), 127.1 (s, C_{Ar}), 124.7 (s, C_{Ar}), 124.2 (d, $J_{P\text{-}C}$ = 8.2 Hz, C_{Ar}), 104.4 (s, C_{Ar}), 32.1 (t, $J_{P\text{-}C}$ = 15.6 Hz, P<u>C</u>H$(CH_3)_2$), 29.2 (s, <u>C</u>H$(CH_3)_2$), 28.9 (s, <u>C</u>H$(CH_3)_2$), 25.8 (s, <u>C</u>H$(CH_3)_2$), 23.7 (s, CH_3), 23.0 (s, CH_3), 16.5 (s, CH_3), 16.0 (s, CH_3); ^{31}P NMR (162 MHz, $CDCl_3$) δ = 174.27 (t, $J_{Pt\text{-}P}$ = 1550.9 Hz, 2P), 39.84 (s, <u>P</u>Ph$_3$); HRMS (MALDI): m/z $[M\text{-}OTf]^+$ calcd. for $C_{64}H_{81}AuN_2O_3P_3Pt^+$: 1410.4773; found: 1410.4375; Anal. calcd. for $C_{65}H_{81}AuF_3N_2O_6P_3PtS$ (1.25 CH_2Cl_2): C, 47.75; H, 5.05; N, 1.68; found: C, 47.95; H, 5.02; N, 1.60.

Cyclization of 1c in presence of PPh_3AuOTf at room temperature:

The mixture of **1c** (100 mg, 0.11 mmol) and PPh_3AuOTf (79 mg, 0.13 mmol) was stirred

in the DCE (3 mL) at room temperature. After stirring for 2 h, all the volatiles were removed under vacuum, and the residue was dissolved in DCM and filtered. After the solvents in the filtrate were evaporated, the crude product was washed twice with diethyl ether to afford a mixture of **2c** and **3c** in the ratio of 28:72 as an orange solid (161 mg, 94%).

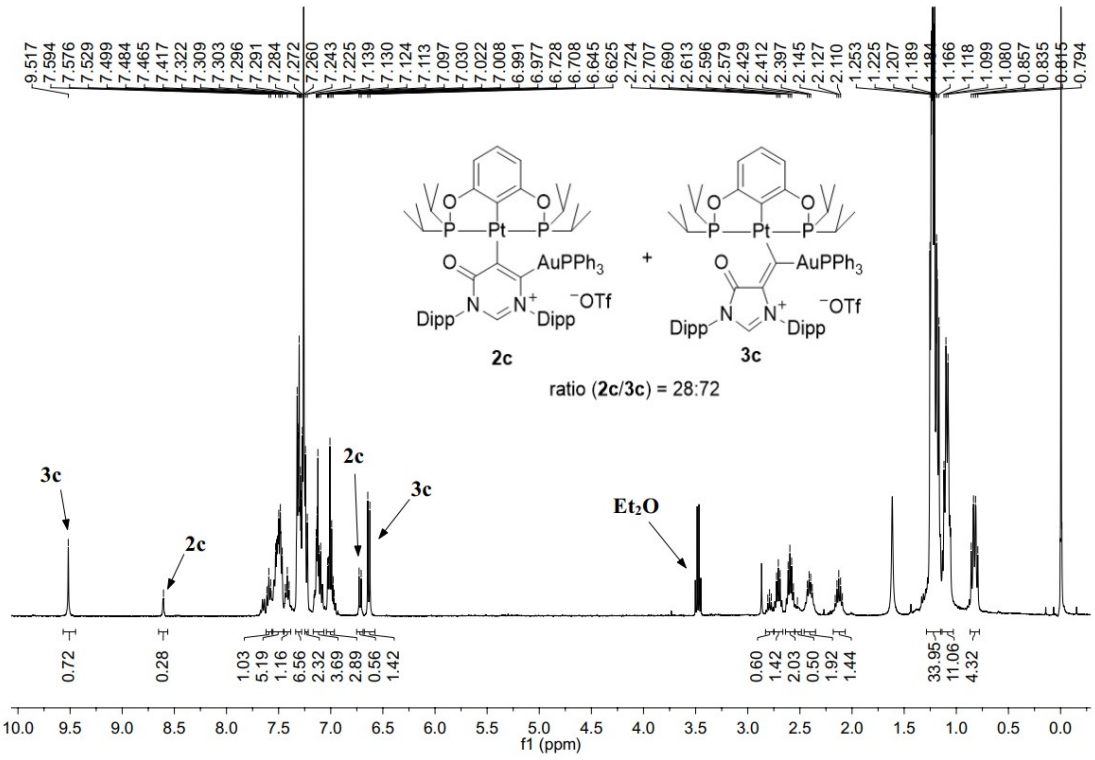


Figure S2. ^{1}H NMR spectra (400 MHz, $CDCl_3$) of the mixtures of **2c** and **3c**.

Synthesis of 2c from the isomerization of 3c at 50 °C:

In a nitrogen-filled round-bottom flask, was charged with **3c** (50 mg, 0.032 mmol) and stirred in the DCE (1 mL) at 50 °C. After stirring for 1 h, the volatiles were removed under vacuum to afford **2c** with a conversion of one hundred percent determinded by ^{1}H NMR analysis. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.61 (d, J = 1.6 Hz, 1H, N-C<u>H</u>=N), 7.56-7.46 (m, 2H, H_{Ar}), 7.45-7.37 (m, 3H, H_{Ar}), 7.31 (dd, J = 8.0, 3.2 Hz, 4H, H_{Ar}), 7.20-7.03 (m, 13H, H_{Ar}), 6.72 (d, J = 8.0 Hz, 2H, PO-C=C<u>H</u>), 2.85-2.73 (m, 2H, C<u>H</u>$(CH_3)_2$), 2.66-2.46 (m, 4H, C<u>H</u>$(CH_3)_2$), 2.45-2.33 (m, 2H, C<u>H</u>$(CH_3)_2$), 1.27-1.06 (m, 48H, CH_3). Our data of **2c** are in full agreement with we previous reported in the literature.[1]

Protodemetalation of 3b in presence of trifluoromethanesulfonic acid:

The mixture of **3b** (100 mg, 0.07 mmol) and trifluoromethanesulfonic acid (12 mg, 0.08 mmol) was stirred in the DCE (3 mL) at 25 °C. After stirring for 4 h, all the volatiles were removed under vacuum, and the residue was dissolved in DCM and filtered. After the solvents in the filtrate were evaporated, the crude product was washed twice with diethyl ether to afford

pure **4** as a yellow solid (63 mg, 88%). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 10.48 (d, J = 2.0 Hz, 1H, N-C<u>H</u>=N), 9.28 (t, J = 2.0 Hz, 1H, C<u>H</u>(Au)), 7.61-7.54 (m, 4H, H_{Ar}), 7.53-7.45 (m, 7H, H_{Ar}), 7.35-7.26 (m, 8H, H_{Ar}), 7.05-6.99 (m, 2H, H_{Ar}), 2.73-2.59 (m, 4H, C<u>H</u>$(CH_3)_2$), 1.30-1.21 (m, CH_3); Our data for **4** are in full agreement we previously reported literature data.[2]

Protodemetalation of 3c in presence of trifluoromethanesulfonic acid:

The mixture of **3c** (100 mg, 0.06 mmol) and trifluoromethanesulfonic acid (11 mg, 0.07 mmol) was stirred in the DCE (3 mL) at 25 °C. After stirring for 4 h, all the volatiles were removed under vacuum, and the residue was dissolved in DCM and filtered. After the solvents in the filtrate were evaporated, the crude product was washed twice with diethyl ether to afford pure **4** as a yellow solid (53 mg, 86%). Our data are in full agreement with we previous reported in the literature.[2]

NMR spectra

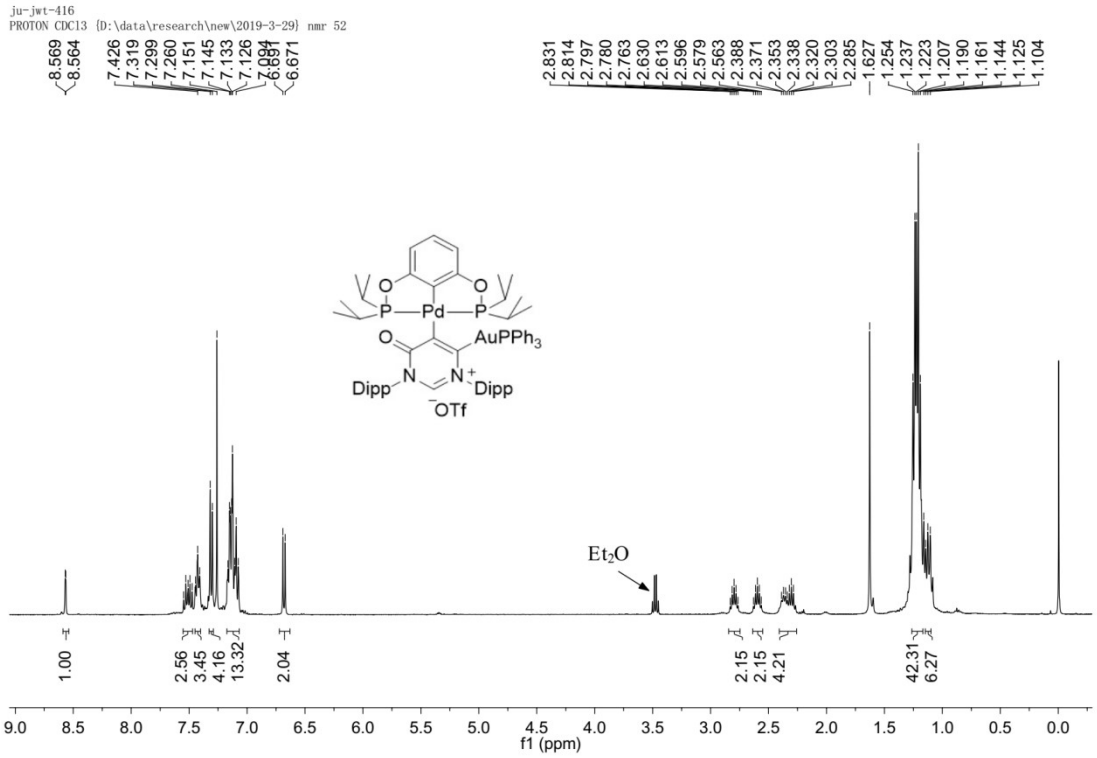


Figure S3. ^{1}H NMR spectra (400 MHz, $CDCl_3$) of **2a**.

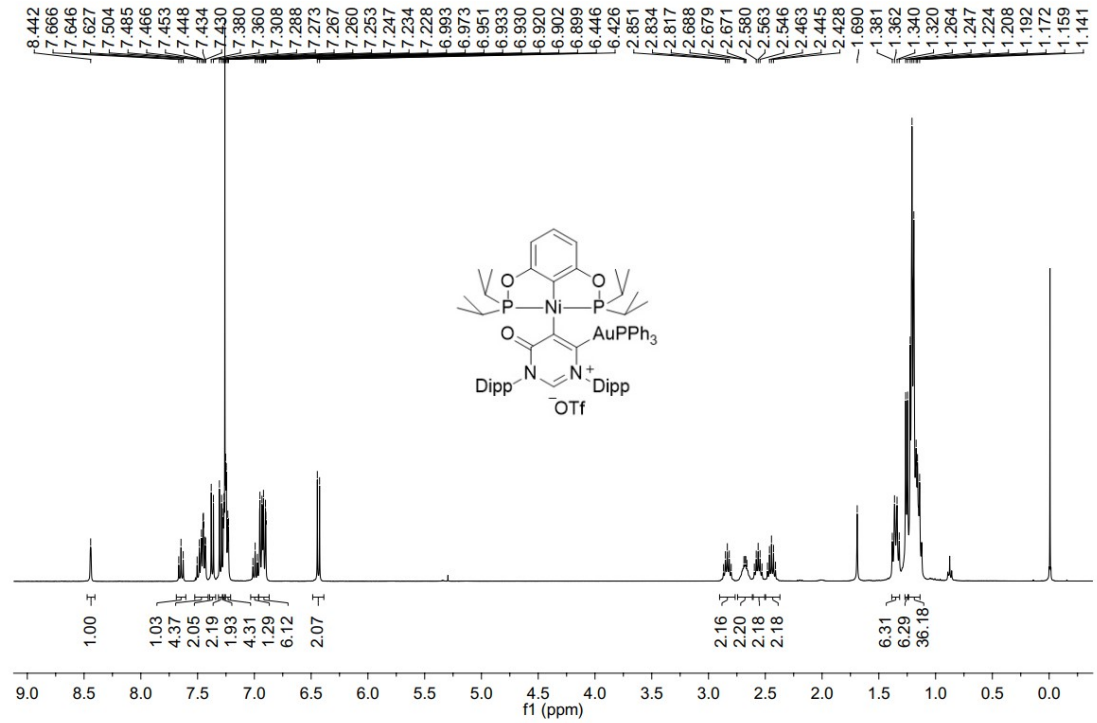


Figure S4. ^{1}H NMR spectra (400 MHz, $CDCl_3$) of **2b**.

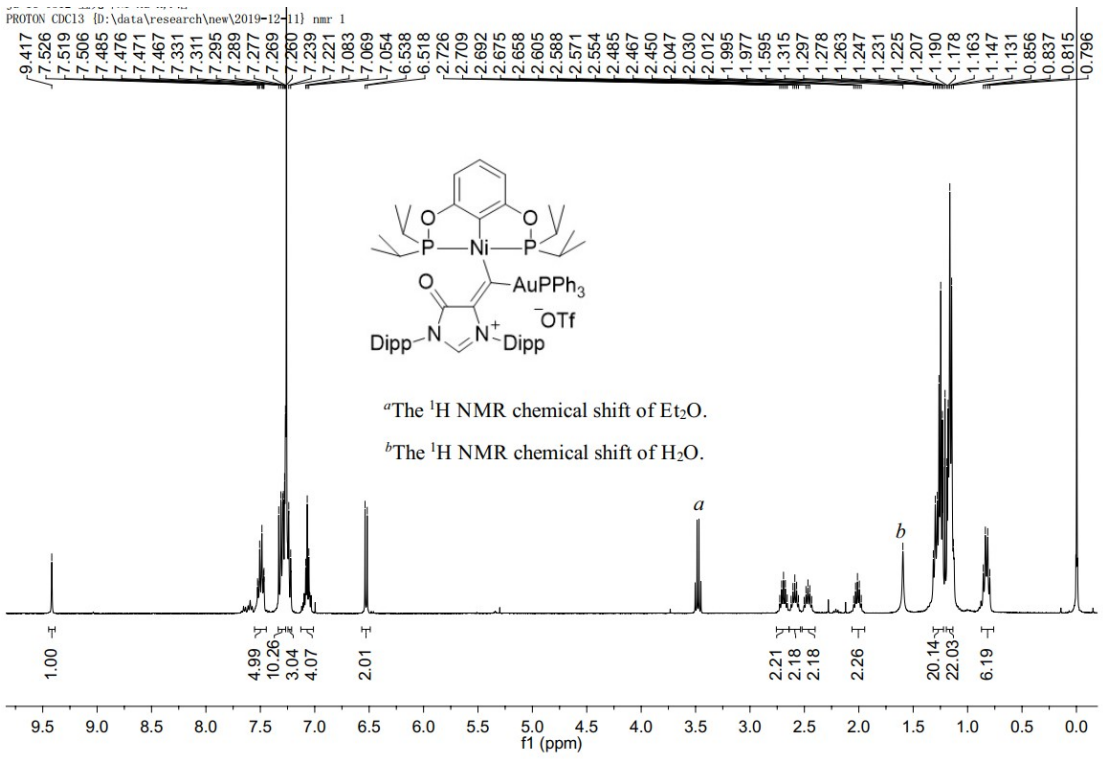


Figure S5. ^{1}H NMR spectra (400 MHz, $CDCl_3$) of **3b**.

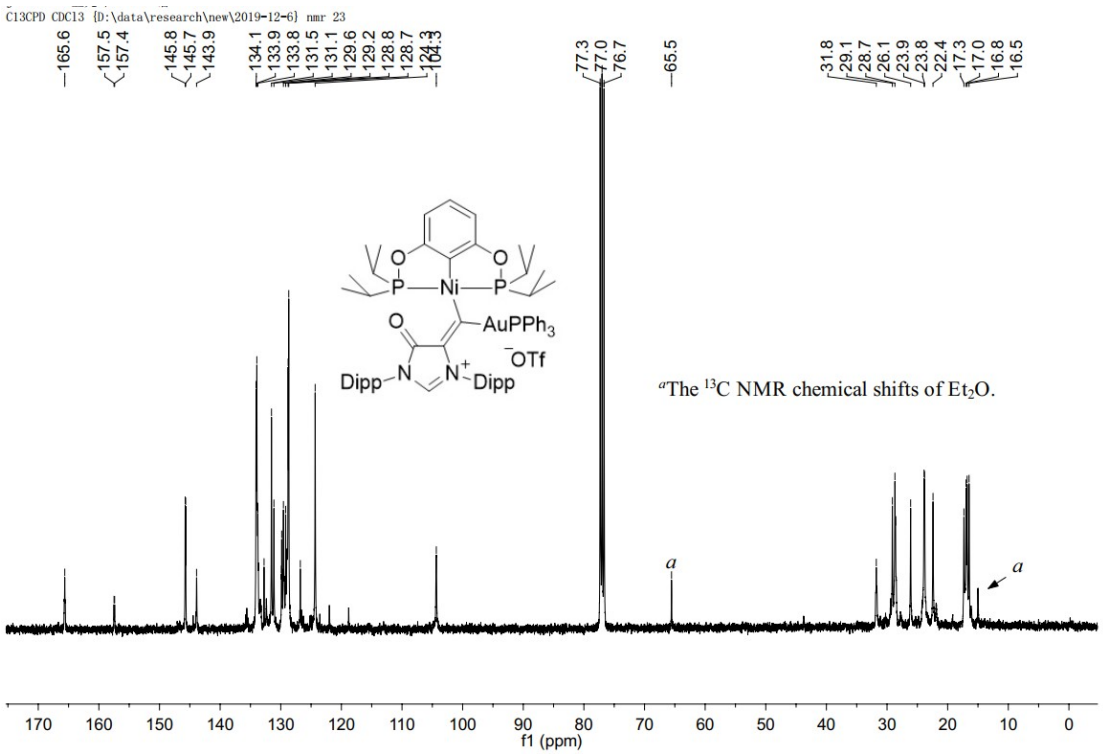


Figure S6. ^{13}C NMR spectra (100 MHz, $CDCl_3$) of **3b**.

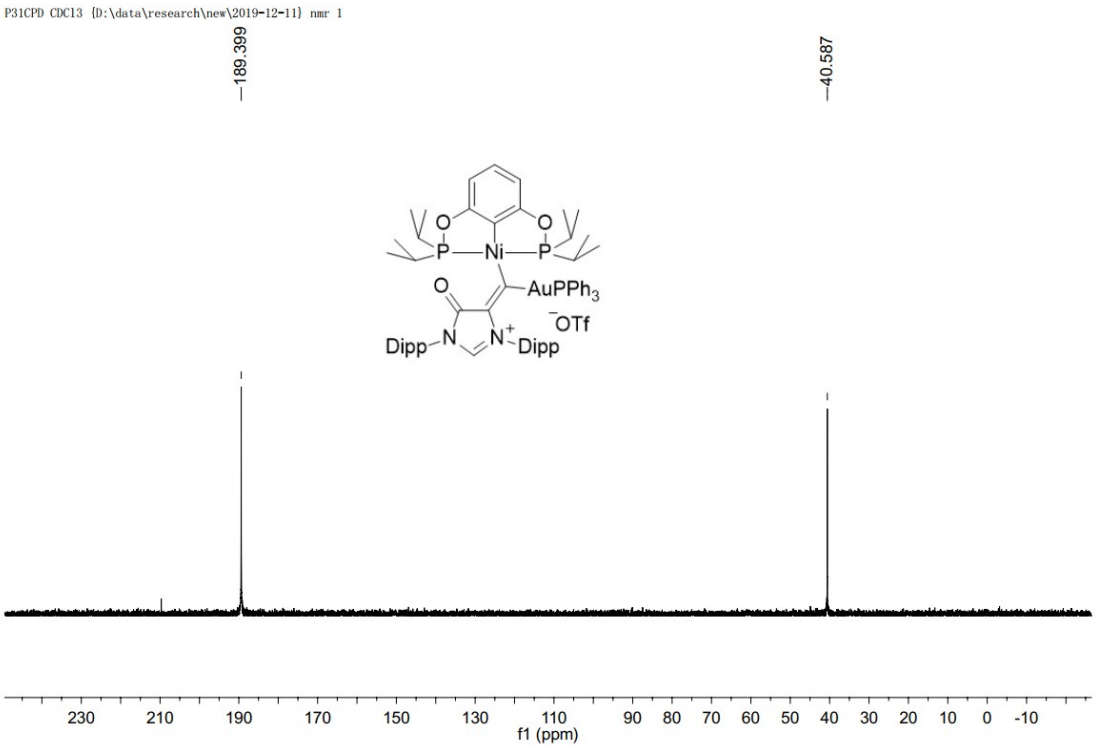


Figure S7. ^{31}P NMR spectra (162 MHz, $CDCl_3$) of **3b**.

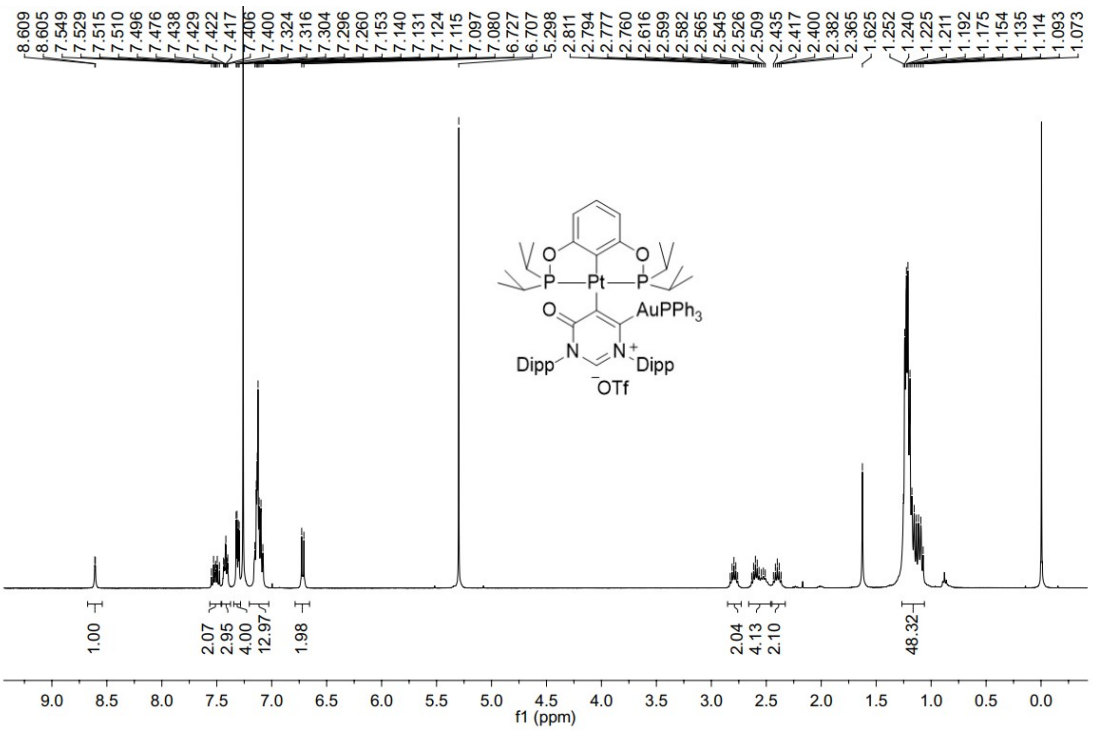


Figure S8. ^{1}H NMR spectra (400 MHz, $CDCl_3$) of **2c**.

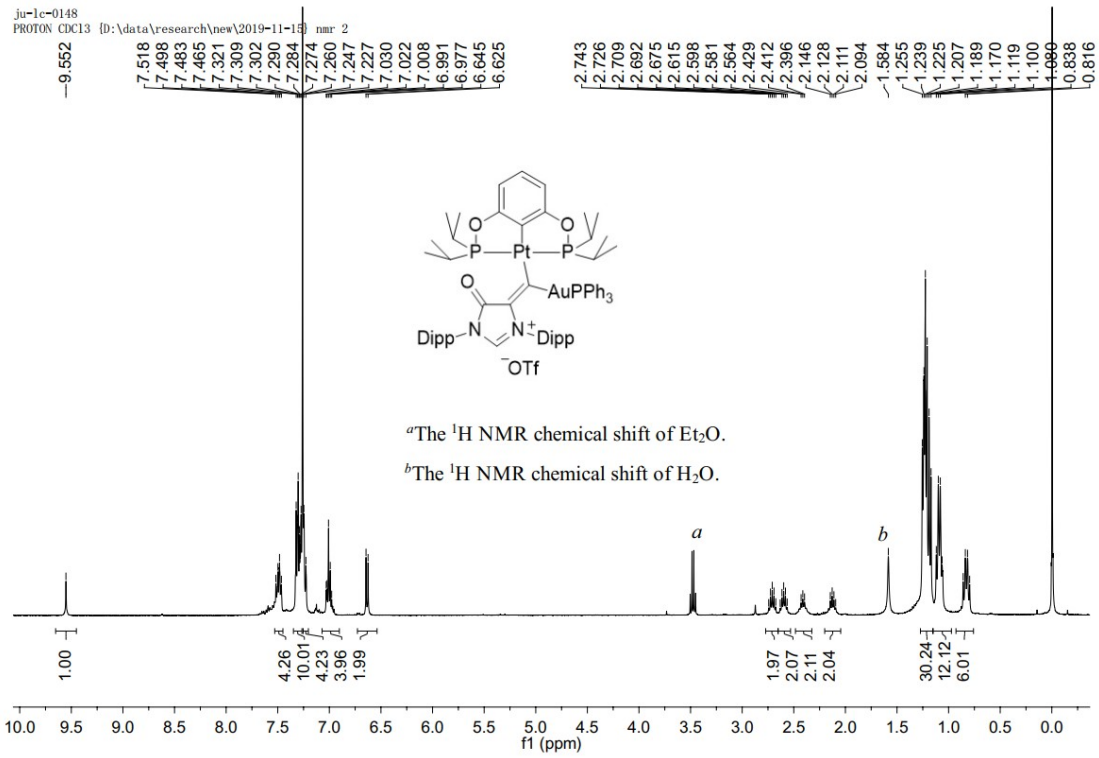


Figure S9. ^{1}H NMR spectra (400 MHz, $CDCl_3$) of **3c**.

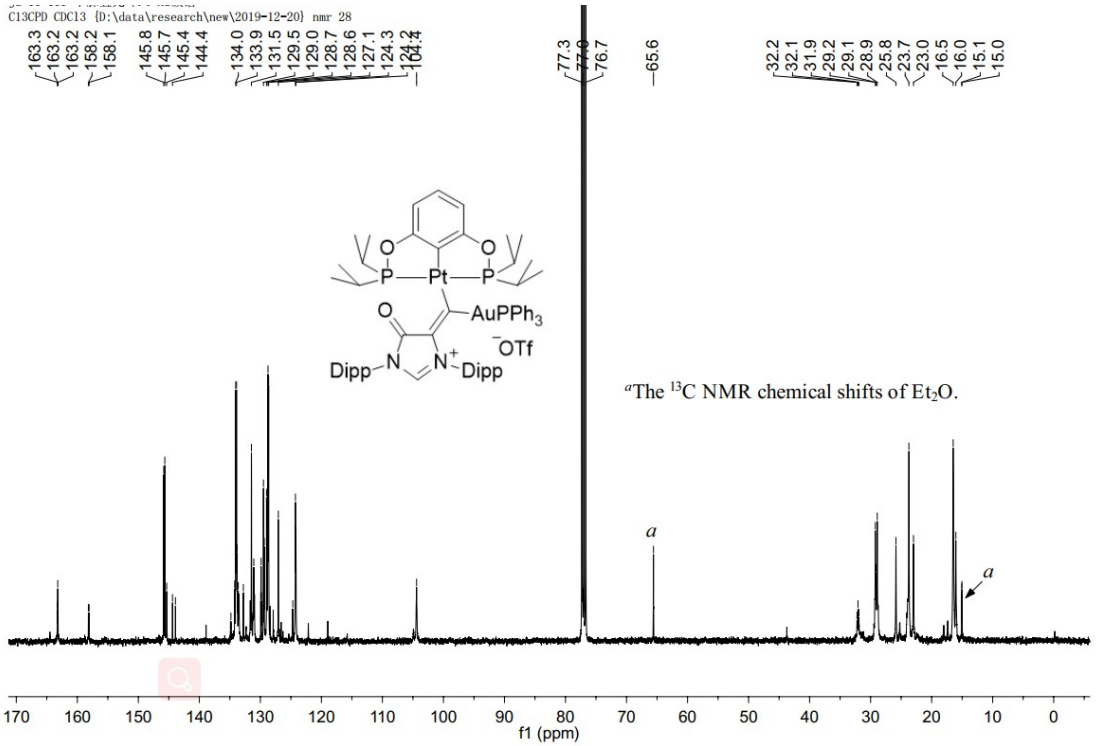


Figure S10. ^{13}C NMR spectra (100 MHz, $CDCl_3$) of **3c**.

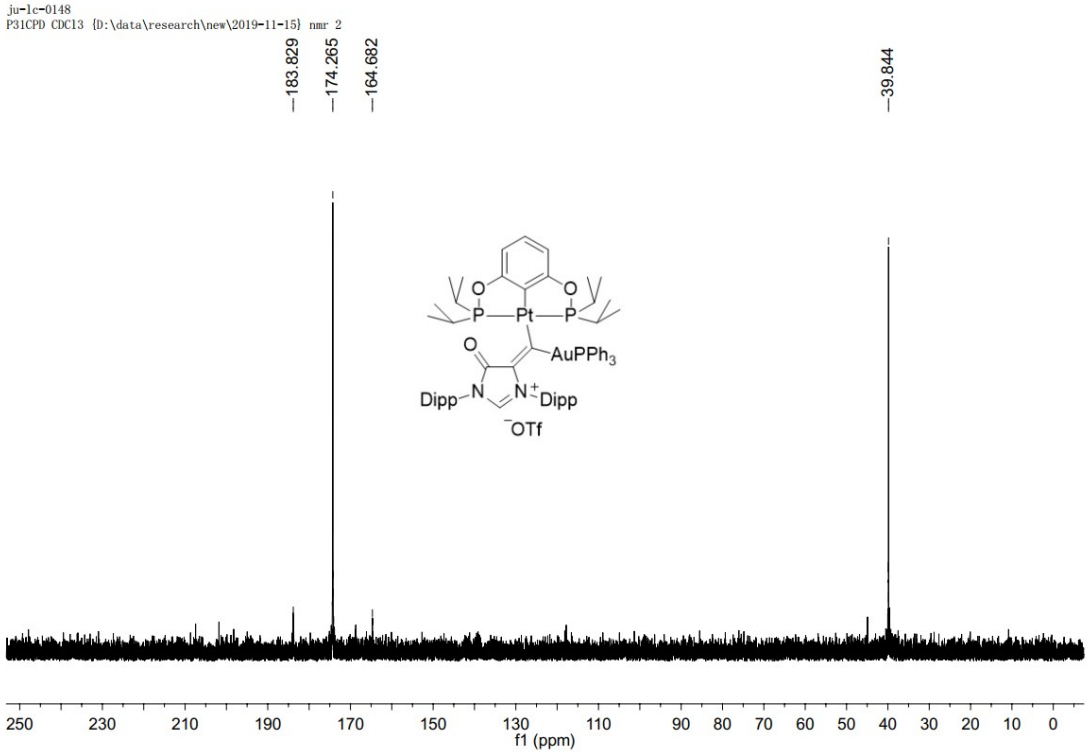


Figure S11. ^{31}P NMR spectra (162 MHz, $CDCl_3$) of **3c**.

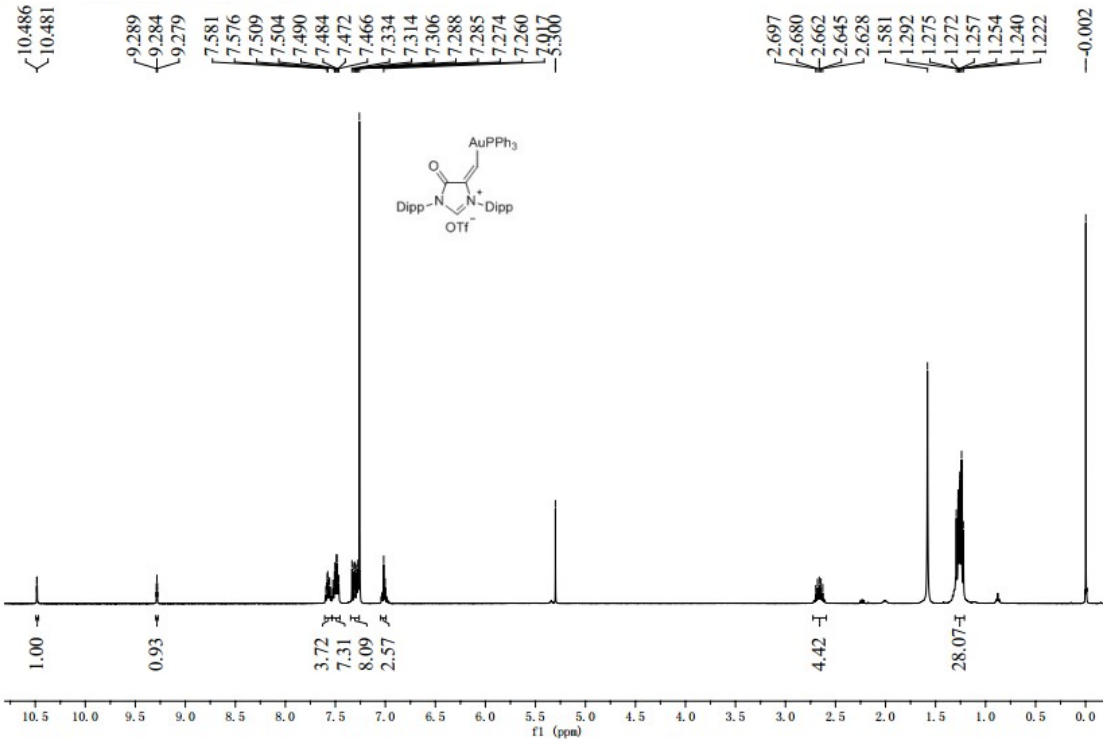


Figure S12. ^{1}H NMR spectra (400 MHz, $CDCl_3$) of **4**.

X-Ray crystallography

Each crystal was mounted on a glass fiber. Crystallographic measurements were made on a Bruker Smart Apex 100 CCD area detector using graphite monochromated Mo-Kαradiation ($\lambda_{\text{Mo-K}\alpha}$ = 0.71073 Å). The structures were solved by directed methods (SHELXS-97) and refined on F^2 by full-matrix least squares (SHELX-97) using all unique data. All the calculations were carried out with the SHELXTL18 program.

Key details of the crystal and structure refinement data are summarized in Table S1. Further crystallographic details may be found in the respective CIF files, which were deposited at the Cambridge Crystallographic Data Centre, Cambridge. CCDC-1977709 (**3b**), CCDC-1977706 (**3c**) contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

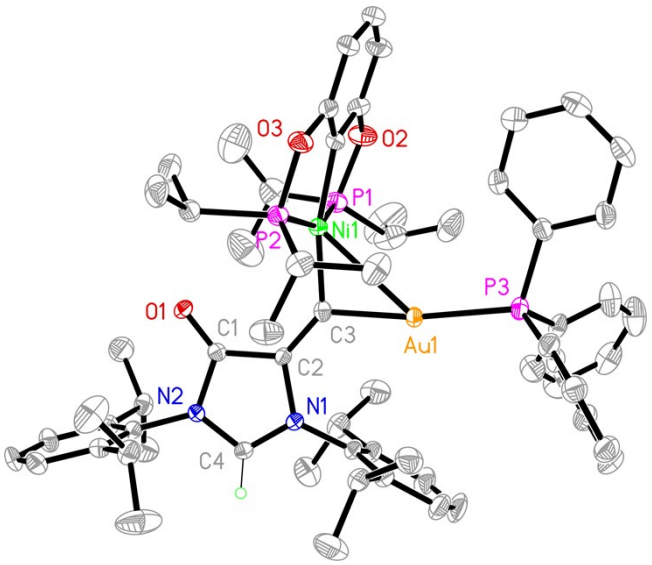


Figure S13. Thermal ellipsoid (30% probability) representation of **3b**. H atoms have been omitted for clarity. Orange cube crystal of **3b** was obtained in *n*-hexane/DCM (v/v, 10:1) at 0 °C.

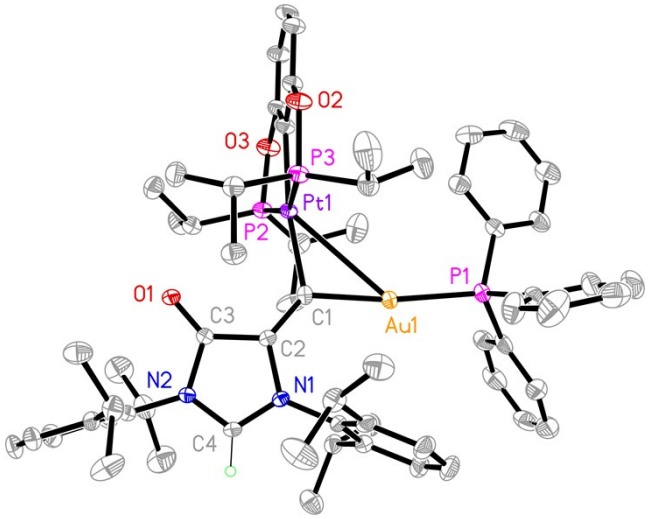


Figure S13. Thermal ellipsoid (30% probability) representation of **3c**. H atoms have been omitted for clarity. Orange cube crystal of **3c** was obtained in *n*-hexane/DCM (v/v, 10:1) at 0 °C.

Table S1. Crystal data, data collection, and structure refinement for **3b** and **3c**.

	3b	**3c**
Identification code	mo_dd19320_0m	mo_d8v19943_0m
Formula	$C_{68}H_{87}AuCl_6F_3N_2NiO_6P_3S$	$C_{68}H_{87}AuCl_6F_3N_2O_6P_3PtS$
Formula weight	1678.74	1815.12
T, K	192(2)	193(2)
crystal system	Monoclinic	Monoclinic
space group	P 21/c	P 21/n
a, Å	15.7638(19)	23.8993(9)
b, Å	13.1411(13)	12.8321(6)
c, Å	36.828(4)	28.1024(12)
α, deg	90	90
β, deg	95.691(4)	114.5080(10)
γ, deg	90	90
Volume, Å ^{3}	7591.4(14)	7841.9(6)
Z	4	4
D_{calc}, Mg / m^3	1.469	1.537
absorption coefficient, mm^{-1}	2.536	3.997
F(000)	3416	3616
crystal size, mm	0.170 x 0.130 x 0.100	0.170 x 0.140 x 0.100
2θ range, deg	2.131 to 26.000	2.175 to 25.999
reflections collected /unique	52996/14912 [R(int) = 0.0530]	116758/15398 [R(int) = 0.0754]
data / restraints/ parameters	14912 / 12 / 836	15398 / 125 / 918
goodness of fit on F^2	1.038	1.034
final R indices [I >2σ(I)][a]	R1 = 0.0443, wR2 = 0.1011	R1 = 0.0359, wR2 = 0.0936
R indices (all data)	R1 = 0.0652, wR2 = 0.1121	R1 = 0.0435, wR2 = 0.0985
largest diff peak and hole, e/Å^3	1.345 and -1.093	1.599 and -1.585

Computational details

All DFT calculations were performed with the Gaussian 09 program package.[3] The structures were fully optimized using B3LYP-D3 functions in combination with the def2-SVP basis and the SMD continuum solvent model of dichloroethane.[4] Vibrational frequencies were calculated at the same level to confirm the optimization of the structures. All minima on the potential energy surface show no imaginary frequency and all transition states show only one imaginary frequency. The electronic energies were obtained using the B3LYP-D3/def2-TZVP to get E_{SCF} energy. The Gcorr is a thermal correction to the free energy in the experimental condition and the Gsolv is the solvation free energy obtained using the SMD continuum model.[5]

I

Geometry with 155 atoms:

C	-0.587829	-1.637234	0.376887
C	0.659719	-1.591106	0.567697
C	3.479083	-0.546885	0.137719
H	4.542344	-0.474380	-0.134354
C	1.864268	-2.374398	0.754674
O	1.784499	-3.520102	1.171464
N	3.114319	-1.861605	0.372757
N	2.747567	0.495832	0.231664
C	-4.281035	-1.799578	-0.300436
C	-4.787562	-1.793134	-1.610332
C	-5.218263	-1.781715	0.745263
C	-6.158794	-1.781258	-1.886382
C	-6.598725	-1.769415	0.518156
C	-7.052467	-1.771659	-0.807373
H	-6.509839	-1.775362	-2.919875
H	-7.293003	-1.753793	1.360297
H	-8.127805	-1.761243	-1.004121
O	-4.740968	-1.751784	2.037761
O	-3.884518	-1.776580	-2.651447
P	-3.053613	-1.726717	2.121451
P	-2.276352	-1.792084	-2.135213
P	-0.787969	2.709524	-0.079527
Ni	-2.395155	-1.738012	0.045866
Au	0.100843	0.567974	0.254119
C	3.359711	1.746728	-0.053858
C	3.491412	2.673622	1.013939
C	3.785451	2.067869	-1.365697
C	4.097239	3.908029	0.749864
C	4.399494	3.314308	-1.570559
C	4.560918	4.225248	-0.530216
H	4.219191	4.634357	1.554628
H	4.745763	3.577650	-2.572501
H	5.038996	5.190713	-0.715344
C	4.182191	-2.840324	0.243416
C	4.399437	-3.420790	-1.026182
C	4.955663	-3.164526	1.373651
C	5.433618	-4.361778	-1.135646
C	5.979750	-4.110333	1.210131
C	6.214447	-4.703839	-0.029375
H	5.634164	-4.837262	-2.097200
H	6.596045	-4.389409	2.067993
H	7.014933	-5.440654	-0.137397
C	-2.607113	2.765857	-0.344807
C	-3.234811	4.004312	-0.575305
C	-3.381113	1.601333	-0.288651
C	-4.617883	4.065148	-0.749740
H	-2.643997	4.922127	-0.622473
C	-4.768242	1.664173	-0.463808

H	-2.905041	0.635391	-0.114437	H	5.015638	1.915868	3.258978
C	-5.386889	2.894882	-0.694156	H	3.699349	1.043797	4.088242
H	-5.098558	5.030075	-0.929799	C	3.596374	1.125200	-2.552808
H	-5.356564	0.746185	-0.421554	C	4.938427	0.547322	-3.030329
H	-6.470076	2.944900	-0.831327	C	2.852564	1.802330	-3.714069
C	-0.109148	3.579450	-1.543556	H	2.969932	0.282011	-2.228074
C	-0.777180	3.475658	-2.777700	H	5.449114	-0.011606	-2.230565
C	1.087179	4.310388	-1.465418	H	4.786888	-0.135293	-3.881160
C	-0.270333	4.123771	-3.906854	H	5.616918	1.351229	-3.360744
H	-1.702075	2.901039	-2.859440	H	1.888016	2.214240	-3.386127
C	1.575762	4.973778	-2.594491	H	3.437200	2.627317	-4.150430
H	1.644653	4.367401	-0.529149	H	2.660117	1.073243	-4.517782
C	0.897771	4.888230	-3.813612	C	4.685966	-2.554323	2.742987
H	-0.798290	4.038336	-4.859920	C	5.925040	-1.849822	3.315448
H	2.501782	5.547007	-2.517750	C	4.139086	-3.615116	3.712392
H	1.286021	5.405719	-4.694411	H	3.905352	-1.789292	2.626501
C	-0.577667	3.794886	1.385958	H	6.314901	-1.090467	2.618914
C	-0.690050	3.175313	2.641324	H	5.674433	-1.343634	4.261812
C	-0.450754	5.191644	1.313626	H	6.737250	-2.564617	3.525529
C	-0.694234	3.938383	3.810027	H	3.232366	-4.084721	3.301665
H	-0.777096	2.089941	2.698722	H	4.883988	-4.406508	3.898430
C	-0.434556	5.950418	2.488399	H	3.885131	-3.157102	4.682804
H	-0.369586	5.694759	0.348686	C	3.521425	-3.075122	-2.226769
C	-0.563830	5.328901	3.735334	C	2.299750	-4.010624	-2.302382
H	-0.786302	3.443573	4.780019	C	4.282913	-3.084716	-3.559162
H	-0.327803	7.036314	2.426087	H	3.141897	-2.052166	-2.081031
H	-0.556318	5.928878	4.648787	H	1.695788	-3.983485	-1.384361
C	3.034092	2.291563	2.417253	H	1.654131	-3.730175	-3.150519
C	2.721213	3.495053	3.311863	H	2.623691	-5.053519	-2.454629
C	4.066267	1.377141	3.103150	H	5.208933	-2.492992	-3.504058
H	2.104435	1.707840	2.298296	H	4.550641	-4.107002	-3.870990
H	2.028529	4.198397	2.827851	H	3.651173	-2.657895	-4.354648
H	2.255109	3.156376	4.249938	C	-1.518872	-0.330307	-2.991541
H	3.635868	4.046565	3.583921	C	-2.252644	0.125847	-4.255759
H	4.285675	0.481655	2.506954	C	-0.015323	-0.548466	-3.212441

H	-1.633840	0.457978	-2.229703
H	-3.311498	0.341554	-4.053361
H	-1.779103	1.048958	-4.628730
H	-2.202664	-0.624255	-5.058922
H	0.488559	-0.936431	-2.314366
H	0.177287	-1.245272	-4.042405
H	0.452922	0.413581	-3.464493
C	-1.642853	-3.364295	-2.865317
C	-1.881003	-3.486977	-4.373093
C	-2.244707	-4.541118	-2.084595
H	-0.559656	-3.325592	-2.658720
H	-1.359973	-2.703899	-4.941878
H	-1.509697	-4.463214	-4.725976
H	-2.955280	-3.428353	-4.607928
H	-2.056566	-4.447634	-1.003834
H	-3.334735	-4.604382	-2.234905
H	-1.799591	-5.487021	-2.432359
C	-2.678488	-0.204214	3.117350
C	-1.332620	-0.355898	3.839234
C	-3.807834	0.250447	4.046306
H	-2.559771	0.552690	2.322584
H	-0.519231	-0.623900	3.146979
H	-1.065113	0.598858	4.318884
H	-1.379230	-1.117634	4.632342
H	-4.758794	0.363209	3.506568
H	-3.965162	-0.451733	4.878759
H	-3.540815	1.229965	4.476619
C	-2.685129	-3.252004	3.093521
C	-2.919089	-4.467964	2.186104
C	-3.464612	-3.345202	4.408564
H	-1.603573	-3.171383	3.300502
H	-2.311839	-4.406955	1.269931
H	-2.645712	-5.392145	2.719792
H	-3.977561	-4.547661	1.889086
H	-3.211047	-2.529592	5.100656
H	-4.550111	-3.319036	4.225190
H	-3.228199	-4.297829	4.910440

3b

Geometry with 155 atoms:

C	-0.844652	3.664584	0.245192
C	-1.281188	4.092264	1.508575
C	-1.257227	4.417646	-0.863781
C	-2.104738	5.211212	1.681238
C	-2.081304	5.543419	-0.742093
C	-2.496815	5.926711	0.540515
H	-2.423299	5.511460	2.681459
H	-2.387484	6.098904	-1.630762
H	-3.141063	6.802817	0.654109
C	0.703328	0.261687	-0.141569
Au	-1.201444	-0.553310	-0.096932
C	1.890813	-0.403992	-0.198543
Ni	0.178171	2.039816	0.039117
P	-3.503749	-1.096624	0.082094
O	-0.868344	3.366357	2.609056
O	-0.836294	4.011200	-2.113248
P	0.099768	2.595420	-2.083105
P	0.305711	2.205466	2.209960
C	3.375422	-2.109721	-0.330127
H	3.794333	-3.109517	-0.435334
C	3.238617	0.128313	0.003048
O	3.644609	1.250440	0.243846
N	4.106202	-1.007457	-0.097907
N	2.092821	-1.829305	-0.394886
C	-3.985047	-1.774085	1.716247
C	-4.881911	-1.113857	2.569875
C	-3.373783	-2.966215	2.141903
C	-5.161446	-1.642750	3.834944
H	-5.361003	-0.184123	2.257300
C	-3.662772	-3.494478	3.401207

H	-2.665223	-3.478607	1.488171	H	-1.669900	-5.502898	-0.945258
C	-4.554847	-2.831176	4.252796	C	5.527608	-0.969166	0.094097
H	-5.858211	-1.120472	4.495526	C	6.024821	-1.118030	1.405616
H	-3.183054	-4.422570	3.722200	C	6.351395	-0.754892	-1.030174
H	-4.775433	-3.240876	5.241833	C	7.415771	-1.052600	1.572139
C	-4.539493	0.402312	-0.139030	C	7.734767	-0.701463	-0.807477
C	-5.814610	0.347846	-0.723469	C	8.258998	-0.849455	0.478295
C	-4.030421	1.637738	0.299201	H	7.844939	-1.156707	2.570366
C	-6.567942	1.517573	-0.866716	H	8.411775	-0.537139	-1.647802
H	-6.221552	-0.603884	-1.072695	H	9.340502	-0.802116	0.630537
C	-4.787409	2.802849	0.158520	C	1.087268	-2.302938	-3.050590
H	-3.029528	1.701046	0.730429	C	0.045134	-2.092044	-4.154497
C	-6.057181	2.743943	-0.426647	C	2.342616	-2.990726	-3.619034
H	-7.558258	1.469460	-1.326919	H	1.386077	-1.304011	-2.694812
H	-4.370441	3.755497	0.492907	H	-0.872870	-1.632541	-3.761585
H	-6.646847	3.656555	-0.546317	H	0.452550	-1.425960	-4.930663
C	-4.091270	-2.309172	-1.158182	H	-0.231529	-3.037746	-4.646899
C	-5.046977	-3.297031	-0.873079	H	3.124636	-3.120774	-2.855664
C	-3.541297	-2.229032	-2.448526	H	2.092428	-3.989494	-4.013330
C	-5.442129	-4.194488	-1.871041	H	2.770122	-2.395859	-4.442598
H	-5.480712	-3.372893	0.126352	C	1.171719	-3.149333	1.984462
C	-3.944573	-3.120260	-3.444519	C	2.217143	-4.186425	2.427085
H	-2.788670	-1.468992	-2.666622	C	0.064423	-2.978333	3.031963
C	-4.893532	-4.108038	-3.155290	H	1.685710	-2.179116	1.911129
H	-6.183168	-4.964686	-1.642394	H	3.042205	-4.261066	1.700720
H	-3.508311	-3.050060	-4.444146	H	2.647043	-3.912152	3.404033
H	-5.204003	-4.812754	-3.930994	H	1.762579	-5.186346	2.523402
C	1.069811	-2.825969	-0.553012	H	-0.688298	-2.250976	2.694665
C	0.552510	-3.065453	-1.843201	H	-0.452285	-3.926843	3.245860
C	0.617128	-3.486768	0.604578	H	0.492929	-2.615330	3.979547
C	-0.442497	-4.045478	-1.956416	C	5.092261	-1.275645	2.603302
C	-0.366258	-4.473080	0.431339	C	4.872051	0.087450	3.286281
C	-0.890031	-4.745460	-0.832662	C	5.570405	-2.334087	3.605485
H	-0.881439	-4.265891	-2.930005	H	4.112420	-1.610635	2.230678
H	-0.732622	-5.026712	1.297930	H	4.510367	0.837066	2.566765

H	4.133534	-0.002314	4.100294
H	5.813541	0.461094	3.721947
H	5.735549	-3.307892	3.117212
H	6.509058	-2.038402	4.101028
H	4.815211	-2.473016	4.395932
C	5.756611	-0.522338	-2.415264
C	6.558476	-1.185408	-3.541978
C	5.583517	0.987870	-2.667387
H	4.751365	-0.971448	-2.429495
H	6.715716	-2.259123	-3.350467
H	6.017430	-1.085371	-4.496774
H	7.545801	-0.715301	-3.676995
H	4.992442	1.462436	-1.870671
H	6.565106	1.489136	-2.702712
H	5.076361	1.164761	-3.630540
C	-0.833239	1.459953	-3.224358
C	-0.599088	1.585684	-4.731265
C	-2.323726	1.545851	-2.879891
H	-0.452478	0.478003	-2.891640
H	0.462207	1.500756	-5.007862
H	-1.139198	0.771661	-5.242567
H	-0.990666	2.535449	-5.126989
H	-2.500916	1.437632	-1.802582
H	-2.742711	2.513961	-3.193428
H	-2.879691	0.747971	-3.396106
C	1.657403	3.137238	-2.940176
C	2.691487	3.613797	-1.914689
C	1.418868	4.206538	-4.014929
H	2.024910	2.206866	-3.410148
H	2.915136	2.837103	-1.172935
H	3.629302	3.883893	-2.427589
H	2.331457	4.507979	-1.380460
H	0.686833	3.908449	-4.775876
H	1.064638	5.140754	-3.553873
H	2.370890	4.421216	-4.527990
C	-0.147694	0.746117	3.274395
C	-1.671525	0.583280	3.319540
C	0.460612	0.654546	4.676341
H	0.270638	-0.075407	2.666552
H	-2.122090	0.598171	2.318097
H	-1.927803	-0.382478	3.781843
H	-2.135640	1.385422	3.912835
H	1.555522	0.762395	4.674388
H	0.035114	1.407909	5.356488
H	0.225451	-0.336900	5.097451
C	1.859661	2.991010	2.866970
C	1.641038	3.766454	4.172670
C	2.482814	3.896208	1.796823
H	2.533234	2.132755	3.038551
H	1.199461	3.163292	4.975654
H	2.611412	4.146149	4.533254
H	0.983550	4.632174	4.000144
H	2.700507	3.334645	0.882837
H	1.815016	4.736248	1.546567
H	3.428523	4.318196	2.175761

II

Geometry with 155 atoms:

C	-1.160713	-3.216108	1.659283
C	-1.573667	-4.428301	1.078356
C	-1.569772	-2.994800	2.985933
C	-2.334710	-5.380724	1.764286
C	-2.326848	-3.919900	3.712853
C	-2.701383	-5.114590	3.087845
H	-2.631679	-6.301663	1.259465
H	-2.608494	-3.697936	4.743700
H	-3.294484	-5.848076	3.640136
C	0.422037	-0.263335	-0.491266
Au	-1.425694	0.557343	-0.652636
C	1.585835	-0.661248	-0.335428

Ni	-0.124419	-1.928770	0.688563	C	-4.073241	-1.220523	0.814858
P	-3.661773	1.198770	-0.490463	C	-5.797323	-0.658539	-0.802099
O	-1.228919	-4.669611	-0.227590	C	-4.709901	-2.433129	1.079204
O	-1.213409	-1.813555	3.587397	H	-3.139165	-0.981685	1.328834
P	-0.115540	-0.902553	2.686857	C	-6.430689	-1.878458	-0.535901
P	-0.576513	-3.317245	-0.993581	H	-6.223261	0.024883	-1.539585
C	3.752152	1.263621	-0.592630	C	-5.888899	-2.765297	0.399707
H	4.566922	1.811807	-1.092583	H	-4.270626	-3.124291	1.801283
C	2.967690	-1.089649	-0.342408	H	-7.349605	-2.136414	-1.068447
O	3.262345	-2.265929	-0.181154	H	-6.381025	-3.721097	0.596791
N	3.945722	-0.126664	-0.621459	C	2.518277	3.191875	0.014606
N	2.761543	1.807302	-0.025557	C	3.000826	3.941992	1.116811
C	-4.408096	1.963420	-1.969191	C	1.664564	3.781723	-0.954616
C	-3.884143	1.627435	-3.229398	C	2.658675	5.299170	1.200156
C	-5.495227	2.847249	-1.875871	C	1.350410	5.141481	-0.823391
C	-4.450297	2.166038	-4.387465	C	1.843787	5.901080	0.239760
H	-3.031887	0.946159	-3.302267	H	3.033434	5.895905	2.034805
C	-6.053636	3.386926	-3.038204	H	0.704382	5.616146	-1.565113
H	-5.904407	3.116123	-0.899127	H	1.587182	6.960505	0.323017
C	-5.534061	3.046524	-4.292256	C	5.272740	-0.605078	-0.960446
H	-4.039638	1.903092	-5.365452	C	5.600987	-0.771913	-2.323373
H	-6.897934	4.076851	-2.963453	C	6.194293	-0.874116	0.074196
H	-5.972506	3.472766	-5.198228	C	6.892341	-1.223100	-2.635049
C	-3.932180	2.344789	0.909398	C	7.467660	-1.336819	-0.289666
C	-4.968860	2.164809	1.837944	C	7.815092	-1.509701	-1.629482
C	-3.044658	3.426387	1.052065	H	7.177687	-1.350255	-3.681567
C	-5.113144	3.061975	2.901801	H	8.197903	-1.565557	0.489426
H	-5.658761	1.323703	1.739375	H	8.814323	-1.867372	-1.892014
C	-3.198700	4.322251	2.111632	C	3.894184	3.288503	2.164220
H	-2.226000	3.562044	0.340217	C	3.575385	3.729504	3.599098
C	-4.231205	4.138902	3.039737	C	5.377916	3.522923	1.834604
H	-5.918461	2.916239	3.626123	H	3.712496	2.204791	2.112040
H	-2.502819	5.157873	2.219104	H	2.504699	3.610163	3.829166
H	-4.345204	4.835165	3.874478	H	4.148396	3.121572	4.318151
C	-4.613743	-0.325835	-0.128111	H	3.843446	4.783490	3.778356

H	5.639587	3.114572	0.845609	H	1.715446	-2.133195	3.417558
H	5.607705	4.601604	1.822622	H	0.395673	-1.714610	5.534827
H	6.028040	3.045324	2.584782	H	2.133723	-1.365310	5.722046
C	1.131110	2.954940	-2.118069	H	0.976108	-0.027305	5.546949
C	2.097599	2.999259	-3.312958	C	-0.873187	0.784386	2.837241
C	-0.288253	3.342941	-2.553035	C	0.069873	1.896337	2.358996
H	1.091377	1.912706	-1.770367	C	-1.494291	1.099914	4.201731
H	3.106442	2.671835	-3.024611	H	-1.693295	0.693972	2.103282
H	1.746828	2.343647	-4.127845	H	0.622925	1.631855	1.447861
H	2.181136	4.024071	-3.712260	H	-0.519066	2.800856	2.146037
H	-0.979997	3.385110	-1.697008	H	0.801340	2.155653	3.136404
H	-0.315752	4.322500	-3.057383	H	-2.170393	0.303247	4.542650
H	-0.682263	2.599569	-3.264525	H	-0.725969	1.258923	4.973115
C	4.624922	-0.437663	-3.444429	H	-2.079301	2.030445	4.113911
C	4.475276	-1.587620	-4.452266	C	-1.999968	-2.730518	-2.048678
C	5.049704	0.860424	-4.152293	C	-2.998257	-3.829726	-2.425436
H	3.635843	-0.265208	-2.994383	C	-1.542837	-1.920606	-3.268506
H	4.247612	-2.537701	-3.947158	H	-2.502345	-2.040301	-1.350102
H	3.658154	-1.371193	-5.159660	H	-3.369929	-4.370025	-1.543887
H	5.394052	-1.731905	-5.043422	H	-3.864030	-3.363694	-2.924980
H	5.155558	1.692506	-3.439134	H	-2.561351	-4.563014	-3.120512
H	6.020547	0.728567	-4.658044	H	-0.760478	-1.185235	-3.026610
H	4.307879	1.153092	-4.912740	H	-1.163800	-2.578242	-4.064802
C	5.837927	-0.703841	1.545078	H	-2.405552	-1.369245	-3.675505
C	6.890135	0.112321	2.311130	C	0.767403	-4.136929	-1.967093
C	5.607610	-2.071127	2.211559	C	1.527629	-3.194131	-2.909575
H	4.892705	-0.146703	1.598024	C	0.309330	-5.410876	-2.687565
H	7.107831	1.065990	1.807272	H	1.452380	-4.414848	-1.146357
H	6.528120	0.338469	3.327371	H	1.739612	-2.216156	-2.460752
H	7.838388	-0.439275	2.416819	H	2.490674	-3.659614	-3.165792
H	4.806970	-2.627069	1.702770	H	0.979188	-3.029663	-3.847398
H	6.526017	-2.680787	2.177805	H	-0.215984	-6.102471	-2.013928
H	5.328603	-1.945616	3.270537	H	-0.353243	-5.176101	-3.535057
C	1.431747	-1.102300	3.696524	H	1.193771	-5.931585	-3.090811
C	1.208784	-1.049208	5.211520	C	2.553498	-0.157434	3.248713

H	3.514980	-0.526784	3.634489
H	2.633843	-0.078621	2.156715
H	2.405654	0.855469	3.646921

2b

Geometry with 155 atoms:

C	1.224273	-3.165147	-0.005687
C	1.757483	-3.630833	1.205066
C	1.946428	-3.443989	-1.176451
C	2.953791	-4.355986	1.267503
C	3.158585	-4.143894	-1.162031
C	3.646153	-4.596751	0.072224
H	3.336160	-4.705763	2.228293
H	3.698463	-4.329827	-2.092390
H	4.589745	-5.148247	0.103326
C	-1.011625	0.604774	-0.069946
Au	1.051640	0.780771	-0.090585
C	-1.625679	-0.625690	-0.050567
Ni	-0.350867	-2.070054	-0.047856
P	3.394505	0.948914	0.023309
O	1.080066	-3.323855	2.367473
O	1.420318	-3.002355	-2.375186
P	-0.139443	-2.351917	-2.194960
P	-0.310243	-2.382329	2.100420
C	-3.128481	1.704808	-0.002033
H	-3.715251	2.624479	0.015932
C	-3.067039	-0.733439	-0.006439
O	-3.735377	-1.758336	0.014268
N	-3.765970	0.534580	0.012513
N	-1.808960	1.774447	-0.040894
C	4.307819	-0.028354	-1.230392
C	3.726674	-0.186058	-2.499886
C	5.571354	-0.587804	-0.973191
C	4.411687	-0.875671	-3.503812
H	2.733594	0.222813	-2.701857
C	6.244915	-1.289222	-1.976537
H	6.030886	-0.484668	0.011730
C	5.668994	-1.430236	-3.243624
H	3.956733	-0.990422	-4.490134
H	7.224136	-1.726657	-1.766081
H	6.197721	-1.978094	-4.027844
C	3.990837	2.674842	-0.146767
C	3.069563	3.730770	-0.049919
C	5.353348	2.959025	-0.345275
C	3.508018	5.055542	-0.143682
H	2.007354	3.522041	0.098852
C	5.785533	4.283568	-0.440828
H	6.080592	2.148249	-0.428637
C	4.864085	5.333373	-0.338683
H	2.782206	5.868129	-0.067229
H	6.845997	4.497368	-0.596800
H	5.205493	6.369026	-0.414837
C	4.004667	0.364981	1.650129
C	4.409737	1.254541	2.657177
C	3.979411	-1.016521	1.909538
C	4.798230	0.761353	3.908244
H	4.426851	2.330526	2.470566
C	4.382240	-1.502184	3.154154
H	3.649301	-1.715311	1.138678
C	4.791379	-0.614555	4.156823
H	5.113411	1.458555	4.688792
H	4.363767	-2.578270	3.341078
H	5.100454	-0.996262	5.133238
C	-1.191775	3.092055	-0.065145
C	-0.950788	3.693847	-1.315207
C	-0.840438	3.694175	1.158694
C	-0.410905	4.988610	-1.311420
C	-0.305528	4.989644	1.106279
C	-0.109892	5.637862	-0.113771
H	-0.218052	5.489668	-2.262588

H	-0.031049	5.491565	2.036715	H	-4.729585	-1.772397	2.360426
H	0.299700	6.650831	-0.132216	H	-4.471960	-1.176132	4.027068
C	-5.214896	0.539537	0.051409	H	-6.126773	-1.361598	3.389619
C	-5.848179	0.490275	1.308239	H	-5.499206	2.409885	3.293774
C	-5.914790	0.580916	-1.170323	H	-6.527880	1.158193	4.035960
C	-7.250562	0.493166	1.318053	H	-4.835093	1.328807	4.546062
C	-7.315710	0.580005	-1.103796	C	-5.191411	0.557642	-2.511950
C	-7.975339	0.538548	0.125949	C	-5.752211	1.570894	-3.518519
H	-7.781523	0.451429	2.271390	C	-5.194423	-0.870537	-3.085716
H	-7.898132	0.604244	-2.026968	H	-4.140855	0.830954	-2.336487
H	-9.068135	0.537173	0.155095	H	-5.772401	2.589450	-3.098508
C	-1.196138	2.966942	-2.630544	H	-5.124894	1.588499	-4.424335
C	0.129292	2.770357	-3.385591	H	-6.776227	1.314412	-3.834380
C	-2.242089	3.676906	-3.502503	H	-4.750949	-1.581970	-2.372675
H	-1.587342	1.966936	-2.401210	H	-6.224599	-1.200505	-3.299288
H	0.867096	2.244916	-2.758293	H	-4.620322	-0.912097	-4.025237
H	-0.030676	2.176644	-4.298850	C	-0.124878	-0.907958	-3.357214
H	0.567678	3.735741	-3.685354	C	-1.567114	-0.522011	-3.713890
H	-3.203759	3.783109	-2.975291	C	0.776575	-1.045490	-4.587320
H	-1.904612	4.684940	-3.794022	H	0.292955	-0.115354	-2.711654
H	-2.423290	3.104639	-4.426866	H	-2.197763	-0.409154	-2.820040
C	-0.972365	2.970720	2.491399	H	-1.572661	0.437199	-4.253413
C	-1.963700	3.667659	3.434495	H	-2.036156	-1.271654	-4.368864
C	0.406304	2.793191	3.149518	H	1.756994	-1.462807	-4.325954
H	-1.361676	1.964372	2.293011	H	0.327332	-1.689540	-5.356339
H	-2.961291	3.759936	2.975596	H	0.933326	-0.050496	-5.036027
H	-2.072973	3.093249	4.368897	C	-1.200124	-3.696688	-2.913597
H	-1.620299	4.680417	3.701807	C	-1.139469	-4.924122	-1.993800
H	1.098001	2.260923	2.477837	C	-0.861074	-4.068800	-4.360861
H	0.861166	3.763492	3.405991	H	-2.218385	-3.272204	-2.863462
H	0.318081	2.209136	4.078783	H	-1.382832	-4.666716	-0.954765
C	-5.055000	0.375963	2.604190	H	-1.857437	-5.684952	-2.340339
C	-5.096381	-1.071640	3.125347	H	-0.135659	-5.378439	-2.002653
C	-5.509536	1.376163	3.675606	H	-1.070622	-3.253047	-5.065854
H	-4.003527	0.605678	2.379703	H	0.199621	-4.349550	-4.458494

H	-1.467403	-4.937047	-4.668505
C	-0.075378	-0.935458	3.247957
C	0.895719	-1.169521	4.407475
C	-1.436014	-0.405998	3.720222
H	0.370472	-0.183326	2.573687
H	1.861958	-1.552170	4.055768
H	1.078139	-0.212269	4.923792
H	0.493518	-1.878853	5.146671
H	-2.134658	-0.248428	2.884846
H	-1.909061	-1.094967	4.435992
H	-1.300803	0.558884	4.231451
C	-1.651734	-3.459262	2.793764
C	-1.298005	-4.080089	4.148191
C	-2.044709	-4.509552	1.748397
H	-2.502463	-2.768208	2.915270
H	-1.120534	-3.318997	4.921569
H	-2.128737	-4.719073	4.490953
H	-0.396221	-4.707014	4.070239
H	-2.415703	-4.025230	0.833233
H	-1.193350	-5.157503	1.484016
H	-2.847513	-5.152634	2.145179

TSI-3b

Geometry with 155 atoms:

C	-0.682337	0.718927	-0.027418
C	-1.911123	0.447417	-0.037401
C	-3.708334	-1.598109	0.338463
H	-4.468991	-2.374071	0.509147
C	-3.316465	0.700388	-0.249168
O	-3.709589	1.812649	-0.582117
N	-4.198221	-0.362660	-0.055817
N	-2.458663	-1.732358	0.473781
C	1.733436	3.728151	-0.174400
C	2.260924	4.207403	-1.385574
C	2.137917	4.391806	0.997156
C	3.166724	5.272296	-1.445883
C	3.042901	5.458664	0.984857
C	3.551053	5.887290	-0.247654
H	3.551902	5.606457	-2.411002
H	3.332024	5.938635	1.921665
H	4.257523	6.721133	-0.275448
O	1.617451	3.963157	2.197733
O	1.867881	3.590376	-2.551258
P	0.527060	2.685154	2.024636
P	0.750244	2.349774	-2.303626
P	3.031364	-1.665540	-0.058725
Ni	0.539261	2.229098	-0.122239
Au	0.969762	-0.583511	0.056996
C	-1.728854	-2.864471	0.833569
C	-1.162496	-2.902347	2.134437
C	-1.473607	-3.884232	-0.124351
C	-0.354249	-3.997632	2.469005
C	-0.632490	-4.938453	0.256123
C	-0.079522	-5.000296	1.537658
H	0.077507	-4.067819	3.468426
H	-0.402175	-5.731339	-0.456285
H	0.571784	-5.834943	1.808948
C	-5.611447	-0.165723	-0.247774
C	-6.171356	-0.510174	-1.496607
C	-6.371930	0.354629	0.818247
C	-7.549641	-0.313312	-1.661197
C	-7.745805	0.538996	0.600961
C	-8.326783	0.208011	-0.623812
H	-8.023125	-0.562780	-2.612689
H	-8.367368	0.949040	1.400030
H	-9.399226	0.358670	-0.773846
C	4.221752	-0.603093	-0.963667
C	4.074398	0.794474	-0.895829
C	5.279987	-1.153287	-1.704954
C	4.977258	1.630382	-1.555503

H	3.234573	1.238157	-0.354750
C	6.178977	-0.311551	-2.367922
H	5.402268	-2.237035	-1.769967
C	6.030618	1.077933	-2.293012
H	4.842612	2.713466	-1.501815
H	6.998025	-0.745039	-2.947347
H	6.732977	1.731422	-2.816739
C	2.984533	-3.266200	-0.941229
C	2.345590	-3.293946	-2.193245
C	3.513899	-4.447651	-0.402326
C	2.241983	-4.492293	-2.900665
H	1.920697	-2.377449	-2.610116
C	3.398489	-5.648527	-1.112049
H	4.008037	-4.438401	0.571442
C	2.764744	-5.673244	-2.358131
H	1.741843	-4.507245	-3.872193
H	3.807447	-6.568140	-0.686085
H	2.674720	-6.613726	-2.907627
C	3.763126	-1.972514	1.587064
C	2.934858	-2.544290	2.566759
C	5.079695	-1.612379	1.910469
C	3.419661	-2.759989	3.857484
H	1.907101	-2.812730	2.317034
C	5.558422	-1.823305	3.208130
H	5.731281	-1.158193	1.161201
C	4.732522	-2.395355	4.181331
H	2.767542	-3.202949	4.614353
H	6.582493	-1.535140	3.458436
H	5.110466	-2.553613	5.194620
C	-1.485864	-1.792232	3.129929
C	-0.443918	-1.635913	4.242549
C	-2.886491	-1.980240	3.743985
H	-1.503057	-0.852160	2.551817
H	0.574551	-1.539096	3.839701
H	-0.660372	-0.735463	4.836793
H	-0.453040	-2.492653	4.935706
H	-3.673078	-2.041836	2.978094
H	-2.926272	-2.907950	4.338688
H	-3.133603	-1.138481	4.412118
C	-2.100170	-3.805264	-1.515737
C	-2.067146	-5.124869	-2.292796
C	-1.461726	-2.679654	-2.345942
H	-3.162725	-3.543747	-1.376698
H	-2.518802	-5.951476	-1.721651
H	-2.629289	-5.017111	-3.234229
H	-1.037538	-5.415918	-2.557576
H	-1.501030	-1.717968	-1.817643
H	-0.405315	-2.908876	-2.550975
H	-1.979316	-2.560020	-3.311815
C	-5.731084	0.746198	2.145033
C	-6.446503	0.122233	3.351987
C	-5.640584	2.277344	2.268691
H	-4.701670	0.358291	2.149681
H	-6.503507	-0.974759	3.263486
H	-5.902424	0.360016	4.280688
H	-7.473114	0.506899	3.464547
H	-5.097221	2.707370	1.413904
H	-6.645466	2.730398	2.301004
H	-5.112354	2.560462	3.194448
C	-5.295085	-1.014147	-2.639062
C	-4.844009	0.165454	-3.520830
C	-5.955814	-2.115381	-3.476888
H	-4.386542	-1.451564	-2.199015
H	-4.356259	0.949523	-2.922067
H	-4.134278	-0.175977	-4.292662
H	-5.709094	0.622176	-4.030035
H	-6.305865	-2.947923	-2.845406
H	-6.817775	-1.738206	-4.050332
H	-5.232385	-2.520375	-4.203163
C	1.487666	0.938278	-3.262432

C	2.446046	1.347880	-4.384047
C	0.386151	-0.019754	-3.726132
H	2.078425	0.427977	-2.485702
H	3.231712	2.024009	-4.019908
H	2.933943	0.441947	-4.780701
H	1.924738	1.841997	-5.217277
H	-0.294058	-0.285985	-2.905665
H	-0.210241	0.412052	-4.544329
H	0.838198	-0.952028	-4.099609
C	-0.758213	2.975809	-3.174861
C	-0.487246	3.457418	-4.603691
C	-1.421699	4.057714	-2.311495
H	-1.424336	2.095470	-3.197522
H	-0.122455	2.650564	-5.254836
H	-1.420799	3.846245	-5.042686
H	0.254812	4.271111	-4.612158
H	-1.703121	3.666135	-1.324571
H	-0.755641	4.924312	-2.168547
H	-2.339136	4.414976	-2.806511
C	1.205377	1.420231	3.192725
C	0.999555	1.690405	4.685139
C	2.684792	1.182220	2.864710
H	0.628564	0.523519	2.907721
H	-0.061532	1.794465	4.953817
H	1.406863	0.843407	5.260710
H	1.534646	2.597779	5.006381
H	2.846820	0.983820	1.796477
H	3.292459	2.057043	3.142772
H	3.056698	0.310728	3.424332
C	-1.054943	3.370374	2.717564
C	-1.941171	3.902545	1.583397
C	-0.827277	4.445959	3.788313
H	-1.541526	2.487547	3.170782
H	-2.190374	3.125213	0.850012
H	-2.885414	4.289268	1.999833
H	-1.444713	4.730271	1.051255
H	-0.201181	4.105441	4.623154
H	-0.350503	5.334833	3.348249
H	-1.802260	4.753466	4.200578

TSII-2b

Geometry with 155 atoms:

C	1.189231	3.763721	0.315686
C	1.686747	4.326650	-0.876133
C	1.827494	4.149474	1.509365
C	2.729731	5.257930	-0.892161
C	2.883935	5.066854	1.534778
C	3.318762	5.620289	0.325328
H	3.070443	5.674835	-1.841437
H	3.349829	5.330935	2.485921
H	4.140580	6.341050	0.329996
C	-0.737223	0.121243	-0.033496
Au	1.165724	-0.520206	-0.217995
C	-1.787595	0.800383	0.122812
Ni	-0.238643	2.487205	0.299290
P	3.413066	-1.192366	-0.217719
O	1.122274	3.926133	-2.065126
O	1.410656	3.577045	2.685815
P	0.205026	2.409004	2.479140
P	-0.308320	3.059116	-1.822736
C	-3.154034	-1.785680	-0.178360
H	-3.850498	-2.588141	-0.469800
C	-3.234040	0.709077	0.204403
O	-3.958906	1.672687	0.410747
N	-3.809545	-0.563533	0.005109
N	-1.911101	-1.959474	-0.024663
C	3.763007	-2.700445	-1.199242
C	3.688387	-2.606343	-2.600593
C	4.033782	-3.939527	-0.600897
C	3.881787	-3.740452	-3.390826

H	3.485564	-1.644022	-3.077427	H	0.318753	-5.668309	1.460679
C	4.225406	-5.073079	-1.398623	H	0.705141	-4.615031	-2.685544
H	4.092317	-4.031327	0.485038	H	1.271455	-6.096506	-0.787949
C	4.147569	-4.977605	-2.790856	C	-5.258318	-0.625981	-0.030672
H	3.821761	-3.658230	-4.478905	C	-5.908051	-0.578755	-1.282015
H	4.434590	-6.035277	-0.924540	C	-5.962177	-0.760969	1.183825
H	4.294971	-5.865966	-3.410187	C	-7.307991	-0.670809	-1.292806
C	3.907629	-1.557228	1.509252	C	-7.361036	-0.845012	1.119748
C	5.119852	-1.115484	2.060717	C	-8.027979	-0.801842	-0.104968
C	3.007286	-2.289520	2.304012	H	-7.842304	-0.630656	-2.244508
C	5.426627	-1.408631	3.393880	H	-7.935921	-0.942413	2.043352
H	5.824917	-0.538322	1.459144	H	-9.118859	-0.868354	-0.133948
C	3.324827	-2.590587	3.629554	C	-0.971609	-2.413120	-2.699571
H	2.055791	-2.623805	1.883237	C	-2.202762	-2.933267	-3.460157
C	4.534124	-2.146705	4.177826	C	0.195486	-2.145200	-3.655608
H	6.369250	-1.056322	3.820114	H	-1.246652	-1.443605	-2.257919
H	2.620758	-3.163166	4.237918	H	-3.063373	-3.071148	-2.788287
H	4.777815	-2.371943	5.219184	H	-2.501263	-2.230334	-4.255162
C	4.553237	0.091985	-0.842668	H	-1.988026	-3.907499	-3.930473
C	4.149566	1.437739	-0.809218	H	1.072968	-1.765740	-3.111394
C	5.831871	-0.241279	-1.322970	H	0.503991	-3.049236	-4.204246
C	5.021389	2.439438	-1.245534	H	-0.092785	-1.392411	-4.406258
H	3.153918	1.708459	-0.446719	C	-1.424090	-3.647101	2.219075
C	6.696968	0.764692	-1.760631	C	-0.515722	-4.039336	3.390170
H	6.151584	-1.285173	-1.358886	C	-2.810267	-4.299183	2.371574
C	6.293299	2.104312	-1.721075	H	-1.568167	-2.554968	2.267362
H	4.696742	3.481010	-1.215310	H	0.495407	-3.619834	3.279195
H	7.689458	0.500440	-2.134259	H	-0.936027	-3.662947	4.336662
H	6.971119	2.889325	-2.066218	H	-0.419195	-5.132750	3.488905
C	-1.173366	-3.124427	-0.256953	H	-3.501136	-3.984080	1.574748
C	-0.829354	-3.944210	0.848133	H	-2.727673	-5.397970	2.324660
C	-0.613854	-3.340353	-1.543215	H	-3.263899	-4.032750	3.339898
C	0.043877	-5.017638	0.628056	C	-5.256492	-0.772517	2.534637
C	0.256512	-4.426747	-1.708331	C	-5.664139	-1.976440	3.397196
C	0.582253	-5.262208	-0.637839	C	-5.499631	0.552816	3.277382

H	-4.174957	-0.854851	2.351261
H	-5.520684	-2.926267	2.859597
H	-5.056164	-2.009793	4.316066
H	-6.720705	-1.917361	3.704753
H	-5.184643	1.409189	2.664141
H	-6.568903	0.676003	3.517336
H	-4.936493	0.576179	4.224427
C	-5.142657	-0.372973	-2.583568
C	-5.303060	1.081376	-3.058664
C	-5.550048	-1.365073	-3.681366
H	-4.073664	-0.533989	-2.382841
H	-5.010542	1.788386	-2.269061
H	-4.680305	1.274279	-3.946928
H	-6.352214	1.290764	-3.325705
H	-5.452488	-2.408043	-3.341237
H	-6.591370	-1.210083	-4.006274
H	-4.907856	-1.235179	-4.567217
C	1.048881	0.888199	3.134323
C	0.044500	-0.232735	3.430367
C	2.028024	1.124755	4.288776
H	1.639902	0.589362	2.250422
H	-0.644312	-0.405863	2.591693
H	0.591995	-1.170261	3.609950
H	-0.548422	-0.013007	4.331349
H	2.729528	1.941841	4.068765
H	1.510893	1.355775	5.230806
H	2.614833	0.204494	4.443103
C	-1.092201	3.062611	3.625502
C	-0.667712	3.131809	5.095225
C	-2.435373	2.351062	3.423461
H	-1.190363	4.092433	3.236265
H	0.307715	3.625044	5.221478
H	-1.415285	3.711651	5.661644
H	-0.615739	2.128234	5.544687
H	-2.764199	2.386828	2.375873
H	-2.394814	1.296776	3.735722
H	-3.205849	2.847229	4.034936
C	-1.543730	4.384010	-2.217789
C	-2.982262	3.991676	-1.868524
C	-1.404173	4.966064	-3.627470
H	-1.214993	5.147174	-1.488655
H	-3.061373	3.519116	-0.878337
H	-3.615510	4.893984	-1.868305
H	-3.401989	3.296829	-2.608234
H	-0.363492	5.239329	-3.857099
H	-1.758975	4.259157	-4.393111
H	-2.019262	5.877923	-3.706432
C	-0.222608	1.737546	-3.119321
C	0.617359	2.099688	-4.348303
C	-1.630339	1.248331	-3.487657
H	0.289895	0.925729	-2.573697
H	1.632943	2.415286	-4.069586
H	0.700284	1.211235	-4.996154
H	0.154860	2.904386	-4.938702
H	-2.235994	1.006207	-2.602691
H	-2.170260	2.001676	-4.079308
H	-1.551936	0.335071	-4.096660

3b'

Geometry with 155 atoms:

C	-2.545723	-2.576247	0.424431
C	-3.262406	-3.127041	-0.647377
C	-3.231064	-2.449908	1.640895
C	-4.599833	-3.526668	-0.538286
C	-4.568454	-2.828448	1.801893
C	-5.241805	-3.367941	0.697133
H	-5.120677	-3.940416	-1.404042
H	-5.060288	-2.709107	2.769201
H	-6.287263	-3.670437	0.801504
C	0.565059	-0.564273	-0.016063

Au	-0.951602	0.908708	-0.027502	H	-1.291124	7.765705	-1.299743
C	1.856261	-0.129880	-0.074782	C	-3.921862	1.767120	-1.471480
Ni	-0.754115	-1.854745	0.201149	C	-4.833182	0.735020	-1.189054
P	-2.790293	2.360778	-0.148397	C	-3.769454	2.207317	-2.797607
O	-2.609186	-3.241722	-1.853852	C	-5.591650	0.165480	-2.215449
O	-2.534100	-1.925646	2.711951	H	-4.948554	0.359541	-0.170259
P	-0.863705	-1.849511	2.412602	C	-4.539166	1.640595	-3.818129
P	-1.136837	-2.399909	-1.878079	H	-3.049744	2.991977	-3.040461
C	4.122817	-0.079231	-0.090538	C	-5.451131	0.619632	-3.530818
H	5.162116	-0.384385	-0.193928	H	-6.292020	-0.640282	-1.982162
C	2.314049	1.249764	0.167705	H	-4.417956	1.995437	-4.844796
O	1.712849	2.287687	0.380052	H	-6.044113	0.172178	-4.332349
N	3.740829	1.176937	0.172402	C	4.613289	2.291844	0.412238
N	3.093988	-0.890423	-0.233394	C	5.038799	2.535883	1.732931
C	-3.799299	2.371837	1.388064	C	4.971675	3.111334	-0.679517
C	-4.567537	3.478119	1.787561	C	5.886439	3.634137	1.942427
C	-3.812602	1.203413	2.170147	C	5.814478	4.199358	-0.413024
C	-5.344308	3.408684	2.947630	C	6.271401	4.454155	0.881738
H	-4.560920	4.399399	1.202421	H	6.241694	3.851943	2.952203
C	-4.602897	1.134223	3.320918	H	6.112989	4.861479	-1.228134
H	-3.207355	0.342057	1.884272	H	6.929485	5.307353	1.066252
C	-5.368694	2.236678	3.712460	C	3.284964	-2.238899	-0.723111
H	-5.935014	4.275905	3.253935	C	3.462778	-2.415672	-2.114746
H	-4.611473	0.215678	3.912382	C	3.386644	-3.298683	0.206134
H	-5.980728	2.186094	4.616755	C	3.725492	-3.716560	-2.570525
C	-2.354498	4.092086	-0.544184	C	3.654613	-4.575182	-0.310113
C	-3.290718	5.009472	-1.055167	C	3.818925	-4.782371	-1.679592
C	-1.029573	4.506181	-0.315656	H	3.864518	-3.897720	-3.637098
C	-2.906534	6.325866	-1.322951	H	3.739343	-5.427232	0.363089
H	-4.317919	4.694988	-1.253396	H	4.024244	-5.788335	-2.054356
C	-0.652510	5.825645	-0.585303	C	3.441612	-1.251421	-3.104309
H	-0.288140	3.796524	0.062433	C	2.828788	-1.621367	-4.464392
C	-1.588701	6.735612	-1.086610	C	4.862181	-0.698438	-3.335386
H	-3.638524	7.033591	-1.720414	H	2.825745	-0.448227	-2.669680
H	0.379609	6.138583	-0.407836	H	1.869330	-2.145787	-4.361460

H	2.658948	-0.708865	-5.056618	C	-1.578631	-1.016088	-3.040100
H	3.502751	-2.266692	-5.049478	C	-2.467934	-1.408952	-4.224110
H	5.342401	-0.343072	-2.413593	C	-0.352803	-0.209635	-3.474927
H	5.509431	-1.480491	-3.764986	H	-2.180493	-0.390132	-2.357620
H	4.833706	0.145248	-4.042241	H	-3.335117	-2.002566	-3.903594
C	3.242226	-3.071220	1.710689	H	-2.844237	-0.491562	-4.703178
C	4.471889	-2.378984	2.332138	H	-1.915872	-1.978844	-4.984812
C	2.969811	-4.366538	2.485007	H	0.322025	0.016976	-2.636180
H	2.375175	-2.402473	1.841812	H	0.217926	-0.742463	-4.247854
H	4.660931	-1.378037	1.926185	H	-0.679794	0.750870	-3.904887
H	4.326449	-2.262608	3.418073	C	-0.009287	-3.646085	-2.637949
H	5.379669	-2.984469	2.175997	C	-0.425056	-4.166854	-4.015530
H	2.117846	-4.925757	2.074654	C	0.182789	-4.779320	-1.620230
H	3.849180	-5.030015	2.477400	H	0.942721	-3.098665	-2.722004
H	2.754180	-4.137102	3.539496	H	-0.389530	-3.383086	-4.784747
C	4.592356	1.673603	2.907894	H	0.266772	-4.967251	-4.326562
C	3.774972	2.497757	3.915640	H	-1.441854	-4.589583	-3.995379
C	5.783748	0.975993	3.582520	H	0.544339	-4.388637	-0.657535
H	3.927351	0.885724	2.525574	H	-0.761124	-5.319232	-1.442149
H	2.894950	2.951353	3.433027	H	0.925341	-5.499298	-1.996780
H	3.423447	1.857235	4.740440	C	-0.384745	-0.328989	3.359859
H	4.378804	3.308273	4.355045	C	1.133617	-0.297650	3.579831
H	6.355112	0.368130	2.862788	C	-1.176847	-0.041244	4.638867
H	6.476150	1.707613	4.030267	H	-0.631802	0.456976	2.624914
H	5.433974	0.309640	4.387609	H	1.686494	-0.453450	2.641974
C	4.416079	2.874679	-2.079380	H	1.424244	0.687507	3.975892
C	5.482485	2.993222	-3.176471	H	1.457135	-1.060551	4.306053
C	3.231900	3.822866	-2.345067	H	-2.259014	-0.139379	4.480590
H	4.026393	1.846592	-2.120831	H	-0.886956	-0.702967	5.467481
H	6.337217	2.325264	-2.984675	H	-0.974719	0.995432	4.955801
H	5.050588	2.721677	-4.153015	C	-0.263454	-3.355569	3.307944
H	5.867876	4.021644	-3.265461	C	-0.613073	-4.607029	2.490338
H	2.452021	3.707253	-1.577479	C	-0.755736	-3.469294	4.754661
H	3.565298	4.874053	-2.339163	H	0.828468	-3.228903	3.310701
H	2.783273	3.614190	-3.330462	H	-0.271656	-4.524143	1.448202

H	-0.139163	-5.492193	2.943934
H	-1.700744	-4.781736	2.472447
H	-0.337178	-2.685516	5.400544
H	-1.854146	-3.415239	4.809680
H	-0.444187	-4.442124	5.170146

2b'

Geometry with 155 atoms:

C	1.509424	-0.458820	0.127649
C	0.870076	0.761774	0.097974
C	3.607911	0.680901	0.016105
H	4.695932	0.648035	-0.023600
C	1.580442	2.012471	0.087546
O	1.121040	3.147800	0.126179
N	3.020455	1.870104	0.034386
N	2.929998	-0.462852	0.051478
Ni	0.085169	-1.767974	0.222974
C	-1.669773	-2.605731	0.193483
P	0.104368	-2.461444	-1.879072
P	-0.391159	-1.695781	2.438947
C	-2.506276	-2.627591	1.321444
C	-2.201393	-3.166460	-0.977895
O	-1.445141	-3.101354	-2.123722
O	-2.047847	-2.043121	2.477533
C	-3.782573	-3.203448	1.313948
C	-3.469621	-3.755652	-1.036995
C	-4.253038	-3.767556	0.121788
H	-4.385178	-3.200750	2.223927
H	-3.831859	-4.174399	-1.976862
H	-5.249444	-4.216371	0.094071
Au	-1.206401	0.932413	-0.061490
P	-3.511697	1.383768	-0.273279
C	-4.471798	0.248180	-1.343213
C	-5.865801	0.097976	-1.225138
C	-3.783090	-0.470810	-2.332746
C	-6.556396	-0.746649	-2.097377
H	-6.414204	0.632634	-0.446715
C	-4.479337	-1.308914	-3.207662
H	-2.696713	-0.393375	-2.406111
C	-5.865355	-1.446099	-3.093827
H	-7.638841	-0.860093	-1.996732
H	-3.930652	-1.872583	-3.965410
H	-6.407773	-2.109035	-3.772935
C	-3.779090	3.077923	-0.943502
C	-2.703859	3.983489	-0.947605
C	-5.033622	3.495336	-1.420719
C	-2.883877	5.288303	-1.419071
H	-1.721451	3.670577	-0.582778
C	-5.207212	4.797837	-1.894340
H	-5.880229	2.805961	-1.430222
C	-4.133662	5.696859	-1.893592
H	-2.040790	5.983938	-1.417013
H	-6.185803	5.112031	-2.266470
H	-4.272616	6.715309	-2.265725
C	-4.352431	1.382980	1.358884
C	-4.818718	0.176199	1.906704
C	-4.400678	2.556073	2.129395
C	-5.338497	0.148643	3.203057
H	-4.767300	-0.747802	1.328755
C	-4.915843	2.521156	3.428794
H	-4.031460	3.499502	1.720505
C	-5.387080	1.319325	3.967967
H	-5.699229	-0.795672	3.618934
H	-4.948772	3.439191	4.021197
H	-5.789713	1.294803	4.983887
C	3.718198	-1.692576	-0.059527
C	4.190170	-2.084131	-1.334573
C	4.034906	-2.410463	1.118645
C	4.907891	-3.288891	-1.415819
C	4.749997	-3.607780	0.972032

C	5.165924	-4.053126	-0.282346	C	4.864574	2.898164	3.591238
H	5.275637	-3.630003	-2.384133	H	3.297640	2.079019	2.400033
H	5.001236	-4.200005	1.851125	H	1.757701	4.022743	2.439388
H	5.717359	-4.992552	-0.371186	H	2.204072	3.506799	4.091099
C	3.839048	3.068068	0.015167	H	2.949150	4.962543	3.379572
C	4.197699	3.643834	1.249008	H	5.678332	2.281331	3.177881
C	4.196440	3.619050	-1.233562	H	5.293988	3.865712	3.897548
C	4.970052	4.814373	1.208860	H	4.490616	2.401651	4.501068
C	4.968849	4.789485	-1.213754	C	3.715552	3.016450	-2.550214
C	5.352911	5.378627	-0.007596	C	4.754514	3.115661	-3.674601
H	5.266468	5.294350	2.143784	C	2.384818	3.660918	-2.983925
H	5.269438	5.253202	-2.154681	H	3.521396	1.946530	-2.380859
H	5.953283	6.292113	-0.017765	H	5.730703	2.709875	-3.367829
C	4.041101	-1.225298	-2.589064	H	4.410200	2.550407	-4.555172
C	3.885207	-2.037003	-3.885970	H	4.905598	4.157611	-3.998728
C	5.264203	-0.300661	-2.757544	H	1.623817	3.591347	-2.194506
H	3.143449	-0.599132	-2.470429	H	2.533309	4.729239	-3.213787
H	3.141375	-2.839129	-3.803192	H	1.996191	3.168531	-3.890528
H	3.579997	-1.368919	-4.706190	C	1.148576	-3.971906	-2.165757
H	4.837964	-2.500378	-4.186449	C	0.945710	-4.644781	-3.526851
H	5.402908	0.397560	-1.922602	C	0.943560	-4.963560	-1.017770
H	6.182692	-0.903900	-2.840644	H	2.174612	-3.577214	-2.095777
H	5.164579	0.294068	-3.677096	H	1.176347	-3.985103	-4.375416
C	3.687893	-1.876498	2.504854	H	1.615162	-5.517907	-3.599985
C	4.575655	-0.677557	2.892782	H	-0.088857	-5.005512	-3.637715
C	3.788809	-2.923352	3.620292	H	1.155240	-4.497450	-0.048850
H	2.647832	-1.523483	2.453910	H	-0.089536	-5.346227	-0.994093
H	4.483958	0.172959	2.208336	H	1.621833	-5.823264	-1.140791
H	4.303339	-0.313687	3.895577	C	0.329151	-1.426712	-3.429103
H	5.636500	-0.974981	2.916766	C	-0.705378	-1.759513	-4.514441
H	3.235482	-3.843461	3.392664	H	-1.695122	-1.367630	-4.242566
H	4.837927	-3.197906	3.814842	H	-0.399361	-1.274637	-5.456049
H	3.389218	-2.505577	4.557294	H	-0.811555	-2.834829	-4.704320
C	3.722340	3.075993	2.581347	C	-0.358160	-0.271502	3.649536
C	2.589342	3.944586	3.155676	C	-1.444598	0.779806	3.410835

H	-1.234929	1.380342	2.512729	H	-0.191238	-4.322491	5.185381
H	-2.438588	0.329245	3.297519	C	1.033511	0.364375	3.742345
H	-1.475069	1.465811	4.273130	H	1.811166	-0.357006	4.030972
C	0.281428	-3.100583	3.465393	H	1.319954	0.830000	2.788541
C	0.710853	-4.261786	2.567887	H	1.020473	1.154672	4.510114
C	-0.689424	-3.565228	4.557516	H	-0.578984	-0.765533	4.610390
H	1.171681	-2.665097	3.944898	H	1.320852	-1.742729	-3.782436
H	1.467058	-3.941284	1.837541	C	0.383876	0.085345	-3.193138
H	1.140530	-5.077544	3.171712	H	-0.572825	0.478541	-2.817583
H	-0.147551	-4.669298	2.011195	H	1.159995	0.371246	-2.473525
H	-1.015544	-2.749161	5.220416	H	0.601469	0.588765	-4.149499
H	-1.587971	-4.025104	4.119264				

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