Electronic Supplementary Information

Bite-Angle Bending as a Key for Understanding Group-10 Metal Reactivity of d^{10}-[M(NHC)$_2$] Complexes with Sterically Modest NHC Ligands

Florian Hering[a], Jörn Nitsch[a], Ursula Paul[a], Andreas Steffen[a], F. Matthias Bickelhaupt[b], and Udo Radius[a]**

[a] F. Hering, U. Paul, H. Schneider, J. Nitsch, Dr. A. Steffen, Prof. Dr. U. Radius, Institut für Anorganische Chemie, Julius-Maximilians-Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany.
[*] Author for correspondence. E-mail: u.radius@uni-wuerzburg.de

[b] Prof. Dr.- F. M. Bickelhaupt, Department of Theoretical Chemistry and Amsterdam Center for Multiscale Modeling, VU University Amsterdam, De Boelelaan 1083, NL-1081 HV Amsterdam, Institute of Molecules and Materials, Radboud University Nijmegen, Heyendaalseweg 135, NL-6525 AJ Nijmegen, The Netherlands. E-mail: F.M.Bickelhaupt@vu.nl
[*] Author for correspondence. E-mail: F.M.Bickelhaupt@vu.nl

The Supporting Information contents:

1. Additional Figures and Tables

Table S1. Energy decomposition analysis [kJ/mol] of the metal–ethylene bond in [M(H_2Im)$_2$(η^2-C_2H_4)] complexes.

M	ΔE_{disp}	ΔV_{elstat}	ΔE_{pauli}	ΔE_{steric}	ΔE_{oi}^{σ}	ΔE_{oi}^{π}	ΔE_{oi}^{δ}	ΔE_{oi}	ΔE_{int}	ΔE_{strain}	ΔE
Ni	-26.3	-543.5	+741.8	+198.4	-98.8	-317.4	-0.8	-417.1	-245.0	+140.8	-104.2
Pd	-24.1	-521.3	+695.7	+174.4	-84.1	-249.6	-0.8	-334.5	-184.2	+159.2	-25.0
Pt	-25.8	-773.2	+1038.2	+265.0	-152.1	-369.0	-2.2	-523.4	-284.1	+263.6	-20.5

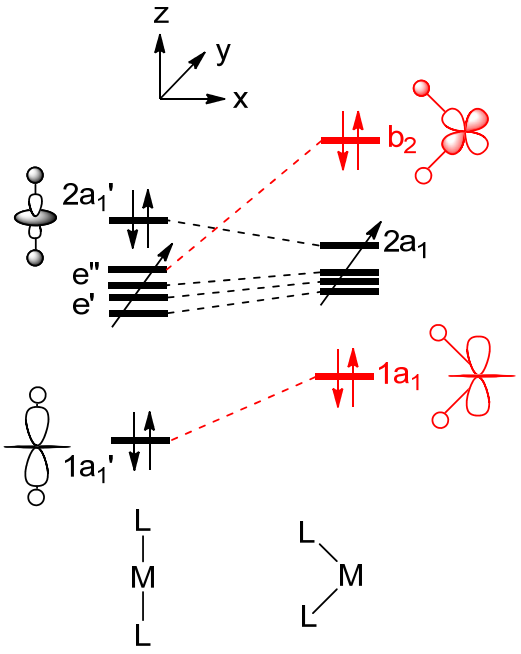
Table S2. Energy decomposition analysis [kJ/mol] of the metal–carbene bond in [M(H_2Im)$_3$] complexes between [M(H_2Im)$_2$] and H_2Im.

M	ΔE_{disp}	ΔV_{elstat}	ΔE_{pauli}	ΔE_{steric}	ΔE_{oi}	ΔE_{int}	ΔE_{strain}	ΔE
Ni	-26.2	-634.0	+757.4	+123.4	-278.5	-181.3	+73.4	-107.9
Pd	-24.9	-596.5	+729.0	+132.4	-224.7	-117.1	+91.5	-25.6
Pt	-27.3	-877.4	+1103.2	+225.8	-357.3	-158.8	+132.3	-26.5

Table S3. Calculated M-L bond energies [kJ/mol] of the complexes [M(*i*Pr$_2$Im)$_2$(L)] (M = Ni, Pd, Pt) (TURBOMOLE, RI-DFT, BP86, def2-TZVPP level) for the ligands *i*Pr$_2$Im, ethylene (C_2H_4), and 2-butyne (Me_2C_2). For comparison, the calculated bond dissociation energies for the dissociation of *i*Pr$_2$Im from linear [M(*i*Pr$_2$Im)$_2$] (D_{2d}) are -222.7 (Ni), -198.7 (Pd), and -243.1 kJ/mol (Pt).

	*i*Pr$_2$Im	C_2H_4	Me_2C_2
[Ni(*i*Pr$_2$Im)$_2$]	-55.3	-66.4	-66.2
[Pd(*i*Pr$_2$Im)$_2$]	+4.4	-8.3	+6.7
[Pt(*i*Pr$_2$Im)$_2$]	+13.1	-2.8	+4.2

Figure S1. Schematic Walsh diagram for the bending of the L–M–L angle of a fourteen-electron dicoordinate group 10 metal complexes d^{10}-ML_2



As the L−M−L angle decreases, the anti-bonding a_1' orbital at the linear geometry is stabilized to the bonding $2a_1$ orbitals, whereas the d_{zx} orbital is remarkably destabilized to an anti-bonding b_2 orbital. The linear geometry is usually favored, because the latter destabilization at the bent geometry is larger in energy compared to the stabilization of the a_1' orbital.

Moreover, bending of the ligands leads to destabilization of the σ-type orbital 1a', which contains metal s and d_{z^2} contributions. The s-d mixing for the $[M(H_2Im)_2]$ fragment increases in the row Ni to Pd to Pt due to the relative energies of the metal n d_{z^2} and (n+1) s orbitals, as does the barrier for bending.

Figure S2. ^{1}H NMR spectrum of [Pd(*i*Pr$_2$Im)$_3$Cl]Cl **1** in dmso-d_6

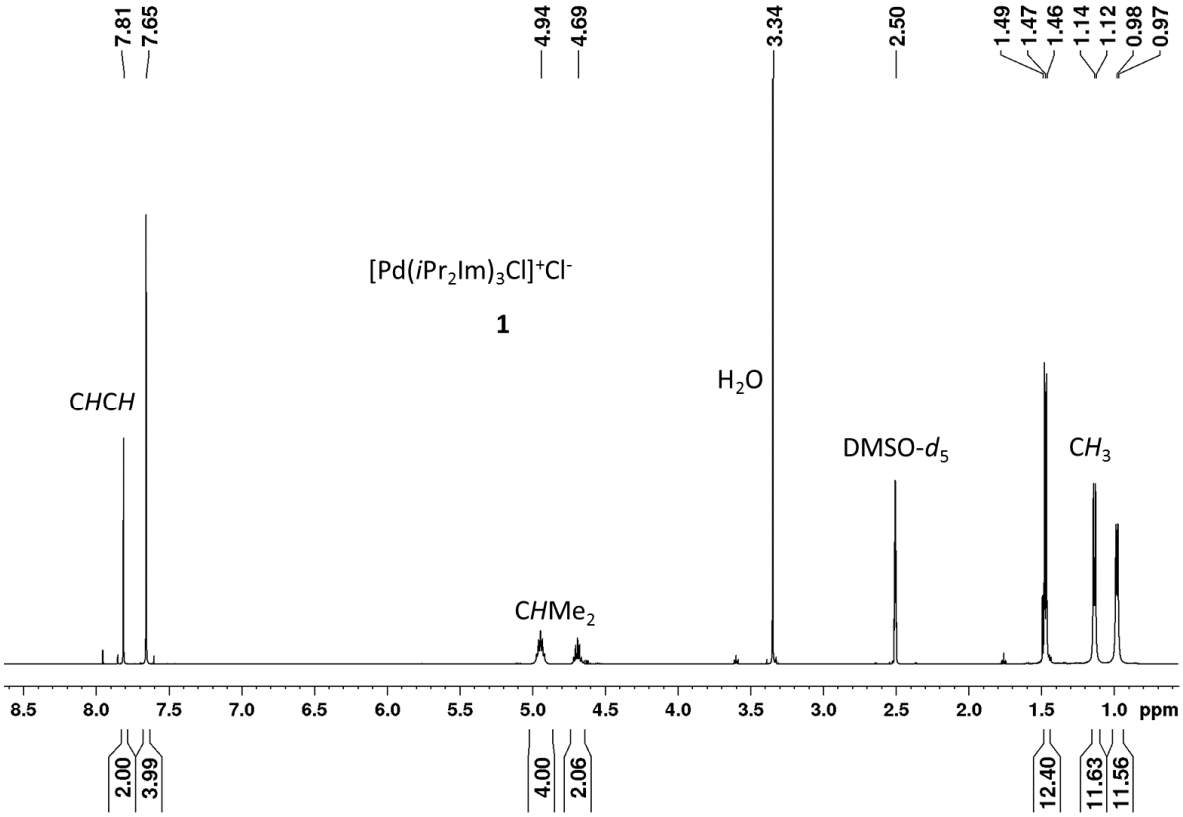


Figure S3. ^{13}C NMR spectrum of [Pd(*i*Pr$_2$Im)$_3$Cl]Cl **1** in dmso-d_6

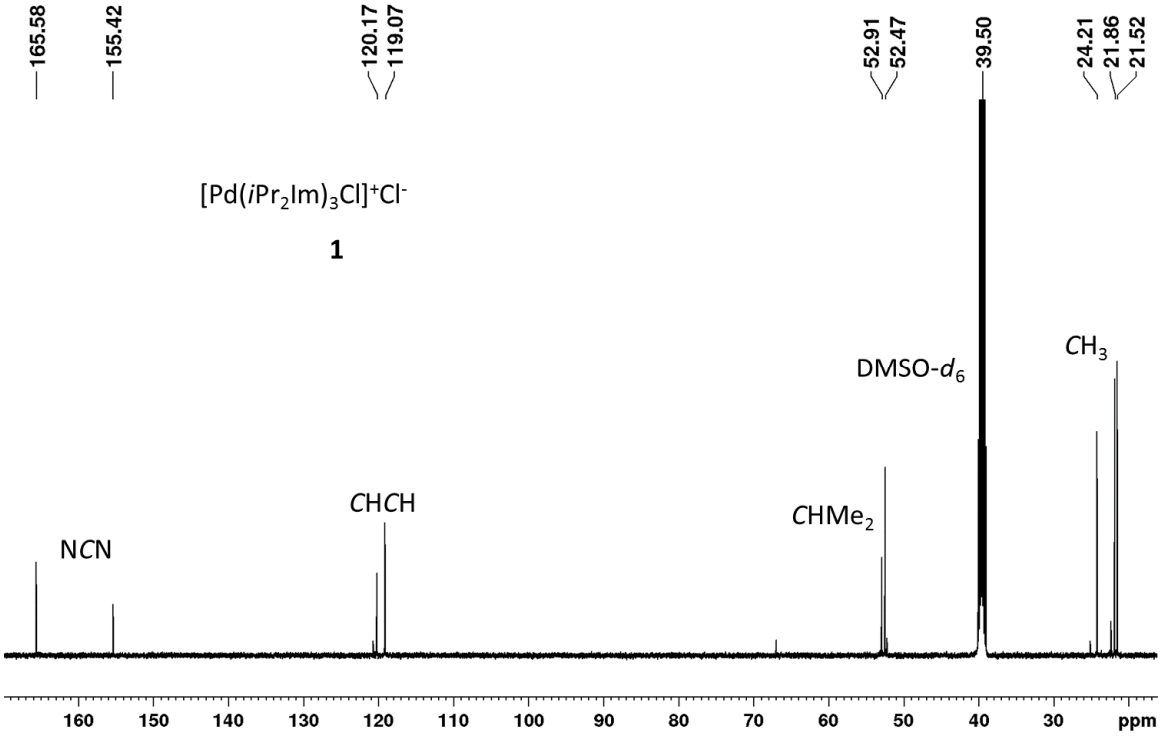


Figure S4. ^{1}H NMR spectrum of [Pt(*i*Pr$_2$Im)$_3$Cl]Cl **2** in dmso-d_6

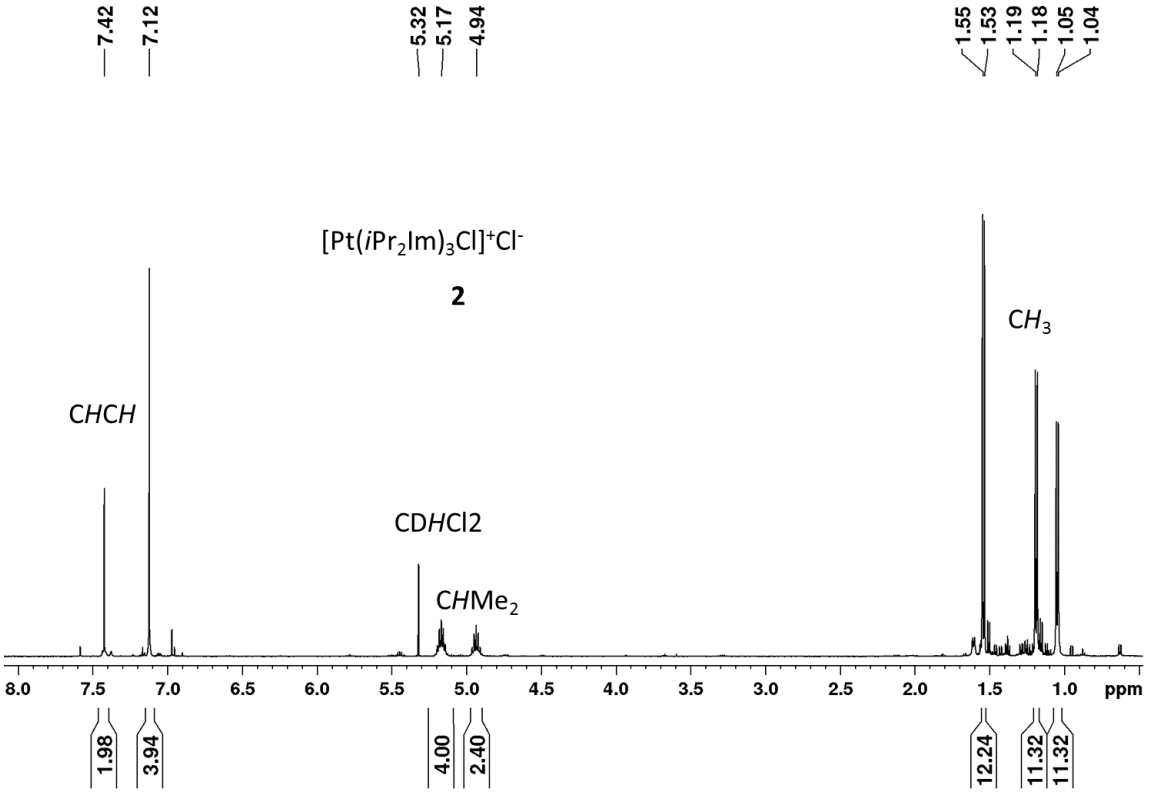


Figure S5. ^{13}C NMR spectrum of [Pt(*i*Pr$_2$Im)$_3$Cl]Cl **2** in dmso-d_6

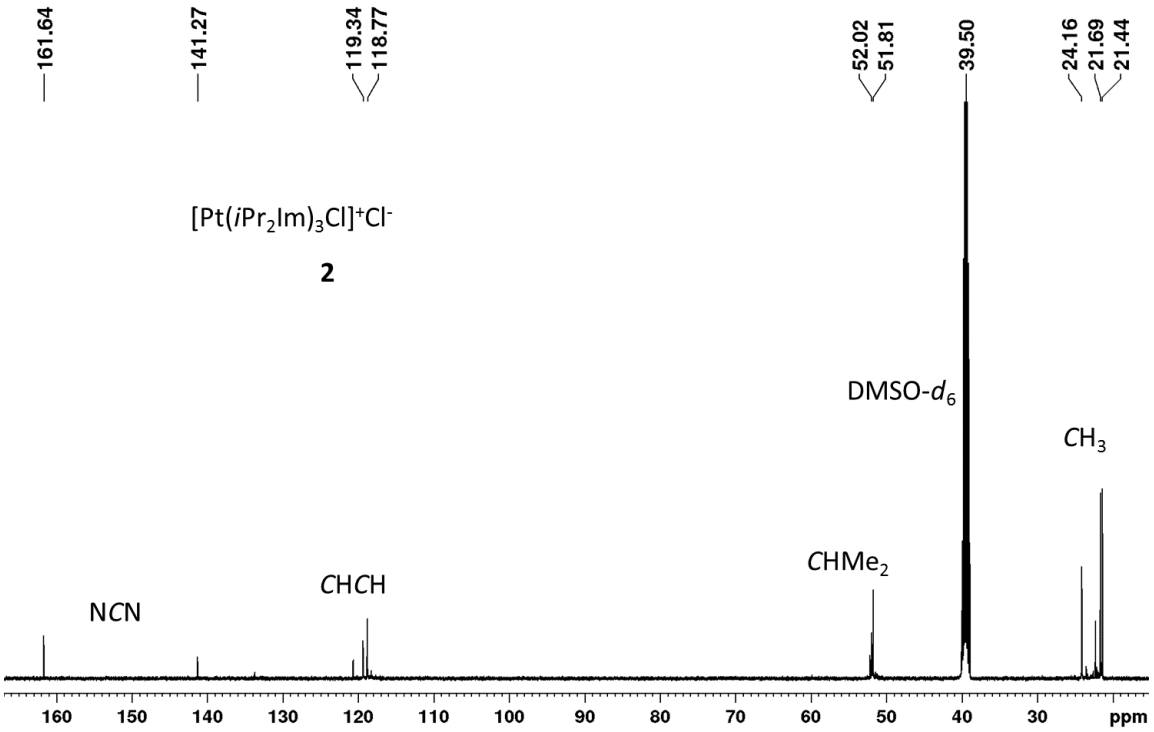
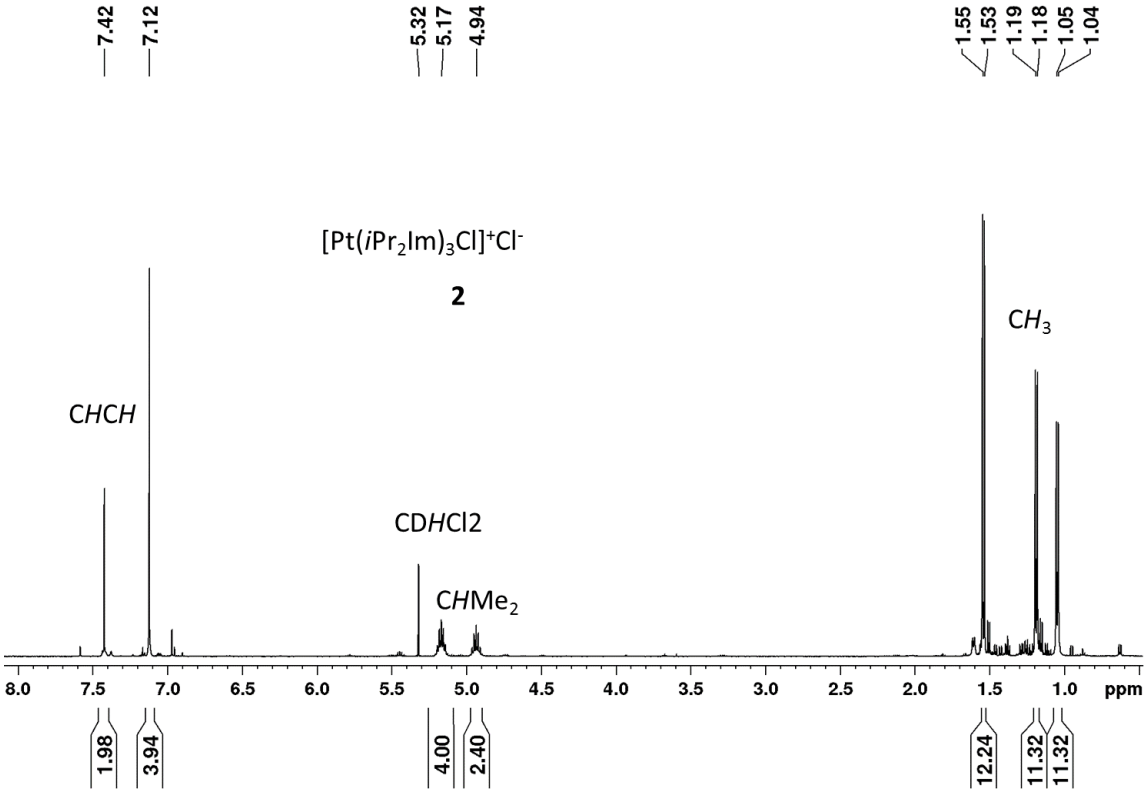


Figure S6. ^{1}H NMR spectrum of [Pt(*i*Pr$_2$Im)$_3$Cl]Cl **2** in CD_2Cl_2



As mentioned in the text, samples of [M(*i*Pr$_2$Im)$_3$Cl]Cl (M = Pd **1**, Pt **2**) prepared from the reaction of pure *i*Pr$_2$Im and MCl_2 may contain the imidazolium salt [*i*Pr$_2$Im-H]Cl as impurity: **^{1}H NMR** (500 MHz, dmso-d_6): δ = 1.48 (d, 12 H, CH_3, $^{3}J_{HH}$ = 6.6 Hz), 4.63 (sept, 2 H, C*H*Me$_2$, $^{3}J_{HH}$ = 6.6 Hz), 7.95 (d, 2 H, C*H*C*H*, $^{4}J_{HH}$ = 1.6 Hz*).* 9.46 (t, 1 H, NC*H*N, $^{4}J_{HH}$ = 1.6 Hz*).* **^{13}C NMR** (126 MHz, dmso-d_6): δ = 22.3 (CH_3), 52.2 (*C*HMe$_2$), 120.6 (*CH*C*H*)*,* 133.8 (N*C*HN).

Figure S7. ^{1}H NMR spectrum of [Pd(*i*Pr$_2$Im)$_2$] **3** in C_6D_6

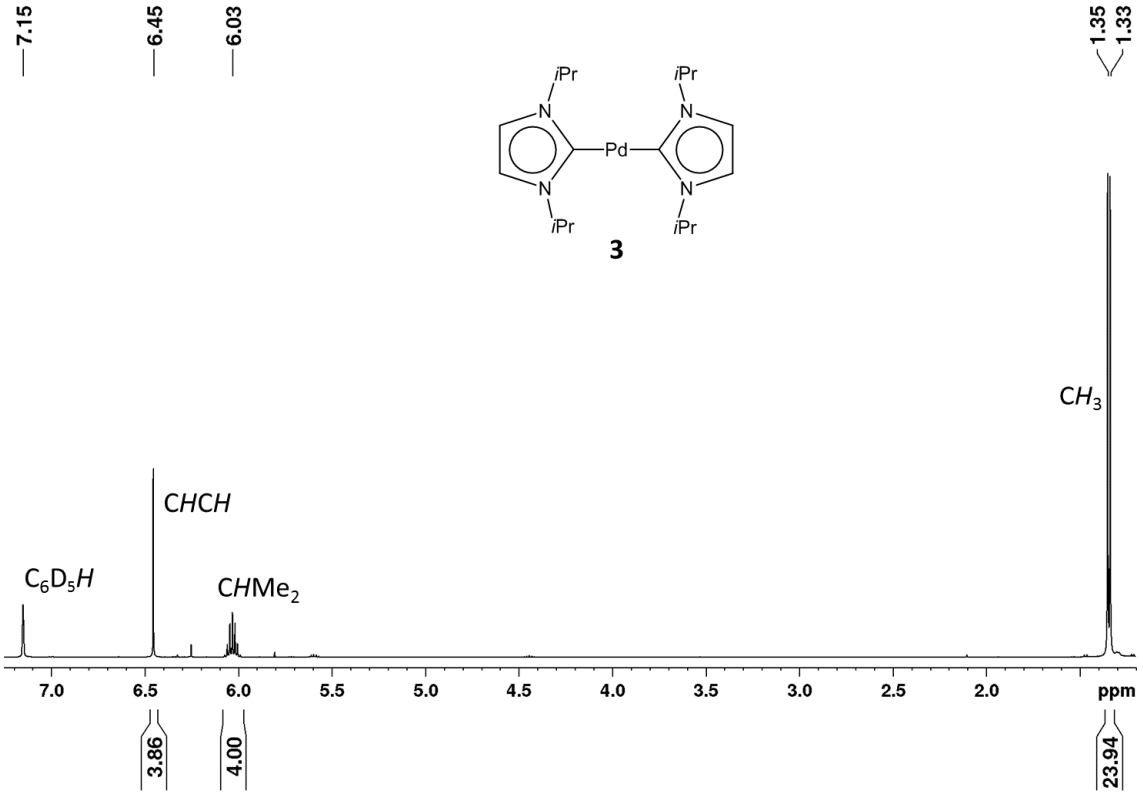


Figure S8. ^{13}C NMR spectrum of [Pd(*i*Pr$_2$Im)$_2$] **3** in C_6D_6

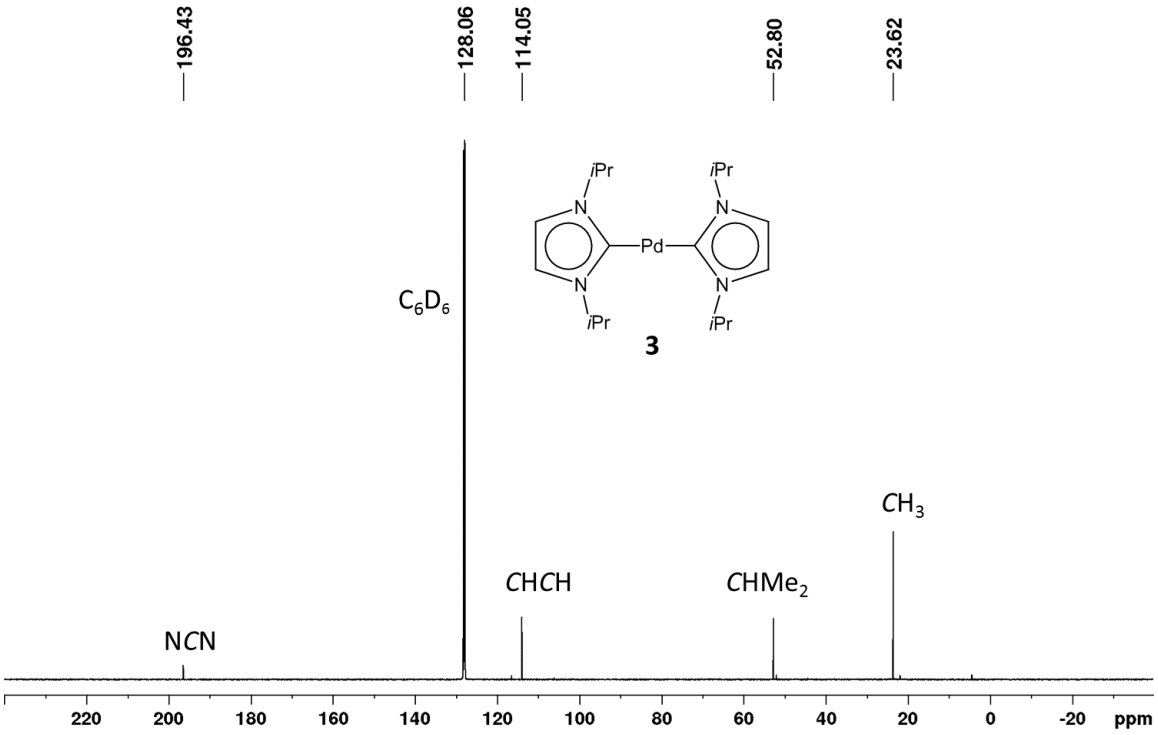


Figure S9. ^{1}H NMR spectrum of [Pt(*i*Pr$_2$Im)$_2$] **4** in C_6D_6

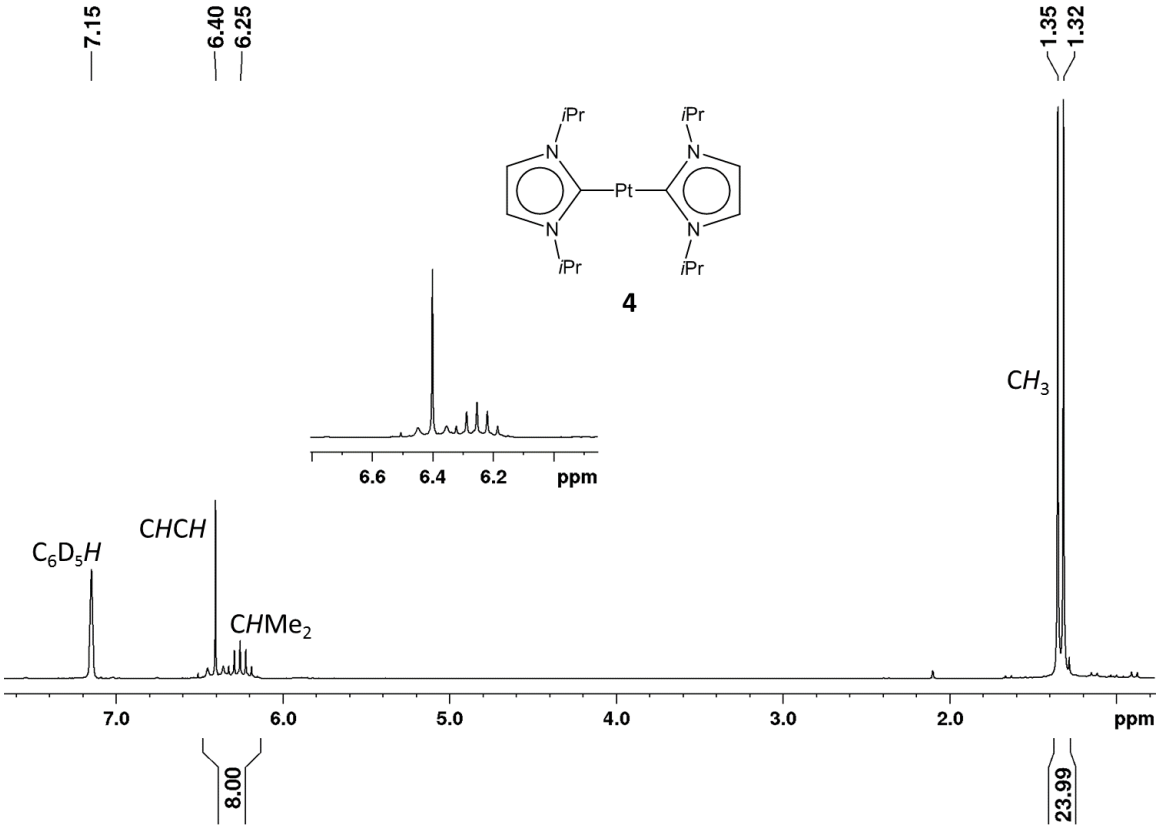


Figure S10. ^{13}C NMR spectrum of [Pt(*i*Pr$_2$Im)$_2$] **4** in C_6D_6

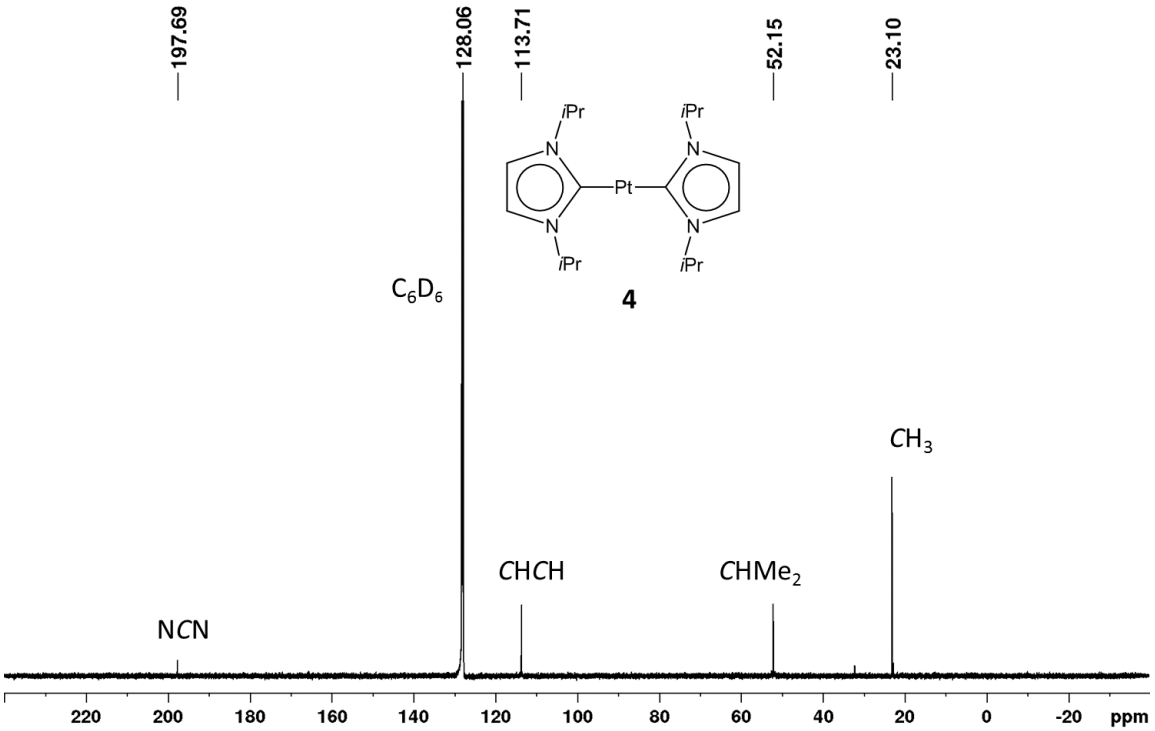


Figure S11. ^{1}H NMR spectrum of [Pt(*i*Pr$_2$Im)$_2$] **4** in thf-d_8

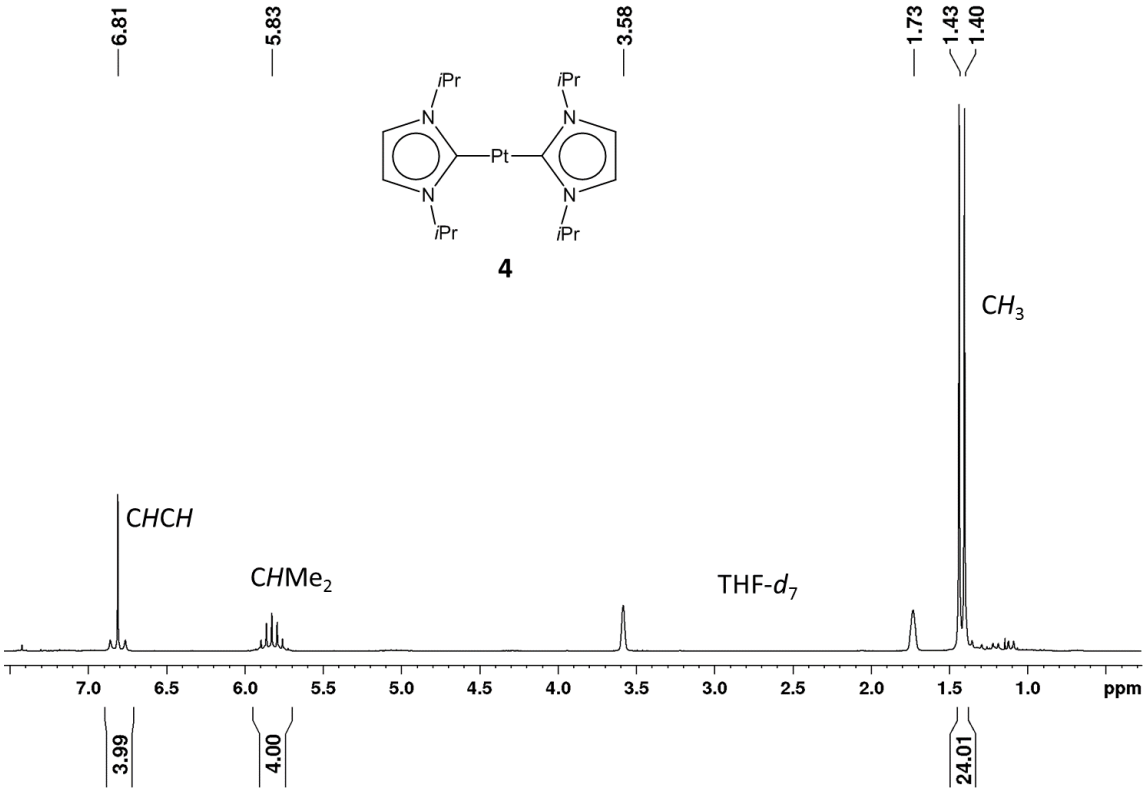


Figure S12. ^{195}Pt NMR spectrum of [Pt(*i*Pr$_2$Im)$_2$] **4** in C_6D_6

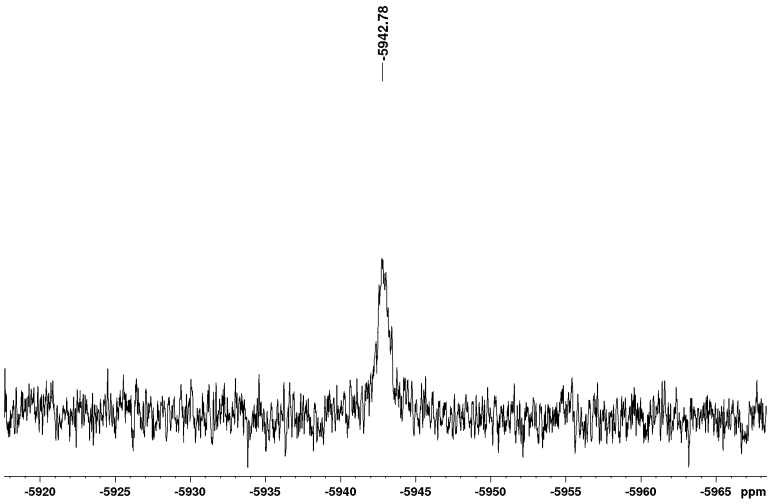


Figure S13. Reaction of [Pd(*i*Pr$_2$Im)$_2$] with ethylene in C_6D_6

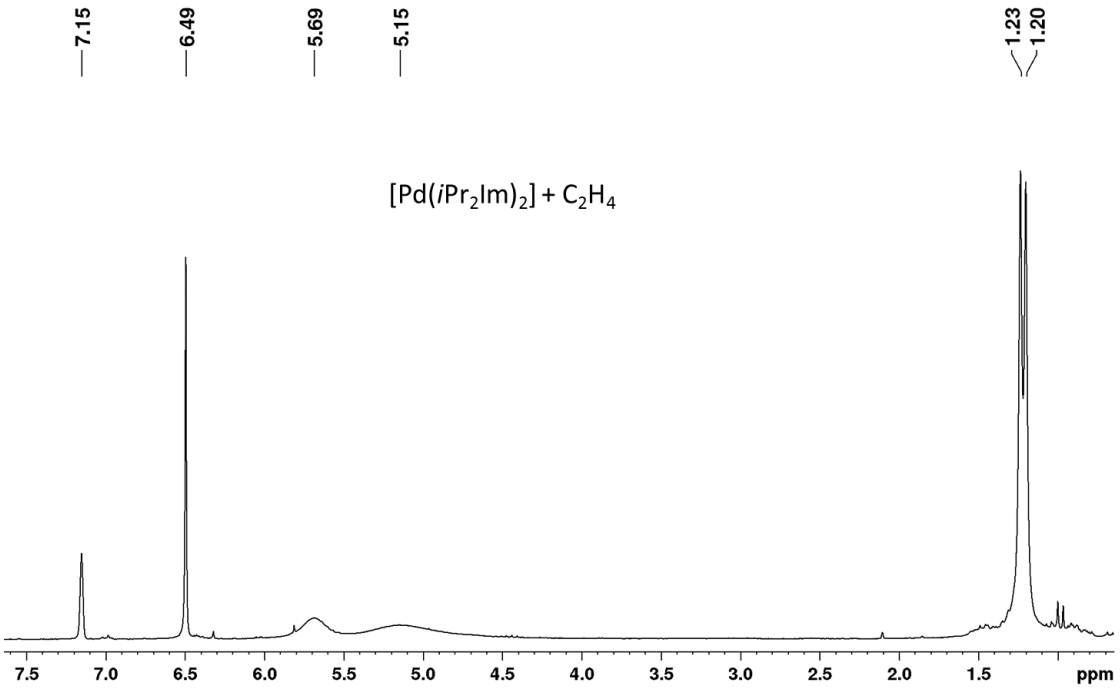


Figure S14. Reaction of [Pd(*i*Pr$_2$Im)$_2$] with ethylene in C_6D_6 after removal of ethylene. Only [Pd(*i*Pr$_2$Im)$_2$] is detected.

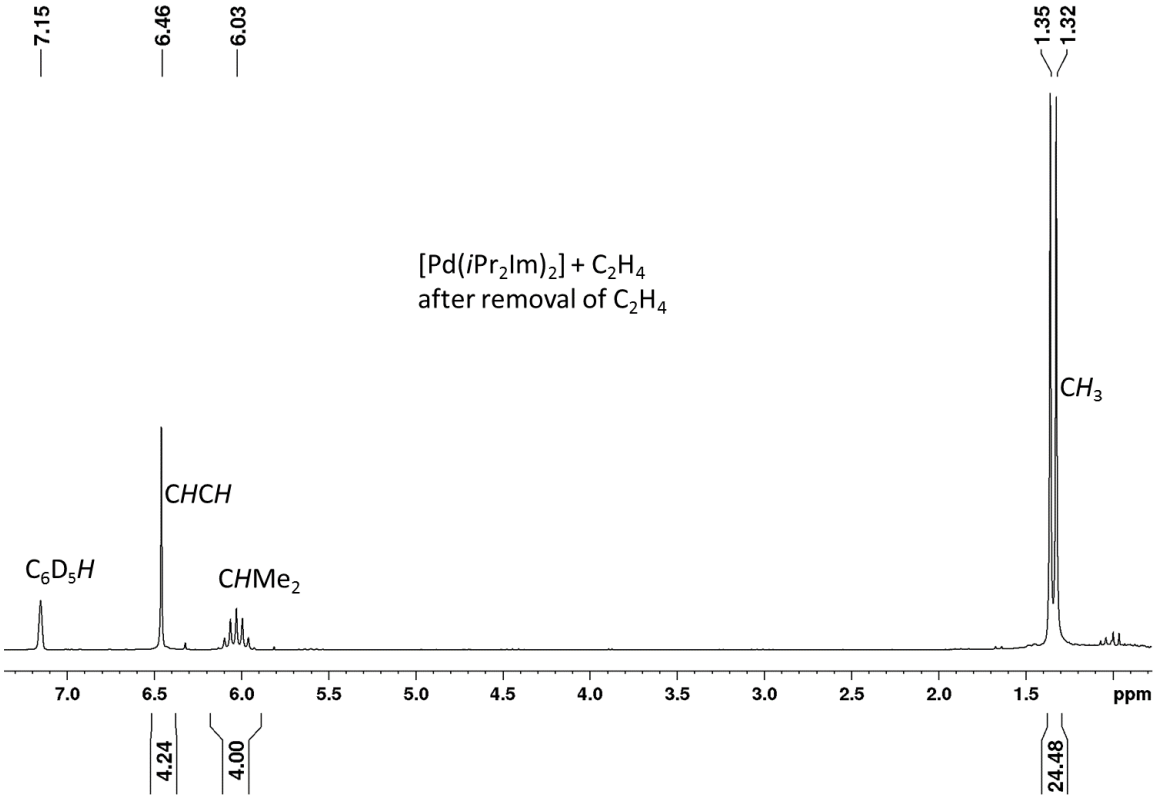


Figure S15. ^{1}H NMR spectrum of [Pt(*i*Pr$_2$Im)$_2$(η^2-C$_2$H$_4$)] **6** in C$_6$D$_6$

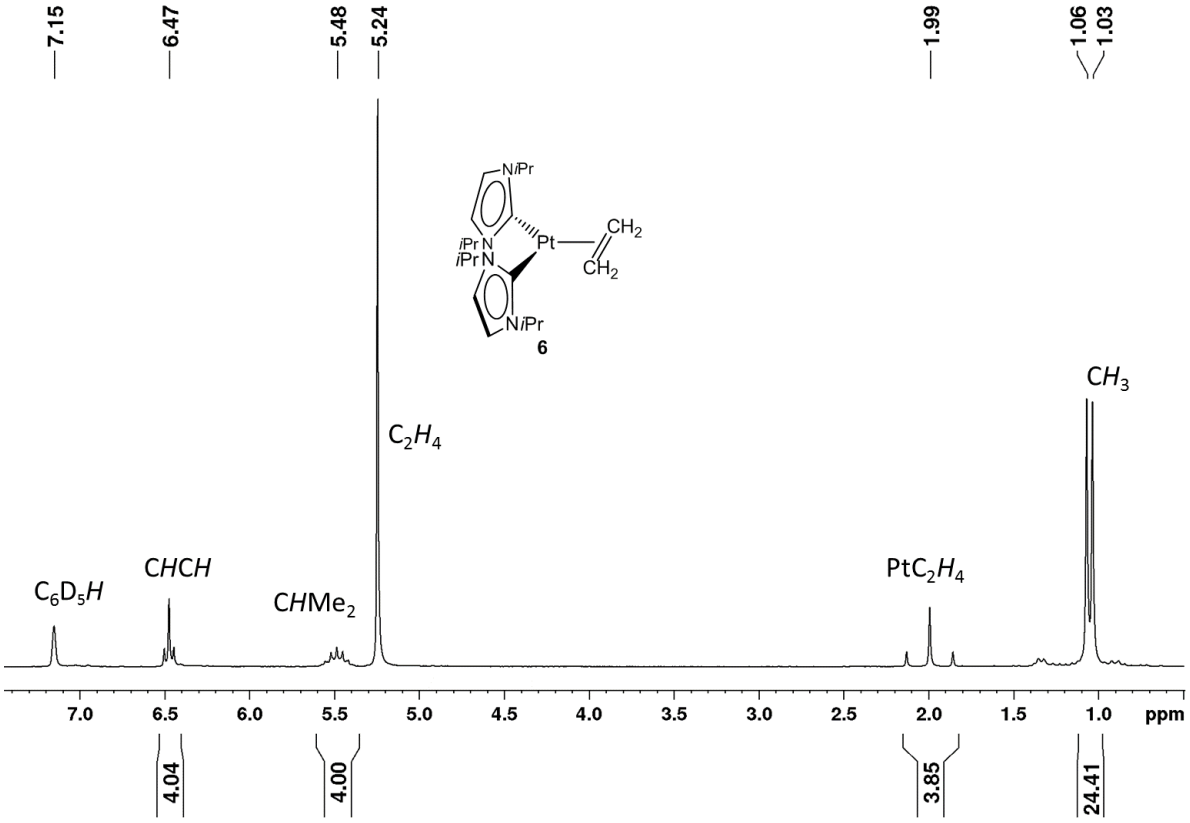


Figure S16. ^{13}C NMR spectrum of [Pt(*i*Pr$_2$Im)$_2$(η^2-C$_2$H$_4$)] **6** in C$_6$D$_6$

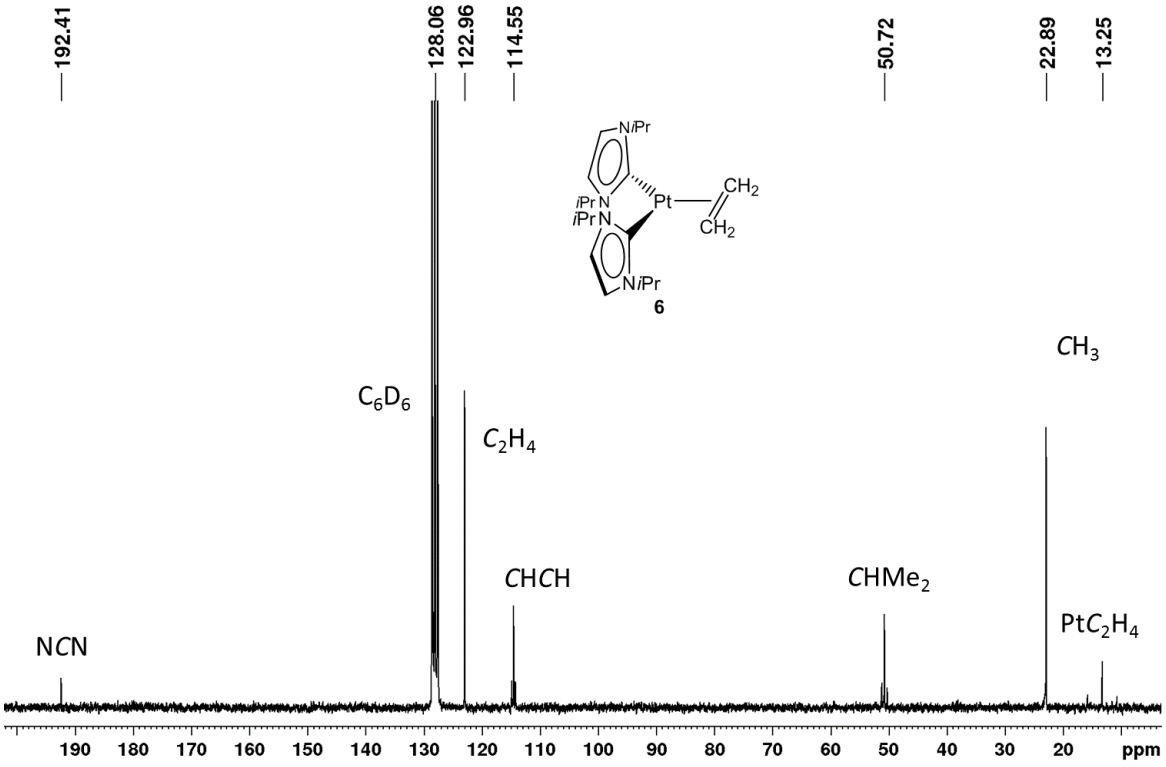


Figure S17. ^{1}H NMR spectrum of [Pt(*i*Pr$_2$Im)$_2$(η^2-HCCPh)] **7** in C_6D_6

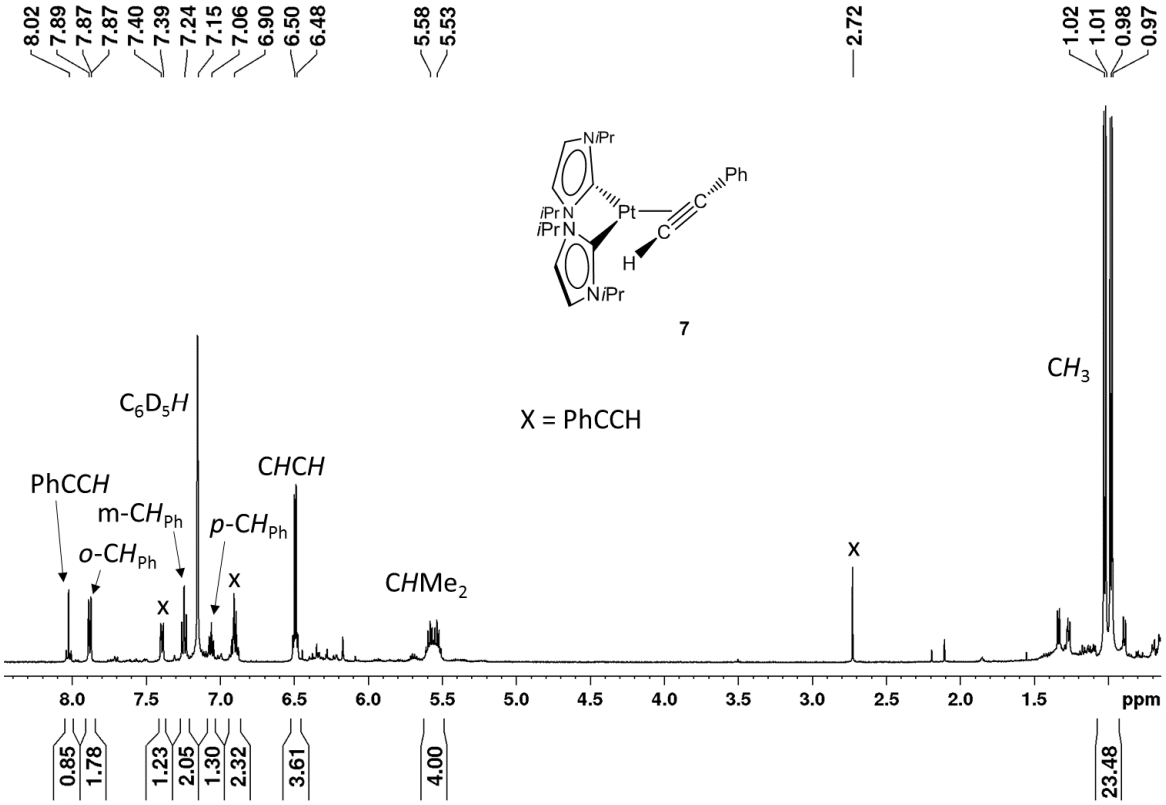


Figure S18. ^{13}C NMR spectrum of [Pt(*i*Pr$_2$Im)$_2$(η^2-HCCPh)] **7** in C_6D_6

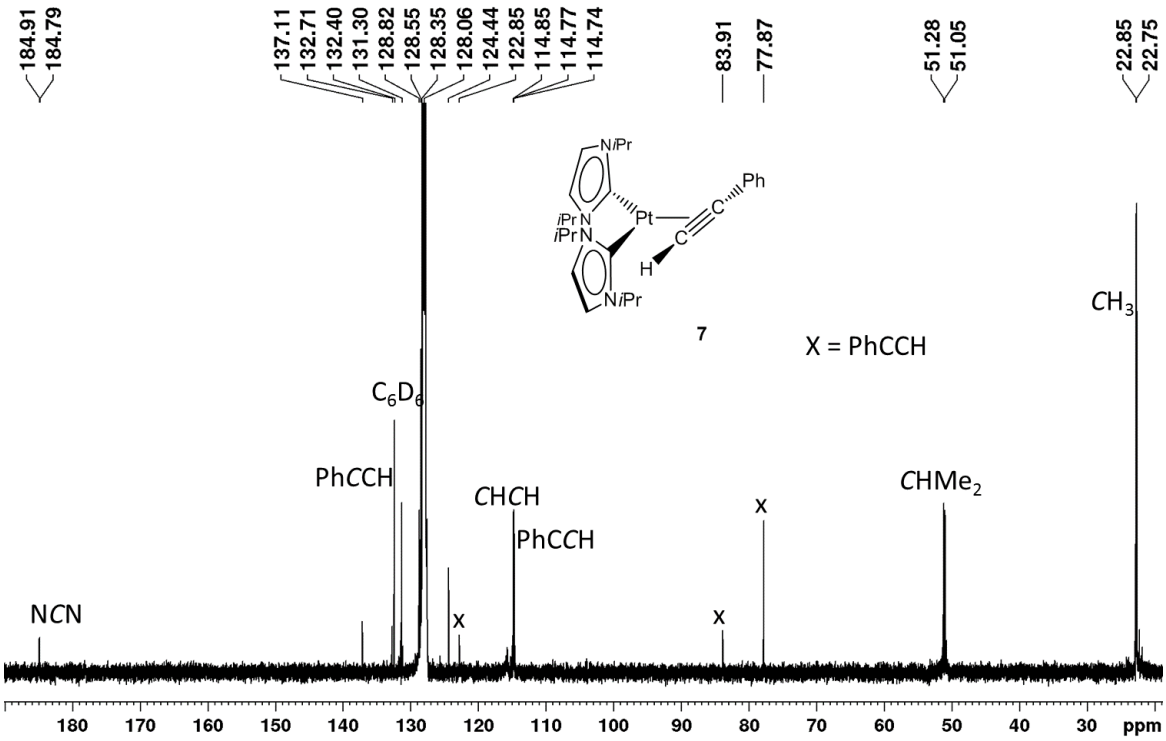


Figure S19. ^{1}H NMR spectrum of [Pt(*i*Pr$_2$Im)$_2$(η^2-PhCCPh)] **8** in C_6D_6

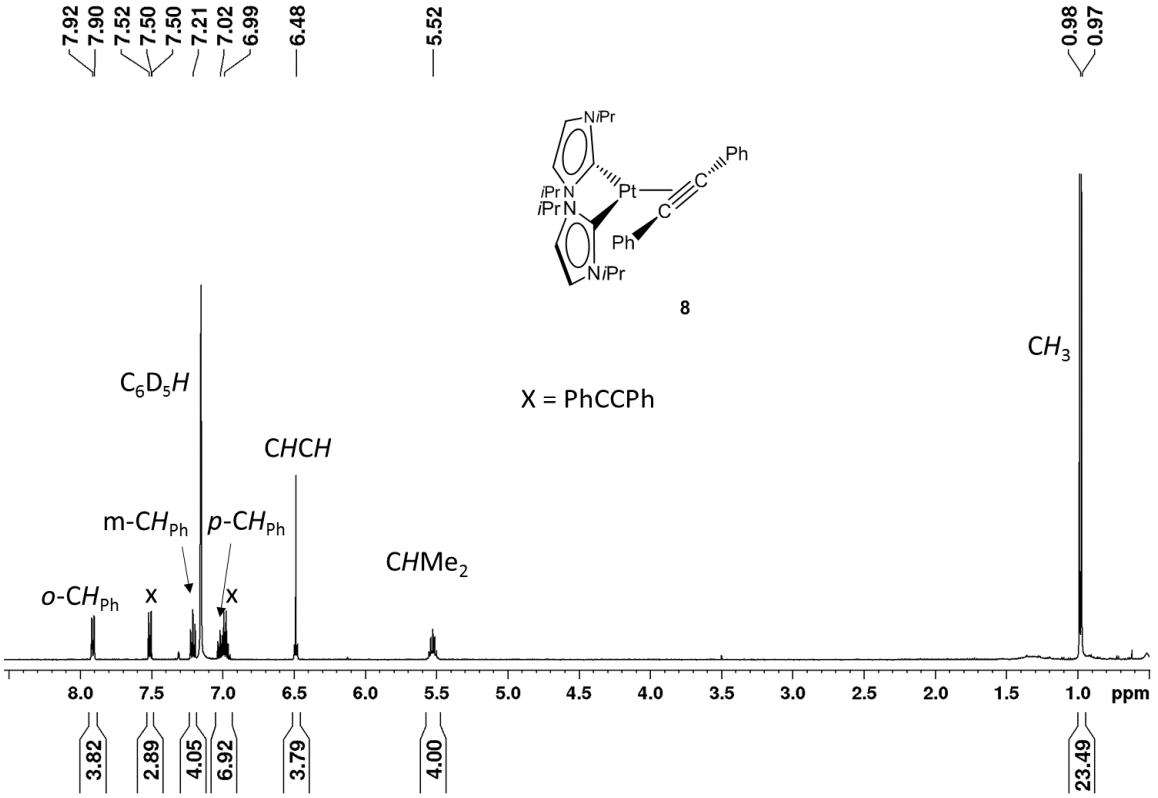


Figure S20. ^{13}C NMR spectrum of [Pt(*i*Pr$_2$Im)$_2$(η^2-PhCCPh)] **8** in C_6D_6

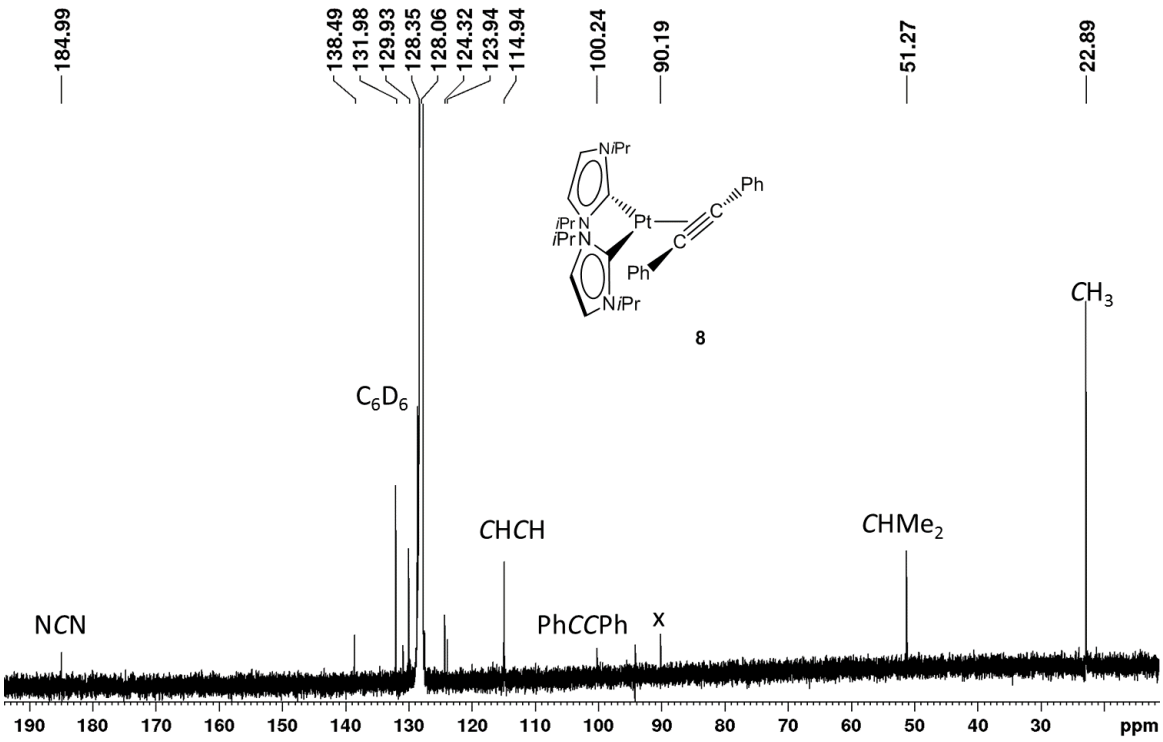


Figure S21. ^{1}H NMR spectrum of [Pt(*i*Pr$_2$Im)$_2$(η^2-MeCCMe)] **9** in C_6D_6 in a mixture with [Pt(*i*Pr$_2$Im)$_2$] **2**.

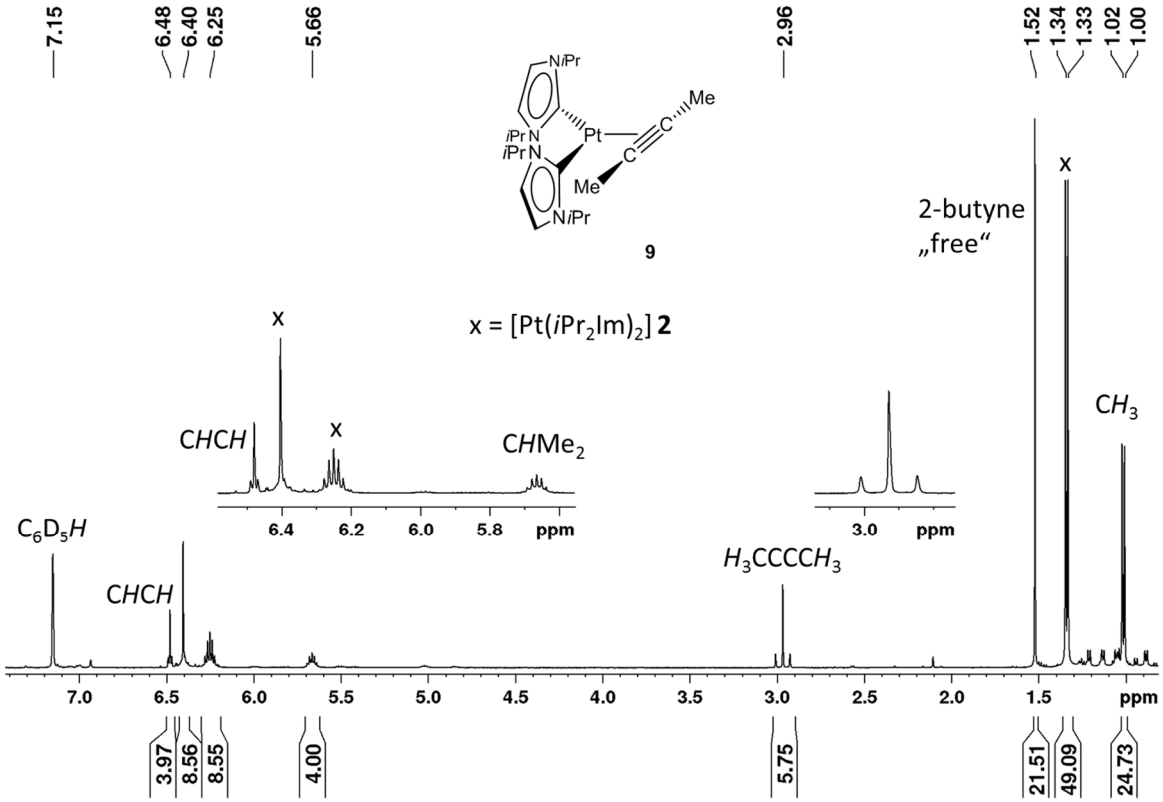


Figure S22. ^{13}C NMR spectrum of [Pt(*i*Pr$_2$Im)$_2$(η^2-MeCCMe)] **9** in C_6D_6 in a mixture with [Pt(*i*Pr$_2$Im)$_2$] **2**.

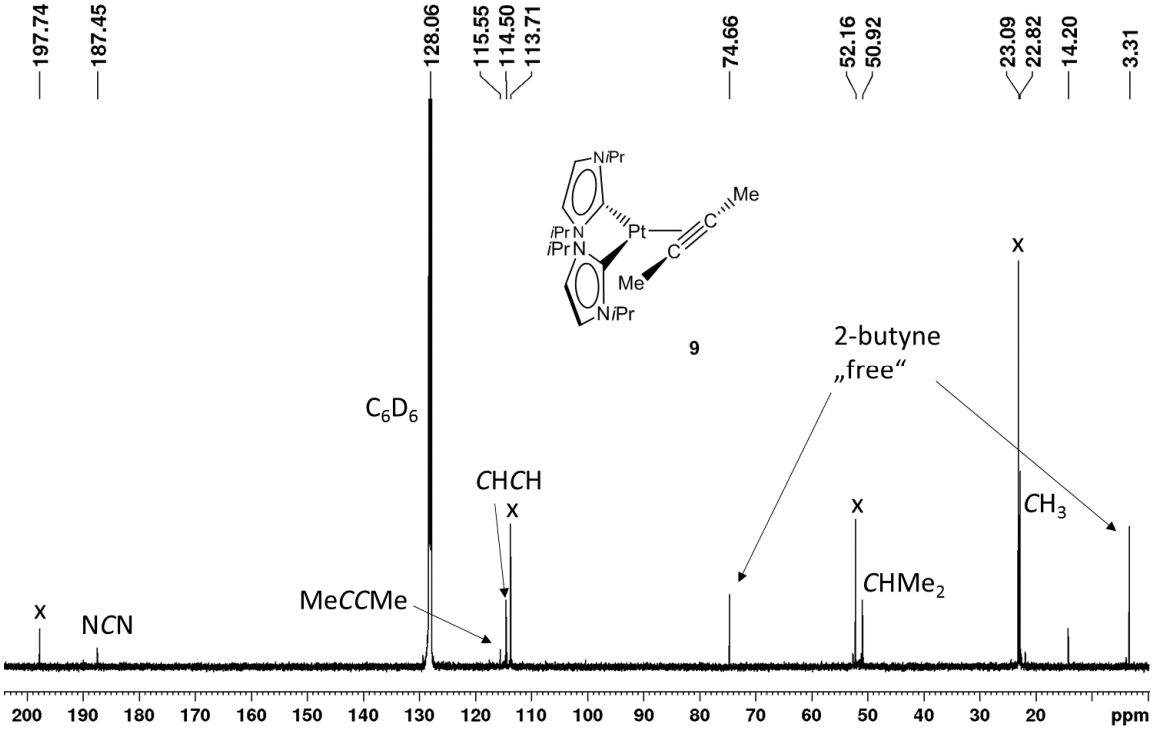


Figure S23. ^{1}H NMR spectrum of [Pt(*i*Pr$_2$Im)$_2$(η^2-H^{2}CCCHMe)] **10** in C_6D_6 in a mixture with [Pt(*i*Pr$_2$Im)$_2$(η^2-MeCCMe)] **9** and [Pt(*i*Pr$_2$Im)$_2$] **2**.

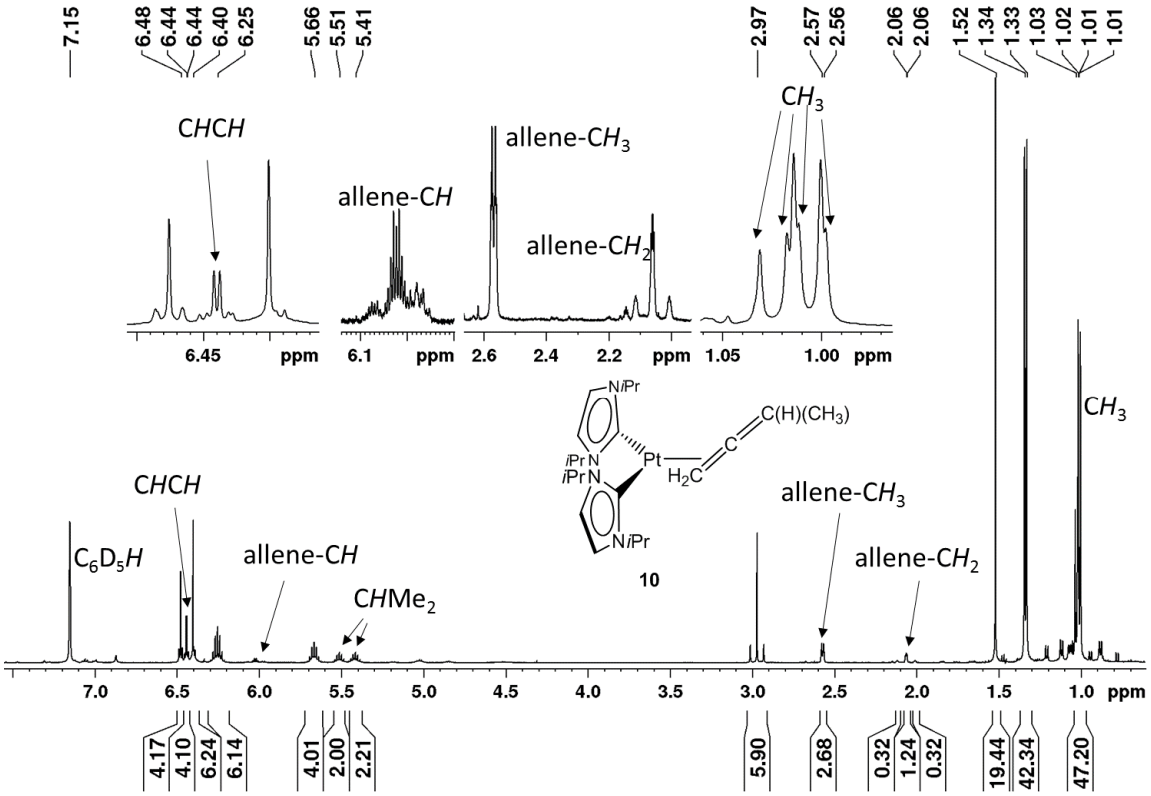


Figure S24. ^{1}H NMR spectrum of [Pt(*i*Pr$_2$Im)$_2$(η^2-H^{2}CCCHMe)] **10** in C_6D_6 in a mixture with [Pt(*i*Pr$_2$Im)$_2$(η^2-MeCCMe)] **9** and [Pt(*i*Pr$_2$Im)$_2$] **4**.

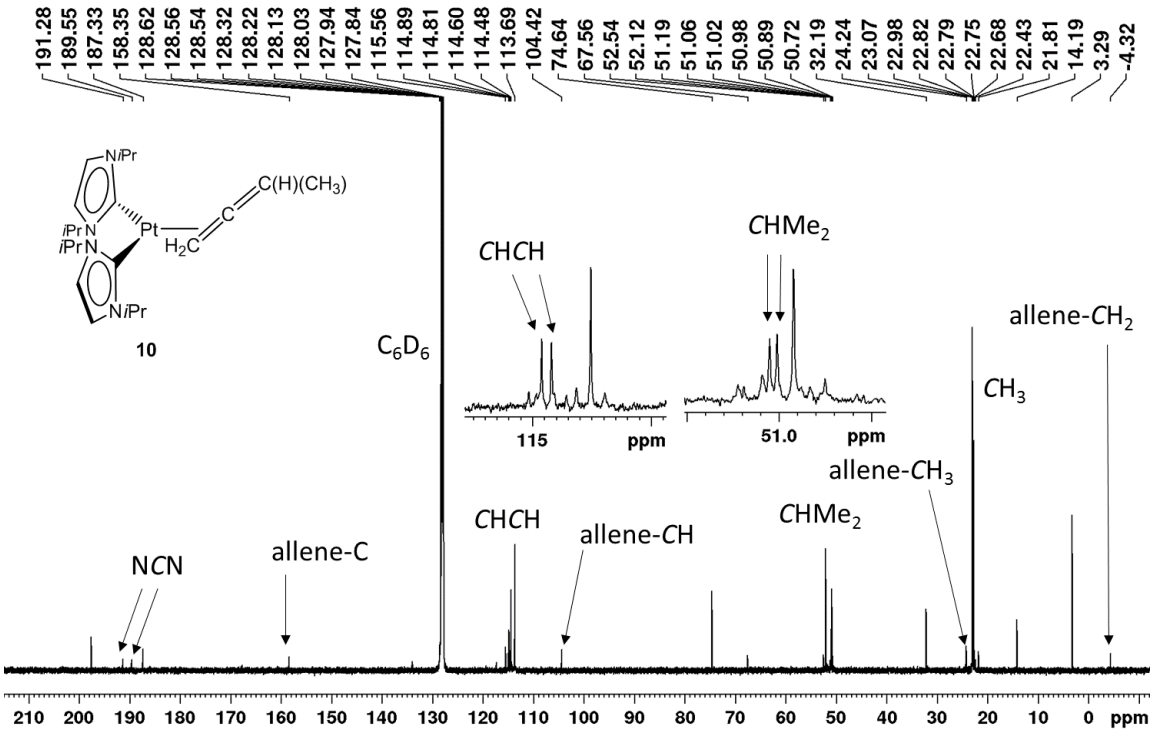


Figure S25. ^{1}H-^{1}H COSY experiment of [Pt(*i*Pr$_2$Im)$_2$(η^2-H$_2$CCCHMe)] **10**. Shown are the resonances of the allene ligand.

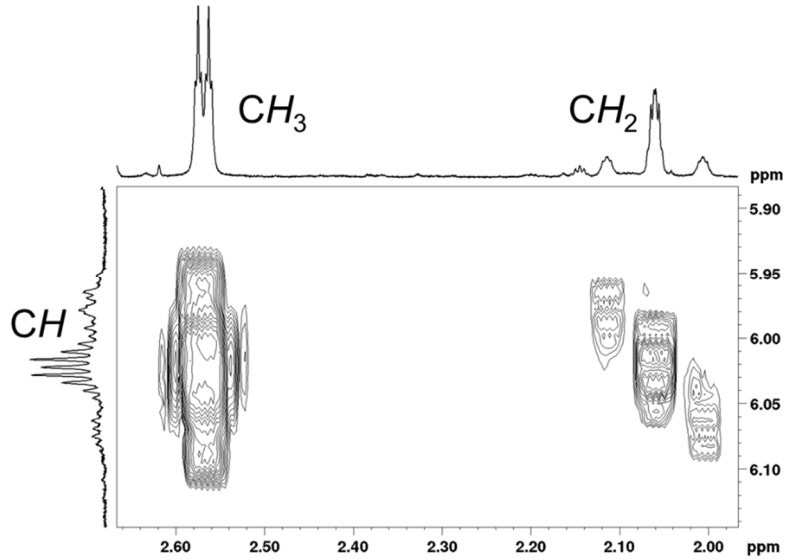


Figure S26. ^{1}H NMR spectrum of [Pt(*i*Pr$_2$Im)$_2$(H)(–CH$_2$-C{O}Ph)] **11** in C_6D_6

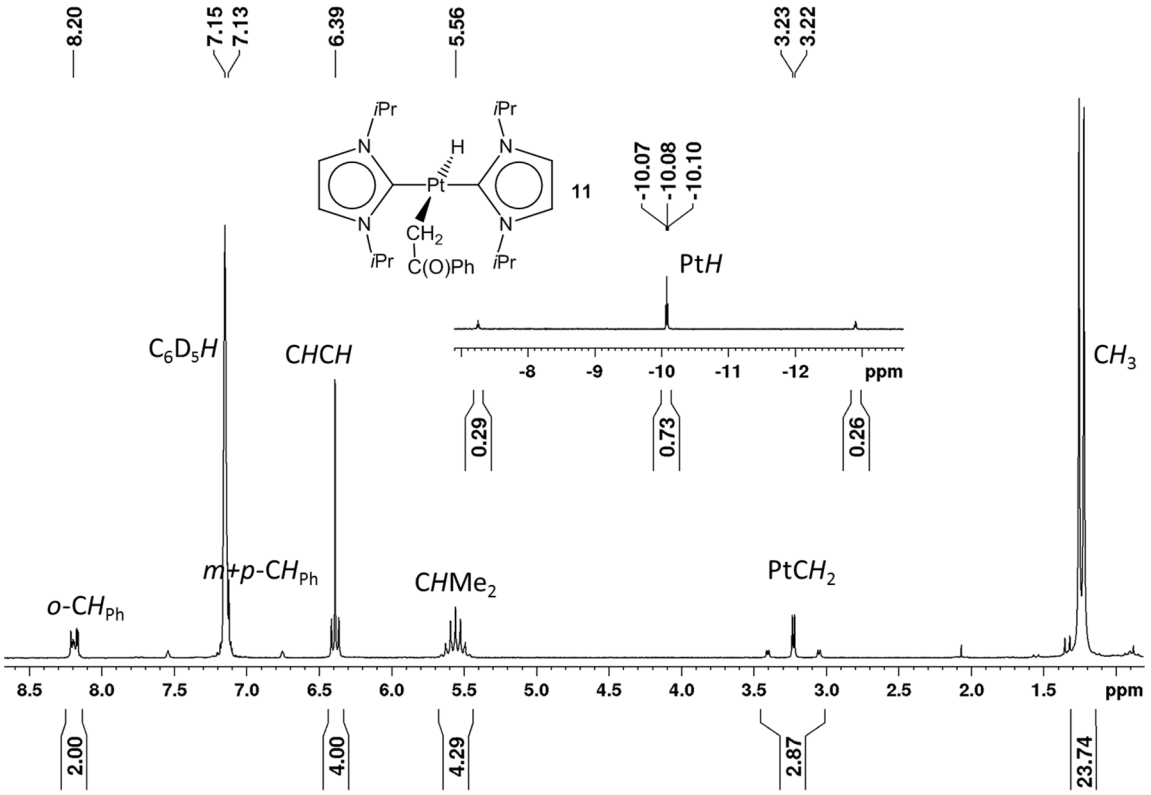


Figure S27. ^{13}C NMR spectrum of [Pt(*i*Pr$_2$Im)$_2$(H)(–CH$_2$-C{O}Ph)] **11** in C_6D_6

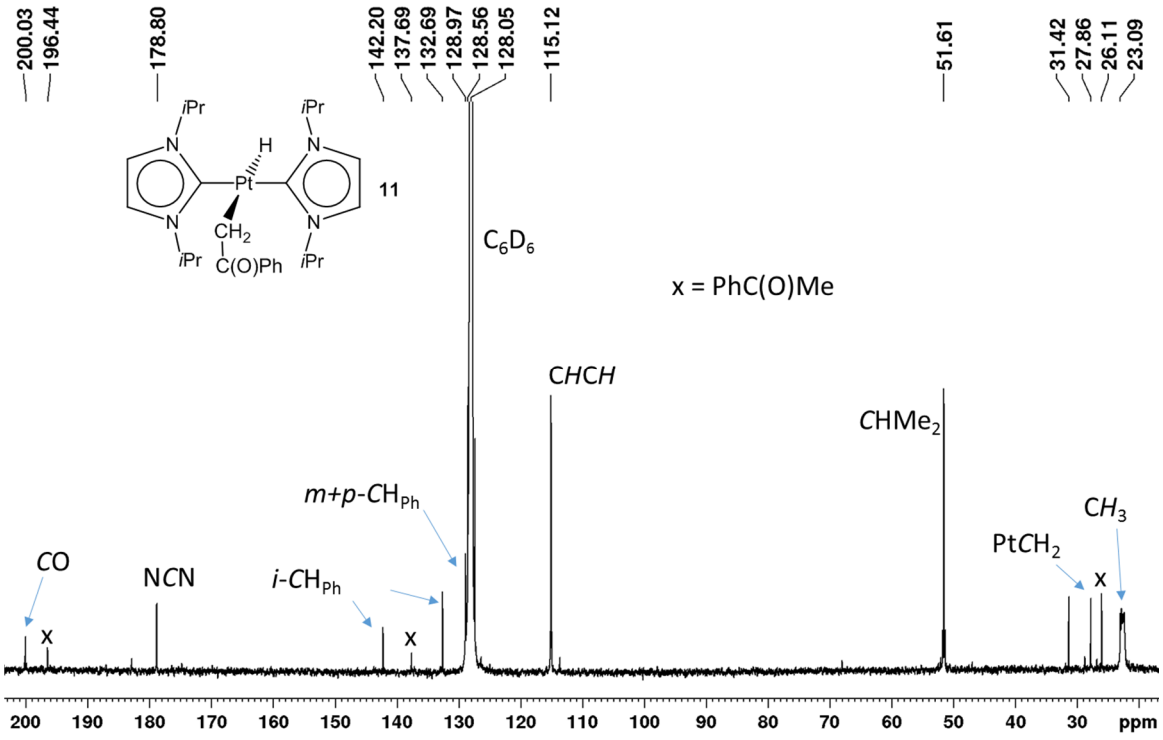


Figure S28. IR spectrum (ATR) of [Pt(*i*Pr$_2$Im)$_2$(H)(–CH$_2$-C{O}Ph)] **11**.

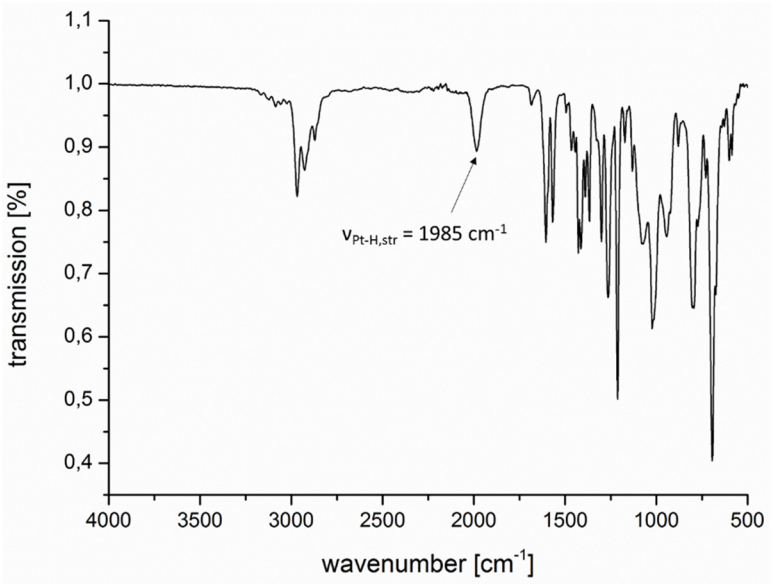
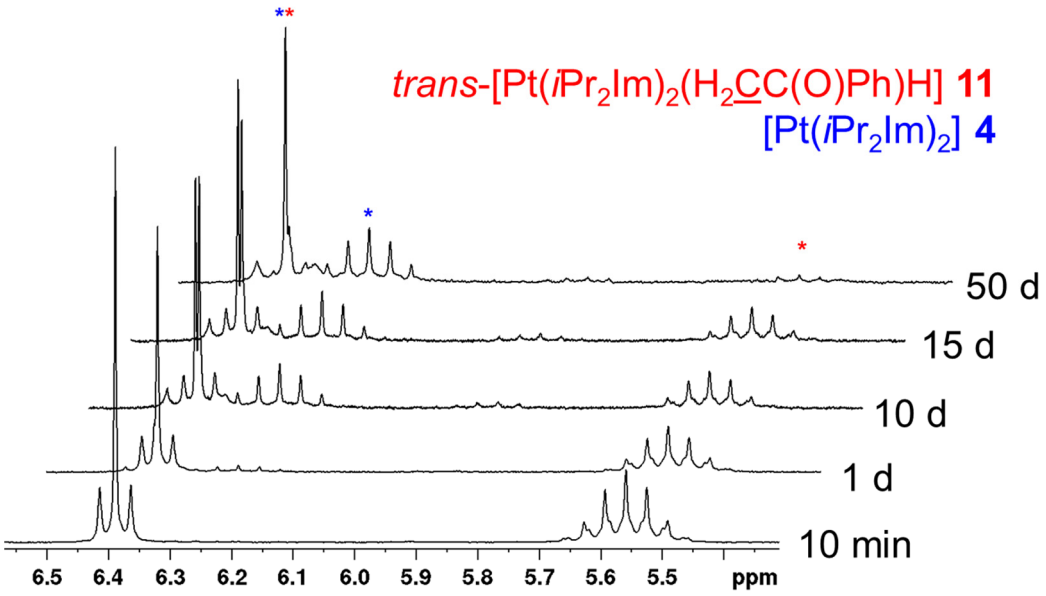


Figure S29. ^{1}H NMR spectra showing the decomposition of a sample of [Pt(*i*Pr$_2$Im)$_2$(C̲H$_2$C(O)Ph)H] (**11**) at room temperature in C_6D_6 (see also Figure S 4).



2. Experimental Details

General Considerations

All reactions and subsequent manipulations involving organometallic reagents were performed under nitrogen or argon atmosphere using standard Schlenk techniques, as reported previousely. [S1] NMR spectra were recorded, if not noted otherwise, on Bruker DRX-300, Bruker Avance 200, Bruker Avance 400, or Bruker Avance 500 spectrometers at 298 K. NMR experiments at variable temperature were conducted on Bruker Avance 200 or Bruker Avance 500 spectrometers and the temperatures were calibrated using a Bruker calibration sample. ^{13}C NMR spectra were broad-band proton-decoupled ($^{13}C\{^{1}H\}$). NMR data are listed in parts per million (ppm) and are reported relative to Tetramethylsilane. Coupling constants are quoted in hertz (Hz). Spectra are referenced internally to residual protio-solvent resonances (^{1}H: C_6D_5H, 7.15 ppm, $CDHCl_2$ 5.32 ppm thf-d_7 3.58, 1.72 ppm, dmso-d_5 2.50 ppm) or natural-abundance carbon resonances (^{13}C: C_6D_6, 128.1 ppm, CD_2Cl_2 53.8 ppm, thf-d_8 67.2, 25.3 ppm, dmso-d_6 39.5 ppm) and external $H_2[PtCl_6]$ 1 M in D_2O (^{195}Pt: 0 ppm) respectively. Elemental analyses were performed in the microanalytical laboratory of the University Würzburg with an Elementar vario micro cube. Infrared spectra were recorded on a Nicolet 380 FT-IR or a Bruker alpha spectrometer as solids by using an ATR unit, or in solution using a cell for measurement and are reported in cm^{-1}. The NHC *i*Pr_2Im was prepared according to a literature procedure. [S2] All other reagents have been obtained from commercial sources and have been used as received.

^{195}Pt satellites of the NHC carbene carbon atoms have usually not been detected in ^{13}C NMR spectra due to line broadening caused by the chemical shift anisotropy (CSA). Intensities of carbene carbon atoms are intrinsically low as they are quaternary carbon atoms bound to two quadrupole cores (^{14}N). ^{195}Pt holds a large anisotropy of its chemical shift and thus induces rapid relaxation of the surrounding nuclei. This effect correlates with B_0^2 causing significant line broadening at high frequencies. [S3, S4]

Synthesis of [Pd(*i*Pr_2Im)$_3$Cl]Cl (1)

6.88 g (45.2 mmol, 4.00 eq) of pure *i*Pr_2Im were added dropwise to a suspension of 2.00 g (11.3 mmol) $PdCl_2$ in 40 mL thf. The resulting mixture was stirred overnight at room temperature. During this time a greyish solid precipitated, which was filtered off, washed twice with 20 mL diethyl ether and dried *in vacuo*. To remove colloidal palladium, the crude product was dissolved in methylene chloride and filtered over a pad of Celite. After removal of the solvent [Pd(*i*Pr_2Im)$_3$Cl]Cl was obtained as a light greyish solid.

Yield: 5.36 g (8.45 mmol, 75 %) of a light greyish solid.

Crystals suitable for x-ray diffraction were grown at room temperature by slow evaporation of the solvent from a solution in dichloromethane.

$C_{27}H_{48}Cl_2N_6Pd$ [634.04 gmol^{-1}] calcd. (found): C, 51.15 (51.27); H, 7.63 (7.64); N, 13.25 (12.94). **IR** (ATR): $\tilde{\nu}$ [cm^{-1}] = 704 (m), 740 (m), 779 (w), 817 (m), 1131 (m), 1180 (w), 1213 (vs), 1282 (w), 1300 (m), 1372 (s), 1398 (s), 1428 (), 1457 (m), 1635 (w), 1653 (w), 1684 (w), 1699 (w), 1717 (w), 1734 (w), 1792 (vw), 1844 (vw), 1928 (m), 2037 (m), 2877 (m), 2936 (m), 2976 (vs), 3054 (s), 3730 (w). **^{1}H NMR** (500 MHz, CD_2Cl_2): δ = 1.04 (d, 12 H, *trans*-CH_3, $^3J_{HH}$ = 6.7 Hz), 1.18 (d, 12 H, *cis*-CH_3, $^3J_{HH}$ = 6.7 Hz), 1.54 (d, 12 H, *cis*-CH_3, $^3J_{HH}$ = 6.7 Hz), 4.93 (sept, 2 H, *trans*-CHMe$_2$, $^3J_{HH}$ = 6.7 Hz), 5.17 (sept, 4 H, *cis*-CHMe$_2$, $^3J_{HH}$ = 6.7 Hz), 7.12 (s, 4 H, *cis*-CHCH), 7.42 (s, 2 H, *trans*-CHCH). **^{1}H NMR** (500 MHz, dmso-d_6): δ = 0.97 (d, 12 H, *trans*-CH_3, $^3J_{HH}$ = 6.7 Hz), 1.13 (d, 12 H, *cis*-CH_3, $^3J_{HH}$ = 6.7 Hz), 1.48 (d, 12 H, *cis*-CH_3, $^3J_{HH}$ = 6.7 Hz), 4.69 (sept, 2 H, *trans*-CHMe$_2$, $^3J_{HH}$ = 6.7 Hz), 4.94 (sept, 4 H, *cis*-CHMe$_2$, $^3J_{HH}$ = 6.7 Hz), 7.65 (s, 4 H, *cis*-CHCH), 7.81 (s, 2 H, *trans*-CHCH). **^{13}C NMR** (126 MHz, dmso-d_6): δ = 21.5 (*cis*-*C*H$_3$), 21.9 (*trans*-*C*H$_3$), 24.2 (*cis*-*CH*$_3$), 52.5 (*cis*-*C*HMe$_2$), 52.9 (*trans*-*C*HMe$_2$), 119.1 (*cis*-*C*H*C*H), 120.2 (*trans*-*C*H*C*H), 155.4 (*trans*-N*C*N), 165.6 (*cis*-N*C*N). [S5]

Synthesis of [Pt(*i*Pr$_2$Im)$_3$Cl]Cl (2)

1.14 g (7.48 mmol, 1.14 mL) of pure *i*Pr$_2$Im were added dropwise to a suspension of 500 mg (1.87 mmol) $PtCl_2$ in 50 mL thf and the resulting mixture was stirred overnight at room temperature. During this time, a colorless solid precipitated, which was filtered off, washed twice with 20 mL diethyl ether and dried *in vacuo*. Yield: 876 mg (1.21 mmol, 65 %) of a colorless solid. $C_{27}H_{48}Cl_2N_6Pt$ [722.71 gmol^{-1}] calcd. (found): C, 44.68 (44.18); H, 7.08 (7.53); N, 11.58 (11.23). **IR** (ATR): $\tilde{\nu}$ [cm^{-1}] = 3164 (vw), 3127 (w), 3094 (w), 3054 (vw), 2975 (s), 2936 (w), 2875 (w), 2160 (w), 1658 (vw), 1565 (vw), 1473 (w), 1457 (w), 1434 (m), 1415 (m), 1395 (m), 1372 (m), 1305 (w), 1282 (w), 1215 (vs), 1179 (w), 1136 (w), 744 (w), 713 (m). **^{1}H NMR** (500 MHz, CD_2Cl_2): δ = 1.04 (d, 12 H, *trans*-CH_3, $^3J_{HH}$ = 6.7 Hz), 1.17 (d, 12 H, *cis*-CH_3, $^3J_{HH}$ = 6.7 Hz), 1.54 (d, 12 H, *cis*-CH_3, $^3J_{HH}$ = 6.7 Hz), 4.93 (sept, 2 H, *trans*-CHMe$_2$, $^3J_{HH}$ = 6.7 Hz), 5.17 (sept, 4 H, *cis*-CHMe$_2$, $^3J_{HH}$ = 6.7 Hz), 7.12 (s, 4 H, *cis*-CHCH), 7.42 (s, 2 H, *trans*-CHCH). **^{1}H NMR** (500 MHz, dmso-d_6): δ = 0.96 (d, 12 H, *trans*-CH_3, $^3J_{HH}$ = 6.5 Hz), 1.12 (d, 12 H, *cis*-CH_3, $^3J_{HH}$ = 6.7 Hz), 1.45 (d, 12 H, *cis*-CH_3, $^3J_{HH}$ = 6.7 Hz), 4.81 (sept, 2 H, *trans*-CHMe$_2$, $^3J_{HH}$ = 6.5 Hz), 5.04 (sept, 4 H, *cis*-CHMe$_2$, $^3J_{HH}$ = 6.5 Hz), 7.65 (s, 4 H, *cis*-CHCH), 7.74 (s, 2 H, *trans*-CHCH). **^{13}C NMR** (126 MHz, dmso-d_6): δ = 21.4 (*cis*-*C*H$_3$), 21.7 (*trans*-*C*H$_3$), 24.2 (*cis*-CH_3), 51.8 (*cis*- *C*HMe$_2$), 52.0 (*trans*-*C*HMe$_2$), 118.8 (*cis*-*C*H*C*H), 119.3 (*trans*-*C*H*C*H), 141.3 (*trans*-N*C*N), 161.6 (*cis*-N*C*N). [S5]

Synthesis of [Pd(*i*Pr$_2$Im)$_2$] (3)

A suspension of 720 mg (1.13 mmol) [Pd(*i*Pr$_2$Im)$_3$Cl]Cl (**1**) and 458 mg (3.39 mmol, 3.00 eq) potassium graphite in 40 mL thf was stirred for 4 d at room temperature resulting in a yellow solution and black graphite. All solid components were removed by filtration over a pad of Celite and the residue was washed with 5 mL portions thf until the eluate is colorless. All volatile material was removed *in vacuo* and the remaining orange colored solid was suspended in a small amount (5 mL) of hexane, filtered off, washed twice with 5 mL hexane and dried *in vacuo*. Yield: 281 mg (0.68 mmol, 54 %) of an orange powder. Single crystals suitable for X-ray diffraction have been obtained by slow diffusion of the solvent from a solution in diethyl ether. $C_{18}H_{32}N_4Pd$ [410.90 g/mol] calcd. (found): C 52.62 (52.80), H 7.85 (7.93), N 13.64 (13.45). **IR** (ATR): $\tilde{\nu}$ [cm^{-1}] = 719 (m), 828 (w), 1014 (m), 1107 (w), 1130 (m), 1220 (vs), 1269 (m), 1301 (w), 1367 (m), 1393 (m), 1422 (m), 1467 (w), 1591 (w), 1659 (w), 2040 (w), 2934 (s), 2972 (vs). **^{1}H NMR** (500 MHz, C_6D_6): δ = 1.34 (d, 24 H, C*H*$_3$, $^3J_{HH}$ = 6.9 Hz), 6.03 (sept, 4 H, C*H*Me$_2$, $^3J_{HH}$ = 6.9 Hz), 6.46 (s, 4 H, C*H*C*H*). **^{1}H NMR** (200 MHz, thf-d_8): δ = 1.42 (d, 24 H, C*H*$_3$, $^3J_{HH}$ = 6.9 Hz), 5.62 (sept, 4 H, C*H*Me$_2$, $^3J_{HH}$ = 6.9 Hz), 6.83 (s, 4 H, C*H*C*H*). **^{13}C NMR** (126 MHz, C_6D_6): δ = 23.6 (*C*H$_3$), 52.8 (*C*HMe$_2$), 114.0 (*C*H*C*H), 196.4 (N*C*N).

Synthesis of [Pt(*i*Pr$_2$Im)$_2$] (4)

A suspension of 651 mg (899 µmol) [Pt(*i*Pr$_2$Im)$_3$Cl]Cl (**2**) and 425 mg (3.15 mmol) potassium graphite in 40 mL thf was stirred for 4 d at room temperature resulting in a yellow solution and black graphite. All solid components were removed by filtration over a large pad of Celite and washed with 5 mL portions of thf until the eluate was colorless. Volatile components have been removed *in vacuo*. The crude product was suspended in small amounts of hexane (5 mL) and filtered off. The yellow solid obtained was washed twice with 5 mL hexane and dried *in vacuo*. Yield: Yield: 233 mg (467 µmol, 52 %) of a yellow solid. $C_{18}H_{32}N_4Pt$ [499.57 g/mol] calcd. (found): C, 43.28 (43.68); H, 6.46 (6.39); N, 11.22 (11.05). **IR** (ATR): $\tilde{\nu}$ [cm^{-1}] = 723 (m), 791 (m), 874 (w), 1020 (m), 1078 (w), 1109 (w), 1131 (m), 1169 (w), 1218 (vs), 1271 (s), 1271 (s), 1304 (m), 1369 (s), 1425 (s), 1457 (s), 1564 (w), 1658 (w), 1980 (w), 1997 (w), 2022 (w), 2932 (s), 2973 (vs), 3056 (m). **^{1}H NMR** (500 MHz, C_6D_6): δ = 1.33 (d, 24 H, C*H*$_3$, $^3J_{HH}$ = 6.8 Hz), 6.26 (sept, 4 H, C*H*Me$_2$, $^3J_{HH}$ = 6.8 Hz), 6.25 (s$_{sat}$, 4 H, C*H*C*H,* $^4J_{PtH}$ = 19.0 Hz). **^{1}H NMR** (200 MHz, thf-d_8): δ = 1.42 (d, 24 H, C*H*$_3$, $^3J_{HH}$ = 6.8 Hz), 5.83 (sept, 4 H, C*H*Me$_2$, $^3J_{HH}$ = 6.8 Hz), 6.81 (s$_{sat}$, 4 H, C*H*C*H,* $^4J_{PtH}$ = 19.3 Hz). **^{13}C NMR** (126 MHz, C_6D_6): δ = 23.1 (*C*H$_3$), 52.2 (sat, *C*HMe$_2$, $^3J_{PtC}$ = 108.5 Hz), 113.7 (sat, *C*H*C*H, $^3J_{PtC}$ = 45.1 Hz), 197.7 (N*C*N). **^{195}Pt NMR** (107 MHz, 23.0 °C, C_6D_6): δ = -5943.

Due to line broadening caused by the large chemical shift anisotropy (CSA) of the ^{195}platinum isotope satellites for the resonance of the backbone protons of **2** only appear as a shoulder.

[S3] Since CSA is proportional to squared frequency, [S4] $^4J_{PtH}$ coupling constant (19.0 Hz) can be determined by recording the spectra at 200 MHz.

Synthesis of [Pd(*i*Pr$_2$Im)$_2$(η^2-C$_2$H$_4$)] (5)

In an NMR tube, 10.0 mg (24.2 µmol) [Pd(*i*Pr$_2$Im)$_2$] (**3**) were dissolved in 0.60 mL of C_6D_6. The solution was degassed by three freeze-pump cycles and the NMR tube was pressurized with 3 bar ethylene. The yellow solution brightened up a little bit after addition of ethylene. The proton NMR spectrum (200 MHz, rt) reveals significantly broadened resonances in the region between 1.5 and 1.0 ppm, at 5.15 ppm and at 5.69 ppm in addition to a fairly sharp doublet at 1.21 ppm and a singlet at 6.49 ppm. This significant broadening of some of the resonances is attributed to an equilibrium between [Pd(*i*Pr$_2$Im)$_2$(η^2-C$_2$H$_4$)], ethylene and [Pd(*i*Pr$_2$Im)$_2$] and a low concentration of **6**. After degassing, pure **1** was detected as the sole component in the ^{1}H NMR spectrum: δ = 1.34 (d, 24 H, C*H*$_3$, $^3J_{HH}$ = 6.9 Hz), 6.03 (sept, 4 H, C*H*Me$_2$, $^3J_{HH}$ = 6.9 Hz), 6.46 (s, 4 H, C*H*C*H*).

Synthesis of [Pt(*i*Pr$_2$Im)$_2$(η^2-C$_2$H$_4$)] (6)

In an NMR tube, 10.0 mg (20.0 µmol) [Pt(*i*Pr$_2$Im)$_2$] (**4**) were dissolved in 0.60 mL of C_6D_6. The solution was degassed by three freeze-pump cycles and the NMR tube was pressurized with 3 bar ethylene. The dark yellow solution brightened up a little bit after addition of ethylene. **^{1}H NMR** (200 MHz, C_6D_6) δ = 1.04 (d, 24 H, C*H*$_3$, $^3J_{HH}$ = 6.8 Hz,), 1.99 (s$_{sat}$, 4 H, C$_2$*H*$_4$, $^2J_{PtH}$ = 54.7 Hz), 5.48 (sept, 4 H, C*H*Me$_2$, $^3J_{HH}$ = 6.8 Hz), 6.47 (s$_{sat}$, 4 H, C*H*C*H*, $^4J_{PtH}$ = 11.3 Hz). **^{13}C NMR** (50.3 MHz, C_6D_6) δ = 13.3 (sat, *C*$_2$H$_4$, $^3J_{PtC}$ = 253.8 Hz,), 22.9 (*C*H$_3$), 50.72 (sat, *C*HMe$_2$, $^4J_{PtC}$ = 46.4 Hz), 114.6 (sat, *C*H*C*H, $^4J_{PtC}$= 32.4 Hz), 192.4 (N*C*N).

To study the decomposition of the resulting complex, the solution was degassed in a freeze-pump circle and argon was added. Proton NMR spectra were measured 10 min and 5 h after exchanging the atmosphere. After that, the solvent was removed *in vacuo*, the remaining solid (starting material) was dried for 2 h *in vacuo* and dissolved in C_6D_6 again.

Synthesis of [Pt(*i*Pr$_2$Im)$_2$(η^2-HCCPh)] (7)

In an NMR tube, 20.0 mg (40.0 µmol) [Pt(*i*Pr$_2$Im)$_2$] (**4**) and 4.10 mg (40.0 µmol, 4.40 µL) phenylacetylene were dissolved in 0.60 mL of C_6D_6. Quantitative conversion to yellow [Pt(*i*Pr$_2$Im)$_2$(η^2-HCCPh)] (**7**) was detected via NMR spectroscopy. **^{1}H NMR** (500 MHz, C_6D_6) δ = 0.97 (d, 12 H, C*H*$_3$, $^3J_{HH}$ = 6.8 Hz), 1.01 (d, 12 H, C*H*$_3$, $^3J_{HH}$ = 6.8 Hz), 5.53 (sept, 2 H, C*H*Me$_2$, $^3J_{HH}$ = 6.8 Hz), 5.58 (sept, 2 H, C*H*Me$_2$, $^3J_{HH}$ = 6.8 Hz), 6.48 (s$_{sat}$, 2 H, C*H*C*H*, $^4J_{HPt}$ = 11.0 Hz), 6.50 (s$_{sat}$, 2 H, C*H*C*H*, $^4J_{HPt}$ = 11.0 Hz), 7.06 (m, 1 H, *p*-CH$_{Ph}$), 7.24 (m, 2 H, *m*-C*H*$_{Ph}$), 7.87 (m, 2 H, *o*-C*H*$_{Ph}$), 8.02 (s$_{sat}$, 1 H, CC*H*, $^2J_{PtH}$ = 16.4 Hz). **^{13}C NMR** (126 MHz, C_6D_6) δ = 22.8 (*C*H$_3$),

22.9 (*C*H_3), 51.05 (sat, *C*HMe_2, $^3J_{PtC}$ = 42.6 Hz), 51.28 (s_{sat}, *C*HMe_2, $^3J_{PtC}$ = 44.2 Hz), 114.7 (C*C*H), 114.8 (*CHC*H), 114.9 (*CHC*H), 124.4 (*p*-*C*H_{Ph}), 128.3 (*m*-*C*H_{Ph}), 131.3 (*o*-*C*H_{Ph}), 137.1 (*i*-*C*H_{Ph}), 132.4 (*C*CH), 184.8 (N*C*N), 184.9 (N*C*N).

Synthesis of [Pt(*i*Pr_2Im)$_2$(η^2-PhCCPh)] (8)

In an NMR tube, 20.0 mg (40.0 µmol) [Pt(*i*Pr_2Im)$_2$] (**4**) and 7.14 mg (40.0 µmol) diphenyacetylene were dissolved in 0.60 mL of C_6D_6. Quantitative conversion to yellow [Pt(*i*Pr_2Im)$_2$(η^2-PhCCPh)] (**8**) was detected via NMR spectroscopy. **^{1}H NMR** (500 MHz, C_6D_6) δ = 0.97 (d, 24 H, C*H*$_3$, $^3J_{HH}$ = 6.8 Hz,), 5.52 (sept, 4 H, C*H*Me_2, $^3J_{HH}$ = 6.8 Hz), 6.48 (s_{sat}, 4 H, C*H*C*H*, $^4J_{PtH}$ = 11.3 Hz), 7.02 (m, 2 H, *p*-C*H*$_{Ph}$), 7.21 (m, 4 H, *m*-C*H*$_{Ph}$), 7.91 (m, 4 H, *o*-C*H*$_{Ph}$). **^{13}C NMR** (126 MHz, C_6D_6) δ = 22.9 (*C*H_3), 51.3 (sat, *C*HMe_2, $^4J_{PtC}$ = 42.0 Hz), 100.2 (Ph*CC*Ph), 114.9 (sat, *C*H*C*H, $^4J_{PtC}$= 31.3 Hz), 124.3 (*p*-*C*H_{Ph}), 128.4 (*m*-*C*H_{Ph}), 130.0 (*o*-*C*H_{Ph}), 138.5 (*i*-*C*$_{Ph}$), 185.0 (N*C*N).

Synthesis of [Pt(*i*Pr_2Im)$_2$(η^2-MeCCMe)] (9) and [Pt(*i*Pr_2Im)$_2$(η^2-H_2CCCHMe)] (10)

In an NMR tube, 10.0 mg (20.0 µmol) [Pt(*i*Pr_2Im)$_2$] (**4**) were dissolved in 0.60 mL of C_6D_6 and 1.19 mg (22.0 µmol, 1.6 µl of 2-butyne were added. Within 2 h the solution brightened up slightly. An equilibrium between the starting material and [Pt(*i*Pr_2Im)$_2$(η^2-MeCCMe)] (**9**) in a ratio of 2/1 was detected. **^{1}H NMR** (500 MHz, C_6D_6) δ = 1.01 (d, 24 H, C*H*$_3$, $^3J_{HH}$ = 6.8 Hz), 2.96 (s_{sat}, 4 H, C*H*$_3$CCC*H*$_3$, $^2J_{PtH}$ = 54.7 Hz), 5.66 (sept, 4 H, C*H*Me_2, $^3J_{HH}$ = 6.8 Hz), 6.48 (s_{sat}, 4 H, C*H*C*H*, $^4J_{PtH}$ = 11.3 Hz). **^{13}C NMR** (126 MHz, C_6D_6) δ = 14.2 (*C*H_3CC*C*H_3), 22.8 (*C*H_3), 50.9 (sat, *C*HMe_2, $^4J_{PtC}$ = 43.2 Hz), 114.5 (sat, *C*H*C*H, $^4J_{PtC}$= 30.8 Hz), 115.6 (Me*CC*Me), 187.5 (N*C*N). After a few weeks the formation of [Pt(*i*Pr_2Im)$_2$(η^2-H_2CCCHMe)] (**10**) can be observed: **^{1}H NMR** (500 MHz, C_6D_6) δ = 1.00 (d, 12 H, C*H*$_3$, $^3J_{HH}$ = 6.8 Hz,), 1.02 (d, 12 H, C*H*$_3$, $^3J_{HH}$ = 6.8 Hz,), 2.06 (m_{sat}, 2 H, =C*H*$_2$, $^2J_{PtH}$ = 54.2 Hz), 2.57 (dt, 3 H, =CHC*H*$_3$, $^3J_{HH}$ = 6.0 Hz, $^5J_{HH}$ = 1.8 Hz), 5.41 (sept, 2 H, C*H*Me_2, $^3J_{HH}$ = 6.8 Hz), 5.51 (sept, 2 H, C*H*Me_2, $^3J_{HH}$ = 6.8 Hz), 6.02 (m_{sat}, 1 H, =C*H*, $^3J_{PtH}$ = 47.0 Hz), 6.43 (s_{sat}, 2 H, C*H*C*H*, $^4J_{PtH}$ = 9.7 Hz), 6.44 (s_{sat}, 2 H, C*H*C*H*, $^4J_{PtH}$ = 11.0 Hz). **^{13}C NMR** (126 MHz, C_6D_6) δ = -4.3 (=*C*H_2), 22.9 (*C*H_3), 23.0 (*C*H_3), 24.3 (=CH*C*H_3), 51.0 (sat, *C*HMe_2, $^4J_{PtC}$ = 45.4 Hz), 51.0 (sat, *C*HMe_2, $^4J_{PtC}$ = 43.5 Hz), 104.5 (=*C*H), 114.9 (sat, *C*H*C*H, $^4J_{PtC}$= 32.0 Hz), 114.9 (sat, *C*H*C*H, $^4J_{PtC}$= 27.0 Hz), 158.4 (H_2C=*C*), 189.6 (N*C*N), 191.3 (N*C*N).

Synthesis of [Pt(*i*Pr_2Im)$_2$(H)(–CH_2-C{O}Ph)] (11)

In an NMR tube, 20.0 mg (40.0 µmol) [Pt(*i*Pr_2Im)$_2$] (**4**) were dissolved in 0.60 mL of C_6D_6 and 6.00 mg (50.0 µmol) acetophenone were added. The solution was heated to 80 °C for 4 d. Quantitative conversion to colorless [Pt(*i*Pr_2Im)$_2$(CH_2C(O)Ph)H] (**11**) was detected via NMR

spectroscopy. Pure samples of **11** slowly decompose at room temperature (see Figure S 28). **IR** (ATR): $\tilde{\nu}$ [cm^{-1}] = 3083 (vw, $\nu_{\text{-C-H,str}}$), 2969 (s, $\nu_{\text{-C-H,str}}$), 2926 (m, $\nu_{\text{-C-H,str}}$), 2869 (m, $\nu_{\text{-C-H,str}}$), 1985 (m, $\nu_{\text{Pt-H,str}}$), 1680 (vw), 1605 (vs), 1568 (s), 1415 (s), 1301 (s), 1264 (vs), 1211 (vs, NHC-$\gamma_{\text{=C-H,oop}}$), 1170 (w), 1129 (w), 1072 (s), 1018 (vs), 946 (m), 879 (w), 793 (vs), 691 (vs), 601 (m). **^{1}H NMR** (500 MHz, C_6D_6) δ = -10.11 (t_{sat}, 1 H, Pt*H*, $^1J_{PtH}$ = 1133.3 Hz, $^3J_{HH}$ = 3.1 Hz), 1.24 (d, 24 H, C*H*$_3$, $^3J_{HH}$ = 7.0 Hz), 3.22 (d_{sat}, 2 H, PtC*H*$_2$, $^2J_{PtH}$ = 70.6 Hz, $^3J_{HH}$ = 3.1 Hz), 5.55 (sept, 2 H, C*H*Me$_2$,$^3J_{HH}$ = 7.0 Hz), 6.40 (s_{sat}, 4 H, C*H*C*H*. $^4J_{PtH}$ = 10.1 Hz), 7.13 (m, 3 H, *m*-C*H*$_{Ph}$ + *p*-C*H*$_{Ph}$), 8.18 (m, 2 H, *o*-C*H*$_{Ph}$). **^{13}C NMR** (126 MHz, C_6D_6) δ = 23.0 (br, *C*H$_3$), 27.9 (sat, Pt*C*H$_2$ $^1J_{PtC}$ = 245.4 Hz), 51.6 (sat, *C*HMe$_2$ $^3J_{PtC}$ = 48.6 Hz), 115.1 (sat, *C*H*C*H, $^3J_{PtC}$ = 29.4 Hz), 128.2 (*o*-*C*H$_{Ph}$), 129.0 (*m*-*C*H$_{Ph}$ + *p*-*C*H$_{Ph}$), 142.2 (*i*-*C*H$_{Ph}$), 178.8 (sat, N*C*N, $^1J_{PtC}$ = 1036.7 Hz), 200.0 (sat, *C*O, $^2J_{PtC}$ = 38.6 Hz).

3. Crystallographic Details

Crystal data collection and processing parameters are given in Table S4. Crystals were immersed in a film of perfluoropolyether oil on a glass fiber and transferred to a Bruker D8 Apex-1 diffractometer with CCD area detector and graphite-monochromated Mo-Kα radiation equipped with a non-commercial low temperature device or a Bruker D8 Apex-2 diffractometer with CCD area detector and graphite-monochromated Mo-Kα radiation equipped with an Oxford Cryosystems low-temperature device. Data were collected at 168 K (Apex-1) and 100 K (Apex-2) respectively. The images were processed with the Bruker software packages and equivalent reflections were merged. Corrections for Lorentz-polarization effects and absorption were performed if necessary and the structures were solved by direct methods. Subsequent difference Fourier syntheses revealed the positions of all other non-hydrogen atoms. Extinction corrections were applied as required. Crystallographic calculations were performed using the SHELXTL software package. [S6] All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were assigned to idealized positions and were included in structure factors calculations.

Crystallographic data (excluding structure factors) for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no.s CCDC 1025171 (**1**) and 1025170 (**3**). Copies of the data can be obtained free of charge on application to CCDC.

Table S4. Crystallographic Data of complexes [Pd(*i*Pr$_2$Im)$_2$] (**3**) and [Pd(*i*Pr$_2$Im)$_3$Cl]$^+$Cl$^-$ (**1**)

	3	**1**
Formula	$C_{18}H_{32}N_4Pd$	$C_{27}H_{48}ClN_6Pd$ Cl x CH_2Cl_2
Formula weight	410.88	634.01
Temperature [K]	168(2)	100(2)
Color, shape	yellow, block	colorless, block
Cryst. size [mm^3]	0.11x0.09x0.05	0.31x0.25x0.15
Crystal system	monoclinic	triclinic
Space group	$P2_1/c$	$P\bar{1}$
a [Å]	9.5147(10)	9.5437(6)
b [Å]	8.7236(9)	19.9675(16)
c [Å]	12.2763(13)	14.7569(10)
α [°]		81.229(2)
β [°]	96.210(2)	83.044(2)
γ [°]		81.137(2)
Volume [Å^3]	1012.98(18)	1731.26(19)
Z	2	2
Density [g·cm^{-3}]	1.347	1.379
μ [mm^{-1}]	0.921	0.871
F (000)	428	748
θ [°]	2.15 – 26.15	2.464 - 26.113
Index	-11 ≤ *h* ≤ 11, -10 ≤ *k* ≤ 10, -15 ≤ *l* ≤ 15	-11 ≤ *h* ≤ 11, -15 ≤ *k* ≤ 15, -18 ≤ *l* ≤ 18
Reflections collected	18273	16737
Indep. Reflections	2018	6825
Observed Reflections [*I*>2*σ*(I)]	1775	5808
R_{int}	0.0283	0.0348
Restraints	0	0
Parameters	110	364
*R*1 / *wR*2 [*I*>2*σ*(I)]	0.0211 / 0.0568	0.0340 / 0.0732
*R*1 /*wR*2 (all data)	0.0254 / 0.0598	0.0444 / 0.0777
Largest diff peak and hole [e·Å^{-3}]	0.397 / -0.215	0.540 / -0.658
GooF	1.074	1.042

4. Computational Details

The calculations on model systems were carried out using the Amsterdam Density Functional (ADF) program developed by Baerends and co-workers. [S7] The integration was performed using a procedure developed by te Velde *et al.* [S8] The MOs were expanded in a large uncontracted set of Slater type orbitals (STOs, no Gaussian functions are involved). A TZ2P basis set [S9] was used and is of triple-ξ quality for all atoms. It has been augmented with two sets of polarization functions, that is, 2p and 3d on H, 3d and 4f on C and N, 4p and 4f on Ni, 5p and 4f on Pd and 6p and 5f on Pt. An auxiliary set of s, p, d, f and g STOs was used to fit the molecular density and to represent the Coulomb and exchange potentials accurately in each self-consistent field (SCF) cycle. All electrons are included in the variational treatment (no frozen-core approximation used). For all calculations, the generalized gradient approximation (GGA) at the BLYP level was used: exchange is described by Slater's Xα potential, [S10] with nonlocal corrections due to Becke [S11] added self-consistently, and correlation is treated using the gradient-corrected functional of Lee, Yang and Parr. [S12] Relativistic effects were included with the scalar-zeroth-order-regular-approximation (ZORA). [S13] This approach has been extensively tested and was shown to agree well with high-level coupled-cluster reference data. [S14] In addition the Grimme3 BJDAMP dispersion correction was used. [S15]

Energy Decomposition Analysis: The method of bond energy decomposition analysis (EDA) was developed by Ziegler and Rauk. [S16] Here the bond energy ΔE between the fragments were decomposed into the preparation energy ΔE_{strain}, which is associated with the geometrical deformation of the fragments as the bond formation takes place and the actual interaction energy ΔE_{int} (Equation 1).

$$\Delta E = \Delta E_{strain} + \Delta E_{int} \quad (1)$$

$$\Delta E_{int} = \Delta V_{elstat} + \Delta E_{Pauli} + \Delta E_{oi} + \Delta E_{disp} \quad (2)$$

$$\Delta E_{steric} = \Delta V_{elstat} + \Delta E_{Pauli} \quad (3)$$

The interaction energy ΔE_{int} of two fragments can be decomposed in ΔV_{elstat}, ΔE_{Pauli}, ΔE_{oi} and ΔE_{disp} (Equation 2). The term ΔV_{elstat} correspond to the classical electrostatic interaction between unperturbed charge distributions $\rho_A(r) + \rho_B(r)$ of the prepared or deformed fragments A and B. The Pauli repulsion term, ΔE_{Pauli} is caused by the destabilizing interactions between two occupied orbitals, i.e. by the fact that two electrons with the same spin cannot occupy the same space; therefore it is responsible for steric repulsion. Dispersive interactions are also included and they are responsible for the last term ΔE_{disp} in Equation 2. The orbital interaction term ΔE_{oi} emerges from charge transfer (interaction between occupied orbitals on one

fragment with unoccupied orbitals on the other fragment, including HOMO-LUMO interactions) and polarization (empty-occupied orbital mixing on one fragment due to the presence of the other fragment).

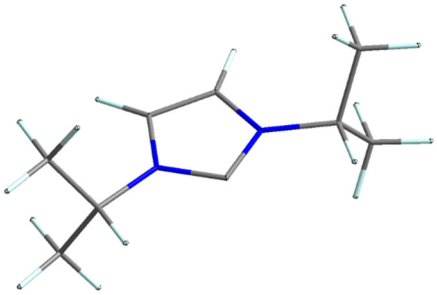
The orbital interaction can be further divided into contributions from each irreducible representation Γ of the interacting systems (Equation 4).

$$\Delta E_{oi} = \sum_{\Gamma} \Delta E_{oi}^{\Gamma} \quad (4)$$

For the EDA the $[M(H_2Im)_2(\eta^2\text{-}C_2H_4)]$ were optimized and analyzed in C_{2v} symmetry, where a_1 corresponds to σ-, b_1 and b_2 to π- and a_2 to orbital interaction with δ-symmetry.

Calculations on the fully substituted systems were carried out with the DFT implementation of TURBOMOLE V6.5 2013, a development of University of Karlsruhe and Forschungszentrum Karlsruhe GmbH, 1989-2007, TURBOMOLE GmbH, since 2007; available from http://www.turbomole.com. [S17] For the DFT calculations we used the BP86 functional, [S11] TZVPP basis sets and the RI-J approximation. [S18, S19] Analytic second derivatives were calculated with the program AOFORCE using the RI-J approximation.

Calculated Compounds



iPr$_2$Im

Def2-SV(P)/BP86

Molecular formula: $C_9H_{16}N_2$

SCF-energy + E(vib0) [h]: -461.4750634

E(vib0) [h]: 0.2320883

Imaginary frequencies: none

Def2-TZVPP/BP86

SCF-energy + E(vib0) [h]: -462.0176462

E(vib0) [h]: 0.2320306

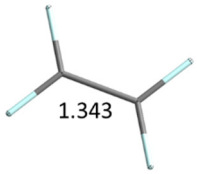
Imaginary frequencies: none

Cartesian coordinates:

C	1.013031	-0.015932	0.013714
N	0.151211	1.057080	-0.021628
C	-1.190525	0.675706	-0.057613
C	-1.194414	-0.696227	-0.045150
N	0.145133	-1.084501	-0.002177
C	0.633422	2.448660	-0.019764
C	0.248782	3.175754	-1.317783
C	0.173616	3.198334	1.240421
C	0.619434	-2.478529	0.025023
C	0.155335	-3.202618	1.298519
C	0.230709	-3.226844	-1.259656
H	-2.028098	1.383548	-0.089046
H	-2.036002	-1.399743	-0.063764
H	1.737295	2.335230	0.013662
H	0.706199	4.189196	-1.341709
H	0.607591	2.611192	-2.205596
H	-0.854049	3.301519	-1.408417
H	0.628272	4.212809	1.272622
H	0.480348	2.650272	2.157590
H	-0.932633	3.323968	1.264361
H	1.723933	-2.370790	0.056573
H	0.604630	-4.218752	1.349408
H	0.464646	-2.639524	2.205646
H	-0.951552	-3.322018	1.324342
H	0.681735	-4.243395	-1.264852

H	0.593406	-2.680884	-2.157458
H	-0.872856	-3.347314	-1.348468

Ethylene



Def2-SV(P)/BP86

Molecular formula: C_2H_4

SCF-energy + E(vib0) [h]: -78.4700988

E(vib0) [h]: 0.0492548

Imaginary frequencies: none

Def2-TZVPP/BP86

SCF-energy + E(vib0) [h]: -78.5707099

E(vib0) [h]: 0.0488093

Imaginary frequencies: none

Cartesian coordinates:

C	-0.581594	-0.335707	0.000000
C	0.581594	0.335707	0.000000
H	-0.614634	-1.440849	0.000000
H	-1.555072	0.188593	0.000000
H	0.614634	1.440849	0.000000
H	1.555072	-0.188593	0.000000

2-Butyne

Def2-SV(P)/BP86

Molecular formula: C_4H_6

SCF-energy + E(vib0) [h]: -155.7710471

E(vib0) [h]: 0.0813944

Imaginary frequencies: none

Def2-TZVPP/BP86

SCF-energy + E(vib0) [h]: -155.9592105

E(vib0) [h]: 0.0812566

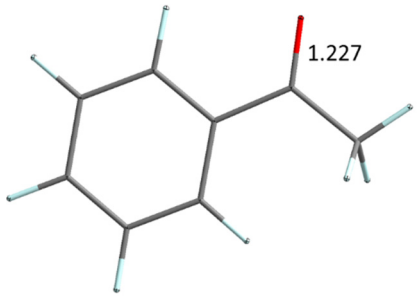
Imaginary frequencies: none

Cartesian coordinates:

C	-0.399006	-0.533091	-0.000039
C	0.661425	0.078966	0.000035
C	1.928050	0.809650	0.000130

C	-1.665195	-1.264153	-0.000130
H	1.765503	1.911996	0.000095
H	2.542104	0.565963	0.897463
H	2.542259	0.565929	-0.897087
H	-2.538563	-0.571991	-0.000105
H	-1.761511	-1.917818	-0.897373
H	-1.761566	-1.917950	0.897011

Acetophenone



Def2-SV(P)/BP86

Molecular formula: C_8H_8O

SCF-energy + E(vib0) [h]: -384.4824686

E(vib0) [h]: 0.1339238

Imaginary frequencies: none

Def2-TZVPP/BP86

SCF-energy + E(vib0) [h]: -384.9235726

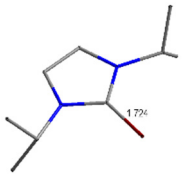
E(vib0) [h]: 0.1327933

Imaginary frequencies: none

Cartesian coordinates:

C	0.970263	2.567022	-0.225209
C	1.547037	1.218198	0.191104
C	0.599041	0.067792	0.420886
C	1.149105	-1.174418	0.812304
C	0.321180	-2.280460	1.042361
C	-1.072908	-2.160817	0.883480
C	-1.632099	-0.931116	0.494296
C	-0.801161	0.177634	0.264199
O	2.756121	1.070228	0.337756
H	0.259999	2.955401	0.539178
H	1.803789	3.287253	-0.347550
H	0.410519	2.489087	-1.184412
H	2.243057	-1.237505	0.928298
H	0.760694	-3.244818	1.347639
H	-1.726443	-3.030814	1.063869
H	-2.723495	-0.834881	0.369323
H	-1.254301	1.134814	-0.039921

{Ni(*i*Pr$_2$Im)}



Def2-SV(P)/BP86

Molecular formula: $C_9H_{16}N_2Ni$

SCF-energy + E(vib0) [h]: -1969.8563103

E(vib0) [h]: 0.2328355

Imaginary frequencies: none

Def2-TZVPP/BP86

SCF-energy + E(vib0) [h]: -1970.6451938

E(vib0) [h]: 0.2332327

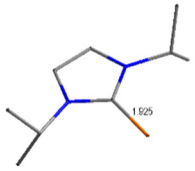
Imaginary frequencies: none

Cartesian coordinates:

C	1.087685	-1.035143	0.229777
C	-0.229459	-1.414388	0.141826
N	-0.957696	-0.281865	-0.206586
C	-0.126239	0.825845	-0.344960
N	1.141537	0.322945	-0.065822
C	2.334484	1.179664	-0.111141
C	-2.408082	-0.184405	-0.420183
C	3.009150	1.279662	1.263414
C	3.294431	0.745443	-1.227106
C	-2.859425	-1.040451	-1.611173
C	-3.187367	-0.479843	0.868147
Ni	-0.561946	2.440710	-0.764759
H	1.976377	-1.626947	0.478316
H	-0.692399	-2.395268	0.300479
H	1.891175	2.172281	-0.375547
H	-2.526968	0.897107	-0.680694
H	3.853328	2.003358	1.226554
H	2.283868	1.629317	2.029682
H	3.420694	0.298937	1.594910
H	4.145169	1.458043	-1.303317
H	2.768483	0.725197	-2.206303
H	3.718052	-0.267488	-1.037100
H	-3.941130	-0.878678	-1.814138
H	-2.289580	-0.766841	-2.525658
H	-2.710578	-2.127834	-1.419692
H	-4.275656	-0.315239	0.706949

H	-2.852083	0.190793	1.688923
H	-3.051223	-1.534312	1.201001

{Pd(*i*Pr$_2$Im)}



Def2-SV(P)/BP86

Molecular formula: $C_9H_{16}N_2Pd$

SCF-energy + E(vib0) [h]: -590.1012507

E(vib0) [h]: 0.2333576

Imaginary frequencies: none

Def2-TZVPP/BP86

SCF-energy + E(vib0) [h]: -590.1012507

E(vib0) [h]: 0.2332444

Imaginary frequencies:

Cartesian coordinates:

C	1.076983	-0.998557	0.214871
C	-0.237738	-1.378007	0.123396
N	-0.962240	-0.243327	-0.223867
C	-0.134047	0.855797	-0.356399
N	1.126358	0.359658	-0.078651
C	2.345699	1.188189	-0.102419
C	-2.420611	-0.187355	-0.432424
C	2.992350	1.262041	1.287900
C	3.312830	0.716051	-1.197039
C	-2.842947	-1.061921	-1.621244
C	-3.177648	-0.516025	0.861671
Pd	-0.621609	2.659072	-0.820554
H	1.967617	-1.587009	0.463336
H	-0.703582	-2.357970	0.277390
H	1.950378	2.195936	-0.374992
H	-2.588721	0.885320	-0.691094
H	3.855566	1.963068	1.269258
H	2.262124	1.630582	2.040354
H	3.372006	0.270139	1.623716
H	4.181695	1.407121	-1.260905
H	2.806921	0.702258	-2.186664
H	3.709101	-0.304560	-0.990645
H	-3.929070	-0.932293	-1.821966

H	-2.284493	-0.772493	-2.537728
H	-2.662875	-2.144044	-1.427375
H	-4.270774	-0.381581	0.707583
H	-2.858102	0.159192	1.684763
H	-3.010572	-1.568682	1.185528

{Pt(*i*Pr$_2$Im)}

Def2-SV(P)/BP86

Molecular formula: $C_9H_{16}N_2Pt$

SCF-energy + E(vib0) [h]: -581.0272712

E(vib0) [h]: 0.2337680

Imaginary frequencies: none

Def2-TZVPP/BP86

SCF-energy + E(vib0) [h]: -581.5768619

E(vib0) [h]: 0.2336403

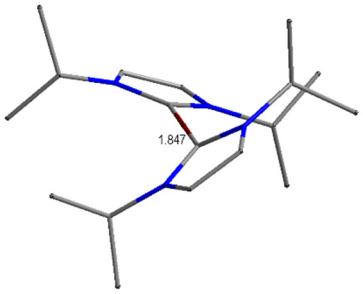
Imaginary frequencies: none

Cartesian coordinates:

C	1.074383	-0.988984	0.212100
C	-0.239246	-1.369113	0.118260
N	-0.970611	-0.239174	-0.229060
C	-0.134922	0.858125	-0.357491
N	1.131099	0.369221	-0.078942
C	2.353666	1.196120	-0.099058
C	-2.430736	-0.188111	-0.438559
C	2.995035	1.264652	1.293978
C	3.321316	0.719052	-1.190968
C	-2.846747	-1.068221	-1.625428
C	-3.184144	-0.518774	0.857061
Pt	-0.610797	2.614212	-0.808221
H	1.965334	-1.575896	0.461194
H	-0.705383	-2.348751	0.270391
H	1.963661	2.204912	-0.371716
H	-2.604358	0.882309	-0.699180
H	3.861124	1.961981	1.278201
H	2.264948	1.636441	2.044712
H	3.369787	0.270809	1.629674
H	4.192863	1.406819	-1.251401

H	2.819712	0.708070	-2.182638
H	3.713152	-0.303042	-0.983210
H	-3.933352	-0.944065	-1.826259
H	-2.290685	-0.778331	-2.543019
H	-2.661973	-2.149052	-1.428592
H	-4.277809	-0.390494	0.702520
H	-2.869298	0.159945	1.678860
H	-3.011417	-1.570061	1.182590

[Ni(*i*Pr$_2$Im)$_2$]



Molecular formula: $C_{18}H_{32}N_4Ni$

SCF-energy + E(vib0) [h]: -2431.4366156

E(vib0) [h]: 0.4661435

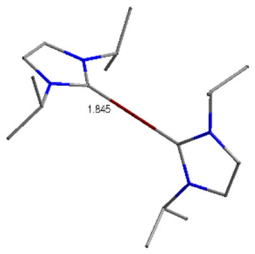
Imaginary frequencies: none

Cartesian coordinates:

N	-0.976521	-0.475559	2.709670
C	-0.617770	-0.301064	4.041574
C	0.617764	0.301238	4.041553
N	0.976539	0.475591	2.709637
C	0.000005	-0.000007	1.846836
Ni	-0.000014	-0.000029	-0.000012
C	-0.000018	0.000004	-1.846859
N	0.976525	-0.475519	-2.709686
C	0.617768	-0.301057	-4.041588
C	-0.617783	0.301212	-4.041578
N	-0.976560	0.475579	-2.709664
C	-2.223044	-1.058140	2.192060
C	2.223100	1.058057	2.191986
C	-2.223121	1.058051	-2.192012
C	2.223064	-1.058050	-2.192060
H	-2.072964	-0.967338	1.086272
C	-2.348940	-2.541200	2.565448
C	-3.444237	-0.225196	2.604069
H	2.073033	0.967151	1.086205
C	2.349062	2.541150	2.565226
C	3.444248	0.225096	2.604093
H	-2.073038	0.967146	-1.086232

C	-2.349079	2.541147	-2.565242
C	-3.444274	0.225091	-2.604102
H	2.072976	-0.967206	-1.086278
C	2.348994	-2.541127	-2.565371
C	3.444243	-0.225097	-2.604085
H	-4.364048	-0.625954	2.123438
H	-3.605565	-0.241811	3.706395
H	-3.317071	0.832791	2.286910
H	-3.250196	-2.984268	2.086800
H	-1.457479	-3.107330	2.217874
H	-2.446545	-2.684042	3.666257
H	3.250339	2.984131	2.086537
H	1.457627	3.107285	2.217592
H	2.446670	2.684099	3.666022
H	4.364085	0.625772	2.123447
H	3.605555	0.241798	3.706421
H	3.317042	-0.832913	2.287022
H	-3.250355	2.984128	-2.086549
H	-1.457641	3.107273	-2.217604
H	-2.446687	2.684100	-3.666037
H	-4.364105	0.625763	-2.123438
H	-3.605598	0.241800	-3.706427
H	-3.317061	-0.832919	-2.287039
H	4.364057	-0.625819	-2.123432
H	3.605584	-0.241747	-3.706407
H	3.317055	0.832898	-2.286965
H	3.250255	-2.984153	-2.086695
H	1.457542	-3.107254	-2.217774
H	2.446608	-2.684020	-3.666171
H	-1.251544	0.611438	-4.880719
H	1.251534	-0.611231	-4.880742
H	1.251513	0.611497	4.880691
H	-1.251532	-0.611236	4.880733

[Ni(*i*Pr$_2$Im)$_2$] (D_{2d})



Def2-SV(P)/BP86

Molecular formula: $C_{18}H_{32}N_4Ni$

SCF-energy + E(vib0) [h]: -2431.4338319

E(vib0) [h]: 0.4648941

Imaginary frequencies: i55.66, i35.16, i35.16, i28.82, i17.22

Def2-TZVPP/BP86

SCF-energy + E(vib0) [h]: -2432.7476707

E(vib0) [h]: 0.4661012

Imaginary frequencies: none

Cartesian coordinates:

N	0.768515	-0.768515	-2.710211
C	0.485612	-0.485612	-4.042466
C	-0.485612	0.485612	-4.042466
N	-0.768515	0.768515	-2.710211
C	0.000000	0.000000	-1.844944
Ni	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.844944
N	0.768515	0.768515	2.710211
C	0.485612	0.485612	4.042466
C	-0.485612	-0.485612	4.042466
N	-0.768515	-0.768515	2.710211
C	-1.744504	-1.744504	2.206266
C	1.744504	1.744504	2.206266
C	-1.744504	1.744504	-2.206266
C	1.744504	-1.744504	-2.206266
H	-1.636064	-1.636064	1.098592
C	-1.364483	-3.176845	2.608091
C	-3.176845	-1.364483	2.608091
H	1.636064	1.636064	1.098592
C	1.364483	3.176845	2.608091
C	3.176845	1.364483	2.608091
H	-3.906235	-2.064407	2.143625
H	-3.323318	-1.407266	3.711786
H	-3.415718	-0.334554	2.264552
H	-2.064407	-3.906235	2.143625
H	-0.334554	-3.415718	2.264552

H	-1.407266	-3.323318	3.711786
H	3.906235	2.064407	2.143625
H	3.323318	1.407266	3.711786
H	3.415718	0.334554	2.264552
H	2.064407	3.906235	2.143625
H	0.334554	3.415718	2.264552
H	1.407266	3.323318	3.711786
H	-1.636064	1.636064	-1.098592
C	-1.364483	3.176845	-2.608091
C	-3.176845	1.364483	-2.608091
H	1.636064	-1.636064	-1.098592
C	1.364483	-3.176845	-2.608091
C	3.176845	-1.364483	-2.608091
H	2.064407	-3.906235	-2.143625
H	0.334554	-3.415718	-2.264552
H	1.407266	-3.323318	-3.711786
H	3.906235	-2.064407	-2.143625
H	3.323318	-1.407266	-3.711786
H	3.415718	-0.334554	-2.264552
H	-2.064407	3.906235	-2.143625
H	-0.334554	3.415718	-2.264552
H	-1.407266	3.323318	-3.711786
H	-3.906235	2.064407	-2.143625
H	-3.323318	1.407266	-3.711786
H	-3.415718	0.334554	-2.264552
H	-0.984340	-0.984340	4.881970
H	0.984340	0.984340	4.881970
H	-0.984340	0.984340	-4.881970
H	0.984340	-0.984340	-4.881970

[Ni(*i*Pr$_2$Im)$_2$] (D$_{2h}$)

Def2-SV(P)/BP86

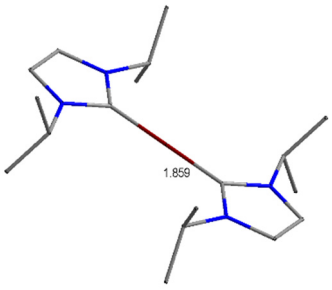
Molecular formula: $C_{18}H_{32}N_4Ni$

SCF-energy + E(vib0) [h]: -2431.4310710

E(vib0) [h]: 0.4649214

Imaginary frequencies: i76.58, i63.94, i13.58, i11.66

Def2-TZVPP/BP86



SCF-energy + E(vib0) [h]: -2432.7440324

E(vib0) [h]: 0.4660560

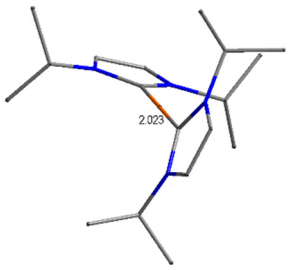
Imaginary frequencies: i15.89

Cartesian coordinates:

N	-1.084625	0.000000	2.730534
C	-0.686523	0.000000	4.061197
C	0.686523	0.000000	4.061197
N	1.084625	0.000000	2.730534
C	0.000000	0.000000	1.858938
Ni	0.000000	0.000000	0.000000
C	0.000000	0.000000	-1.858938
N	1.084625	0.000000	-2.730534
C	0.686523	0.000000	-4.061197
C	-0.686523	0.000000	-4.061197
N	-1.084625	0.000000	-2.730534
C	-2.469600	0.000000	2.244238
C	2.469600	0.000000	2.244238
C	-2.469600	0.000000	-2.244238
C	2.469600	0.000000	-2.244238
H	-2.325571	0.000000	1.136338
C	-3.208239	-1.281785	2.653123
C	-3.208239	1.281785	2.653123
H	2.325571	0.000000	1.136338
C	3.208239	1.281785	2.653123
C	3.208239	-1.281785	2.653123
H	-2.325571	0.000000	-1.136338
C	-3.208239	1.281785	-2.653123
C	-3.208239	-1.281785	-2.653123
H	2.325571	0.000000	-1.136338
C	3.208239	-1.281785	-2.653123
C	3.208239	1.281785	-2.653123
H	-4.224149	1.302712	2.200378
H	-3.330554	1.355455	3.758113
H	-2.652470	2.179116	2.303687
H	-4.224149	-1.302712	2.200378
H	-2.652470	-2.179116	2.303687
H	-3.330554	-1.355455	3.758113

H	4.224149	1.302712	2.200378
H	2.652470	2.179116	2.303687
H	3.330554	1.355455	3.758113
H	4.224149	-1.302712	2.200378
H	3.330554	-1.355455	3.758113
H	2.652470	-2.179116	2.303687
H	-4.224149	1.302712	-2.200378
H	-2.652470	2.179116	-2.303687
H	-3.330554	1.355455	-3.758113
H	-4.224149	-1.302712	-2.200378
H	-3.330554	-1.355455	-3.758113
H	-2.652470	-2.179116	-2.303687
H	4.224149	1.302712	-2.200378
H	3.330554	1.355455	-3.758113
H	2.652470	2.179116	-2.303687
H	4.224149	-1.302712	-2.200378
H	2.652470	-2.179116	-2.303687
H	3.330554	-1.355455	-3.758113
H	-1.392645	0.000000	-4.899786
H	1.392645	0.000000	-4.899786
H	1.392645	0.000000	4.899786
H	-1.392645	0.000000	4.899786

[Pd(*i*Pr$_2$Im)$_2$]



Molecular formula: $C_{18}H_{32}N_4Pd$

SCF-energy + E(vib0) [h]: -1051.0791044

E(vib0) [h]: 0.4669416

Imaginary frequencies: none

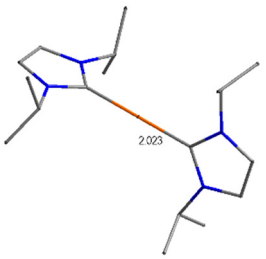
Cartesian coordinates:

N	-0.837536	-0.681470	2.882947
C	-0.524254	-0.433785	4.215256
C	0.543966	0.427312	4.213211
N	0.849054	0.678845	2.879728
C	0.003204	-0.000181	2.023454
Pd	-0.001655	0.001098	0.000008
C	-0.005457	0.001334	-2.023446
N	0.837280	-0.677679	-2.882795

C	0.525557	-0.428362	-4.215160
C	-0.543709	0.431434	-4.213311
N	-0.851054	0.680468	-2.879872
C	-1.923938	-1.553160	2.403875
C	1.932764	1.551600	2.396480
C	-1.935734	1.552120	-2.396842
C	1.924030	-1.548827	-2.403508
H	-1.825258	-1.480107	1.294074
C	-1.697071	-3.009851	2.832671
C	-3.297120	-1.007653	2.821336
H	1.825190	1.484327	1.287149
C	1.711502	3.006283	2.834754
C	3.308458	1.001965	2.799947
H	-1.832856	1.479274	-1.287417
C	-1.710489	3.008762	-2.826684
C	-3.310453	1.006546	-2.809065
H	1.823358	-1.477957	-1.293739
C	1.699896	-3.004999	-2.835448
C	3.297179	-1.000669	-2.817536
H	-4.105899	-1.628020	2.376160
H	-3.432054	-1.020794	3.927212
H	-3.426106	0.037806	2.466035
H	-2.475299	-3.665564	2.383704
H	-0.702403	-3.366803	2.488075
H	-1.750063	-3.132709	3.938926
H	2.486756	3.663285	2.382562
H	0.714415	3.366422	2.500611
H	1.774218	3.123437	3.941139
H	4.114599	1.623737	2.351931
H	3.452044	1.008575	3.904778
H	3.433091	-0.041616	2.437626
H	-2.487212	3.664518	-2.375186
H	-0.714667	3.365807	-2.485534
H	-1.767239	3.131371	-3.932784
H	-4.117540	1.626836	-2.360722
H	-3.449695	1.019806	-3.914401
H	-3.438058	-0.038956	-2.453385

H	4.106045	-1.620853	-2.372252
H	3.433990	-1.011380	-3.923203
H	3.424147	0.044236	-2.459883
H	2.478124	-3.660520	-2.386208
H	0.705043	-3.363922	-2.493434
H	1.755185	-3.125763	-3.941828
H	-1.096510	0.874769	-5.049667
H	1.075516	-0.871648	-5.053412
H	1.097351	0.870111	5.049460
H	-1.072634	-0.878835	5.053610

[Pd(*i*Pr$_2$Im)$_2$] (D_{2d})



Def2-SV(P)/BP86

Molecular formula: $C_{18}H_{32}N_4Pd$

SCF-energy + E(vib0) [h]: -1051.0795223

E(vib0) [h]: 0.4665872

Imaginary frequencies: i3.98

Def2-TZVPP/BP86

SCF-energy + E(vib0) [h]: -1052.1945794

E(vib0) [h]: 0.4666658

Imaginary frequencies: none

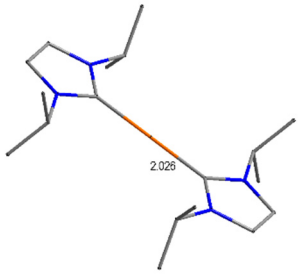
Cartesian coordinates:

N	0.766145	0.766145	2.881156
C	0.485114	0.485114	4.214117
C	-0.485114	-0.485114	4.214117
N	-0.766145	-0.766145	2.881156
C	0.000000	0.000000	2.023399
Pd	0.000000	0.000000	0.000000
C	0.000000	0.000000	-2.023399
N	0.766145	-0.766145	-2.881156
C	0.485114	-0.485114	-4.214117
C	-0.485114	0.485114	-4.214117
N	-0.766145	0.766145	-2.881156
C	-1.750539	1.750539	-2.399910
C	1.750539	-1.750539	-2.399910

C	-1.750539	-1.750539	2.399910
C	1.750539	1.750539	2.399910
H	-1.662620	1.662620	-1.290243
C	-1.362797	3.175150	-2.822207
C	-3.175150	1.362797	-2.822207
H	1.662620	-1.662620	-1.290243
C	1.362797	-3.175150	-2.822207
C	3.175150	-1.362797	-2.822207
H	-3.910957	2.065818	-2.373327
H	-3.306422	1.398355	-3.928122
H	-3.419358	0.335914	-2.473806
H	-2.065818	3.910957	-2.373327
H	-0.335914	3.419358	-2.473806
H	-1.398355	3.306422	-3.928122
H	3.910957	-2.065818	-2.373327
H	3.306422	-1.398355	-3.928122
H	3.419358	-0.335914	-2.473806
H	2.065818	-3.910957	-2.373327
H	0.335914	-3.419358	-2.473806
H	1.398355	-3.306422	-3.928122
H	-1.662620	-1.662620	1.290243
C	-1.362797	-3.175150	2.822207
C	-3.175150	-1.362797	2.822207
H	1.662620	1.662620	1.290243
C	1.362797	3.175150	2.822207
C	3.175150	1.362797	2.822207
H	2.065818	3.910957	2.373327
H	0.335914	3.419358	2.473806
H	1.398355	3.306422	3.928122
H	3.910957	2.065818	2.373327
H	3.306422	1.398355	3.928122
H	3.419358	0.335914	2.473806
H	-2.065818	-3.910957	2.373327

H	-0.335914	-3.419358	2.473806
H	-1.398355	-3.306422	3.928122
H	-3.910957	-2.065818	2.373327
H	-3.306422	-1.398355	3.928122
H	-3.419358	-0.335914	2.473806
H	-0.985334	0.985334	-5.051562
H	0.985334	-0.985334	-5.051562
H	-0.985334	-0.985334	5.051562
H	0.985334	0.985334	5.051562

[Pd(*i*Pr$_2$Im)$_2$] (D$_{2h}$)



Def2-SV(P)/BP86

Molecular formula: $C_{18}H_{32}N_4Pd$

SCF-energy + E(vib0) [h]: -1051.0778229

E(vib0) [h]: 0.4666572

Imaginary frequencies: i11.47

Def2-TZVPP/BP86

SCF-energy + E(vib0) [h]: -1052.1928543

E(vib0) [h]: 0.4664808

Imaginary frequencies: i15.24

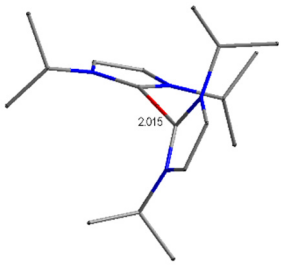
Cartesian coordinates:

N	-1.082822	0.000000	2.886254
C	-0.685951	0.000000	4.218454
C	0.685951	0.000000	4.218454
N	1.082822	0.000000	2.886254
C	0.000000	0.000000	2.025822
Pd	0.000000	0.000000	0.000000
C	0.000000	0.000000	-2.025822
N	1.082822	0.000000	-2.886254
C	0.685951	0.000000	-4.218454
C	-0.685951	0.000000	-4.218454
N	-1.082822	0.000000	-2.886254
C	-2.476659	0.000000	2.412347
C	2.476659	0.000000	2.412347
C	-2.476659	0.000000	-2.412347
C	2.476659	0.000000	-2.412347

H	-2.355596	0.000000	1.302770
C	-3.207214	-1.281729	2.837343
C	-3.207214	1.281729	2.837343
H	2.355596	0.000000	1.302770
C	3.207214	1.281729	2.837343
C	3.207214	-1.281729	2.837343
H	-2.355596	0.000000	-1.302770
C	-3.207214	1.281729	-2.837343
C	-3.207214	-1.281729	-2.837343
H	2.355596	0.000000	-1.302770
C	3.207214	-1.281729	-2.837343
C	3.207214	1.281729	-2.837343
H	-4.228009	1.304283	2.396239
H	-3.317622	1.350427	3.943862
H	-2.656338	2.180501	2.484318
H	-4.228009	-1.304283	2.396239
H	-2.656338	-2.180501	2.484318
H	-3.317622	-1.350427	3.943862
H	4.228009	1.304283	2.396239
H	2.656338	2.180501	2.484318
H	3.317622	1.350427	3.943862
H	4.228009	-1.304283	2.396239
H	3.317622	-1.350427	3.943862
H	2.656338	-2.180501	2.484318
H	-4.228009	1.304283	-2.396239
H	-2.656338	2.180501	-2.484318
H	-3.317622	1.350427	-3.943862
H	-4.228009	-1.304283	-2.396239
H	-3.317622	-1.350427	-3.943862
H	-2.656338	-2.180501	-2.484318
H	4.228009	1.304283	-2.396239
H	3.317622	1.350427	-3.943862
H	2.656338	2.180501	-2.484318
H	4.228009	-1.304283	-2.396239
H	2.656338	-2.180501	-2.484318
H	3.317622	-1.350427	-3.943862
H	-1.393359	0.000000	-5.055703

H	1.393359	0.000000	-5.055703
H	1.393359	0.000000	5.055703
H	-1.393359	0.000000	5.055703

[Pt(*i*Pr$_2$Im)$_2$]



Molecular formula: $C_{18}H_{32}N_4Pt$

SCF-energy + E(vib0) [h]: -1042.5935797

E(vib0) [h]: 0.4673302

Imaginary frequencies: none

Cartesian coordinates:

N	-0.849264	-0.677696	2.871781
C	-0.537422	-0.427411	4.203745
C	0.533867	0.429408	4.204047
N	0.846897	0.679176	2.872279
C	-0.000792	0.000586	2.015142
Pt	0.000051	0.000116	0.000015
C	0.000783	-0.000500	-2.015113
N	0.849041	-0.679349	-2.871479
C	0.537079	-0.429750	-4.203527
C	-0.534087	0.427219	-4.204191
N	-0.846933	0.677750	-2.872514
C	-1.937544	-1.547077	2.391383
C	1.935652	1.548303	2.392535
C	-1.935465	1.547367	-2.393124
C	1.937228	-1.548654	-2.390772
H	-1.834664	-1.476889	1.281980
C	-1.716708	-3.003048	2.825814
C	-3.309584	-0.995453	2.804548
H	1.833718	1.477779	1.283069
C	1.714600	3.004437	2.826305
C	3.307298	0.996683	2.807014
H	-1.833850	1.476908	-1.283622
C	-1.713638	3.003377	-2.826960
C	-3.307221	0.996310	-2.807976
H	1.834297	-1.478158	-1.281398
C	1.716344	-3.004735	-2.824808
C	3.309331	-0.997228	-2.803985

H	-4.119400	-1.613829	2.358524
H	-3.447487	-1.006359	3.910169
H	-3.434553	0.049611	2.447083
H	-2.495830	-3.657342	2.376399
H	-0.722521	-3.365151	2.485667
H	-1.774110	-3.122280	3.932347
H	2.494162	3.658502	2.377321
H	0.720735	3.366530	2.485218
H	1.771098	3.124021	3.932840
H	4.117540	1.614812	2.361424
H	3.444305	1.007968	3.912740
H	3.432442	-0.048519	2.450023
H	-2.493225	3.657797	-2.378531
H	-0.719835	3.365134	-2.485329
H	-1.769420	3.122805	-3.933551
H	-4.117323	1.614839	-2.362692
H	-3.443899	1.007570	-3.913745
H	-3.432948	-0.048809	-2.450947
H	4.119080	-1.615622	-2.357869
H	3.447240	-1.008286	-3.909601
H	3.434393	0.047869	-2.446657
H	2.495358	-3.658953	-2.375100
H	0.722088	-3.366674	-2.484695
H	1.773892	-3.124303	-3.931293
H	-1.086652	0.869310	-5.041104
H	1.090166	-0.872441	-5.039778
H	1.086377	0.871891	5.040787
H	-1.090690	-0.869563	5.040164

[Pt(*i*Pr$_2$Im)$_2$] (D$_{2d}$)

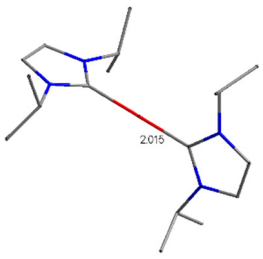
Def2-SV(P)/BP86

Molecular formula: $C_{18}H_{32}N_4Pt$

SCF-energy + E(vib0) [h]: -1042.5939860

E(vib0) [h]: 0.4669817

Imaginary frequencies: i1.54



Def2-TZVPP/BP86

SCF-energy + E(vib0) [h]: -1043.6870846

E(vib0) [h]: 0.4670754

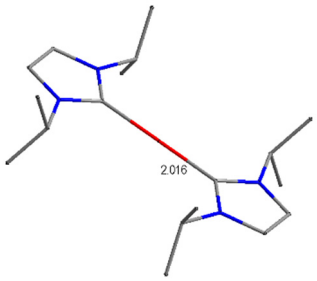
Imaginary frequencies: none

Cartesian coordinates:

N	0.768043	0.768043	2.871856
C	0.485015	0.485015	4.203796
C	-0.485015	-0.485015	4.203796
N	-0.768043	-0.768043	2.871856
C	0.000000	0.000000	2.015153
Pt	0.000000	0.000000	0.000000
C	0.000000	0.000000	-2.015153
N	0.768043	-0.768043	-2.871856
C	0.485015	-0.485015	-4.203796
C	-0.485015	0.485015	-4.203796
N	-0.768043	0.768043	-2.871856
C	-1.753060	1.753060	-2.391662
C	1.753060	-1.753060	-2.391662
C	-1.753060	-1.753060	2.391662
C	1.753060	1.753060	2.391662
H	-1.665429	1.665429	-1.282160
C	-1.364988	3.177044	-2.815890
C	-3.177044	1.364988	-2.815890
H	1.665429	-1.665429	-1.282160
C	1.364988	-3.177044	-2.815890
C	3.177044	-1.364988	-2.815890
H	-3.913058	2.068576	-2.368276
H	-3.306992	1.400579	-3.922060
H	-3.422726	0.338631	-2.467472
H	-2.068576	3.913058	-2.368276
H	-0.338631	3.422726	-2.467472
H	-1.400579	3.306992	-3.922060
H	3.913058	-2.068576	-2.368276
H	3.306992	-1.400579	-3.922060
H	3.422726	-0.338631	-2.467472
H	2.068576	-3.913058	-2.368276
H	0.338631	-3.422726	-2.467472
H	1.400579	-3.306992	-3.922060
H	-1.665429	-1.665429	1.282160

C	-1.364988	-3.177044	2.815890
C	-3.177044	-1.364988	2.815890
H	1.665429	1.665429	1.282160
C	1.364988	3.177044	2.815890
C	3.177044	1.364988	2.815890
H	2.068576	3.913058	2.368276
H	0.338631	3.422726	2.467472
H	1.400579	3.306992	3.922060
H	3.913058	2.068576	2.368276
H	3.306992	1.400579	3.922060
H	3.422726	0.338631	2.467472
H	-2.068576	-3.913058	2.368276
H	-0.338631	-3.422726	2.467472
H	-1.400579	-3.306992	3.922060
H	-3.913058	-2.068576	2.368276
H	-3.306992	-1.400579	3.922060
H	-3.422726	-0.338631	2.467472
H	-0.985619	0.985619	-5.040534
H	0.985619	-0.985619	-5.040534
H	-0.985619	-0.985619	5.040534
H	0.985619	0.985619	5.040534

[Pt(*i*Pr$_2$Im)$_2$] (D$_{2h}$)



Def2-SV(P)/BP86

Molecular formula: $C_{18}H_{32}N_4Pt$

SCF-energy + E(vib0) [h]: -1042.5924292

E(vib0) [h]: 0.4671047

Imaginary frequencies: i9.76

Def2-TZVPP/BP86

SCF-energy + E(vib0) [h]: -1043.6854082

E(vib0) [h]: 0.4669638

Imaginary frequencies: i13.98

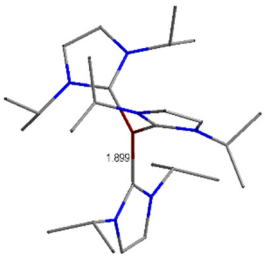
Cartesian coordinates:

N	-1.085577	0.000000	2.875761
C	-0.685913	0.000000	4.206562
C	0.685913	0.000000	4.206562
N	1.085577	0.000000	2.875761

C	0.000000	0.000000	2.015877
Pt	0.000000	0.000000	0.000000
C	0.000000	0.000000	-2.015877
N	1.085577	0.000000	-2.875761
C	0.685913	0.000000	-4.206562
C	-0.685913	0.000000	-4.206562
N	-1.085577	0.000000	-2.875761
C	-2.480318	0.000000	2.403181
C	2.480318	0.000000	2.403181
C	-2.480318	0.000000	-2.403181
C	2.480318	0.000000	-2.403181
H	-2.359984	0.000000	1.293852
C	-3.209830	-1.281658	2.830379
C	-3.209830	1.281658	2.830379
H	2.359984	0.000000	1.293852
C	3.209830	1.281658	2.830379
C	3.209830	-1.281658	2.830379
H	-2.359984	0.000000	-1.293852
C	-3.209830	1.281658	-2.830379
C	-3.209830	-1.281658	-2.830379
H	2.359984	0.000000	-1.293852
C	3.209830	-1.281658	-2.830379
C	3.209830	1.281658	-2.830379
H	-4.231047	1.304640	2.390319
H	-3.319526	1.349034	3.937134
H	-2.659780	2.180938	2.477804
H	-4.231047	-1.304640	2.390319
H	-2.659780	-2.180938	2.477804
H	-3.319526	-1.349034	3.937134
H	4.231047	1.304640	2.390319
H	2.659780	2.180938	2.477804
H	3.319526	1.349034	3.937134
H	4.231047	-1.304640	2.390319
H	3.319526	-1.349034	3.937134
H	2.659780	-2.180938	2.477804
H	-4.231047	1.304640	-2.390319
H	-2.659780	2.180938	-2.477804

H	-3.319526	1.349034	-3.937134
H	-4.231047	-1.304640	-2.390319
H	-3.319526	-1.349034	-3.937134
H	-2.659780	-2.180938	-2.477804
H	4.231047	1.304640	-2.390319
H	3.319526	1.349034	-3.937134
H	2.659780	2.180938	-2.477804
H	4.231047	-1.304640	-2.390319
H	2.659780	-2.180938	-2.477804
H	3.319526	-1.349034	-3.937134
H	-1.393677	0.000000	-5.043269
H	1.393677	0.000000	-5.043269
H	1.393677	0.000000	5.043269
H	-1.393677	0.000000	5.043269

[Ni(*i*Pr$_2$Im)$_3$]



Def2-SV(P)/BP86

Molecular formula: $C_{27}H_{48}N_6Ni$

SCF-energy + E(vib0) [h]: -2892.9590237

E(vib0) [h]: 0.6982237

Imaginary frequencies: none

Def2-TZVPP/BP86

SCF-energy + E(vib0) [h]: -2894.7863913

E(vib0) [h]: 0.6952634

Imaginary frequencies: none

Cartesian coordinates:

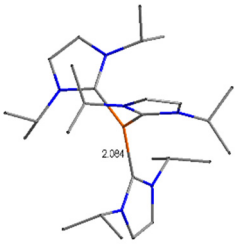
Ni	0.318033	0.123593	0.043341
C	-1.408599	0.434008	-0.683397
C	1.587255	1.534729	0.101577
C	0.773380	-1.594254	0.713395
N	1.130914	-1.968924	2.012251
C	1.395084	-3.332462	2.117810
C	1.212595	-3.866487	0.869261
N	0.837695	-2.815476	0.035624
N	-2.654884	0.359576	-0.053367
C	-3.704992	0.667009	-0.915305

C	-3.144731	0.945943	-2.134238
N	-1.767227	0.804528	-1.983045
N	1.523042	2.752934	0.784949
C	2.656890	3.536405	0.581465
C	3.481810	2.825960	-0.250564
N	2.830897	1.626545	-0.530505
C	-2.796518	-0.058901	1.343870
C	-3.571596	-1.380985	1.458874
C	-3.397246	1.056249	2.213251
C	-0.767247	1.059337	-3.023368
C	-0.799565	2.523949	-3.487340
C	-0.894844	0.066189	-4.188556
C	0.349345	3.143263	1.570750
C	-0.337036	4.383911	0.978610
C	0.692092	3.310760	3.058823
C	3.372702	0.533641	-1.342546
C	4.655731	-0.043894	-0.724483
C	3.559350	0.953980	-2.808439
C	1.254253	-0.992277	3.097869
C	2.696856	-0.911849	3.621082
C	0.233787	-1.254468	4.215984
C	0.490878	-2.936931	-1.382930
C	-0.724411	-3.854455	-1.589809
C	1.701738	-3.360117	-2.228131
H	1.686430	-3.817737	3.057182
H	1.322351	-4.900329	0.520928
H	-4.756809	0.668707	-0.605188
H	-3.619895	1.228492	-3.081336
H	2.793840	4.524700	1.036208
H	4.466707	3.085288	-0.657297
H	-1.738636	-0.236462	1.649390
H	-3.087858	-2.167452	0.839828
H	-3.586607	-1.731678	2.514694

H	-4.627931	-1.271167	1.123708
H	-2.803923	1.991565	2.119127
H	-3.404501	0.754361	3.284190
H	-4.447999	1.284763	1.921213
H	0.192024	0.875505	-2.484525
H	-0.676643	3.207256	-2.619257
H	0.027610	2.722287	-4.204355
H	-1.756862	2.775405	-3.998436
H	-0.847827	-0.981485	-3.819356
H	-0.069746	0.216032	-4.919789
H	-1.856755	0.194942	-4.735779
H	-0.327666	2.265878	1.444230
H	-0.594963	4.210980	-0.088625
H	-1.277082	4.608297	1.530291
H	0.313642	5.285814	1.040364
H	1.170309	2.390207	3.458286
H	-0.228766	3.509932	3.651119
H	1.390846	4.162136	3.226884
H	2.566927	-0.235690	-1.278261
H	4.470203	-0.361649	0.324281
H	4.999238	-0.931721	-1.300467
H	5.485728	0.699171	-0.723600
H	2.608798	1.349273	-3.227861
H	3.878870	0.085020	-3.426037
H	4.337255	1.745014	-2.914405
H	1.004388	-0.032752	2.587121
H	3.399590	-0.694738	2.787718
H	2.791565	-0.098478	4.374547
H	3.014663	-1.861752	4.108423
H	-0.799001	-1.287433	3.805968
H	0.278985	-0.448646	4.982284
H	0.429578	-2.221550	4.733711
H	0.201651	-1.893193	-1.649212

H	-1.584737	-3.500565	-0.981309
H	-1.032752	-3.853508	-2.658741
H	-0.502782	-4.907838	-1.303294
H	2.554125	-2.664317	-2.069468
H	1.444098	-3.354044	-3.310615
H	2.044092	-4.388170	-1.968947

[Pd(*i*Pr$_2$Im)$_3$]



Def2-SV(P)/BP86

Molecular formula: $C_{27}H_{48}N_6Pd$

SCF-energy + E(vib0) [h]: -1512.5617837

E(vib0) [h]: 0.6978200

Imaginary frequencies: none

Def2-TZVPP/BP86

SCF-energy + E(vib0) [h]: -1514.2105427

E(vib0) [h]: 0.6951811

Imaginary frequencies: none

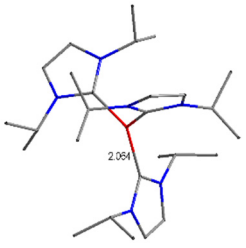
Cartesian coordinates:

Pd	0.323606	0.123363	0.042990
C	-1.572456	0.460379	-0.753588
C	1.712904	1.673921	0.099139
C	0.816190	-1.761423	0.782312
N	1.152198	-2.128845	2.081203
C	1.414033	-3.492870	2.192293
C	1.249448	-4.026469	0.941184
N	0.887404	-2.973447	0.103629
N	-2.809544	0.379004	-0.122354
C	-3.861741	0.686143	-0.982332
C	-3.302012	0.969150	-2.200515
N	-1.923983	0.831718	-2.047137
N	1.643711	2.883013	0.783682
C	2.773150	3.672281	0.575912
C	3.594875	2.966831	-0.263307
N	2.944980	1.765713	-0.540221
C	-2.955731	-0.025311	1.281106
C	-3.778886	-1.316859	1.408067

C	-3.511417	1.120156	2.141075
C	-0.927890	1.078952	-3.096493
C	-0.999845	2.527181	-3.605055
C	-1.036061	0.045415	-4.227912
C	0.481441	3.266777	1.593620
C	-0.190024	4.534246	1.043016
C	0.847711	3.386613	3.080751
C	3.486926	0.683078	-1.370086
C	4.795646	0.131289	-0.783452
C	3.629380	1.116649	-2.837116
C	1.252106	-1.156707	3.176558
C	2.679145	-1.099070	3.743499
C	0.193105	-1.417816	4.258442
C	0.573965	-3.098067	-1.324912
C	-0.617826	-4.040089	-1.556338
C	1.813994	-3.497809	-2.138495
H	1.691985	-3.977827	3.135850
H	1.362666	-5.060240	0.593791
H	-4.913406	0.683835	-0.671856
H	-3.777262	1.252546	-3.147331
H	2.908711	4.660235	1.031732
H	4.576187	3.229895	-0.676203
H	-1.904536	-0.238729	1.586064
H	-3.330941	-2.124770	0.789700
H	-3.795699	-1.659961	2.466144
H	-4.834598	-1.171444	1.084135
H	-2.881638	2.030185	2.036542
H	-3.525703	0.828157	3.214663
H	-4.553581	1.386075	1.849999
H	0.037906	0.935870	-2.557471
H	-0.896716	3.241351	-2.759437
H	-0.175676	2.723104	-4.326033
H	-1.960624	2.738553	-4.127751
H	-0.960753	-0.987390	-3.823744
H	-0.216688	0.191578	-4.966252
H	-2.002699	0.132715	-4.775068
H	-0.212012	2.404667	1.453133

H	-0.460371	4.397176	-0.026392
H	-1.121685	4.754121	1.610198
H	0.472339	5.425925	1.126065
H	1.314858	2.446527	3.446283
H	-0.062316	3.582762	3.690329
H	1.562503	4.221575	3.263515
H	2.700339	-0.104034	-1.292594
H	4.642631	-0.191563	0.269011
H	5.140323	-0.749097	-1.369798
H	5.612527	0.888643	-0.802606
H	2.660304	1.493135	-3.230503
H	3.951160	0.257333	-3.466690
H	4.387952	1.924247	-2.957272
H	1.029319	-0.189367	2.668263
H	3.410240	-0.886594	2.933755
H	2.759536	-0.290389	4.503577
H	2.970407	-2.054384	4.237033
H	-0.825550	-1.435043	3.813850
H	0.222179	-0.617924	5.031605
H	0.361509	-2.390820	4.774732
H	0.270264	-2.061423	-1.601447
H	-1.497960	-3.704648	-0.966033
H	-0.902909	-4.042688	-2.631562
H	-0.381879	-5.089966	-1.268016
H	2.647058	-2.783924	-1.959199
H	1.582568	-3.496493	-3.226888
H	2.170429	-4.518883	-1.870691

[Pt(*i*Pr$_2$Im)$_3$]



Def2-SV(P)/BP86

Molecular formula: $C_{27}H_{48}N_6Pt$

SCF-energy + E(vib0) [h]: -1504.0702015

E(vib0) [h]: 0.6979245

Imaginary frequencies: none

Def2-TZVPP/BP86

SCF-energy + E(vib0) [h]: -1505.6997547

E(vib0) [h]: 0.6952903

Imaginary frequencies: none

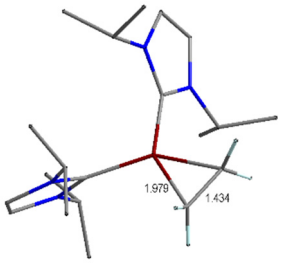
Cartesian coordinates:

Pt	0.327162	0.122609	0.049078
C	-1.553561	0.459648	-0.737394
C	1.703175	1.660318	0.094861
C	0.810479	-1.747291	0.777467
N	1.081265	-2.131084	2.090971
C	1.363894	-3.492084	2.189353
C	1.280491	-4.005964	0.923246
N	0.944818	-2.948042	0.080666
N	-2.788190	0.436397	-0.088928
C	-3.839559	0.722238	-0.957449
C	-3.286702	0.930951	-2.192437
N	-1.909735	0.773052	-2.048804
N	1.660680	2.849555	0.822443
C	2.780338	3.645484	0.588157
C	3.564907	2.970363	-0.307966
N	2.908908	1.775401	-0.597128
C	-2.937385	0.091711	1.329198
C	-3.783558	-1.178835	1.509424
C	-3.469555	1.280842	2.143776
C	-0.923875	0.964601	-3.118227
C	-0.977743	2.395271	-3.677453
C	-1.064367	-0.106374	-4.210587
C	0.530013	3.217652	1.681308
C	-0.155841	4.499583	1.183442
C	0.949109	3.301832	3.157057
C	3.429670	0.719084	-1.471591
C	4.761578	0.163018	-0.943400
C	3.519292	1.190312	-2.931371
C	1.118226	-1.179879	3.207432
C	2.520954	-1.106393	3.831294
C	0.022866	-1.483500	4.241380
C	0.697787	-3.064286	-1.360676
C	-0.475113	-4.014195	-1.651555
C	1.976417	-3.448064	-2.120716
H	1.599718	-3.987692	3.138586

H	1.431905	-5.031072	0.565519
H	-4.887693	0.756322	-0.637873
H	-3.764954	1.176860	-3.147968
H	2.933211	4.619022	1.068376
H	4.526881	3.248753	-0.754413
H	-1.890291	-0.129696	1.641114
H	-3.352913	-2.018467	0.921971
H	-3.802999	-1.479595	2.580389
H	-4.837742	-1.026835	1.183479
H	-2.823713	2.174398	2.002125
H	-3.488018	1.032574	3.228292
H	-4.507053	1.554184	1.843147
H	0.046718	0.824964	-2.587780
H	-0.851282	3.137102	-2.859425
H	-0.160093	2.551012	-4.415645
H	-1.941685	2.604435	-4.195132
H	-1.002568	-1.125657	-3.771490
H	-0.252642	-0.001054	-4.964366
H	-2.036334	-0.020860	-4.748565
H	-0.172181	2.362176	1.546243
H	-0.463287	4.388232	0.121106
H	-1.066383	4.708975	1.787777
H	0.512050	5.387370	1.264119
H	1.425220	2.352193	3.484543
H	0.062659	3.488214	3.803283
H	1.673991	4.129649	3.332733
H	2.653183	-0.076784	-1.387847
H	4.646936	-0.186758	0.105256
H	5.092278	-0.699760	-1.563267
H	5.572115	0.926850	-0.971689
H	2.534836	1.567860	-3.283561
H	3.827883	0.350542	-3.593022
H	4.266285	2.008043	-3.055464
H	0.897470	-0.206330	2.711096
H	3.277985	-0.862044	3.055412
H	2.555164	-0.313843	4.611849
H	2.812034	-2.066750	4.314961

H	-0.977178	-1.512151	3.757035
H	0.005492	-0.700062	5.031547
H	0.191051	-2.463688	4.744080
H	0.397143	-2.029183	-1.644773
H	-1.383284	-3.689357	-1.099217
H	-0.711696	-4.012833	-2.738658
H	-0.243454	-5.063855	-1.358973
H	2.794799	-2.728883	-1.900233
H	1.793580	-3.443031	-3.218284
H	2.329215	-4.467723	-1.842962

[Ni(*i*Pr$_2$Im)$_2$(η^2-C$_2$H$_4$)]



Def2-SV(P)/BP86

Molecular formula: $C_{20}H_{36}N_4Ni$

SCF-energy + E(vib0) [h]: -2509.9528002

E(vib0) [h]: 0.5183527

Imaginary frequencies: none

Def2-TZVPP/BP86

SCF-energy + E(vib0) [h]: -2511.3436523

E(vib0) [h]: 0.5163969

Imaginary frequencies: none

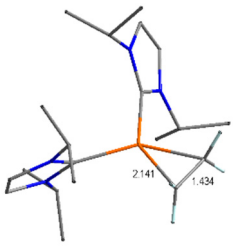
Cartesian coordinates:

Ni	-1.101719	0.238040	-0.393959
C	0.175276	1.586862	0.006041
C	-2.909007	-0.114901	-1.120094
C	-2.593057	1.283237	-1.167406
C	-0.490957	-1.502030	0.064419
N	-0.231914	-2.587843	-0.763797
C	0.127639	-3.723641	-0.042078
C	0.103899	-3.372052	1.281379
N	-0.264912	-2.029733	1.328870
C	2.032277	2.954819	-0.102855
C	1.205992	3.466905	0.861935
N	0.091544	2.632846	0.917756

N	1.400355	1.819409	-0.604837
C	-0.395215	-2.538172	-2.223724
C	-1.540964	-3.450943	-2.687493
C	0.925255	-2.835344	-2.949924
C	-0.461523	-1.247313	2.555461
C	0.804944	-1.230364	3.423308
C	-1.707037	-1.719473	3.321287
C	-1.076574	2.851632	1.782383
C	-1.807743	4.151844	1.413871
C	-0.696112	2.792649	3.269668
C	1.910140	0.976472	-1.693461
C	3.299187	0.410054	-1.365041
C	1.868201	1.720649	-3.037277
H	-2.932052	-0.701470	-2.061517
H	-3.627217	-0.490599	-0.362378
H	-3.092639	1.979876	-0.462999
H	-2.347803	1.759095	-2.139516
H	0.373307	-4.681331	-0.515311
H	0.320103	-3.967318	2.175977
H	3.005806	3.308419	-0.461209
H	1.328758	4.346339	1.504381
H	-0.687387	-1.480336	-2.407052
H	-2.478544	-3.203412	-2.145776
H	-1.722608	-3.317541	-3.776846
H	-1.307938	-4.526041	-2.512036
H	1.733236	-2.156253	-2.601248
H	0.801400	-2.695663	-4.046355
H	1.260891	-3.883963	-2.781630
H	-0.649546	-0.221526	2.163931

H	1.677636	-0.865458	2.839591
H	0.663995	-0.554868	4.295663
H	1.050136	-2.240751	3.822770
H	-2.602581	-1.685835	2.663612
H	-1.894873	-1.064001	4.200466
H	-1.587580	-2.762345	3.694523
H	-1.735376	1.990041	1.535449
H	-2.074767	4.156827	0.335721
H	-2.744796	4.246367	2.005445
H	-1.181994	5.049040	1.624204
H	-0.172169	1.842016	3.508995
H	-1.608039	2.857326	3.902819
H	-0.026935	3.635049	3.557413
H	1.172700	0.142488	-1.722703
H	3.282518	-0.138217	-0.398395
H	3.622640	-0.297341	-2.160038
H	4.071128	1.210637	-1.298696
H	0.839590	2.086794	-3.245305
H	2.172129	1.044012	-3.866374
H	2.557398	2.595936	-3.042712

[Pd(*i*Pr$_2$Im)$_2$(η^2-C$_2$H$_4$)]



Def2-SV(P)/BP86

Molecular formula: $C_{20}H_{36}N_4Pd$

SCF-energy + E(vib0) [h]: -1129.5575838

E(vib0) [h]: 0.5181743

Imaginary frequencies: none

Def2-TZVPP/BP86

SCF-energy + E(vib0) [h]: -1130.7684613

E(vib0) [h]: 0.5163374

Imaginary frequencies: none

Cartesian coordinates:

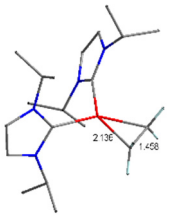
Pd	-1.183018	0.252403	-0.434381
C	0.235977	1.712732	0.011745
C	-3.136986	-0.073043	-1.245994
C	-2.836262	1.328715	-1.264066
C	-0.487044	-1.641765	0.086557
N	-0.230128	-2.723352	-0.737188
C	0.120614	-3.859321	-0.011526
C	0.092078	-3.502719	1.311028
N	-0.271598	-2.158597	1.350978
C	2.079075	3.085679	-0.111527
C	1.254117	3.595713	0.856297
N	0.146311	2.753450	0.919005
N	1.450759	1.944971	-0.606490
C	-0.381324	-2.671473	-2.200581
C	-1.535333	-3.570992	-2.668932
C	0.942956	-2.985733	-2.912267
C	-0.463709	-1.368680	2.576661
C	0.800701	-1.367085	3.447781
C	-1.716798	-1.827619	3.337817
C	-1.019897	2.959645	1.793029
C	-1.769538	4.247743	1.420375
C	-0.623128	2.912426	3.276317
C	1.964903	1.096805	-1.692640
C	3.368039	0.562040	-1.370964
C	1.895668	1.827754	-3.042335
H	-3.127847	-0.645822	-2.193947
H	-3.845927	-0.472112	-0.494783
H	-3.328861	2.002352	-0.535524
H	-2.582894	1.823330	-2.221983
H	0.362844	-4.820081	-0.480361
H	0.301891	-4.095519	2.208807
H	3.048995	3.443778	-0.475252
H	1.373867	4.478430	1.494861
H	-0.659191	-1.609904	-2.388779
H	-2.474752	-3.303478	-2.139725
H	-1.703175	-3.442236	-3.760954

H	-1.321113	-4.648397	-2.483646
H	1.754891	-2.314082	-2.557819
H	0.830418	-2.845881	-4.009816
H	1.265634	-4.037845	-2.740236
H	-0.638496	-0.340776	2.184912
H	1.682215	-1.023700	2.864251
H	0.667678	-0.679159	4.311500
H	1.026538	-2.376914	3.859843
H	-2.609871	-1.779619	2.677949
H	-1.897618	-1.170605	4.217147
H	-1.611418	-2.872303	3.710301
H	-1.670283	2.087766	1.556688
H	-2.051331	4.236593	0.345874
H	-2.699962	4.336900	2.022947
H	-1.152341	5.154834	1.613112
H	-0.086887	1.968236	3.514921
H	-1.530242	2.968987	3.916976
H	0.038396	3.763926	3.555190
H	1.244549	0.247672	-1.707098
H	3.375533	0.034923	-0.392441
H	3.689574	-0.158168	-2.155069
H	4.128697	1.375356	-1.335424
H	0.857066	2.167101	-3.245291
H	2.207612	1.148962	-3.866551
H	2.565875	2.717357	-3.061978

[Pt(*i*Pr$_2$Im)$_2$(η^2-C$_2$H$_4$)]

Def2-SV(P)/BP86

Molecular formula: $C_{20}H_{36}N_4Pt$



SCF-energy + E(vib0) [h]: -1121.0661366

E(vib0) [h]: 0.5188833

Imaginary frequencies: none

Def2-TZVPP/BP86

SCF-energy + E(vib0) [h]: -1122.2588437

E(vib0) [h]: 0.5168294

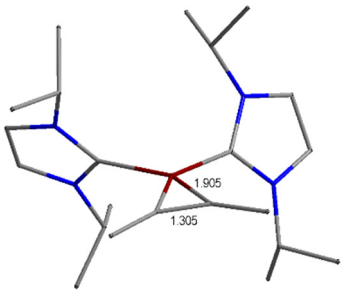
Imaginary frequencies: none

Cartesian coordinates:

Pt	-1.200379	0.256486	-0.436493
C	0.403199	1.570003	-0.393462
C	-3.225043	-0.039610	-1.049029
C	-2.773445	1.288253	-1.448851
C	-0.631551	-1.499491	0.505772
N	0.245083	-2.475292	0.063084
C	0.266465	-3.576793	0.915486
C	-0.606051	-3.301111	1.934508
N	-1.139700	-2.041101	1.675222
C	2.043732	3.034102	-1.066120
C	1.925103	3.151611	0.293266
N	0.933778	2.255174	0.686189
N	1.119361	2.072945	-1.467398
C	0.999413	-2.365513	-1.195197
C	0.422090	-3.304428	-2.265575
C	2.504512	-2.567412	-0.966958
C	-2.181595	-1.385876	2.483788
C	-1.703768	-1.143404	3.923143
C	-3.502324	-2.168227	2.418568
C	0.447421	2.084384	2.063877
C	-0.363334	3.308175	2.516457
C	1.594161	1.734973	3.023827
C	0.864101	1.683661	-2.864184
C	2.119535	1.085071	-3.516498
C	0.280308	2.857520	-3.665560
H	-3.365691	-0.814469	-1.829233
H	-3.966200	-0.125870	-0.227991
H	-3.169419	2.172786	-0.910684
H	-2.598267	1.489959	-2.525428
H	0.892261	-4.458671	0.737553
H	-0.879757	-3.896740	2.812882
H	2.708461	3.552635	-1.766383
H	2.465348	3.793164	0.998595
H	0.813231	-1.313208	-1.507167
H	-0.659012	-3.097462	-2.418274
H	0.946247	-3.154493	-3.235327
H	0.538516	-4.374364	-1.978048

H	2.885628	-1.869099	-0.190639
H	3.060693	-2.374265	-1.910454
H	2.744673	-3.607636	-0.649412
H	-2.323324	-0.408166	1.969842
H	-0.750776	-0.571249	3.936449
H	-2.466469	-0.561711	4.486039
H	-1.540680	-2.098677	4.472367
H	-3.819445	-2.304308	1.362812
H	-4.303443	-1.612024	2.953299
H	-3.411458	-3.171963	2.893046
H	-0.239664	1.212803	1.980231
H	-1.199108	3.500649	1.810034
H	-0.794064	3.134881	3.527604
H	0.270336	4.222947	2.569346
H	2.153293	0.843103	2.666629
H	1.187774	1.507737	4.033761
H	2.315605	2.575796	3.139884
H	0.083180	0.895476	-2.769018
H	2.515223	0.236023	-2.917573
H	1.878270	0.709849	-4.535160
H	2.931993	1.839910	-3.622751
H	-0.633991	3.247911	-3.170288
H	0.004235	2.522090	-4.689435
H	1.011235	3.692153	-3.767669

[Ni(*i*Pr$_2$Im)$_2$(η^2 MeCCMe)]



Def2-SV(P)/BP86

Molecular formula: $C_{22}H_{38}N_4Ni$

SCF-energy + E(vib0) [h]: -2587.2562652

E(vib0) [h]: 0.5499715

Imaginary frequencies: none

Def2-TZVPP/BP86

SCF-energy + E(vib0) [h]: -2588.7320955

E(vib0) [h]: 0.5484550

Imaginary frequencies: none

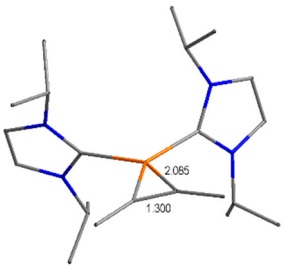
Cartesian coordinates:

N	0.008193	-0.285420	0.240843

C	-0.070014	-0.025246	1.601847
N	1.268205	0.100984	1.959984
C	2.119260	-0.077015	0.871997
C	1.323247	-0.317320	-0.215879
Ni	-1.620682	0.193937	2.690274
C	-2.603194	-1.439112	2.750382
N	-3.907577	-1.685783	2.334393
C	-4.299943	-2.996541	2.594094
C	-3.236732	-3.614359	3.196329
N	-2.222522	-2.664047	3.280942
C	-4.771085	-0.667301	1.716678
C	-5.076883	-1.005704	0.248967
C	-0.915438	-2.880122	3.914164
C	-1.059495	-3.072062	5.431692
C	1.719967	0.414768	3.324463
C	2.488902	-0.761576	3.946396
C	-1.182407	-0.428524	-0.606407
C	-1.333049	0.770477	-1.555635
C	-2.583580	1.395801	3.817196
C	-3.727054	1.564696	4.760261
C	-1.586467	2.017810	3.250229
C	-0.897883	3.336407	3.139134
C	-6.053291	-0.450931	2.534871
C	-0.142912	-4.019622	3.234745
C	-1.194576	-1.778949	-1.336930
C	2.538763	1.714973	3.356778
H	-5.290802	-3.386744	2.334806
H	-3.130535	-4.640406	3.566953
H	3.210877	-0.021796	0.951575
H	1.591074	-0.502409	-1.262410
H	-3.550198	2.389557	5.493007
H	-4.669089	1.819730	4.216981
H	-3.941328	0.639442	5.342825
H	-1.585115	4.190517	3.355521
H	-0.052756	3.417398	3.864979
H	-0.459905	3.505994	2.128921
H	-4.148676	0.254742	1.762902

H	-5.813933	-0.233987	3.596886
H	-6.626249	0.410288	2.126014
H	-6.719754	-1.342799	2.500945
H	-4.139762	-1.154393	-0.328733
H	-5.649546	-0.178879	-0.225964
H	-5.686918	-1.933494	0.161013
H	-0.393294	-1.915672	3.724280
H	-0.042524	-3.831159	2.143967
H	0.878458	-4.102940	3.667173
H	-0.644738	-5.004339	3.374096
H	-1.594936	-2.208717	5.882162
H	-0.057732	-3.147181	5.909700
H	-1.622998	-4.001108	5.677491
H	-2.011969	-0.402535	0.135948
H	-1.107023	-2.618295	-0.613416
H	-2.146203	-1.903284	-1.899043
H	-0.361370	-1.863773	-2.071682
H	-1.352604	1.720477	-0.978925
H	-2.282454	0.692757	-2.130271
H	-0.496165	0.823572	-2.289383
H	0.766174	0.569984	3.878069
H	1.979230	2.546725	2.879956
H	2.757350	2.001365	4.408997
H	3.514427	1.603092	2.830773
H	1.882491	-1.691944	3.922805
H	2.742329	-0.538995	5.006350
H	3.442993	-0.959104	3.405902

[Pd(*i*Pr$_2$Im)$_2$(η^2-MeCCMe)]



Def2-SV(P)/BP86

Molecular formula: $C_{22}H_{38}N_4Pd$

SCF-energy + E(vib0) [h]: -1206.8535287

E(vib0) [h]: 0.5498141

Imaginary frequencies: none

Def2-TZVPP/BP86

SCF-energy + E(vib0) [h]: -1208.1512566

E(vib0) [h]: 0.5480415

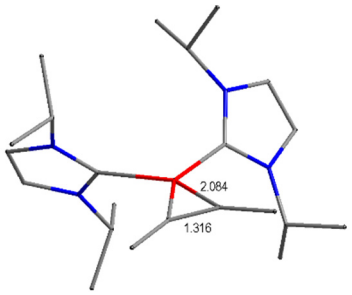
Imaginary frequencies: none

Cartesian coordinates:

N	-1.350858	0.368064	-1.936397
C	-0.303673	0.735339	-1.111532
N	0.577747	1.347398	-1.985690
C	0.092906	1.358726	-3.291412
C	-1.130003	0.742760	-3.259863
Pd	-0.165951	0.611631	0.964417
C	0.283836	-1.337840	1.548259
N	-0.550897	-2.257967	2.158311
C	0.133471	-3.409808	2.539468
C	1.439673	-3.229235	2.169079
N	1.511167	-1.974380	1.567810
C	-1.983533	-2.017804	2.395479
C	-2.850719	-3.009895	1.605354
C	2.747057	-1.345982	1.076084
C	3.658463	-0.937370	2.243472
C	1.859027	1.936027	-1.563682
C	3.045977	1.181925	-2.182715
C	-2.576731	-0.272682	-1.436669
C	-3.750787	0.718141	-1.427572
C	-0.291952	1.741792	2.711742
C	-0.139579	1.666147	4.190502
C	-0.557633	2.520827	1.706113
C	-0.933648	3.901986	1.297879
C	-2.309846	-2.019104	3.896536
C	3.455488	-2.236004	0.044485
C	-2.887833	-1.563934	-2.206511
C	1.903959	3.443678	-1.854660
H	-0.350987	-4.258547	3.035769
H	2.306846	-3.889102	2.286883
H	0.645499	1.793198	-4.132365
H	-1.844665	0.545798	-4.067099

H	-0.313136	2.653097	4.686423
H	-0.851285	0.937445	4.645035
H	0.879374	1.319863	4.482091
H	-1.070198	4.581723	2.175065
H	-0.161438	4.364272	0.638847
H	-1.882379	3.914954	0.712527
H	-2.136754	-0.988500	1.998209
H	-1.671028	-1.288737	4.437147
H	-3.372749	-1.733275	4.055933
H	-2.159144	-3.023925	4.353417
H	-2.592133	-2.990074	0.524949
H	-3.926958	-2.749993	1.712340
H	-2.719789	-4.053603	1.972172
H	2.376186	-0.423010	0.576699
H	2.767207	-2.505488	-0.785785
H	4.328635	-1.699189	-0.386499
H	3.838696	-3.178527	0.498201
H	3.112185	-0.267596	2.941651
H	4.550939	-0.392059	1.864330
H	4.017947	-1.824600	2.812937
H	-2.316798	-0.522720	-0.383918
H	-2.019134	-2.257426	-2.186643
H	-3.757343	-2.081497	-1.745766
H	-3.149055	-1.364713	-3.271050
H	-3.490613	1.617472	-0.828827
H	-4.651353	0.247511	-0.974777
H	-4.019455	1.045144	-2.458135
H	1.856159	1.785066	-0.459977
H	1.033896	3.957611	-1.393646
H	2.831884	3.885648	-1.430000
H	1.899536	3.656181	-2.948023
H	2.991349	0.096547	-1.949569
H	4.005141	1.577457	-1.781955

H	3.072323	1.295370	-3.290756



[Pt(*i*Pr$_2$Im)$_2$(η^2-MeCCMe)]

Def2-SV(P)/BP86

Molecular formula: $C_{22}H_{38}N_4Pt$

SCF-energy + E(vib0) [h]: -1198.3638609

E(vib0) [h]: 0.5501489

Imaginary frequencies: none

Def2-TZVPP/BP86

SCF-energy + E(vib0) [h]: -1199.6447138

E(vib0) [h]: 0.5484328

Imaginary frequencies: none

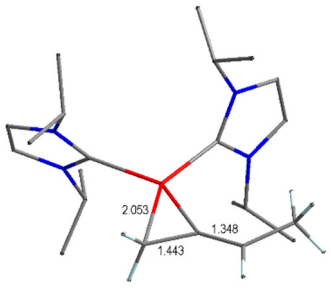
Cartesian coordinates:

Pt	-0.197025	0.743825	1.069936
C	-0.128568	0.764440	-1.004017
C	-0.416253	1.840558	2.828305
C	-0.546208	2.661784	1.808434
C	0.106067	-1.263209	1.499171
N	-0.727385	-2.110175	2.215069
C	-0.162756	-3.372200	2.378187
C	1.058612	-3.341633	1.760217
N	1.205742	-2.062066	1.230855
N	0.732971	1.489284	-1.814225
C	0.435429	1.320784	-3.163696
C	-0.639291	0.475092	-3.229030
N	-0.967510	0.145552	-1.916367
C	-0.421716	1.816995	4.319636
C	-0.811393	4.093252	1.484601
C	-2.028838	-1.703134	2.773669
C	-2.032551	-1.824931	4.305014
C	-3.184410	-2.478403	2.122741

C	2.411963	-1.574188	0.543889
C	2.744423	-2.434115	-0.683440
C	3.587282	-1.446822	1.525117
C	-2.108904	-0.697244	-1.525733
C	-1.997511	-2.103896	-2.130785
C	-3.440373	-0.004772	-1.853410
C	1.797578	2.369032	-1.300824
C	1.557783	3.826698	-1.723557
C	3.188821	1.862593	-1.711500
H	-0.665755	-4.185835	2.913011
H	1.822082	-4.121449	1.659835
H	1.002529	1.808089	-3.964960
H	-1.187282	0.090525	-4.096665
H	-0.511448	2.841073	4.758310
H	-1.269352	1.212014	4.720458
H	0.507749	1.356400	4.728603
H	-1.024616	4.700686	2.398255
H	0.056514	4.568395	0.968713
H	-1.680336	4.205767	0.795095
H	-2.101180	-0.627551	2.495312
H	-1.180793	-1.265054	4.745761
H	-2.975170	-1.403379	4.717700
H	-1.965368	-2.886082	4.638270
H	-3.166791	-2.367190	1.016906
H	-4.159629	-2.092635	2.492452
H	-3.139233	-3.565652	2.361323
H	2.113551	-0.555644	0.211210
H	1.873763	-2.496990	-1.372035
H	3.594602	-1.985855	-1.243229

H	3.042282	-3.470042	-0.402153
H	3.308844	-0.791641	2.378488
H	4.468134	-0.997175	1.015908
H	3.897849	-2.438096	1.928127
H	-2.002597	-0.762227	-0.420184
H	-1.026937	-2.574556	-1.861663
H	-2.813951	-2.752057	-1.743013
H	-2.082863	-2.089670	-3.241314
H	-3.485648	0.995296	-1.371435
H	-4.292800	-0.611239	-1.475330
H	-3.578917	0.126108	-2.951046
H	1.685124	2.288462	-0.196008
H	0.541840	4.159371	-1.423288
H	2.299660	4.492226	-1.230557
H	1.662201	3.963743	-2.824446
H	3.344882	0.812263	-1.383410
H	3.977260	2.491125	-1.242587
H	3.335426	1.905074	-2.815068

[Pt(*i*Pr$_2$Im)$_2$(η^2-H$_2$CCCHMe)]]



Def2-SV(P)/BP86

Molecular formula: $C_{22}H_{38}N_4Pt$

SCF-energy + E(vib0) [h]: -1198.3706547

E(vib0) [h]: 0.5505885

Imaginary frequencies: none

Def2-TZVPP/BP86

SCF-energy + E(vib0) [h]: -1199.6516101

E(vib0) [h]: 0.5485398

Imaginary frequencies: none

Cartesian coordinates:

C	1.117431	-2.607294	-0.736071
C	0.934408	-1.668503	-1.817083

N	-1.629502	1.425947	-1.222438
C	-1.721308	2.771931	-1.568918
C	-0.544382	3.358752	-1.187531
N	0.234217	2.356255	-0.613631
C	-0.413646	1.134868	-0.628288
N	-0.860769	-1.165738	2.802071
C	-0.471576	-1.378581	4.122744
C	0.888236	-1.222703	4.159982
C	0.220622	-0.887336	1.987776
N	1.292532	-0.924333	2.861474
Pt	0.321062	-0.726787	-0.098677
H	2.149419	-2.865740	-0.414489
H	0.415733	-3.462792	-0.633807
C	1.187572	-1.535416	-3.134439
C	0.941006	-0.307439	-3.973115
C	1.606490	2.536287	-0.113388
C	1.667614	3.624930	0.967742
C	2.586407	2.780080	-1.270871
C	-2.668073	0.416252	-1.495096
C	-2.885779	0.231808	-3.003926
C	-3.968533	0.745994	-0.747332
C	2.693812	-0.752266	2.439409
C	3.486506	-2.055696	2.619057
C	3.346000	0.444711	3.146904
C	-2.236714	-1.305236	2.299654
C	-3.213339	-0.421544	3.089151
C	-2.658574	-2.782432	2.262229
H	-2.604543	3.204503	-2.052254
H	-0.207970	4.397342	-1.279804
H	-1.179402	-1.618002	4.924041
H	1.586941	-1.297845	5.000902
H	1.634397	-2.400343	-3.673180
H	0.509492	0.511330	-3.356972
H	1.884609	0.073757	-4.435301
H	0.244345	-0.509241	-4.823654
H	1.839226	1.549345	0.343873
H	0.953666	3.407669	1.791599

H	2.691572	3.676581	1.398053
H	1.429879	4.633283	0.558607
H	2.526875	1.950853	-2.008030
H	3.629454	2.831543	-0.888140
H	2.369321	3.737302	-1.797693
H	-2.226152	-0.520103	-1.086174
H	-1.930721	-0.027446	-3.506612
H	-3.607599	-0.594567	-3.184883
H	-3.299391	1.151931	-3.476299
H	-3.783514	0.882105	0.340141
H	-4.703274	-0.078830	-0.876264
H	-4.441151	1.677250	-1.134681
H	2.607435	-0.539348	1.349760
H	2.990013	-2.889069	2.077984
H	4.513037	-1.937508	2.207960
H	3.581314	-2.337538	3.692494
H	2.753183	1.371669	2.990528
H	4.369751	0.613703	2.746505
H	3.440354	0.276303	4.244009
H	-2.165286	-0.932829	1.254604
H	-2.880717	0.639095	3.089033
H	-4.224646	-0.469484	2.630132
H	-3.315551	-0.753969	4.147204
H	-1.939306	-3.373636	1.655887
H	-3.667328	-2.884554	1.804457
H	-2.702185	-3.221632	3.284978

[Pt(*i*Pr$_2$Im)$_2$(η^2-H$_2$CCCHMe)]

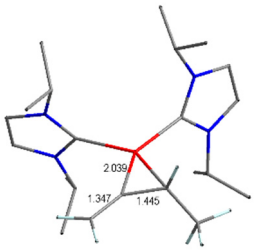
Def2-SV(P)/BP86

Molecular formula: $C_{22}H_{38}N_4Pt$

SCF-energy + E(vib0) [h]: -1198.3676969

E(vib0) [h]: 0.5500311

Imaginary frequencies: none



Def2-TZVPP/BP86

SCF-energy + E(vib0) [h]: -1199.6480111

E(vib0) [h]: 0.5480542

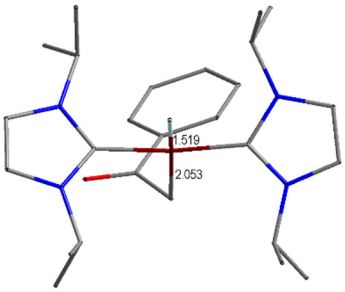
Imaginary frequencies: none

Cartesian coordinates:

C	0.826415	1.250712	-0.527333
C	-0.418555	-1.843278	0.188663
N	-0.068627	-3.044871	-0.402359
C	-0.021544	-4.082267	0.525875
C	-0.351370	-3.539881	1.738829
N	-0.584792	-2.184139	1.519168
N	1.947459	1.358161	-1.328270
C	2.700765	2.485854	-1.009463
C	2.055891	3.108720	0.025495
N	0.923518	2.349013	0.307454
C	-2.107437	1.140823	-1.816633
C	-2.814544	-0.087793	-1.537751
C	-2.241668	2.299138	-2.490893
H	-3.179278	2.560222	-3.026206
Pt	-0.808831	-0.008710	-0.743459
C	0.199280	-3.198721	-1.841982
C	-0.772243	-4.197360	-2.487995
C	1.671474	-3.561129	-2.093334
C	-0.098652	2.707131	1.307124
C	-0.844876	3.986107	0.900812
C	0.505495	2.784185	2.717231
C	2.221175	0.451438	-2.455686
C	3.675397	-0.040498	-2.441378
C	1.816579	1.101441	-3.787685
C	-1.023563	-1.230774	2.550943
C	-0.030401	-1.178601	3.721263
C	-2.463695	-1.526264	2.996649
H	0.238989	-5.112399	0.257822
H	-0.437566	-4.009658	2.725191
H	3.626368	2.753314	-1.531195
H	2.315767	4.018583	0.578033
H	-3.568225	-0.034555	-0.720911
C	-3.230704	-1.035873	-2.656836
H	-1.422828	3.042890	-2.548304
H	-0.008252	-2.183306	-2.249666
H	-1.825222	-3.901479	-2.296098

H	-0.616075	-4.220898	-3.588601
H	-0.619778	-5.231957	-2.104588
H	2.349807	-2.819618	-1.619129
H	1.882034	-3.580366	-3.185076
H	1.921157	-4.567262	-1.685632
H	-0.815234	1.856817	1.253118
H	-1.314434	3.857187	-0.098313
H	-1.650426	4.205514	1.635604
H	-0.164463	4.867672	0.869463
H	1.033414	1.841330	2.978419
H	-0.297811	2.953327	3.467324
H	1.230482	3.624526	2.812796
H	1.539291	-0.406118	-2.265486
H	3.938580	-0.488804	-1.458492
H	3.819734	-0.814564	-3.226366
H	4.397800	0.780055	-2.654008
H	0.745755	1.397737	-3.759678
H	1.960411	0.384906	-4.626511
H	2.432170	2.005100	-4.000982
H	-1.012282	-0.255606	2.016171
H	0.998179	-0.962137	3.359453
H	-0.323996	-0.378436	4.435196
H	-0.004722	-2.136671	4.288620
H	-3.148297	-1.523093	2.121448
H	-2.811883	-0.751047	3.714237
H	-2.541646	-2.516045	3.501406
H	-3.429115	-2.063733	-2.273921
H	-2.447904	-1.109613	-3.443879
H	-4.168848	-0.688479	-3.159309

trans-[Ni(*i*Pr$_2$Im)$_2$(C̲H$_2$C(O)Ph)H]



Def2-SV(P)/BP86

Molecular formula: $C_{26}H_{40}N_4NiO$

SCF-energy + E(vib0) [h]: -2815.9372178

E(vib0) [h]: 0.5996325

Imaginary frequencies: none

Def2-TZVPP/BP86

SCF-energy + E(vib0) [h]: -2817.6697979

E(vib0) [h]: 0.5996325

Imaginary frequencies: none

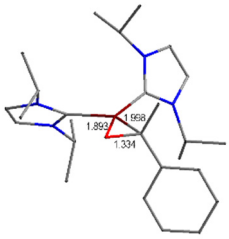
Cartesian coordinates:

C	-3.104425	-5.582933	2.595813
C	-2.107746	-4.741830	2.052833
C	-2.334970	-4.168782	0.781456
C	-3.525012	-4.424635	0.078970
C	-4.507678	-5.265196	0.632556
C	-4.291216	-5.846001	1.895311
C	-0.830650	-4.536690	2.863483
O	-0.830128	-4.918324	4.052284
C	0.320271	-3.901704	2.214343
Ni	0.300779	-1.892208	2.632270
C	0.211912	-2.088884	4.510711
N	-0.880377	-1.925011	5.325524
C	-0.536529	-2.053927	6.667771
C	0.808285	-2.309249	6.705560
N	1.246366	-2.322728	5.383912
C	-2.238618	-1.667898	4.817131
C	-2.673384	-0.227200	5.123690
C	2.602935	-2.683182	4.941640
C	3.652334	-1.704458	5.485327
C	0.416718	-1.285089	0.854450
N	-0.463525	-0.436322	0.213283
C	-0.046398	-0.149236	-1.082465
C	1.128629	-0.826541	-1.276355
N	1.393734	-1.514127	-0.093905
C	-1.627143	0.166978	0.888857
C	-1.457473	1.688789	1.004913

C	2.619914	-2.287345	0.171707
C	2.814447	-3.410950	-0.855730
C	3.838060	-1.355766	0.275541
C	-2.947387	-0.246220	0.227630
C	-3.223886	-2.730618	5.321545
C	2.898946	-4.153760	5.276870
H	0.401551	-0.420848	2.994941
H	2.546309	-2.571152	3.836086
H	1.782642	-0.874817	-2.154048
H	-0.613731	0.496137	-1.762165
H	-1.265715	-1.966467	7.480490
H	1.473493	-2.492227	7.556400
H	-2.127321	-1.782081	3.715936
H	3.726714	-1.754902	6.595216
H	3.404796	-0.659054	5.199252
H	4.655331	-1.951622	5.072749
H	2.431287	-2.736407	1.169562
H	-1.562766	-0.269353	1.910793
H	-2.765796	-0.055062	6.220051
H	-3.664654	-0.017557	4.664333
H	-1.934828	0.498257	4.718517
H	-2.289556	2.119812	1.603520
H	-1.465829	2.185879	0.008498
H	-0.500293	1.934162	1.513884
H	3.012328	-4.305378	6.374471
H	3.844269	-4.481584	4.790535
H	2.064547	-4.797569	4.923135
H	3.666674	-0.571161	1.043855
H	4.052991	-0.852678	-0.694547
H	4.742394	-1.935935	0.563168
H	1.919137	-4.067303	-0.902481
H	3.686686	-4.038131	-0.569877
H	3.011365	-3.012136	-1.876705
H	-3.805453	0.171797	0.798551
H	-3.055515	-1.351984	0.207779
H	-3.022752	0.134815	-0.816488
H	-4.204648	-2.612610	4.811299

H	-3.401075	-2.641753	6.417757
H	-2.823720	-3.743292	5.100129
H	0.350580	-4.061206	1.117680
H	1.261669	-4.254005	2.688725
H	-1.575553	-3.504121	0.339818
H	-3.686197	-3.966879	-0.912323
H	-5.438868	-5.470245	0.077279
H	-5.054515	-6.511389	2.334246
H	-2.906675	-6.031301	3.583255

[Ni(*i*Pr$_2$Im)$_2$(MeC(O)Ph)]



Def2-SV(P)/BP86

Molecular formula: $C_{26}H_{40}N_4NiO$

SCF-energy + E(vib0) [h]: -2815.9644944

E(vib0) [h]: 0.6023964

Imaginary frequencies: none

Def2-TZVPP/BP86

SCF-energy + E(vib0) [h]: -2817.6929947

E(vib0) [h]: 0.5996385

Imaginary frequencies: none

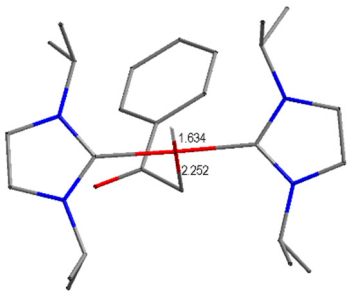
Cartesian coordinates:

C	0.594092	-2.200918	-1.011594
O	0.834741	-1.176114	-1.831700
N	-1.789667	-1.196835	1.992727
C	-3.058419	-1.380660	2.537274
C	-3.953881	-1.241130	1.510544
N	-3.209138	-0.972089	0.366923
C	-1.845027	-0.932671	0.630931
N	-0.740536	1.623741	-2.629854
C	-0.751369	3.009346	-2.750395
C	-0.712559	3.516805	-1.477899
C	-0.696626	1.224341	-1.306659
N	-0.681479	2.422741	-0.618147
Ni	-0.518006	-0.581059	-0.648792
C	-3.766635	-0.790827	-0.981717
C	-4.711379	0.417849	-1.040197
C	-4.415966	-2.085329	-1.493187

C	-0.535635	-1.323319	2.756315
C	-0.402680	-2.725298	3.368632
C	-0.409562	-0.218907	3.817492
C	-0.555938	2.504543	0.845083
C	-1.743074	3.249866	1.470962
C	0.804034	3.094698	1.248423
C	-0.712425	0.687153	-3.771621
C	0.604725	0.813123	-4.549802
C	-1.956601	0.853873	-4.656110
C	-0.182948	-3.391352	-1.574806
C	1.642496	-2.487813	0.019830
H	-0.895338	-3.036311	-2.349145
H	-0.765369	-3.931953	-0.796255
H	0.501115	-4.133314	-2.058876
C	1.731830	-3.724037	0.709498
C	2.743604	-3.961031	1.656274
H	-3.226081	-1.598628	3.598049
H	-5.046979	-1.318501	1.508184
H	-0.783931	3.524662	-3.717160
H	-0.700989	4.555133	-1.127901
H	-2.861461	-0.573985	-1.594226
H	-4.195415	1.336948	-0.687230
H	-5.048737	0.590721	-2.085853
H	-5.621237	0.265661	-0.415900
H	-3.691412	-2.927338	-1.457367
H	-4.749770	-1.959188	-2.546620
H	-5.307809	-2.366847	-0.887798
H	0.257670	-1.189128	1.989967
H	-0.517056	-3.506569	2.588784
H	0.604590	-2.845670	3.821156
H	-1.163060	-2.900817	4.163728
H	-0.502794	0.790309	3.362090
H	0.582038	-0.282620	4.316170
H	-1.191261	-0.315395	4.605300
H	-0.586295	1.436500	1.153714
H	-2.706038	2.783885	1.169107
H	-1.675298	3.214703	2.580419

H	-1.765018	4.322306	1.171465
H	1.632387	2.509475	0.794134
H	0.923913	3.065711	2.353862
H	0.906245	4.155652	0.925182
H	-0.716146	-0.311942	-3.288577
H	1.462360	0.629322	-3.869843
H	0.640124	0.049658	-5.358007
H	0.717695	1.815799	-5.022476
H	-2.889253	0.753858	-4.058423
H	-1.967915	0.071477	-5.446651
H	-1.978394	1.843616	-5.166739
C	3.701189	-2.972468	1.940720
C	3.639132	-1.744529	1.251430
C	2.634019	-1.509773	0.304040
H	1.004432	-4.523732	0.496010
H	2.788371	-4.936834	2.170802
H	4.497866	-3.161050	2.680045
H	4.397045	-0.965827	1.447367
H	2.597793	-0.563464	-0.258403

trans-[Pt(*i*Pr$_2$Im)$_2$(C̲H$_2$C(O)Ph)H]



Def2-SV(P)/BP86

Molecular formula: $C_{26}H_{40}N_4PtO$

SCF-energy + E(vib0) [h]: -1427.0781461

E(vib0) [h]: 0.6003082

Imaginary frequencies: none

Def2-TZVPP/BP86

SCF-energy + E(vib0) [h]: -1428.6110258

E(vib0) [h]: 0.5970411

Imaginary frequencies: none

Cartesian coordinates:

N	-0.441492	-0.392521	-0.103135
C	0.466783	-1.146915	0.606407
N	1.501949	-1.344238	-0.280585
C	1.247350	-0.722699	-1.499625
C	0.021641	-0.121503	-1.387099
Pt	0.339085	-1.751921	2.549926

C	0.293332	-3.923611	1.954037
C	2.748851	-2.058201	0.057924
C	3.931812	-1.080565	0.125299
C	-1.688952	0.143884	0.478175
C	-2.905523	-0.191686	-0.394108
C	0.239258	-2.178609	4.549732
N	-0.833298	-1.995986	5.387476
C	-0.508629	-2.328311	6.698157
C	0.800767	-2.729452	6.688736
N	1.240919	-2.627458	5.374014
C	-2.156089	-1.522199	4.938959
C	-3.237850	-2.572741	5.224679
C	2.572234	-3.048916	4.897230
C	2.728502	-4.570315	5.042069
C	3.686953	-2.243105	5.578489
C	-2.472511	-0.141623	5.532695
C	2.994522	-3.236304	-0.894423
C	-1.546437	1.646650	0.761784
H	0.485307	-0.173841	2.982543
H	2.550268	-2.785388	3.816882
H	1.944068	-0.761149	-2.344163
H	-0.552036	0.461521	-2.115653
H	-1.226552	-2.263821	7.522904
H	1.441026	-3.086004	7.502489
H	-2.029541	-1.420294	3.837844
H	3.736710	-2.447643	6.672130
H	3.536462	-1.151249	5.432635
H	4.672591	-2.520613	5.144519
H	2.551000	-2.448702	1.079452
H	-1.769750	-0.394228	1.448702
H	-2.570025	-0.183276	6.641384
H	-3.435690	0.236457	5.124977
H	-1.674095	0.588555	5.277336
H	-2.460409	2.028904	1.267108
H	-1.407842	2.228923	-0.177481
H	-0.676968	1.832509	1.428222
H	2.815584	-4.868648	6.112030

H	3.649535	-4.914017	4.520894
H	1.840914	-5.079898	4.604524
H	3.720032	-0.258955	0.842781
H	4.152554	-0.631169	-0.869729
H	4.847401	-1.612243	0.465507
H	2.123120	-3.925537	-0.906591
H	3.884396	-3.812894	-0.559907
H	3.189938	-2.896399	-1.936891
H	-3.836172	0.132805	0.120130
H	-2.979191	-1.285293	-0.576419
H	-2.871854	0.328486	-1.377919
H	-4.202633	-2.257749	4.770618
H	-3.407154	-2.703907	6.317817
H	-2.949988	-3.554361	4.791550
C	-0.713465	-4.665730	2.724039
H	0.140340	-3.972948	0.857147
H	1.307629	-4.290232	2.220501
O	-0.491034	-5.170288	3.843055
C	-2.115180	-4.829242	2.145166
C	-2.578714	-4.146570	0.998911
C	-3.878112	-4.363773	0.510088
C	-4.734587	-5.274174	1.154902
C	-4.283391	-5.961855	2.296313
C	-2.988552	-5.735244	2.786624
H	-1.917475	-3.426621	0.490717
H	-4.227028	-3.820225	-0.385100
H	-5.752419	-5.449025	0.766464
H	-4.947852	-6.681249	2.805342
H	-2.607159	-6.257212	3.679451

[Pt(*i*Pr$_2$Im)$_2$(Me<u>C</u>(<u>O</u>)Ph)]]

Def2-SV(P)/BP86

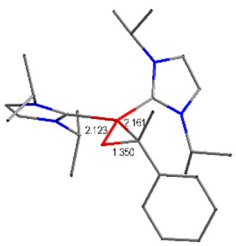
Molecular formula: $C_{26}H_{40}N_4PtO$

SCF-energy + E(vib0) [h]: -1427.0621723

E(vib0) [h]: 0.6022814

Imaginary frequencies: none

Def2-TZVPP/BP86



SCF-energy + E(vib0) [h]: -1428.5951603

E(vib0) [h]: 0.5991885

Imaginary frequencies: none

Cartesian coordinates:

C	2.809255	-1.753983	0.294597
C	1.768741	-2.670882	-0.009026
C	1.750220	-3.896916	0.702456
C	2.710464	-4.182133	1.689138
C	3.721989	-3.253561	1.990844
C	3.764151	-2.036747	1.281132
C	0.767618	-2.329588	-1.080933
C	0.029262	-3.502326	-1.732762
O	1.106574	-1.309947	-1.898284
Pt	-0.462463	-0.605852	-0.652710
C	-0.704775	1.351252	-1.382691
N	-0.638346	1.709871	-2.713442
C	-0.749005	3.086394	-2.874008
C	-0.882329	3.622741	-1.620206
N	-0.856492	2.555320	-0.726912
C	-0.442098	0.753437	-3.826563
C	-1.697392	0.677731	-4.706702
C	-0.877965	2.694378	0.740546
C	0.446669	3.285796	1.247700
C	-1.866920	-0.847694	0.744548
N	-1.713230	-1.098734	2.100716
C	-2.945444	-1.190472	2.741859
C	-3.908439	-1.004734	1.786677
N	-3.245123	-0.792301	0.581061
C	-0.409646	-1.314823	2.758357
C	-0.063685	-0.159744	3.709979
C	-3.902104	-0.643391	-0.728276
C	-4.450620	-1.992443	-1.220030
C	-4.968993	0.459586	-0.702267
C	-0.365927	-2.681268	3.457246
C	-2.105096	3.486249	1.212839
C	0.829591	1.088790	-4.617867
H	-0.656424	-3.114478	-2.515027

H	-0.577665	-4.085683	-1.006514
H	0.747923	-4.207168	-2.221148
H	-3.041260	-1.380095	3.816643
H	-5.000730	-1.009343	1.871917
H	-0.722032	3.575797	-3.854168
H	-0.987263	4.666068	-1.302522
H	-3.068721	-0.333577	-1.397756
H	-4.542260	1.419650	-0.339163
H	-5.366210	0.624986	-1.727457
H	-5.833267	0.193636	-0.052269
H	-3.638662	-2.750151	-1.257619
H	-4.874960	-1.887700	-2.242963
H	-5.257420	-2.372885	-0.552699
H	0.314217	-1.320701	1.914168
H	-0.646198	-3.492253	2.752717
H	0.667056	-2.885398	3.810484
H	-1.046271	-2.722243	4.338813
H	-0.056157	0.812351	3.171673
H	0.947585	-0.317762	4.143865
H	-0.789503	-0.088669	4.552336
H	-0.959204	1.645362	1.096373
H	-3.044335	3.035481	0.825130
H	-2.153646	3.479503	2.323417
H	-2.068154	4.550700	0.888483
H	1.303436	2.662193	0.913821
H	0.452275	3.319137	2.359182
H	0.600746	4.324291	0.875958
H	-0.274728	-0.221193	-3.319413
H	1.710498	1.118282	-3.942131
H	1.012805	0.297097	-5.376134
H	0.753185	2.062117	-5.155242
H	-2.590774	0.409468	-4.101731
H	-1.564823	-0.101519	-5.488650
H	-1.903949	1.643032	-5.223650
H	0.974919	-4.647981	0.480756
H	2.672037	-5.148529	2.221806
H	4.478776	-3.480453	2.760772

H	4.562997	-1.304520	1.492759
H	2.846468	-0.815070	-0.279221

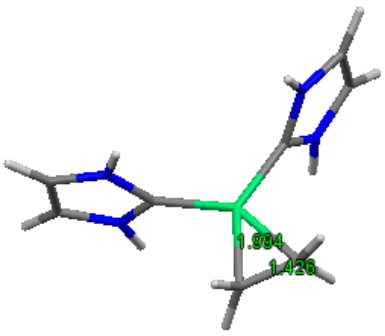
[Ni(H_2Im)$_2$(η^2-C_2H_4)] (C_{2v})

Molecular formula: $C_8H_{12}N_4Ni$

ZORA-BLYP/TZ2P DFTB-D3-BJ

TBE [h]: -5.35478555

Imaginary frequencies [cm^{-1}]: -1.88, -26.12, -36.25

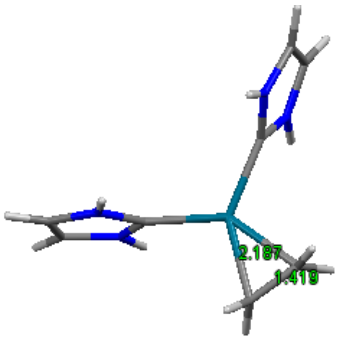


Cartesian coordinates:

Ni	0.000000	0.000000	0.758188
C	-1.575906	0.000000	-0.251421
C	1.575906	0.000000	-0.251421
N	-2.338384	-1.068249	-0.693472
N	-2.338384	1.068249	-0.693472
N	2.338384	-1.068249	-0.693472
N	2.338384	1.068249	-0.693472
C	3.505716	0.679695	-1.358255
H	4.215033	1.383154	-1.765092
C	3.505716	-0.679695	-1.358255
H	4.215033	-1.383154	-1.765092
C	-3.505716	-0.679695	-1.358255
H	-4.215033	-1.383154	-1.765092
C	-3.505716	0.679695	-1.358255
H	-4.215033	1.383154	-1.765092
H	-2.064370	-2.022338	-0.511604
H	-2.064370	2.022338	-0.511604
H	2.064370	-2.022338	-0.511604
H	2.064370	2.022338	-0.511604
C	-0.712836	0.000000	2.620217
C	0.712836	0.000000	2.620217
H	1.262086	0.913888	2.854818
H	1.262086	-0.913888	2.854818
H	-1.262086	-0.913888	2.854818

H -1.262086 0.913888 2.854818

[Pd(H_2Im)$_2$(η^2-C_2H_4)] (C_{2v})



Molecular formula: $C_8H_{12}N_4Pd$

ZORA-BLYP/TZ2P DFTB-D3-BJ

TBE [h]: -5.28451427

Imaginary frequencies: none

Cartesian coordinates:

Pd	0.000000	0.000000	0.849884
C	-1.719408	0.000000	-0.313807
C	1.719408	0.000000	-0.313807
N	-2.458135	-1.065463	-0.784258
N	-2.458135	1.065463	-0.784258
N	2.458135	-1.065463	-0.784258
N	2.458135	1.065463	-0.784258
C	3.593409	0.680129	-1.504276
H	4.283197	1.384300	-1.942619
C	3.593409	-0.680129	-1.504276
H	4.283197	-1.384300	-1.942619
C	-3.593409	-0.680129	-1.504276
H	-4.283197	-1.384300	-1.942619
C	-3.593409	0.680129	-1.504276
H	-4.283197	1.384300	-1.942619
H	-2.185020	-2.018460	-0.593782
H	-2.185020	2.018460	-0.593782
H	2.185020	-2.018460	-0.593782
H	2.185020	2.018460	-0.593782
C	-0.709310	0.000000	2.918650
C	0.709310	0.000000	2.918650
H	1.255911	0.916849	3.138359
H	1.255911	-0.916849	3.138359
H	-1.255911	-0.916849	3.138359
H	-1.255911	0.916849	3.138359

[Pt(H_2Im)$_2$(η^2-C_2H_4)] (C_{2v})

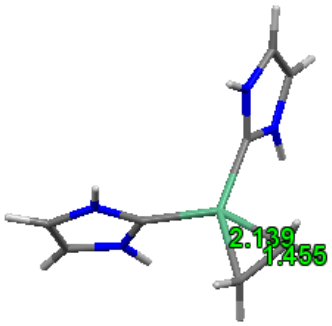
Molecular formula: $C_8H_{12}N_4Pt$

ZORA-BLYP/TZ2P DFTB-D3-BJ

TBE [h]: -5.37312991

Imaginary frequencies: none

Cartesian coordinates:



Pt	0.000000	0.000000	0.855882
C	-1.651782	0.000000	-0.330590
C	1.651782	0.000000	-0.330590
N	-2.388032	-1.068476	-0.801122
N	-2.388032	1.068476	-0.801122
N	2.388032	-1.068476	-0.801122
N	2.388032	1.068476	-0.801122
C	3.525303	0.680040	-1.514263
H	4.216586	1.383836	-1.950276
C	3.525303	-0.680040	-1.514263
H	4.216586	-1.383836	-1.950276
C	-3.525303	-0.680040	-1.514263
H	-4.216586	-1.383836	-1.950276
C	-3.525303	0.680040	-1.514263
H	-4.216586	1.383836	-1.950276
H	-2.117532	-2.019973	-0.600073
H	-2.117532	2.019973	-0.600073
H	2.117532	-2.019973	-0.600073
H	2.117532	2.019973	-0.600073
C	-0.727596	0.000000	2.867052
C	0.727596	0.000000	2.867052
H	1.257371	0.910426	3.152605
H	1.257371	-0.910426	3.152605
H	-1.257371	-0.910426	3.152605
H	-1.257371	0.910426	3.152605

[Ni(H_2Im)$_3$]

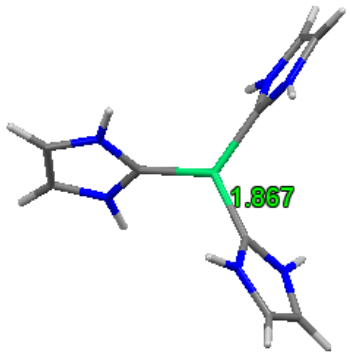
Molecular formula: $C_9H_{12}N_6Ni$

ZORA-BLYP/TZ2P DFTB-D3-BJ

TBE [h]: -6.21054895

Imaginary frequencies : none

Cartesian coordinates:



Ni	0.891389	-0.326492	-0.107637
C	0.765022	-1.052211	-1.824227
N	-0.092106	-0.720221	-2.874768
N	1.504452	-2.075163	-2.420223
C	0.112864	-1.484102	-4.027487
C	1.123949	-2.346979	-3.737688
H	-0.461871	-1.357593	-4.932011
H	1.591045	-3.107387	-4.344396
C	0.550707	-1.389156	1.390319
N	-0.624368	-2.032394	1.782632
N	1.398024	-1.759380	2.436044
C	-0.500740	-2.743691	2.979766
C	0.782216	-2.567162	3.396561
H	-1.311727	-3.298658	3.425657
H	1.292185	-2.941905	4.270621
C	1.359805	1.468010	0.110915
N	0.626000	2.524875	0.652443
N	2.542424	2.130998	-0.221533
C	1.313229	3.742331	0.651517
C	2.528384	3.493105	0.092977
H	0.893385	4.659853	1.034085
H	3.360082	4.153682	-0.097753
H	2.181912	-2.602896	-1.890575
H	-0.725415	0.061753	-2.801182
H	-1.439862	-2.032278	1.188538
H	2.333258	-1.386890	2.503584
H	-0.277149	2.368139	1.073986
H	3.281152	1.657588	-0.719638

[Pd(H_2Im)$_3$]

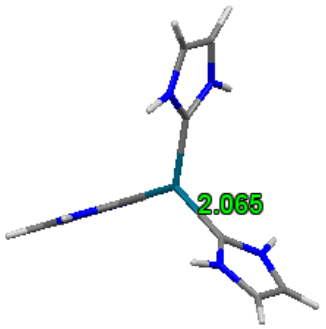
Molecular formula: $C_9H_{12}N_6Pd$

ZORA-BLYP/TZ2P DFTB-D3-BJ

TBE [h]: -6.13910722

Imaginary frequencies: none

Cartesian coordinates:



Pd	0.892340	-0.322000	-0.107292
C	0.753445	-1.128613	-2.002871
N	-0.336710	-1.199849	-2.858137
N	1.724410	-1.749795	-2.775113
C	-0.053010	-1.824760	-4.077308
C	1.259930	-2.175083	-4.024418
H	-0.786404	-1.963672	-4.856511
H	1.883181	-2.675974	-4.748981
C	0.513132	-1.499383	1.545922
N	-0.680666	-1.731470	2.213745
N	1.381254	-2.278330	2.297330
C	-0.553421	-2.597478	3.305175
C	0.760032	-2.945824	3.358425
H	-1.382472	-2.884595	3.933327
H	1.288162	-3.592885	4.041603
C	1.410386	1.661991	0.134601
N	0.601947	2.787778	0.198072
N	2.663639	2.239597	0.278569
C	1.313473	3.980069	0.369984
C	2.626771	3.630875	0.421245
H	0.840486	4.947436	0.439319
H	3.510762	4.237427	0.543545
H	2.666998	-1.866984	-2.435870
H	-1.235043	-0.825578	-2.593165
H	-1.541086	-1.299672	1.912882
H	2.362586	-2.334769	2.071295
H	-0.401380	2.716384	0.123731
H	3.501828	1.678596	0.275862

[Pt(H_2Im)$_3$]

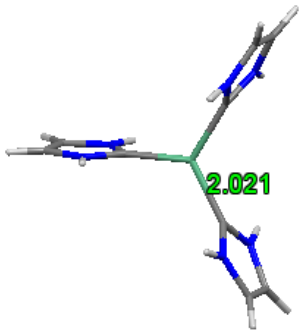
Molecular formula: $C_9H_{12}N_6Pt$

ZORA-BLYP/TZ2P DFTB-D3-BJ

TBE [h]: -6.22972385

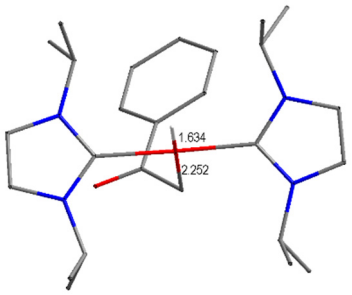
Imaginary frequencies: none

Cartesian coordinates:



Pt	0.891675	-0.325539	-0.114360
C	0.755931	-1.114334	-1.970646
N	-0.339148	-1.185217	-2.827768
N	1.732036	-1.735949	-2.745044
C	-0.049728	-1.809190	-4.045320
C	1.262896	-2.158207	-3.992890
H	-0.781965	-1.948611	-4.825204
H	1.885364	-2.657826	-4.718646
C	0.520509	-1.478163	1.504213
N	-0.678196	-1.709186	2.174069
N	1.392987	-2.260027	2.256835
C	-0.545368	-2.575265	3.263923
C	0.767245	-2.924353	3.316384
H	-1.373256	-2.862460	3.893195
H	1.294081	-3.571832	3.999814
C	1.399016	1.616935	0.121545
N	0.586415	2.745967	0.183680
N	2.657555	2.194973	0.265954
C	1.302609	3.934804	0.354729
C	2.615199	3.585610	0.406877
H	0.831035	4.902667	0.423129
H	3.498303	4.193091	0.529075
H	2.674552	-1.852570	-2.406386
H	-1.237630	-0.812306	-2.562647
H	-1.538322	-1.276960	1.874100
H	2.373840	-2.317399	2.030445
H	-0.416579	2.674976	0.108933
H	3.495520	1.634228	0.264276

trans-[Pt(*i*Pr$_2$Im)$_2$(C̲H$_2$C(O)Ph)H]



Def2-SV(P)/BP86

Molecular formula: $C_{26}H_{40}N_4PtO$

SCF-energy + E(vib0) [h]: -1427.0781461

E(vib0) [h]: 0.6003082

Imaginary frequencies: none

Def2-TZVPP/BP86

SCF-energy + E(vib0) [h]: -1428.6110258

E(vib0) [h]: 0.5970411

Imaginary frequencies: none

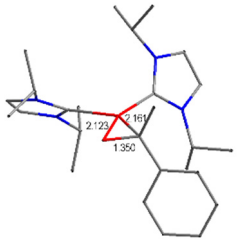
Cartesian coordinates:

N	-0.441492	-0.392521	-0.103135
C	0.466783	-1.146915	0.606407
N	1.501949	-1.344238	-0.280585
C	1.247350	-0.722699	-1.499625
C	0.021641	-0.121503	-1.387099
Pt	0.339085	-1.751921	2.549926
C	0.293332	-3.923611	1.954037
C	2.748851	-2.058201	0.057924
C	3.931812	-1.080565	0.125299
C	-1.688952	0.143884	0.478175
C	-2.905523	-0.191686	-0.394108
C	0.239258	-2.178609	4.549732
N	-0.833298	-1.995986	5.387476
C	-0.508629	-2.328311	6.698157
C	0.800767	-2.729452	6.688736
N	1.240919	-2.627458	5.374014
C	-2.156089	-1.522199	4.938959
C	-3.237850	-2.572741	5.224679
C	2.572234	-3.048916	4.897230

C	2.728502	-4.570315	5.042069
C	3.686953	-2.243105	5.578489
C	-2.472511	-0.141623	5.532695
C	2.994522	-3.236304	-0.894423
C	-1.546437	1.646650	0.761784
H	0.485307	-0.173841	2.982543
H	2.550268	-2.785388	3.816882
H	1.944068	-0.761149	-2.344163
H	-0.552036	0.461521	-2.115653
H	-1.226552	-2.263821	7.522904
H	1.441026	-3.086004	7.502489
H	-2.029541	-1.420294	3.837844
H	3.736710	-2.447643	6.672130
H	3.536462	-1.151249	5.432635
H	4.672591	-2.520613	5.144519
H	2.551000	-2.448702	1.079452
H	-1.769750	-0.394228	1.448702
H	-2.570025	-0.183276	6.641384
H	-3.435690	0.236457	5.124977
H	-1.674095	0.588555	5.277336
H	-2.460409	2.028904	1.267108
H	-1.407842	2.228923	-0.177481
H	-0.676968	1.832509	1.428222
H	2.815584	-4.868648	6.112030
H	3.649535	-4.914017	4.520894
H	1.840914	-5.079898	4.604524
H	3.720032	-0.258955	0.842781
H	4.152554	-0.631169	-0.869729
H	4.847401	-1.612243	0.465507

H	2.123120	-3.925537	-0.906591
H	3.884396	-3.812894	-0.559907
H	3.189938	-2.896399	-1.936891
H	-3.836172	0.132805	0.120130
H	-2.979191	-1.285293	-0.576419
H	-2.871854	0.328486	-1.377919
H	-4.202633	-2.257749	4.770618
H	-3.407154	-2.703907	6.317817
H	-2.949988	-3.554361	4.791550
C	-0.713465	-4.665730	2.724039
H	0.140340	-3.972948	0.857147
H	1.307629	-4.290232	2.220501
O	-0.491034	-5.170288	3.843055
C	-2.115180	-4.829242	2.145166
C	-2.578714	-4.146570	0.998911
C	-3.878112	-4.363773	0.510088
C	-4.734587	-5.274174	1.154902
C	-4.283391	-5.961855	2.296313
C	-2.988552	-5.735244	2.786624
H	-1.917475	-3.426621	0.490717
H	-4.227028	-3.820225	-0.385100
H	-5.752419	-5.449025	0.766464
H	-4.947852	-6.681249	2.805342
H	-2.607159	-6.257212	3.679451

[Pt(*i*Pr$_2$Im)$_2$(MeC(O)Ph)]]



Def2-SV(P)/BP86

Molecular formula: $C_{26}H_{40}N_4PtO$

SCF-energy + E(vib0) [h]: -1427.0621723

E(vib0) [h]: 0.6022814

Imaginary frequencies: none

Def2-TZVPP/BP86

SCF-energy + E(vib0) [h]: -1428.5951603

E(vib0) [h]: 0.5991885

Imaginary frequencies: none

Cartesian coordinates:

C	2.809255	-1.753983	0.294597
C	1.768741	-2.670882	-0.009026
C	1.750220	-3.896916	0.702456
C	2.710464	-4.182133	1.689138
C	3.721989	-3.253561	1.990844
C	3.764151	-2.036747	1.281132
C	0.767618	-2.329588	-1.080933
C	0.029262	-3.502326	-1.732762
O	1.106574	-1.309947	-1.898284
Pt	-0.462463	-0.605852	-0.652710
C	-0.704775	1.351252	-1.382691
N	-0.638346	1.709871	-2.713442
C	-0.749005	3.086394	-2.874008
C	-0.882329	3.622741	-1.620206
N	-0.856492	2.555320	-0.726912
C	-0.442098	0.753437	-3.826563
C	-1.697392	0.677731	-4.706702
C	-0.877965	2.694378	0.740546
C	0.446669	3.285796	1.247700
C	-1.866920	-0.847694	0.744548
N	-1.713230	-1.098734	2.100716
C	-2.945444	-1.190472	2.741859
C	-3.908439	-1.004734	1.786677
N	-3.245123	-0.792301	0.581061
C	-0.409646	-1.314823	2.758357
C	-0.063685	-0.159744	3.709979

C	-3.902104	-0.643391	-0.728276
C	-4.450620	-1.992443	-1.220030
C	-4.968993	0.459586	-0.702267
C	-0.365927	-2.681268	3.457246
C	-2.105096	3.486249	1.212839
C	0.829591	1.088790	-4.617867
H	-0.656424	-3.114478	-2.515027
H	-0.577665	-4.085683	-1.006514
H	0.747923	-4.207168	-2.221148
H	-3.041260	-1.380095	3.816643
H	-5.000730	-1.009343	1.871917
H	-0.722032	3.575797	-3.854168
H	-0.987263	4.666068	-1.302522
H	-3.068721	-0.333577	-1.397756
H	-4.542260	1.419650	-0.339163
H	-5.366210	0.624986	-1.727457
H	-5.833267	0.193636	-0.052269
H	-3.638662	-2.750151	-1.257619
H	-4.874960	-1.887700	-2.242963
H	-5.257420	-2.372885	-0.552699
H	0.314217	-1.320701	1.914168
H	-0.646198	-3.492253	2.752717
H	0.667056	-2.885398	3.810484
H	-1.046271	-2.722243	4.338813
H	-0.056157	0.812351	3.171673
H	0.947585	-0.317762	4.143865
H	-0.789503	-0.088669	4.552336
H	-0.959204	1.645362	1.096373
H	-3.044335	3.035481	0.825130
H	-2.153646	3.479503	2.323417
H	-2.068154	4.550700	0.888483
H	1.303436	2.662193	0.913821
H	0.452275	3.319137	2.359182
H	0.600746	4.324291	0.875958
H	-0.274728	-0.221193	-3.319413
H	1.710498	1.118282	-3.942131
H	1.012805	0.297097	-5.376134

H	0.753185	2.062117	-5.155242
H	-2.590774	0.409468	-4.101731
H	-1.564823	-0.101519	-5.488650
H	-1.903949	1.643032	-5.223650
H	0.974919	-4.647981	0.480756
H	2.672037	-5.148529	2.221806
H	4.478776	-3.480453	2.760772
H	4.562997	-1.304520	1.492759
H	2.846468	-0.815070	-0.279221

5. References

[S1] J. Attner, U. Radius, *Chem. Eur. J.* **2001**, *7*, 783.

[S2] T. Schaub, U. Radius, A. Brucks, M. P. Choules, M. T. Olsen, T. B. Rauchfuss, *Inorg. Synth.* **2010**, *35*, 78–83.

[S3] (a) P. S. Pregosin, *NMR in Organometallic Chemistry, Vol. 1*, Wiley-VCH, Weinheim, **2012**, pp. 15; (b) P. S. Pregosin, *Group 10: Nickel to Platinum,* in: *Transition Metal Nuclear Magnetic Resonance*, Elsevier, Amsterdam, **1991**.

[S4] N. Juranic, *J. Chem. Soc., Dalton Trans.* **1984**, 1537-1540.

[S5] The ^{13}C NHC carbene carbon atom assignment and the unusual shift for a typical NHC coordinated to a transition metal is in accordance with work reported earlier, see for example: (a) A. M. Voutchkova, M. Feliz, E. Clot, O. Eisenstein, R. H. Crabtree, *J. Am. Chem. Soc.* **2007**, *129*, 12834-12846 ([$Pt(Me_2Im)_3Cl]Cl$: 146.35 and 145.56 ppm); (b) S. Fantasia, A. Pasini, S. P. Nolan, *Dalton Trans.* **2009**, 8107-8110 (*cis*-[$Pt(Cy_2Im)_2Cl_2$]: 145.79 ppm).

[S6] G. M. Sheldrick, *Acta Crystallogr. A* **2008**, *64*, 112.

[S7] (a) G. te Velde, F. M. Bickelhaupt, E. J. Baerends, C. Fonseca Guerra, S. J. A. van Gisbergen, J. G. Snijders, T. Ziegler, *J. Comp. Chem.* **2001**, *22*, 931-967; (b) T. Z. E. J. Baerends, J. Autschbach, D. Bashford, A. Bérces, F.M. Bickelhaupt, C. Bo, P. M. Boerrigter, L. Cavallo, D. P. Chong, L. Deng, R. M. Dickson, D. E. Ellis, M. van Faassen, L. Fan, T. H. Fischer, C. Fonseca Guerra, A. Ghysels, A. Giammona, S. J. A. van Gisbergen, A. W. Götz, J. A. Groeneveld, O. V. Gritsenko, M. Grüning, S. Gusarov, F. E. Harris, P. van den Hoek, C. R. Jacob, H. Jacobsen, L. Jensen, J. W. Kaminski, G. van Kessel, F. Kootstra, A. Kovalenko, M. V. Krykunov, E. van Lenthe, D. A. McCormack, A. Michalak, M. Mitoraj, J. Neugebauer, V. P. Nicu, L. Noodleman, V. P. Osinga, S. Patchkovskii, P. H. T. Philipsen, D. Post, C. C. Pye, W. Ravenek, J. I. Rodríguez, P. Ros, P. R. T. Schipper, G. Schreckenbach, J. S. Seldenthuis, M. Seth, J. G. Snijders, M. Solà, M. Swart, D. Swerhone, G. te Velde, P. Vernooijs, L. Versluis, L. Visscher, O. Visser, F. Wang, T.A. Wesolowski, E. M. van Wezenbeek, G. Wiesenekker, S. K. Wolff, T. K. Woo, A. L. Yakovlev, *ADF2010, SCM, Theoretical Chemistry; Vrije Universiteit, Amsterdam, The Netherlands; http://www.scm.com/*; (c) C. Fonseca Guerra, J. G. Snijders, G. te Velde, E. J. Baerends, *Theoretical Chem. Acc.* **1998**, *99*, 391-403.

[S8] (a) P. M. Boerrigter, G. Te Velde, E. J. Baerends, *Int. J. Quant. Chem.* **1988**, *33*, 87-113; (b) G. Te Velde, E. J. Baerends, *J. Comp. Phys.* **1992**, *99*, 84-98.

[S9] E. Van Lenthe, E. J. Baerends, *J. Comp. Phys.* **2003**, *24*, 1142-1156.

[S10] J. C. Slater, *Quantum Theory of Molecules and Solids, Vol. 4*, McGraw-Hill, New York, **1974**.

[S11] (a) A. D. Becke, *J. Chem. Phys.* **1986**, *84*, 4524; (b) A. D. Becke, *Phys. Rev. A* **1988**, *38*, 3098-3100; (c) Perdew, J. P. *Phys. Rev. B* **1986**, *33*, 8822; *erratum*: Perdew, J. P. *Phys. Rev. B* **1986**, *34*, 7406.

[S12] (a) C. Lee, W. Yang, R. G. Parr, *Phys. Rev. B* **1988**, *37*, 785-789; (b) B. G. Johnson, P. M. W. Gill, J. A. Pople, *J. Chem. Phys.* **1993**, *98*, 5612; (c) T. V. Russo, R. L. Martin, P. J. Hay, *J. Chem. Phys.* **1994**, *101*, 7729.

[S13] (a) E. van Lenthe, A. Ehlers, E.-J. Baerends, *J. Chem. Phys.* **1999**, *110*, 8943; (b) E. v. Lenthe, E. J. Baerends, J. G. Snijders, *J. Chem. Phys.* **1993**, *99*, 4597; (c) E. van Lenthe, E. J. Baerends, J. G. Snijders, *J. Chem. Phys.* **1994**, *101*, 9783; (d) E. van Lenthe, J. G. Snijders, E. J. Baerends, *J. Chem. Phys.* **1996**, *105*, 6505.

[S14] (a) G. T. de Jong, F. M. Bickelhaupt, *J. Chem. Theor. Comp.* **2006**, *2*, 322-335; (b) G. T. de Jong, F. M. Bickelhaupt, *J. Phys. Chem. A* **2005**, *109*, 9685-9699; (c) G. T. de Jong, D. P. Geerke, A. Diefenbach, F. Matthias Bickelhaupt, *Chem. Phys.* **2005**, *313*, 261-270; (d) G. T. De Jong, D. P. Geerke, A. Diefenbach, M. Solà, F. M. Bickelhaupt, *J. Comp. Chem.* **2005**, *26*, 1006-1020; (e) G. T. de Jong, M. Solà, L. Visscher, F. M. Bickelhaupt, *J. Chem. Phys.* **2004**, *121*, 9982.

[S15] S. Grimme, S. Ehrlich, L. Goerigk, *J. Comp. Chem.* **2011**, *32*, 1456-1465.

[S16] T. Ziegler, A. Rauk, *Inorg. Chem.* **1979**, *18*, 1755-1759.

[S17] (a) F. Furche, R. Ahlrichs, C. Hättig, W. Klopper, M. Sierka, F. Weigend, *WIREs Comput. Mol. Sci.* **2014**, *4*, 91-100; (b) R. Ahlrichs, M. Bär, M. Häser, H. Horn, C. Kölmel, *Chem. Phys. Lett.* **1989**, *162*, 165-169.

[S18] (a) M. Häser, R. Ahlrichs, *J. Comput. Chem.* **1989**, *10*, 104-111; (b) O. Treutler, R. Ahlrichs, *J. Chem. Phys.* **1995**, *102*, 346-354; (c) K. Eichkorn, O. Treutler, H. Öhm, M. Häser, R. Ahlrichs, *Chem. Phys. Lett.* **1995**, *242*, 652-660 (d) K. Eichkorn, F. Weigend, O. Treutler, R. Ahlrichs, *Theor. Chem. Acc.* **1997**, *97*, 119-124; (e) M. von Arnim, R. Ahlrichs, *J. Comput. Chem.* **1998**, *19*, 1746-1757; (f) M. von Arnim, R. Ahlrichs, *J. Chem. Phys.* **1999**, *111*, 9183-9190; (g) F. Weigend, *Phys. Chem. Chem. Phys.* **2002**, *4*, 4285-4291; (h) P. Deglmann, K. May, F. Furche, R. Ahlrichs, *Chem. Phys. Letters* **2004**, *384*, 103-107; (i) R. Ahlrichs, *Phys. Chem. Chem. Phys.* **2004**, *6*, 5119-5121.

[S19] (a) A. Schäfer, H. Horn, R. Ahlrichs, *J. Chem. Phys.* **1992**, *97*, 2571-2577; (b) F. Weigend, M. Häser, H. Patzelt, R. Ahlrichs, *Chem. Phys. Lett.* **1998**, *294*, 143-152; (c) F. Weigend, R. Ahlrichs, *Phys. Chem. Chem. Phys.* **2005**, *7*, 3297-3305; (d) F. Weigend, *Phys. Chem. Chem. Phys.* **2006**, *8*, 1057-1065.