

Supporting Information

Tridentate Diarylamido-based Pincer Complexes of Nickel and Palladium: Sidearm Effects in Polymerization of Norbornene

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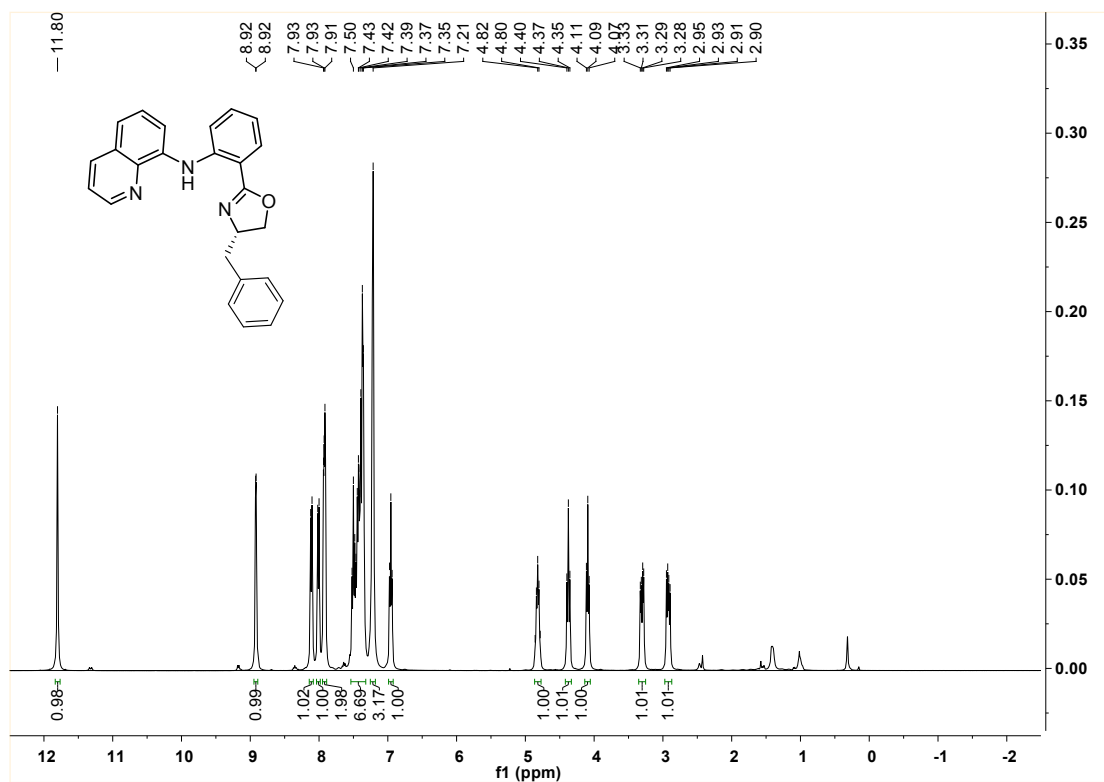


Figure S1 ¹H NMR spectrum of **L1** (400 MHz, CDCl₃, 25 °C)

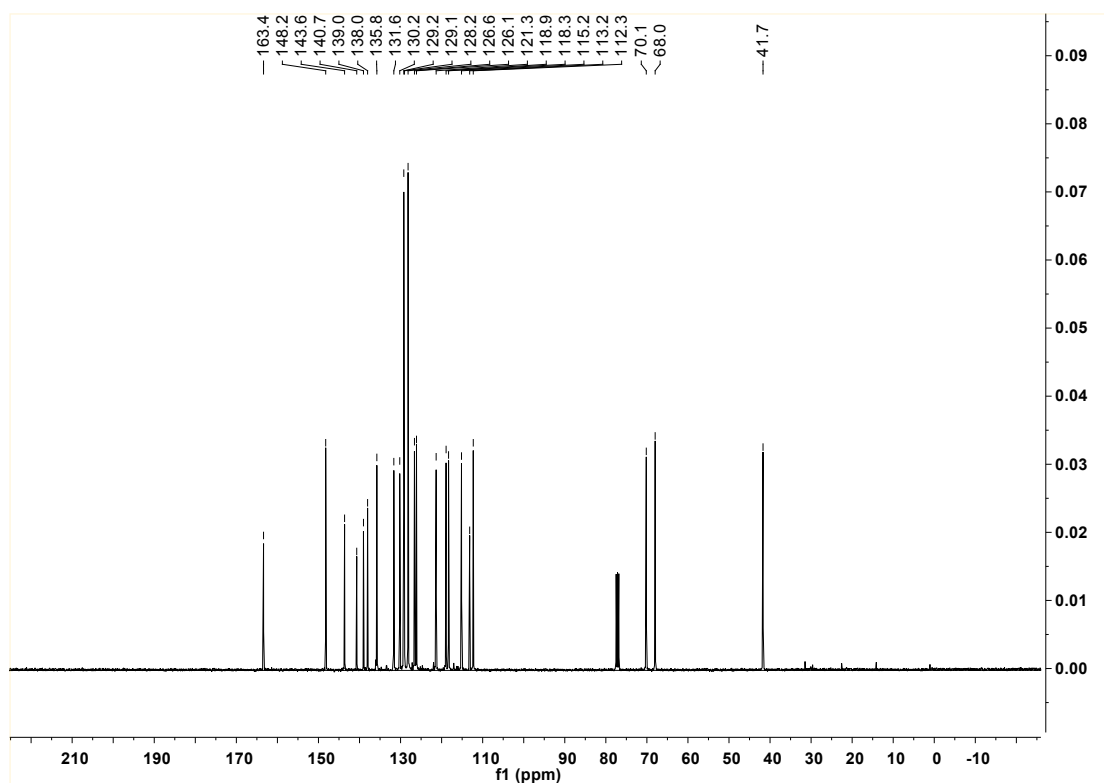


Figure S2 ¹³C NMR spectrum of **L1** (101 MHz, CDCl₃, 25 °C)

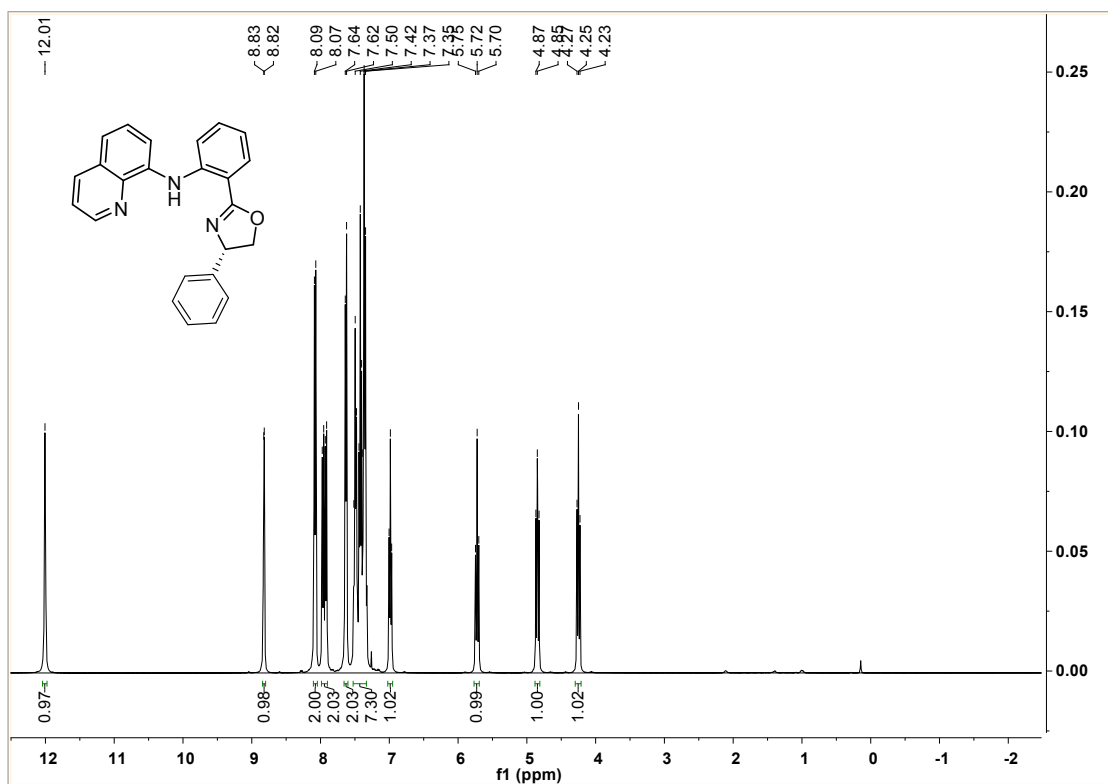


Figure S3 ¹H NMR spectrum of **L2** (400 MHz, CDCl₃, 25 °C)

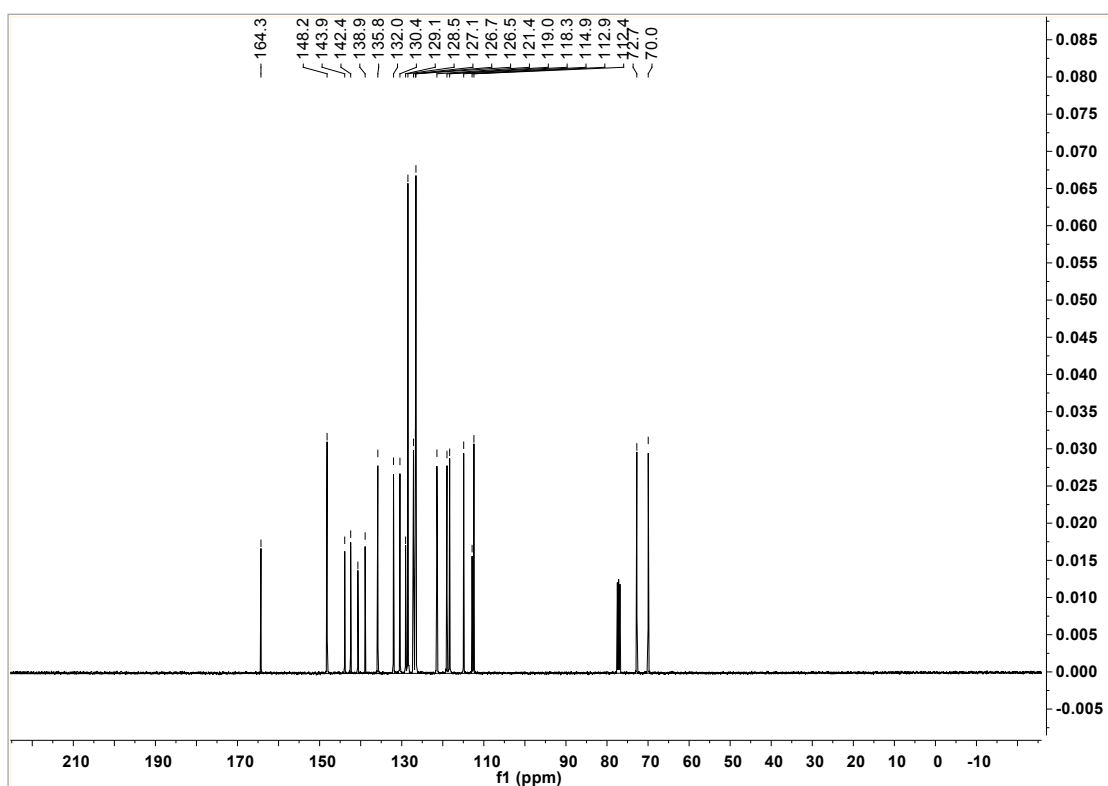


Figure S4 ¹³C NMR spectrum of **L2** (101 MHz, CDCl₃, 25 °C)

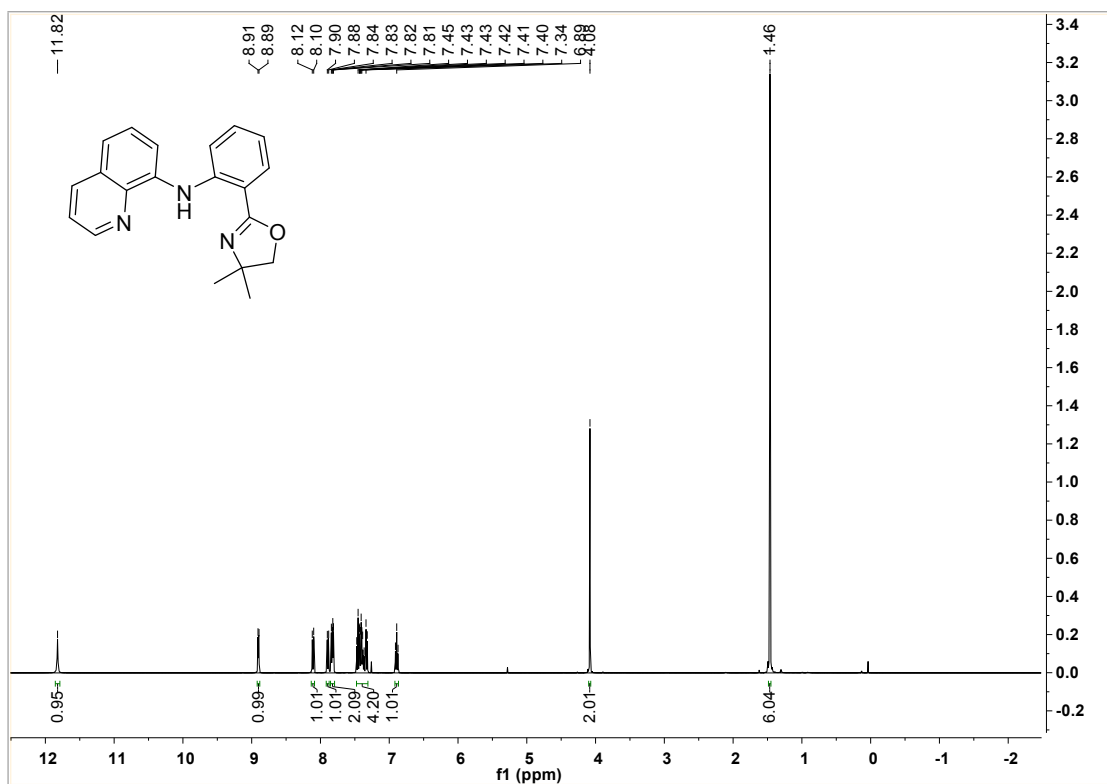


Figure S5 ¹H NMR spectrum of L3 (400 MHz, CDCl₃, 25 °C)

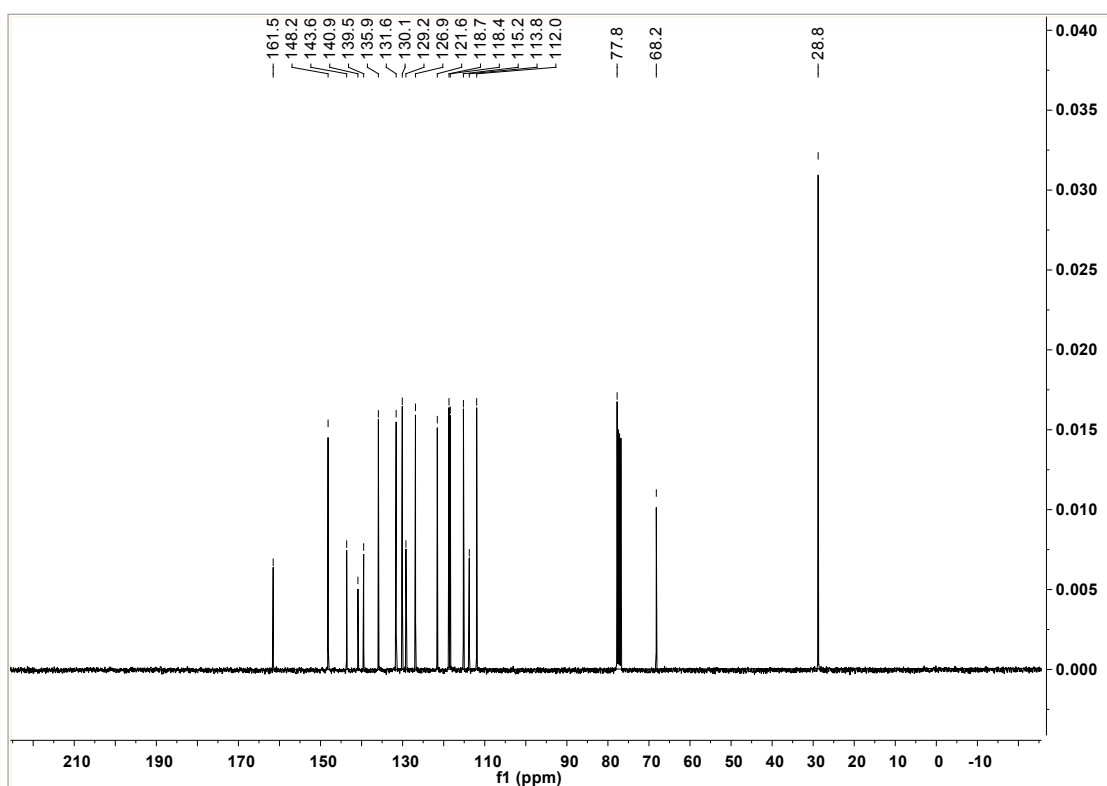


Figure S6 ¹³C NMR spectrum of L3 (101 MHz, CDCl₃, 25 °C)

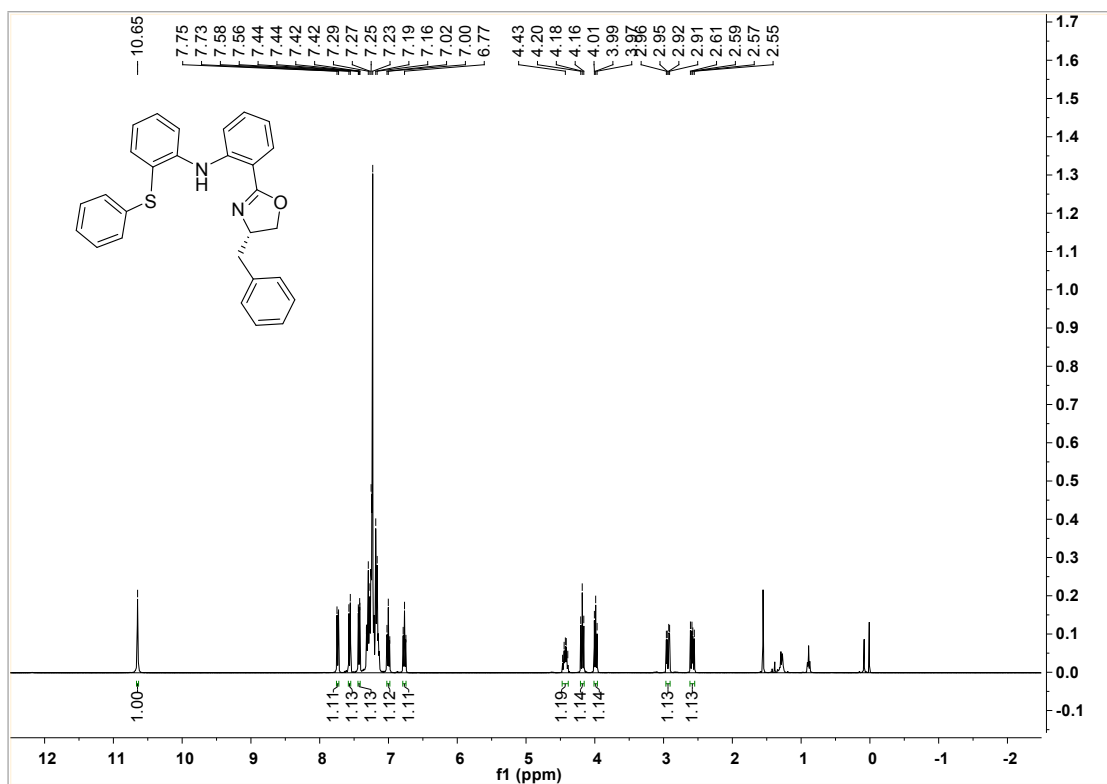


Figure S7 ^1H NMR spectrum of **L4** (400 MHz, CDCl_3 , 25 $^\circ\text{C}$)

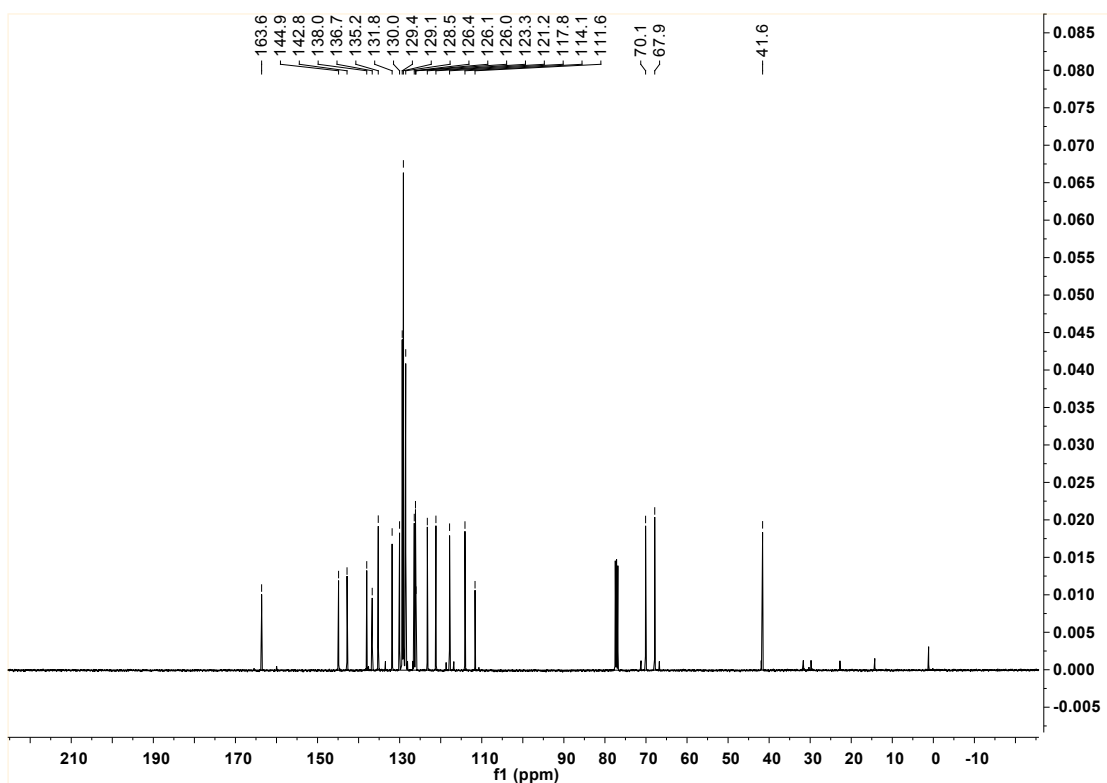


Figure S8 ^{13}C NMR spectrum of **L4** (101 MHz, CDCl_3 , 25 $^\circ\text{C}$)

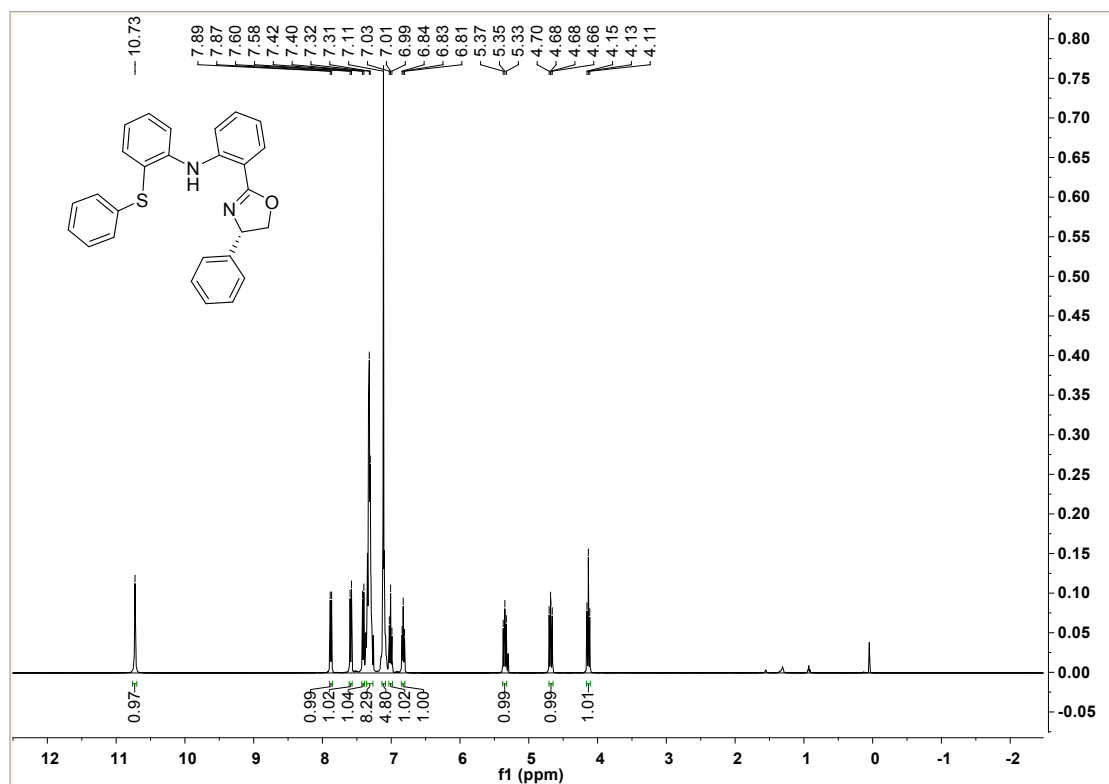


Figure S9 ¹H NMR spectrum of L5 (400 MHz, CDCl₃, 25 °C)

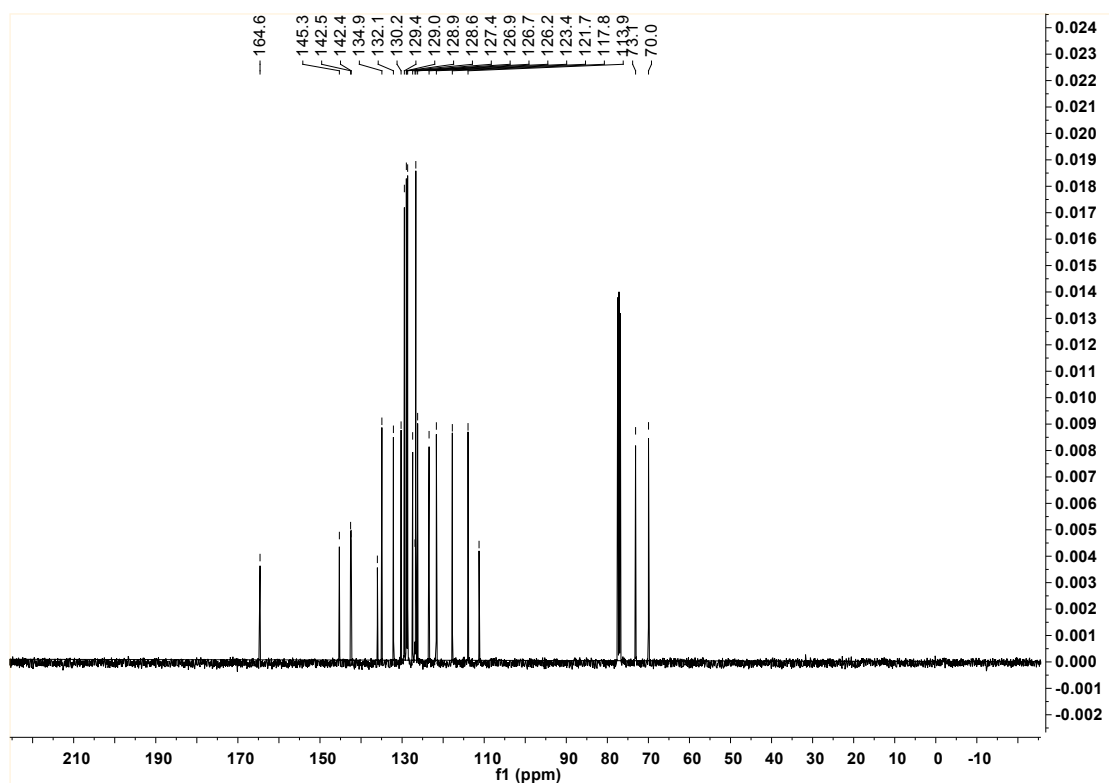


Figure S10 ¹³C NMR spectrum of L5 (101 MHz, CDCl₃, 25 °C)

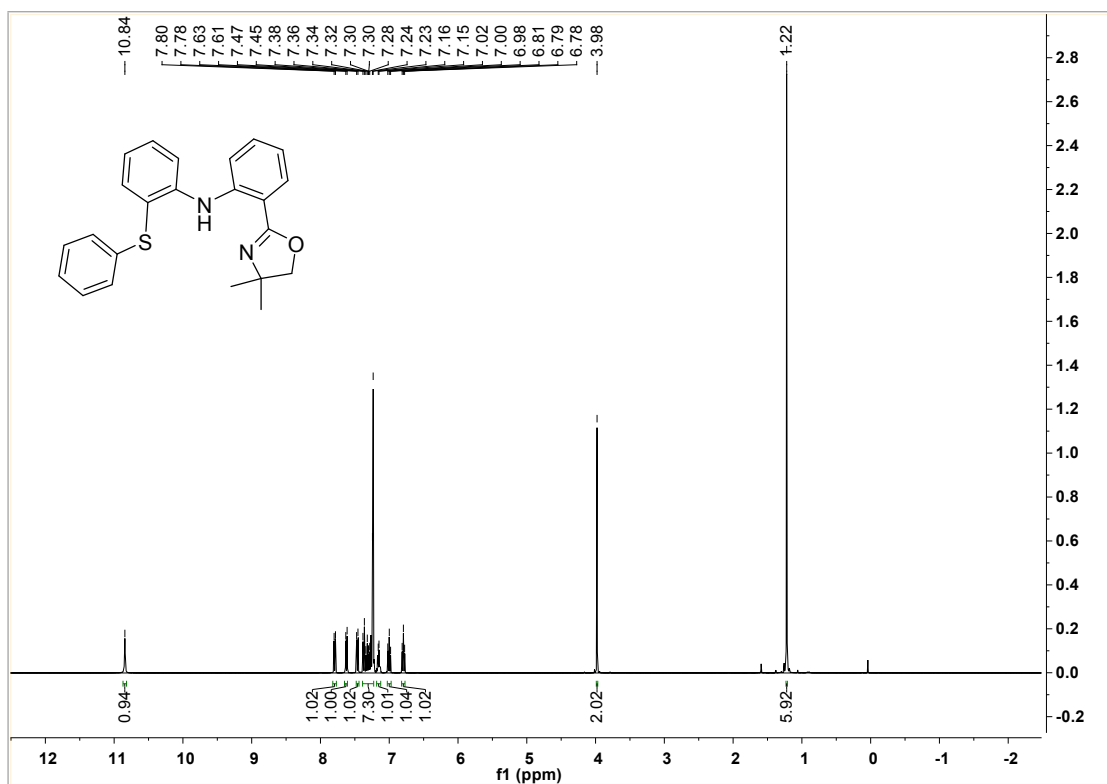


Figure S11 ¹H NMR spectrum of **L6** (400 MHz, CDCl₃, 25 °C)

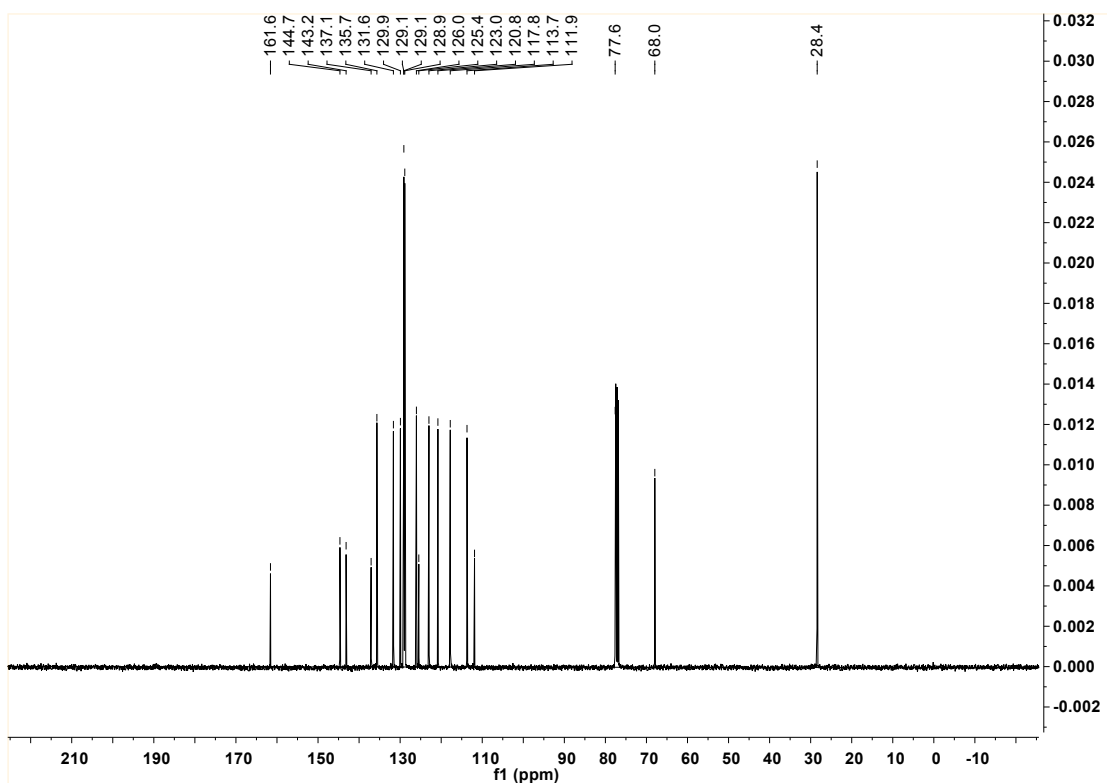


Figure S12 ¹³C NMR spectrum of **L6** (101 MHz, CDCl₃, 25 °C)

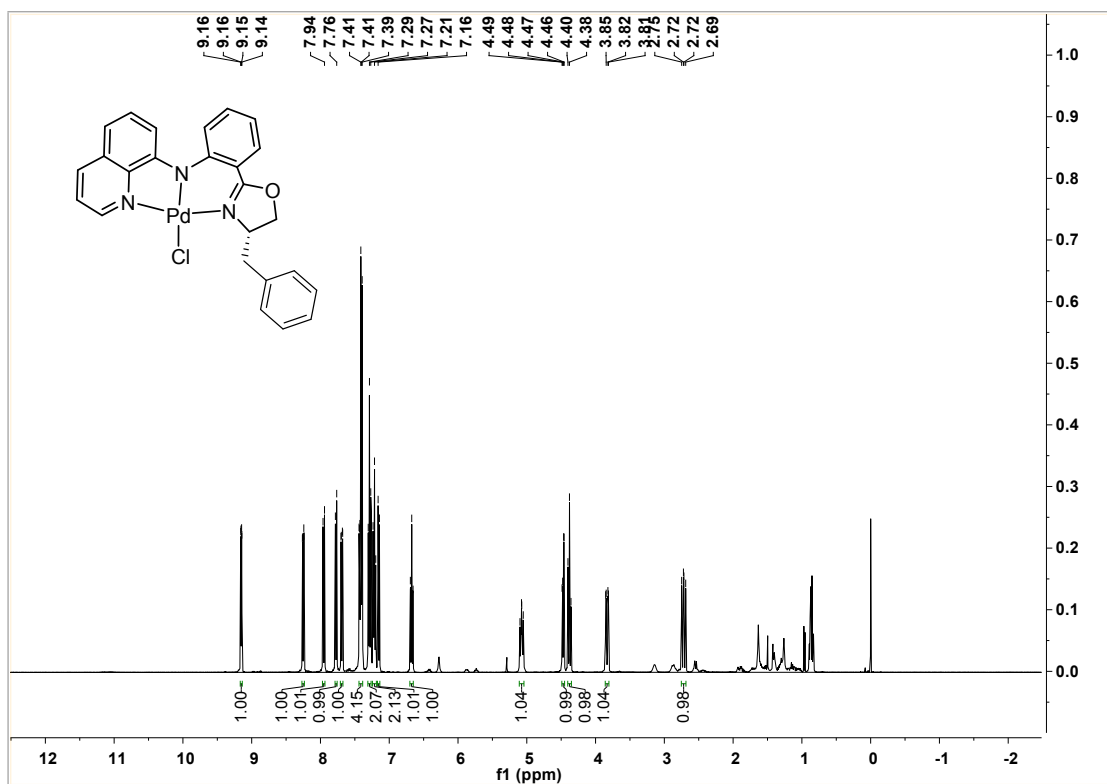


Figure S13 ^1H NMR spectrum of **Pd1** (400 MHz, CDCl_3 , 25 °C)

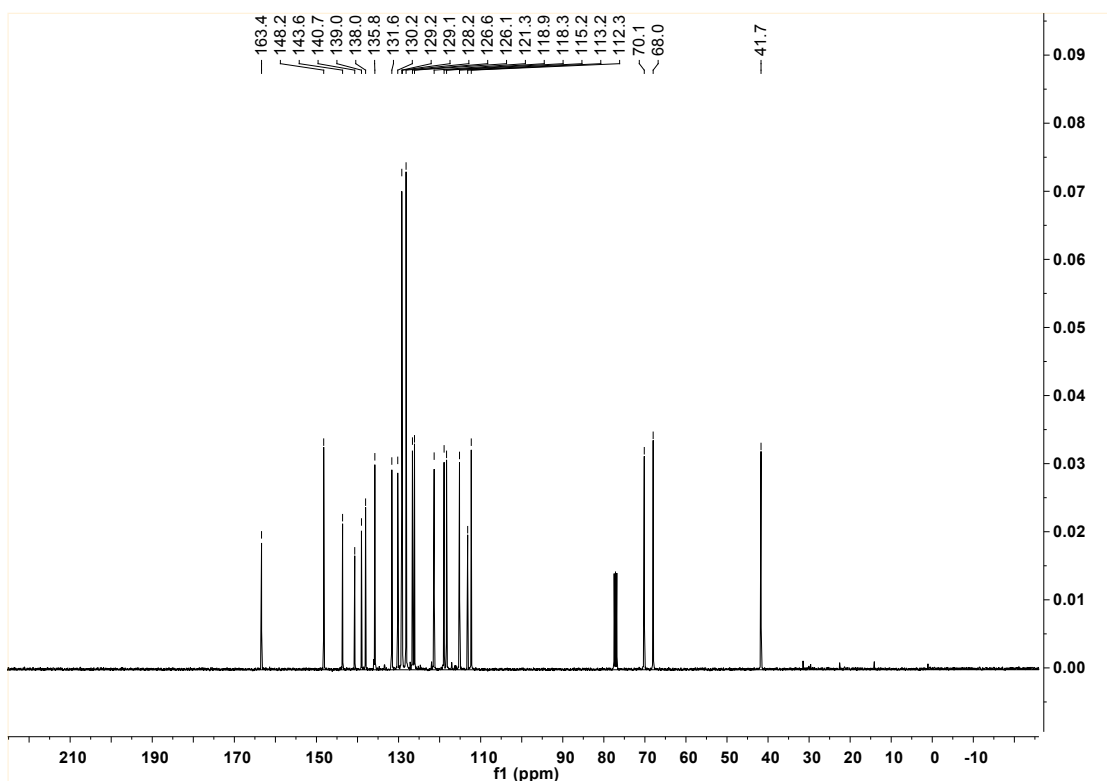


Figure S14 ^{13}C NMR spectrum of **Pd1** (101 MHz, CDCl_3 , 25 °C)

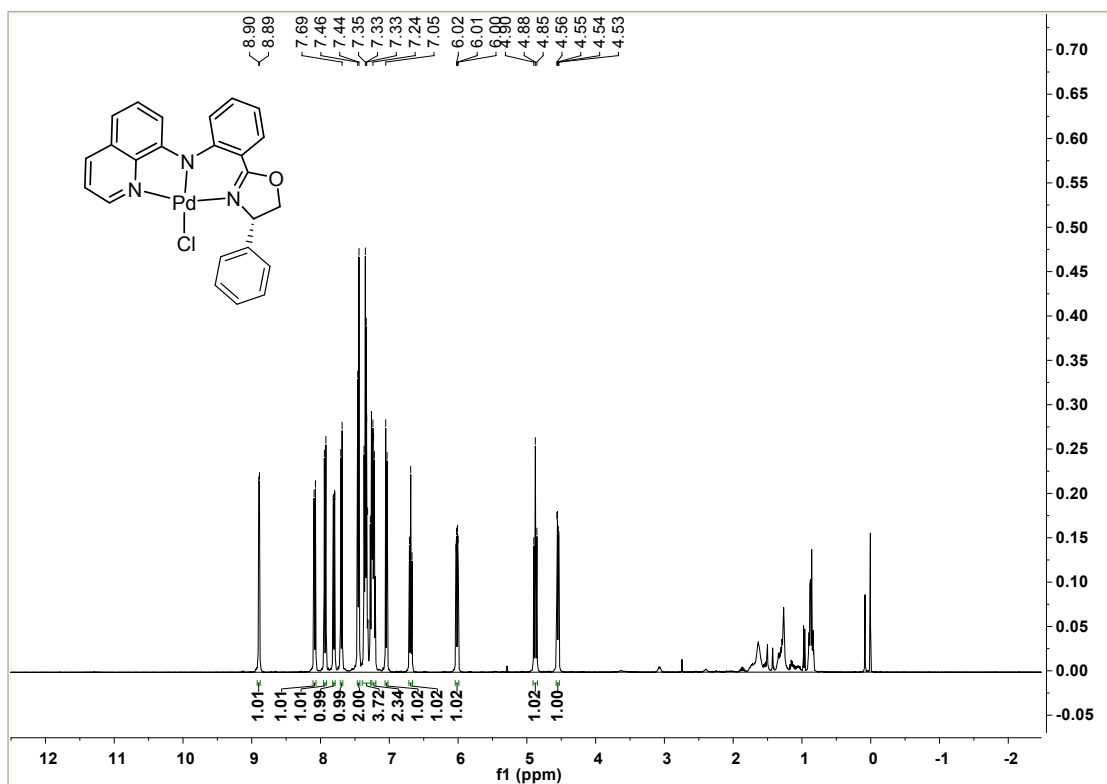


Figure S15 ¹H NMR spectrum of **Pd2** (400 MHz, CDCl₃, 25 °C)

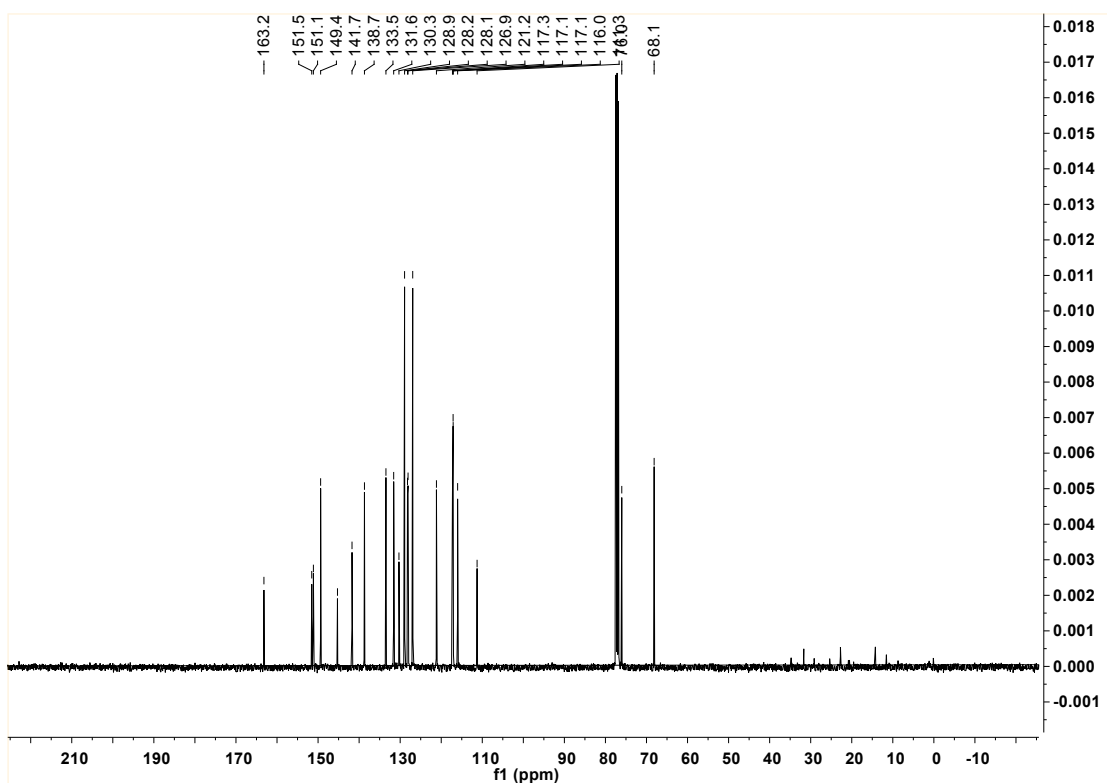


Figure S16 ¹³C NMR spectrum of **Pd2** (101 MHz, CDCl₃, 25 °C)

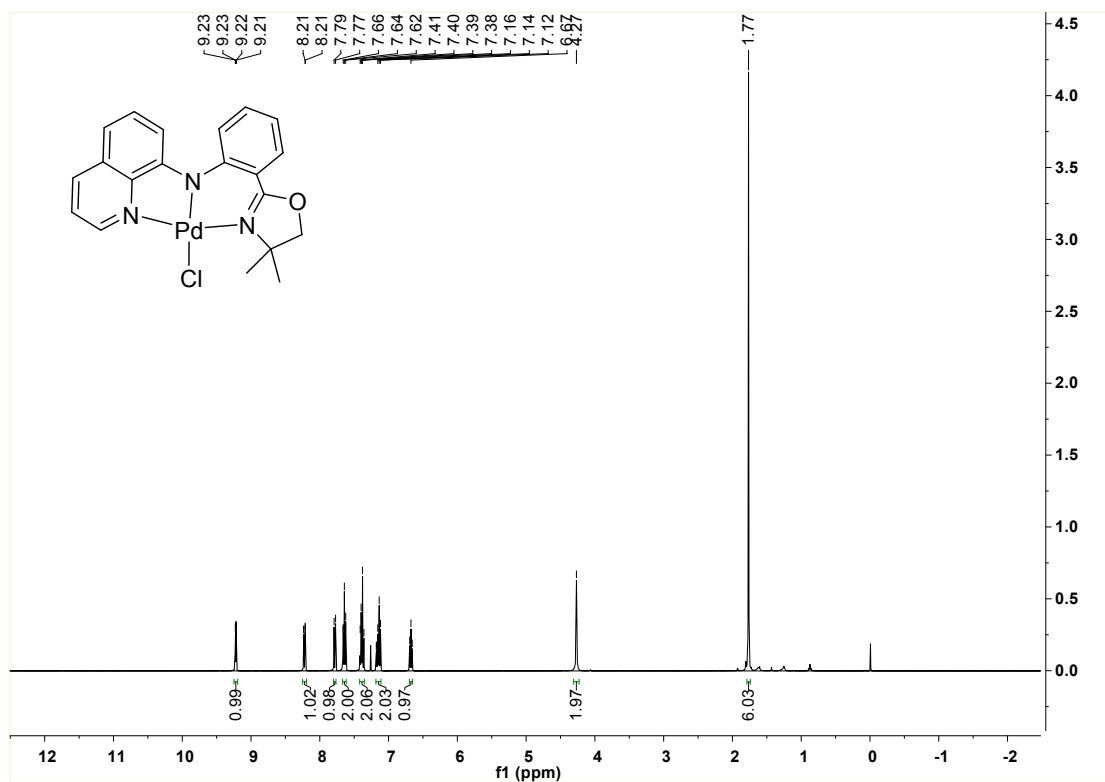


Figure S17 ¹H NMR spectrum of **Pd3** (400 MHz, CDCl₃, 25 °C)

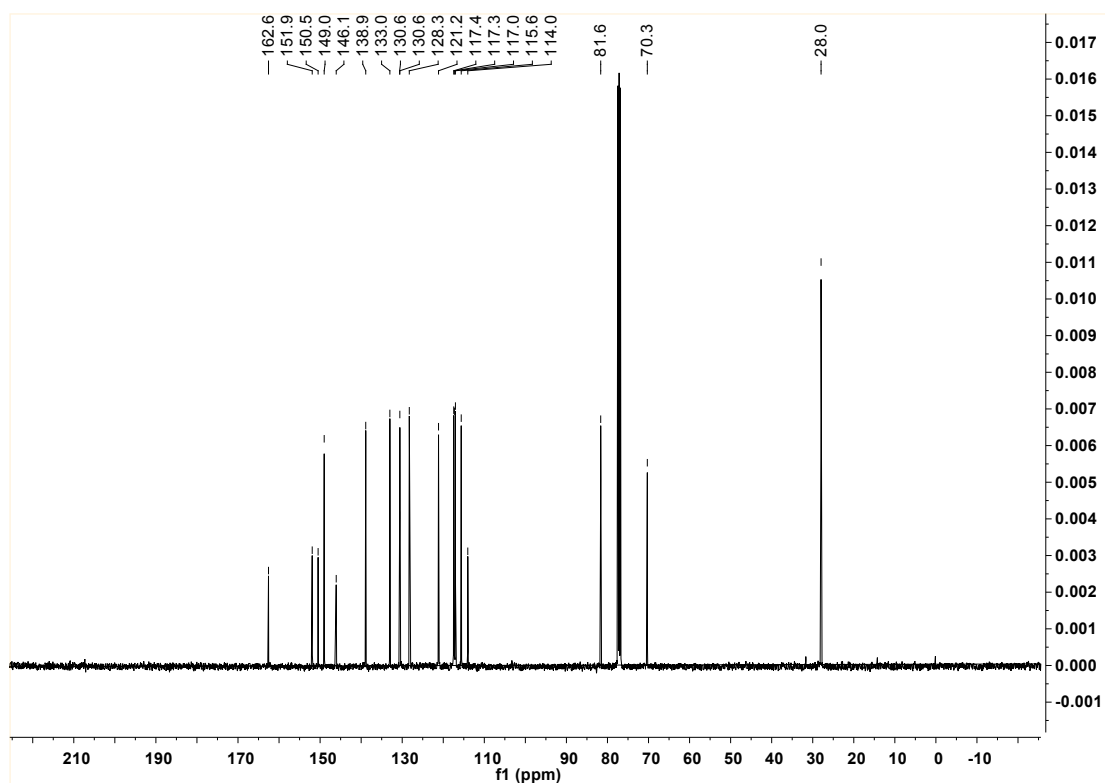


Figure S18 ¹³C NMR spectrum of **Pd3** (101 MHz, CDCl₃, 25 °C)

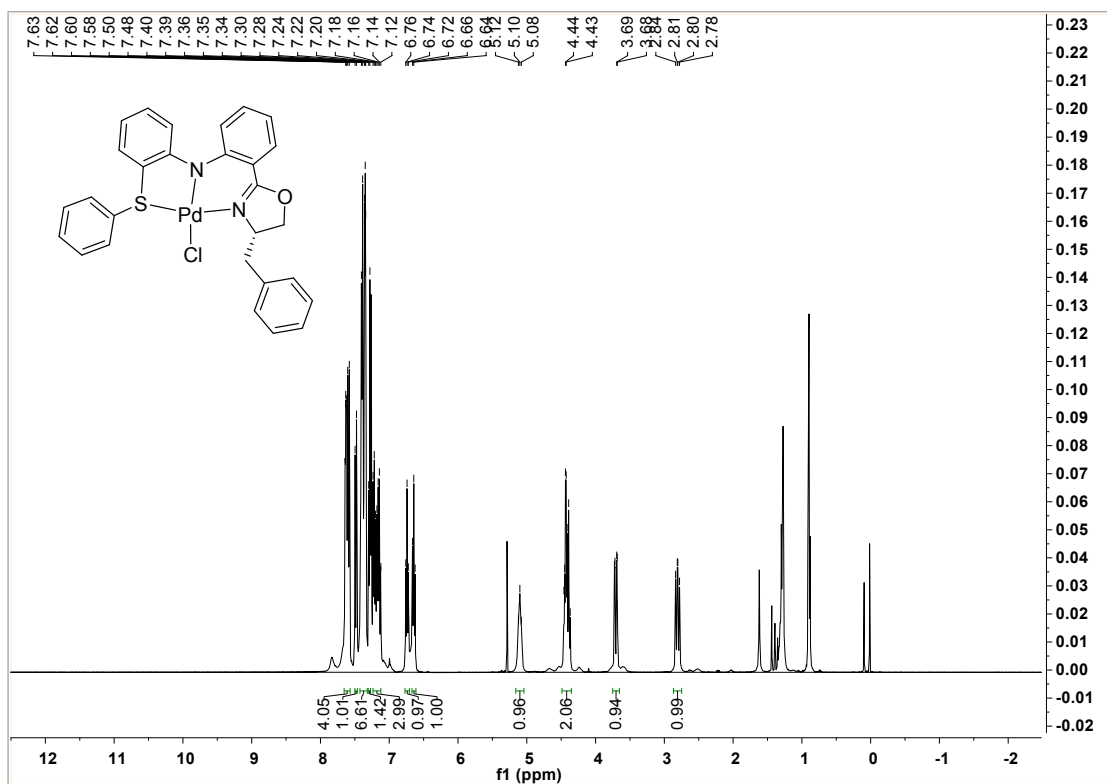


Figure S19 ^1H NMR spectrum of **Pd4** (400 MHz, CDCl_3 , 25 °C)

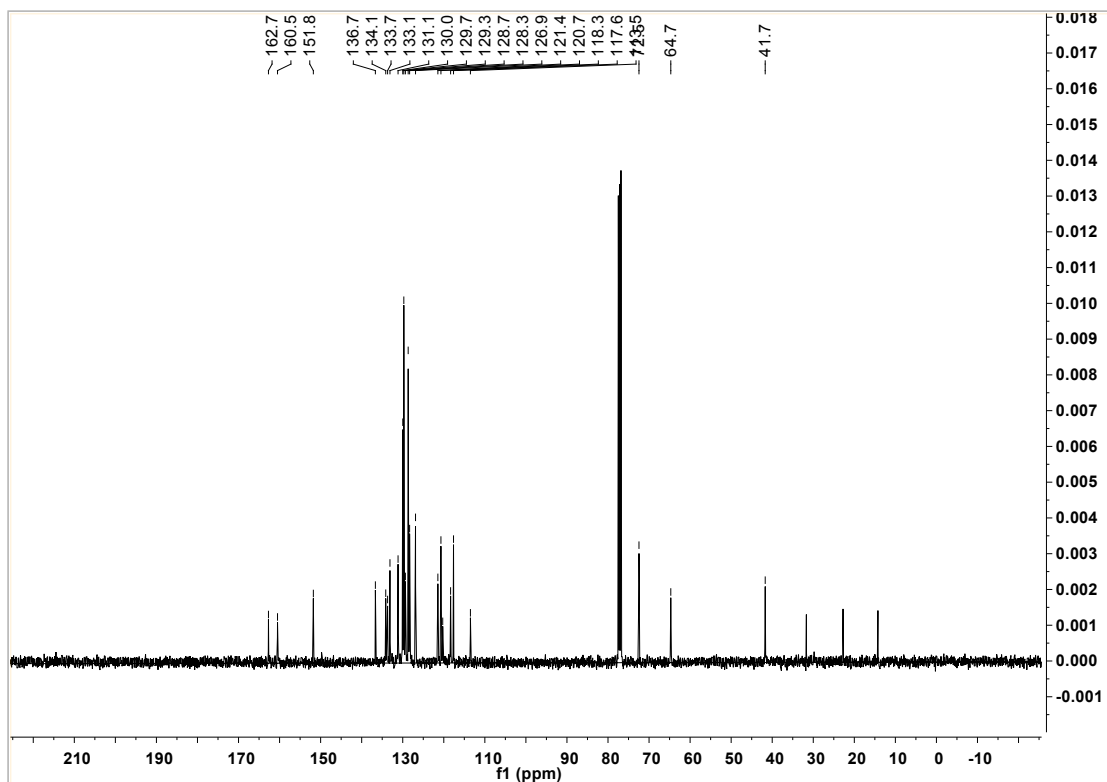


Figure S20 ^{13}C NMR spectrum of **Pd4** (101 MHz, CDCl_3 , 25 °C)

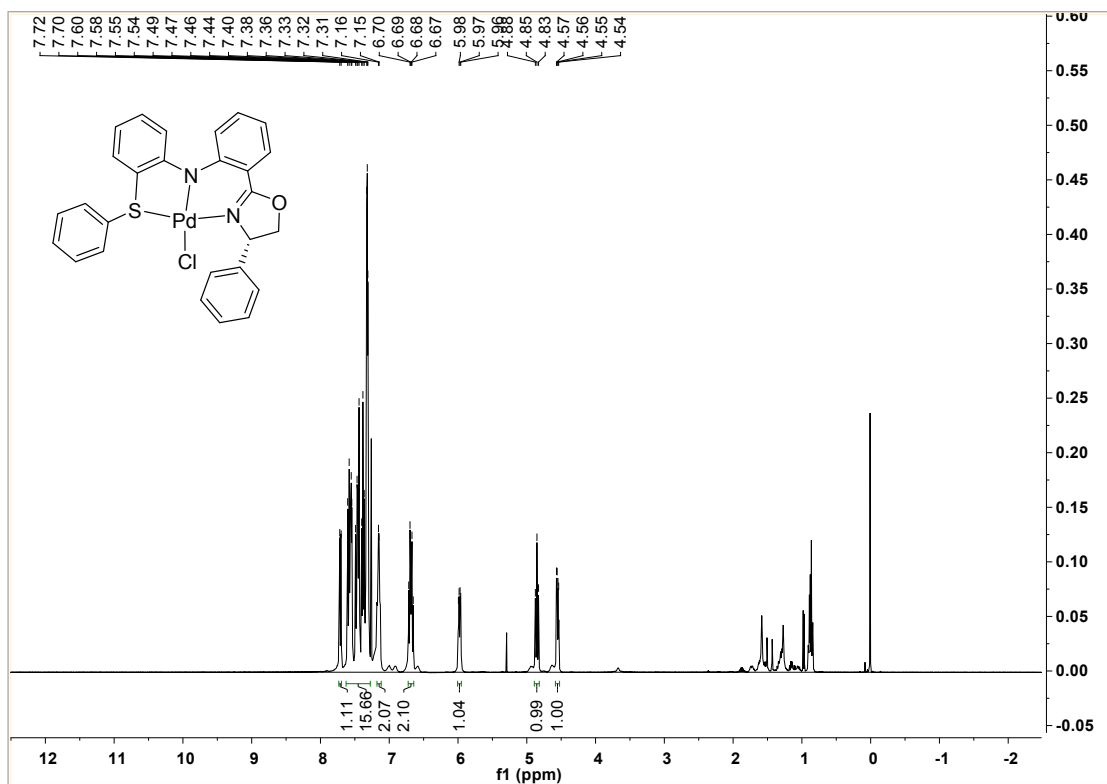


Figure S21 ¹H NMR spectrum of **Pd5** (400 MHz, CDCl₃, 25 °C)

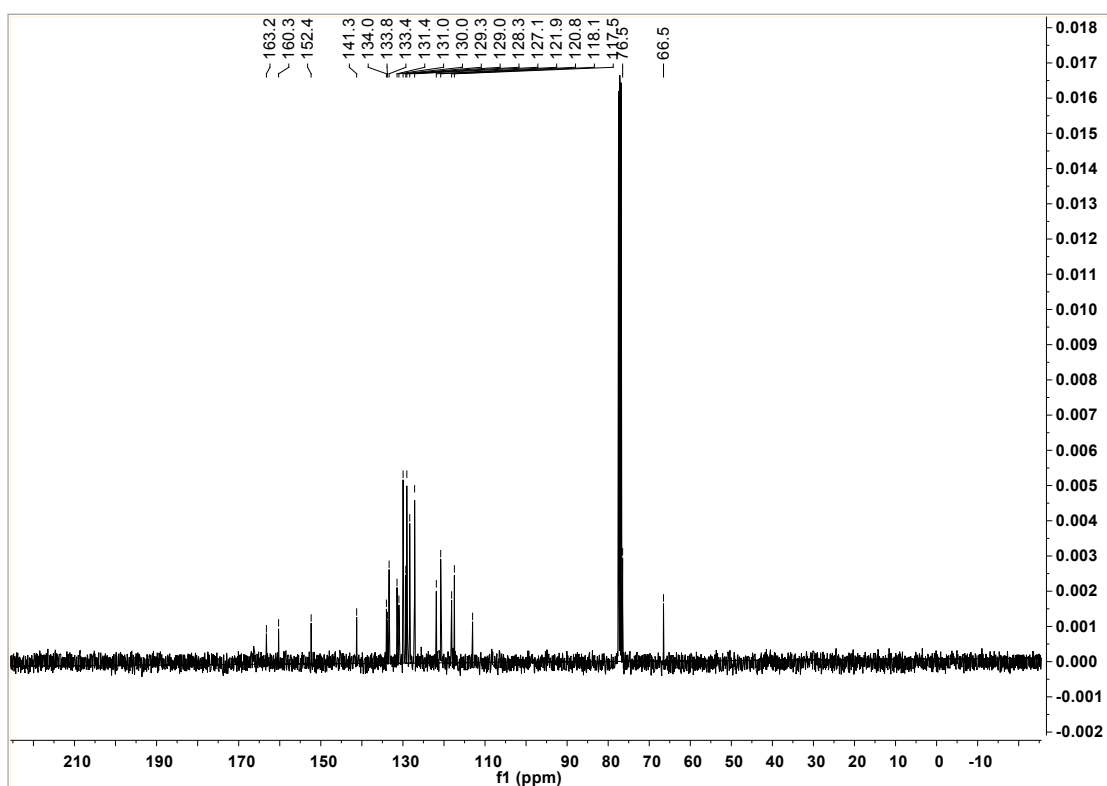


Figure S22 ¹³C NMR spectrum of **Pd5** (101 MHz, CDCl₃, 25 °C)

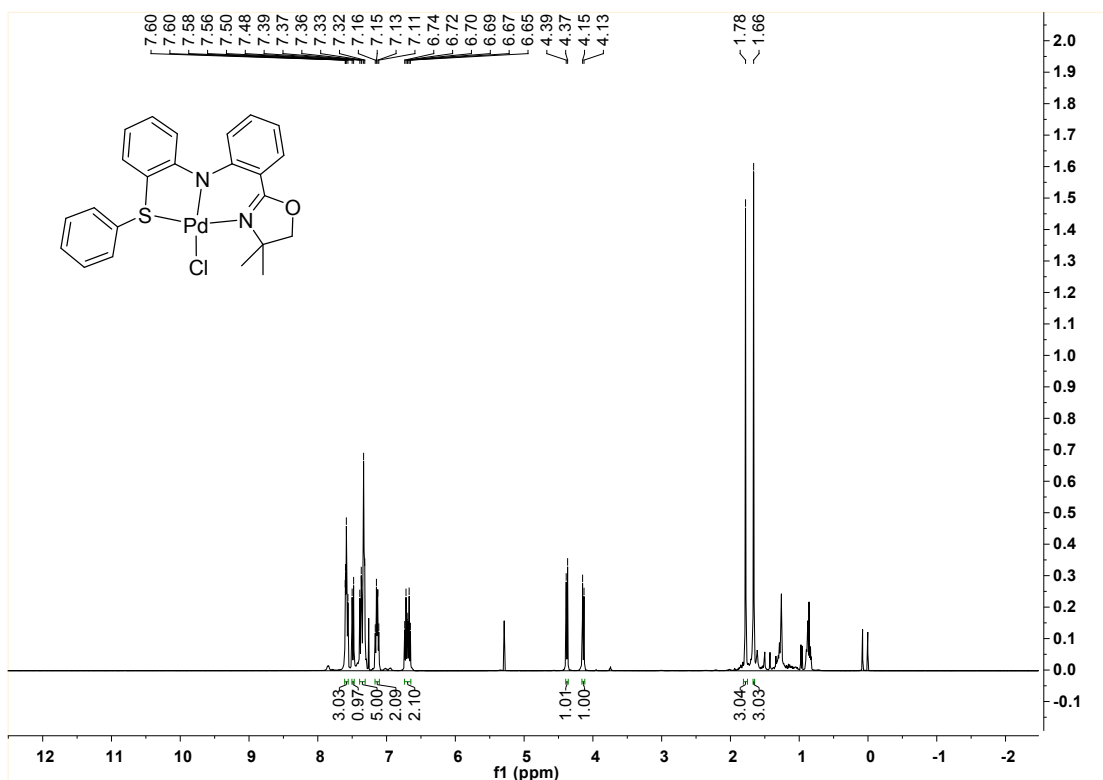


Figure S23 ¹H NMR spectrum of **Pd6** (400 MHz, CDCl₃, 25 °C)

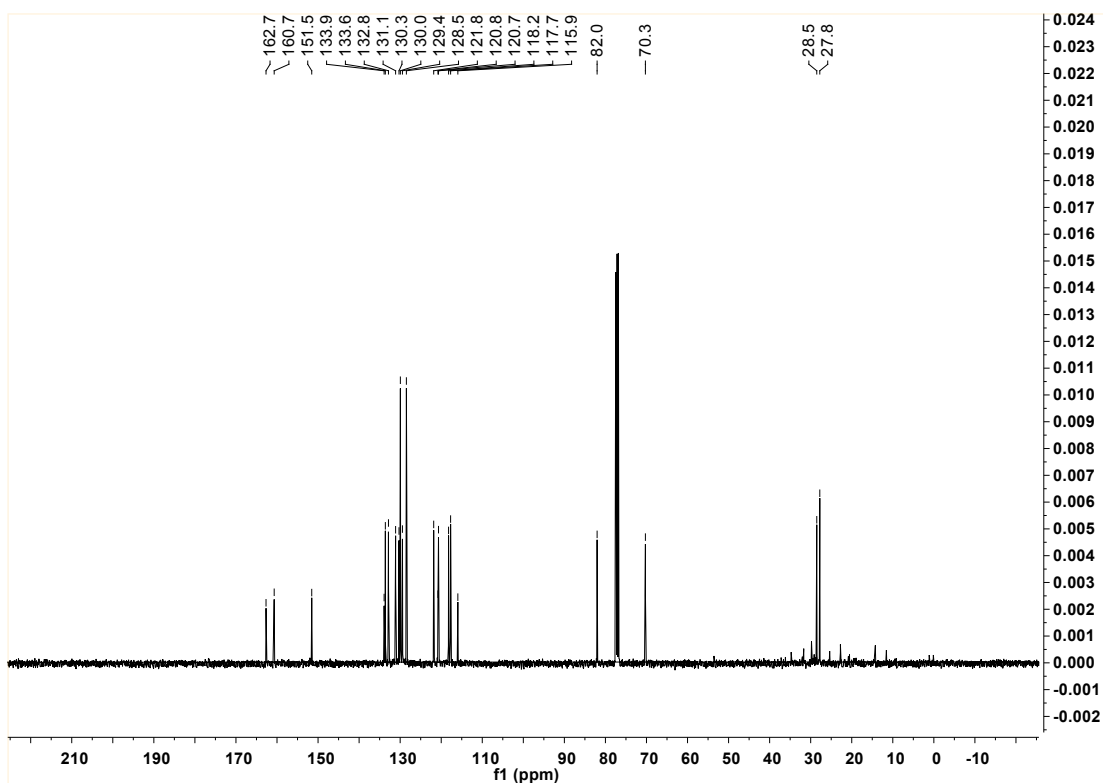


Figure S24 ¹³C NMR spectrum of **Pd6** (101 MHz, CDCl₃, 25 °C)

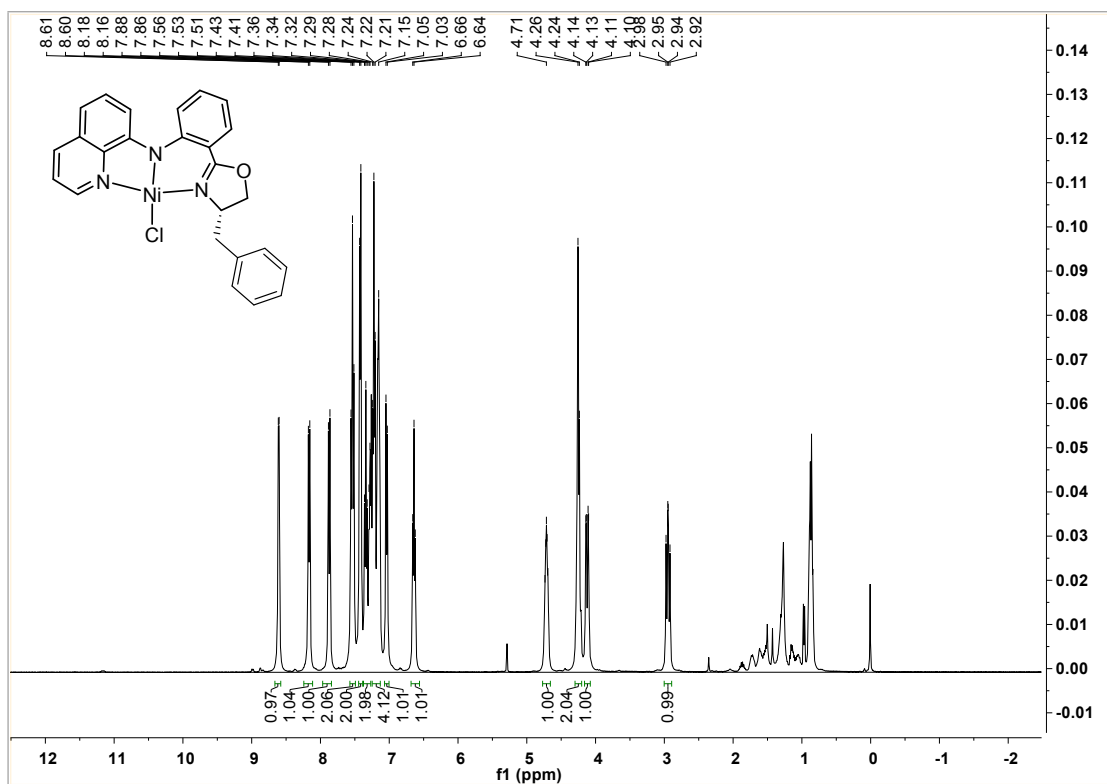


Figure S25 ¹H NMR spectrum of Ni1 (400 MHz, CDCl₃, 25 °C)

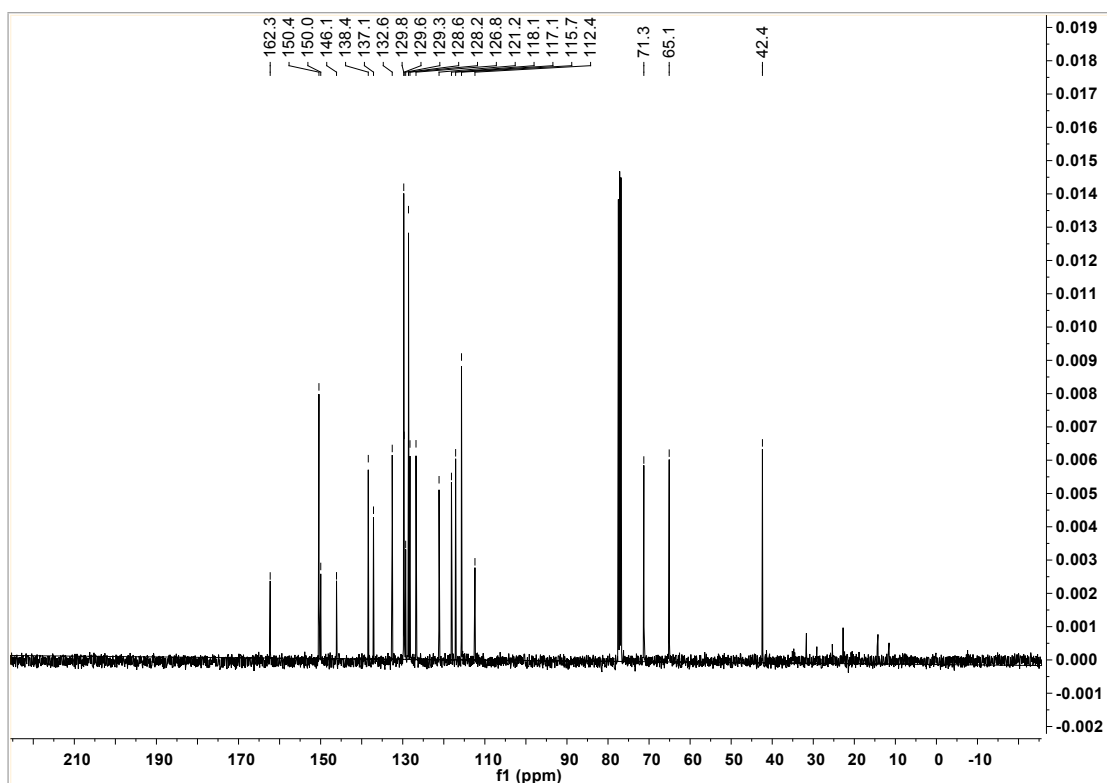


Figure S26 ¹³C NMR spectrum of Ni1 (101 MHz, CDCl₃, 25 °C)

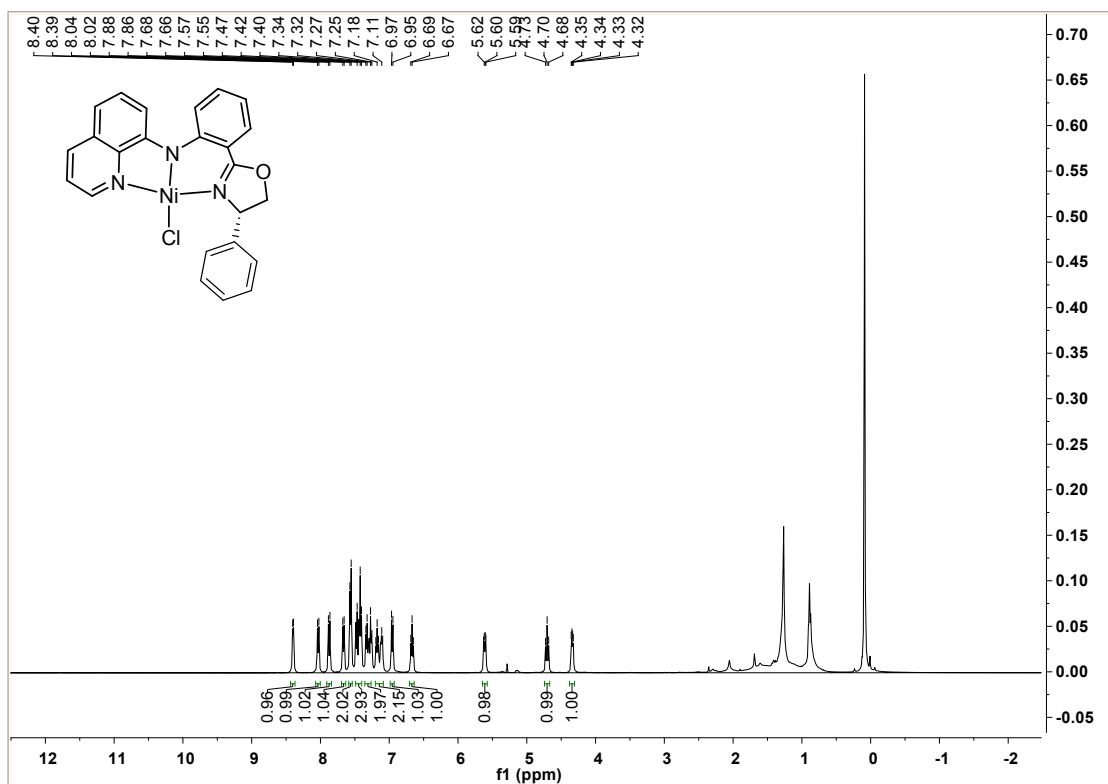


Figure S27 ¹H NMR spectrum of Ni2 (400 MHz, CDCl₃, 25 °C)

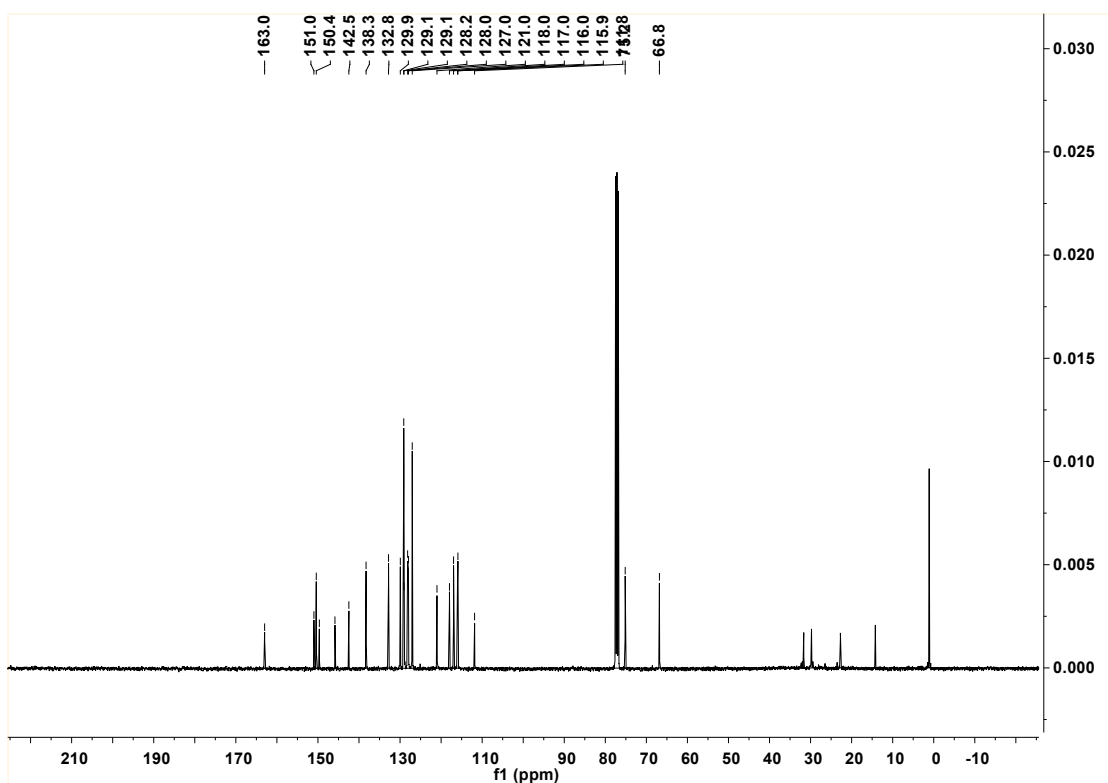


Figure S28 ¹³C NMR spectrum of Ni2 (101 MHz, CDCl₃, 25 °C)

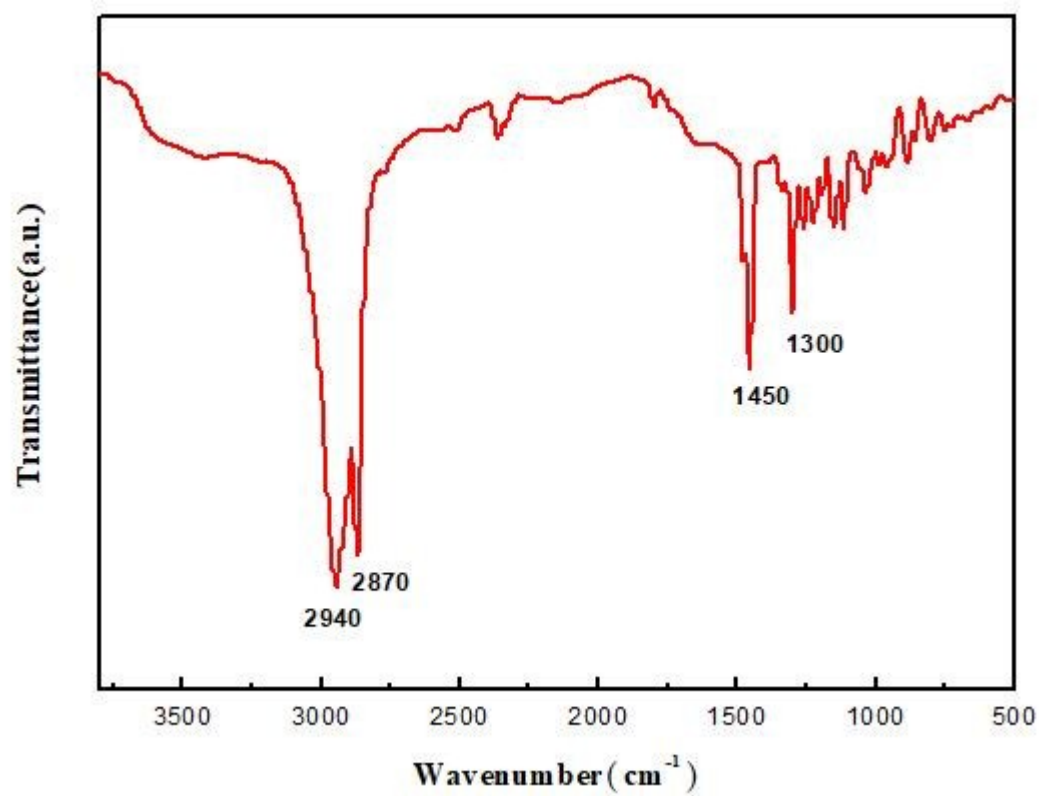


Figure S29 Infrared spectroscopy of **PNB** catalyzed by **Pd1**

Table S1. Summary of the crystallographic data for Pd3, Pd5 and Ni2

	Pd3	Pd5	Ni2
Empirical formula	C ₂₀ H ₁₈ ClN ₃ OPd	C ₂₇ H ₂₃ ClN ₂ O ₃ PdS	C ₂₄ H ₁₈ ClN ₃ NiO
Formula weight	458.22	597.38	458.57
Temperature/K	296(2)	296(2)	296(2)
Wavelength/ Å	0.71073	0.71073	0.71073
Crystal system	Monoclinic	Orthorhombic	Monoclinic
Space group	P2(1)/c	C222(1)	P2(1)
a/Å	10.032(7)	10.9254(10)	9.180(3)
b/Å	14.426(10)	16.9935(15)	9.941(3)
c/Å	12.576(9)	28.235(3)	11.212(4)
α /°	90	90	90
β /°	100.732(8)	90	102.531(3)
γ /°	90	90	90
V/Å ³	1788(2)	5242.2(8)	998.8(6)
Z	4	8	2
D _c /Mg m ⁻³	1.702	1.514	1.525
μ /mm ⁻¹	1.201	0.920	1.127
F(000)	920	2416	472
Crystal size/mm ³	0.22 x 0.19 x 0.15	0.19 x 0.08 x 0.05	0.12 x 0.10 x 0.06
2 θ range for data collection/°	2.170 to 27.651	2.22 to 25.05	2.27 to 25.05
Limiting indices(<i>hkl</i>)	-13, 11; -18, 18; - 13, 16	-12, 13; -20, 14; - 32, 33	-10, 10; -11, 6; -13, 13
Reflections collected	10481	13684	5176
Independent reflections	4028	4588	2484
R _{int}	0.0204	0.0247	0.0200
Completeness to θ /°	25.242 (97.9 %)	25.05 (99.7%)	25.05 (99.7%)
Data/restraints/parameters	4028 / 0 / 236	4588 / 0 / 322	2484 / 1 / 272
Goodness-of-fit on F ²	0.945	1.059	1.043
Final R indexes [$I \geq 2\sigma(I)$]	R1 = 0.0277, wR2 = 0.1162	R1 = 0.0273, wR2 = 0.0653	R1 = 0.0207, wR2 = 0.0496
Final R indexes [all data]	R1 = 0.0309, wR2 = 0.1245	R1 = 0.0303, wR2 = 0.0671	R1 = 0.0221, wR2 = 0.0504
Largest diff. peak/hole / e Å ⁻³	0.552, -0.860	0.608, -0.291	0.178, -0.142

$$R_I = \Sigma ||F_o| - |F_c|| / \Sigma |F_o|; wR_2 = [\Sigma w(F_o^2 - F_c^2)^2 / \Sigma w(F_o^2)^2]^{1/2}$$

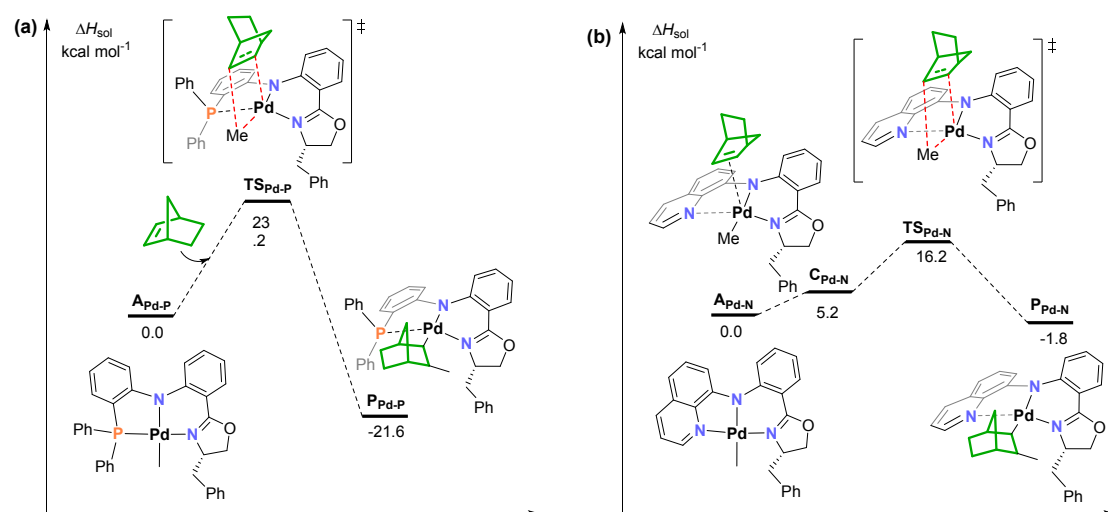


Figure S30. Energy profiles (kcal mol⁻¹) for the norbornene insertion into active species of [PNN^{ox}]-ligated **A_{Pd-P}** and [NNN^{ox}]-ligated **A_{Pd-N}** species, respectively.

Optimized Cartesian coordinates and single-point calculation energies for all of the stationary as well as the imaginary frequencies of transition states

Norbornene, $E_{(\text{SCF Done})} = -272.5852548$ a.u.

C	1.280804000	0.669970000	-0.505411000
C	0.087776000	1.128310000	0.322979000
C	0.087147000	-1.128318000	0.323090000
C	1.280262000	-0.670680000	-0.505590000
C	0.036861000	0.000067000	1.381500000
H	-0.885450000	0.000369000	1.976344000
H	0.905199000	-0.000141000	2.047957000
C	-1.189499000	0.781467000	-0.518827000
H	-2.086936000	1.179006000	-0.030939000
H	-1.142101000	1.207596000	-1.525354000
C	-1.190037000	-0.780923000	-0.518584000
H	-2.087662000	-1.177739000	-0.030449000
H	-1.143041000	-1.207379000	-1.524990000
H	0.119264000	2.157227000	0.689619000
H	0.118139000	-2.157213000	0.689833000
H	1.920836000	-1.329497000	-1.083629000
H	1.921860000	1.328418000	-1.083331000

A_{Pd-P}, $E_{(\text{SCF Done})} = -2005.697722$ a.u.

Pd	0.037658000	-0.219277000	-1.076709000
P	2.019581000	-0.131186000	-0.036931000
C	-1.472172000	2.072296000	0.340776000

C	-1.372255000	3.336524000	0.987781000
H	-0.513630000	3.518905000	1.624381000
C	-2.307940000	4.338193000	0.804029000
H	-2.169492000	5.290515000	1.310903000
C	-3.413859000	4.147210000	-0.040103000
H	-4.149334000	4.932682000	-0.182660000
C	-3.534655000	2.940292000	-0.704782000
H	-4.371740000	2.770575000	-1.373205000
C	-2.585990000	1.905351000	-0.551172000
C	-2.823577000	0.680317000	-1.294592000
C	-4.086495000	-0.735566000	-2.510353000
H	-4.198008000	-0.411669000	-3.551525000
H	-4.933370000	-1.360755000	-2.223449000
C	-2.710772000	-1.366138000	-2.231211000
H	-2.223628000	-1.697592000	-3.151894000
C	-2.741194000	-2.560070000	-1.237161000
H	-3.299299000	-3.374068000	-1.718565000
H	-1.708758000	-2.902704000	-1.113585000
C	-3.344737000	-2.228470000	0.109723000
C	-2.561511000	-1.637948000	1.113427000
H	-1.508745000	-1.451555000	0.930167000
C	-3.124872000	-1.257601000	2.331451000
H	-2.495902000	-0.789357000	3.083966000
C	-4.483526000	-1.474294000	2.572791000
H	-4.925389000	-1.178485000	3.520676000
C	-5.270203000	-2.082027000	1.591985000
H	-6.325509000	-2.266775000	1.775672000
C	-4.702844000	-2.455993000	0.372098000
H	-5.321770000	-2.938351000	-0.382189000
C	0.199247000	0.964892000	1.694923000
C	-0.287437000	1.302337000	2.982334000
H	-1.282160000	1.725201000	3.074726000
C	0.474301000	1.069589000	4.122346000
H	0.059311000	1.329705000	5.093434000
C	1.745558000	0.486683000	4.044648000
H	2.325937000	0.297517000	4.942500000
C	2.238444000	0.124668000	2.792209000
H	3.206476000	-0.363974000	2.708670000
C	1.487684000	0.357732000	1.635144000
C	3.018388000	-1.651767000	0.169142000
C	2.350966000	-2.886606000	0.168105000
H	1.278980000	-2.912780000	-0.008125000
C	3.059871000	-4.068638000	0.378270000
H	2.535288000	-5.020241000	0.374683000

C	4.442051000	-4.029754000	0.581899000
H	4.994804000	-4.951949000	0.739824000
C	5.113398000	-2.805471000	0.573375000
H	6.188967000	-2.771959000	0.725087000
C	4.406454000	-1.619044000	0.366787000
H	4.935155000	-0.670311000	0.354150000
C	3.207229000	1.130728000	-0.635702000
C	3.878768000	2.000797000	0.234241000
H	3.684417000	1.955306000	1.301730000
C	4.786309000	2.933948000	-0.272458000
H	5.301269000	3.607966000	0.406908000
C	5.026855000	3.004735000	-1.646047000
H	5.730743000	3.734092000	-2.037863000
C	4.353475000	2.144291000	-2.517919000
H	4.529493000	2.204901000	-3.588493000
C	3.443793000	1.213782000	-2.017211000
H	2.904194000	0.557162000	-2.694437000
N	-0.533817000	1.087098000	0.522999000
N	-1.968889000	-0.225449000	-1.672344000
O	-4.105730000	0.439596000	-1.667835000
C	0.600183000	-1.490650000	-2.604670000
H	0.134845000	-2.473972000	-2.453295000
H	0.221888000	-1.060832000	-3.542002000
H	1.680167000	-1.646934000	-2.700130000

TS_{Pd-P}, $E_{(\text{SCF Done})} = -2278.247368$ a.u., Imaginary frequency = $i373.81$ cm⁻¹

Pd	-0.860293000	-0.784828000	-0.738746000
N	0.076343000	-1.040488000	1.102165000
N	1.030602000	-1.643085000	-1.497058000
C	1.011121000	-3.198193000	0.415012000
C	-0.216968000	-3.040317000	2.499327000
H	-0.792218000	-2.450413000	3.205597000
C	0.364771000	-0.041159000	2.001812000
C	0.475858000	2.335983000	2.618659000
C	0.723202000	-5.168703000	1.815137000
H	0.887911000	-6.226857000	1.993615000
C	0.291535000	-2.389039000	1.351897000
C	0.172164000	1.344071000	1.667298000
C	1.277825000	0.698859000	4.165424000
H	1.738850000	0.432565000	5.114319000
C	1.226592000	-4.563027000	0.670664000
H	1.790867000	-5.142301000	-0.053222000
C	-0.009896000	-4.395764000	2.724708000
H	-0.431688000	-4.858106000	3.613934000

C	1. 001338000	2. 038870000	3. 869889000
H	1. 221673000	2. 828858000	4. 581510000
C	0. 984008000	-0. 307798000	3. 259250000
H	1. 243738000	-1. 328739000	3. 511735000
O	2. 617454000	-3. 228344000	-1. 378760000
C	1. 920420000	-1. 344509000	-2. 626742000
C	1. 526212000	-2. 636523000	-0. 833337000
C	2. 662164000	-0. 000119000	-2. 412148000
H	3. 158717000	0. 263524000	-3. 354782000
H	1. 897044000	0. 762442000	-2. 221450000
C	2. 835826000	-2. 590356000	-2. 663978000
H	2. 554752000	-3. 303316000	-3. 446687000
H	3. 899093000	-2. 354556000	-2. 737380000
H	1. 319105000	-1. 260904000	-3. 538605000
C	3. 672251000	-0. 021757000	-1. 286921000
C	3. 247102000	-0. 047564000	0. 050390000
C	5. 048667000	-0. 032044000	-1. 549297000
C	4. 169264000	-0. 077950000	1. 096362000
H	2. 188437000	-0. 044964000	0. 270877000
C	5. 976460000	-0. 067130000	-0. 505016000
H	5. 398168000	-0. 001082000	-2. 579723000
C	5. 538984000	-0. 089984000	0. 821003000
H	3. 804984000	-0. 082788000	2. 120148000
H	7. 040281000	-0. 070685000	-0. 728745000
H	6. 260731000	-0. 111165000	1. 633311000
H	0. 319677000	3. 376528000	2. 347399000
C	0. 694527000	3. 435164000	-0. 230737000
C	0. 113305000	4. 694024000	-0. 447718000
C	2. 098679000	3. 338819000	-0. 236497000
C	0. 911782000	5. 820858000	-0. 665577000
H	-0. 966214000	4. 804926000	-0. 439880000
C	2. 892862000	4. 464195000	-0. 445265000
H	2. 576270000	2. 380201000	-0. 059732000
C	2. 302466000	5. 712425000	-0. 665101000
H	0. 440286000	6. 787404000	-0. 827037000
H	3. 975384000	4. 363888000	-0. 437401000
H	2. 921209000	6. 590299000	-0. 832156000
C	-1. 717323000	-0. 776690000	-2. 822529000
H	-0. 971345000	-0. 013775000	-3. 063783000
H	-1. 362043000	-1. 784118000	-3. 050608000
H	-2. 590693000	-0. 575355000	-3. 439120000
C	-2. 750069000	-0. 741611000	0. 056651000
C	-3. 282703000	-2. 081123000	0. 574560000
C	-3. 966373000	-1. 938291000	-1. 581063000

C	-3.160511000	-0.666046000	-1.329728000
C	-4.819304000	-1.870960000	0.718294000
H	-5.283950000	-2.738115000	1.201747000
H	-5.059644000	-0.987331000	1.318480000
C	-5.285444000	-1.734221000	-0.768479000
H	-6.008073000	-2.512688000	-1.035827000
H	-5.752596000	-0.766305000	-0.979791000
H	-4.123367000	-2.203450000	-2.629687000
H	-2.783839000	-2.470162000	1.463937000
C	-3.234256000	-2.966535000	-0.690859000
H	-3.794866000	-3.901585000	-0.579381000
H	-2.217282000	-3.191719000	-1.025059000
H	-3.535397000	0.280589000	-1.706351000
H	-2.871021000	0.127730000	0.697986000
P	-0.270126000	1.854236000	-0.046340000
C	-1.997071000	2.508895000	0.062330000
C	-2.691613000	2.688920000	1.267102000
C	-2.666836000	2.777593000	-1.144033000
C	-4.021973000	3.117317000	1.264698000
H	-2.192302000	2.480482000	2.208447000
C	-3.989756000	3.221914000	-1.147671000
H	-2.145563000	2.630525000	-2.087946000
C	-4.674813000	3.385591000	0.059864000
H	-4.547441000	3.243964000	2.207975000
H	-4.488396000	3.430675000	-2.091010000
H	-5.708967000	3.719682000	0.060298000

P_{Pd-P}, $E_{\text{(SCF Done)}} = -2278.322934$ a.u.

Pd	-0.027656000	-0.443099000	0.448652000
N	1.077106000	1.418985000	0.604683000
N	1.847339000	-1.397659000	0.710076000
C	2.904475000	0.480475000	1.940333000
C	2.161053000	2.748810000	2.355240000
H	1.477309000	3.567152000	2.158551000
C	0.590047000	2.510791000	-0.088909000
C	-1.265256000	3.532987000	-1.342282000
C	3.999171000	1.835221000	3.649998000
H	4.748488000	1.943337000	4.427815000
C	2.024254000	1.556024000	1.590170000
C	-0.744459000	2.478074000	-0.578894000
C	0.842767000	4.676457000	-1.199210000
H	1.478827000	5.519778000	-1.458400000
C	3.881502000	0.651091000	2.943146000
H	4.543080000	-0.181115000	3.159640000

C	3. 113757000	2. 882810000	3. 349762000
H	3. 161918000	3. 812062000	3. 913024000
C	-0. 485284000	4. 642828000	-1. 650482000
H	-0. 890515000	5. 454962000	-2. 246236000
C	1. 374002000	3. 641262000	-0. 442097000
H	2. 411249000	3. 677434000	-0. 126427000
O	4. 035521000	-1. 480759000	1. 195324000
C	2. 345482000	-2. 581628000	-0. 012481000
C	2. 864202000	-0. 801184000	1. 259406000
C	2. 333692000	-2. 360403000	-1. 548102000
H	2. 672013000	-3. 295351000	-2. 014803000
H	1. 289985000	-2. 210894000	-1. 840076000
C	3. 744465000	-2. 766341000	0. 602268000
H	3. 757746000	-3. 520515000	1. 397521000
H	4. 529936000	-2. 980507000	-0. 123973000
H	1. 704759000	-3. 432990000	0. 212501000
C	3. 176234000	-1. 198541000	-2. 023704000
C	2. 647050000	0. 100639000	-2. 040408000
C	4. 508243000	-1. 379872000	-2. 421751000
C	3. 432847000	1. 190979000	-2. 414264000
H	1. 619597000	0. 260041000	-1. 732882000
C	5. 298038000	-0. 292588000	-2. 801052000
H	4. 929407000	-2. 383220000	-2. 445616000
C	4. 763811000	0. 997745000	-2. 791451000
H	2. 999603000	2. 187536000	-2. 402014000
H	6. 328704000	-0. 454410000	-3. 106203000
H	5. 378958000	1. 845111000	-3. 082757000
H	-2. 286167000	3. 467920000	-1. 710448000
C	-2. 581037000	0. 630886000	-1. 784537000
C	-1. 830052000	0. 678309000	-2. 972704000
C	-3. 929713000	0. 261123000	-1. 847995000
C	-2. 416544000	0. 355048000	-4. 193612000
H	-0. 783441000	0. 967805000	-2. 937464000
C	-4. 513730000	-0. 068380000	-3. 074071000
H	-4. 534308000	0. 235649000	-0. 947963000
C	-3. 760630000	-0. 026398000	-4. 247304000
H	-1. 822879000	0. 396563000	-5. 102728000
H	-5. 561637000	-0. 354267000	-3. 107920000
H	-4. 217172000	-0. 284271000	-5. 198971000
C	-1. 563511000	-2. 731284000	-1. 806893000
H	-1. 387358000	-1. 700867000	-2. 115110000
H	-0. 615832000	-3. 269399000	-1. 906736000
H	-2. 274657000	-3. 180411000	-2. 512427000
C	-1. 263575000	-2. 106302000	0. 743852000

C	-0.686818000	-3.308940000	1.556808000
C	-2.166643000	-4.264186000	0.136295000
C	-2.112722000	-2.798721000	-0.375031000
C	-1.823120000	-3.767216000	2.506909000
H	-1.471332000	-4.561942000	3.177727000
H	-2.197831000	-2.950235000	3.133173000
C	-2.894722000	-4.314085000	1.504977000
H	-3.189891000	-5.338873000	1.756467000
H	-3.808237000	-3.707164000	1.495773000
H	-2.566194000	-4.966260000	-0.603617000
H	0.256113000	-3.108387000	2.072338000
C	-0.698549000	-4.485955000	0.557395000
H	-0.526617000	-5.457021000	1.038587000
H	0.002934000	-4.389143000	-0.274960000
H	-3.123744000	-2.365066000	-0.398924000
H	-1.954974000	-1.593095000	1.422283000
P	-1.689665000	0.966740000	-0.209636000
C	-2.987550000	1.402498000	1.015426000
C	-3.113794000	2.708417000	1.511088000
C	-3.833302000	0.397333000	1.517617000
C	-4.074577000	3.004155000	2.480128000
H	-2.459553000	3.491605000	1.142076000
C	-4.797343000	0.699286000	2.479112000
H	-3.739579000	-0.623435000	1.160627000
C	-4.919359000	2.003773000	2.963941000
H	-4.160758000	4.019831000	2.856855000
H	-5.446937000	-0.086880000	2.854398000
H	-5.665977000	2.237192000	3.718104000

Apd-N, $E_{(\text{SCF Done})} = -1371.479032$ a.u.

Pd	0.593486000	-1.050606000	-0.963813000
N	0.758795000	0.951517000	-0.334794000
N	-1.421025000	-0.805231000	-1.186779000
N	2.575451000	-1.045797000	-0.385119000
C	-1.412089000	1.690991000	-1.177418000
C	0.391643000	3.299803000	-0.941766000
H	1.431565000	3.525089000	-0.738490000
C	1.904180000	1.139160000	0.403820000
C	4.131169000	0.187347000	1.033386000
C	-1.782612000	4.048043000	-1.712324000
H	-2.438828000	4.841421000	-2.055807000
C	-0.056934000	1.958670000	-0.779442000
C	2.885085000	0.080242000	0.344296000
C	3.406007000	2.285891000	1.970449000

H	3.571853000	3.138969000	2.623623000
C	-2.243641000	2.748198000	-1.610547000
H	-3.266828000	2.514960000	-1.882216000
C	-0.440733000	4.307912000	-1.393111000
H	-0.037786000	5.310985000	-1.512837000
C	4.383815000	1.319186000	1.846905000
H	5.328427000	1.396093000	2.376938000
C	2.188424000	2.204740000	1.270059000
H	1.446253000	2.981451000	1.412093000
O	-3.357006000	0.314699000	-1.155736000
C	3.465085000	-2.024278000	-0.500883000
H	3.160795000	-2.886365000	-1.082146000
C	4.733097000	-1.968779000	0.109741000
H	5.423168000	-2.795431000	-0.023723000
C	-2.450145000	-1.845937000	-1.005748000
C	5.056591000	-0.876104000	0.881056000
H	6.016797000	-0.815667000	1.387321000
C	-2.002446000	0.363214000	-1.163276000
C	-2.392113000	-2.453623000	0.420381000
H	-3.126027000	-3.269162000	0.459597000
H	-1.399600000	-2.901368000	0.537093000
C	-3.738677000	-1.068961000	-1.319047000
H	-4.075305000	-1.210527000	-2.352386000
H	-4.560226000	-1.267917000	-0.629126000
H	-2.284241000	-2.646958000	-1.728440000
C	-2.661893000	-1.454947000	1.524153000
C	-1.652839000	-0.587204000	1.971375000
C	-3.938619000	-1.340964000	2.092152000
C	-1.921934000	0.381378000	2.938513000
H	-0.657129000	-0.660018000	1.545463000
C	-4.209953000	-0.375681000	3.064007000
H	-4.727544000	-2.021078000	1.776070000
C	-3.202341000	0.493700000	3.485625000
H	-1.126918000	1.048257000	3.261996000
H	-5.206728000	-0.305049000	3.491744000
H	-3.411741000	1.248332000	4.239121000
C	0.601447000	-3.009930000	-1.591335000
H	1.383387000	-3.124920000	-2.355444000
H	0.827870000	-3.678333000	-0.748305000
H	-0.345536000	-3.328301000	-2.040156000

C_{Pd-N}, $E_{(\text{SCF Done})} = -1644.057893$ a.u.

Pd	-0.946404000	-0.434879000	-0.925390000
N	-0.134386000	0.181161000	0.993868000

N	0.706927000	-1.743390000	-0.883683000
N	-0.388573000	2.234605000	-0.855650000
C	0.457510000	-2.115444000	1.545457000
C	-0.716251000	-0.774670000	3.184677000
H	-1.182265000	0.163553000	3.468630000
C	0.258176000	1.444024000	1.340321000
C	0.579347000	3.848411000	0.691480000
C	-0.120037000	-3.068336000	3.706485000
H	-0.119348000	-3.907315000	4.395451000
C	-0.124381000	-0.862935000	1.903070000
C	0.127326000	2.523227000	0.369788000
C	1.325841000	3.080723000	2.843523000
H	1.804889000	3.263330000	3.802980000
C	0.466688000	-3.188200000	2.453682000
H	0.935437000	-4.119861000	2.153353000
C	-0.720215000	-1.852061000	4.061342000
H	-1.202074000	-1.747990000	5.030608000
C	1.169652000	4.120961000	1.947353000
H	1.500778000	5.128906000	2.180781000
C	0.893491000	1.777657000	2.553971000
H	1.082975000	0.997823000	3.281692000
O	2.059962000	-3.209164000	0.139875000
C	-0.504211000	3.186280000	-1.761932000
H	-0.913724000	2.885732000	-2.726162000
C	-0.120531000	4.527047000	-1.530974000
H	-0.243628000	5.273375000	-2.310363000
C	1.593534000	-2.213326000	-1.961044000
C	0.420906000	4.845836000	-0.307577000
H	0.745746000	5.860675000	-0.088822000
C	1.057114000	-2.308281000	0.228871000
C	2.453412000	-1.067938000	-2.549926000
H	3.024954000	-1.486008000	-3.389038000
H	1.761261000	-0.327628000	-2.966915000
C	2.394324000	-3.338094000	-1.264579000
H	2.095878000	-4.339595000	-1.590308000
H	3.475981000	-3.225767000	-1.354961000
H	0.974347000	-2.618073000	-2.766354000
C	3.379372000	-0.411175000	-1.553039000
C	2.887973000	0.580145000	-0.692925000
C	4.723242000	-0.793168000	-1.439810000
C	3.710197000	1.165343000	0.269936000
H	1.853686000	0.886475000	-0.780204000
C	5.551467000	-0.210538000	-0.477465000
H	5.129339000	-1.541893000	-2.117899000

C	5.044773000	0.766488000	0.382301000
H	3.301659000	1.926067000	0.928897000
H	6.591961000	-0.516653000	-0.403827000
H	5.689004000	1.219837000	1.131232000
C	-1.384805000	-1.175548000	-2.809246000
H	-2.221751000	-0.706995000	-3.331230000
H	-0.480157000	-1.014763000	-3.408449000
H	-1.578258000	-2.251915000	-2.722971000
C	-2.832987000	0.494787000	0.089371000
C	-3.762193000	-0.499745000	0.765231000
C	-4.235146000	-0.542525000	-1.447022000
C	-3.100786000	0.459172000	-1.258872000
C	-5.164740000	0.197716000	0.695910000
H	-5.897919000	-0.378206000	1.271134000
H	-5.143206000	1.211414000	1.108537000
C	-5.489840000	0.169465000	-0.834030000
H	-6.391576000	-0.418264000	-1.038146000
H	-5.644237000	1.168273000	-1.254360000
H	-4.380000000	-0.928124000	-2.457558000
H	-3.458342000	-0.837223000	1.757589000
C	-3.932667000	-1.570507000	-0.334322000
H	-4.771874000	-2.248382000	-0.140523000
H	-3.022645000	-2.148103000	-0.517292000
H	-2.887717000	1.260783000	-1.957636000
H	-2.375416000	1.318865000	0.619308000

TS_{Pd-N}, $E_{(\text{SCF Done})} = -1644.039136$ a.u., Imaginary frequency = $i377.25$ cm⁻¹

Pd	-1.043274000	-0.436115000	-0.729231000
N	-0.110217000	0.219162000	1.034055000
N	0.702491000	-1.727128000	-0.863514000
N	-0.250756000	2.180950000	-0.947016000
C	0.665947000	-2.034676000	1.582212000
C	-0.528029000	-0.749003000	3.253698000
H	-1.057823000	0.154411000	3.538132000
C	0.258577000	1.501401000	1.327287000
C	0.490565000	3.897850000	0.609902000
C	0.277652000	-2.971597000	3.794403000
H	0.381727000	-3.790139000	4.500042000
C	0.011565000	-0.818439000	1.949464000
C	0.138359000	2.538004000	0.305270000
C	1.221190000	3.231564000	2.798534000
H	1.666698000	3.464547000	3.763315000
C	0.803616000	-3.078643000	2.513179000
H	1.321302000	-3.981853000	2.206634000

C	-0.402355000	-1.800498000	4.153324000
H	-0.844262000	-1.710940000	5.142849000
C	1.016757000	4.239761000	1.877026000
H	1.274587000	5.272475000	2.094237000
C	0.866219000	1.899303000	2.536051000
H	1.074464000	1.153714000	3.293498000
O	2.194051000	-3.118833000	0.074592000
C	-0.374914000	3.098710000	-1.886599000
H	-0.676837000	2.742548000	-2.871585000
C	-0.124849000	4.472220000	-1.666486000
H	-0.256875000	5.189530000	-2.471434000
C	1.525020000	-2.181402000	-1.993270000
C	0.315251000	4.858303000	-0.422018000
H	0.551752000	5.899145000	-0.211957000
C	1.170425000	-2.244741000	0.226147000
C	2.333398000	-1.013850000	-2.615776000
H	2.838373000	-1.399764000	-3.511087000
H	1.606929000	-0.262754000	-2.948449000
C	2.383832000	-3.296255000	-1.351588000
H	2.041019000	-4.302741000	-1.614511000
H	3.451774000	-3.202536000	-1.555233000
H	0.864874000	-2.585875000	-2.768670000
C	3.333993000	-0.391202000	-1.669935000
C	2.901687000	0.531119000	-0.707197000
C	4.688886000	-0.748417000	-1.698407000
C	3.793948000	1.070111000	0.219298000
H	1.859058000	0.816818000	-0.686191000
C	5.587586000	-0.208534000	-0.774971000
H	5.046344000	-1.445973000	-2.454119000
C	5.140513000	0.697530000	0.189421000
H	3.427835000	1.775265000	0.960668000
H	6.635898000	-0.494086000	-0.811473000
H	5.839608000	1.115443000	0.909213000
C	-1.905637000	-1.334232000	-2.596123000
H	-2.779580000	-1.472801000	-3.228873000
H	-1.123632000	-0.875052000	-3.209953000
H	-1.615823000	-2.323339000	-2.229766000
C	-2.820778000	0.500259000	-0.344535000
C	-3.689816000	-0.132582000	0.746263000
C	-4.373728000	-1.061848000	-1.203124000
C	-3.237905000	-0.114225000	-1.587909000
C	-5.105848000	0.485194000	0.555532000
H	-5.774410000	0.180735000	1.369137000
H	-5.079086000	1.579698000	0.541243000

C	-5.561658000	-0.126364000	-0.810227000
H	-6.476064000	-0.718899000	-0.698849000
H	-5.757151000	0.634222000	-1.574031000
H	-4.631649000	-1.822520000	-1.944609000
H	-3.285953000	-0.060981000	1.758454000
C	-3.923097000	-1.555459000	0.189224000
H	-4.714507000	-2.097583000	0.719250000
H	-3.016488000	-2.167306000	0.163818000
H	-3.357203000	0.508241000	-2.471961000
H	-2.645519000	1.573238000	-0.302947000

P_{Pd-N}, $E_{\text{(SCF Done)}} = -1644.070267$ a.u.

Pd	-0.936116000	-0.465308000	-0.831465000
N	-0.113742000	0.053608000	1.003962000
N	0.937507000	-1.624278000	-1.056276000
N	-0.336798000	2.122007000	-0.856852000
C	0.866274000	-2.156409000	1.357770000
C	-0.485239000	-1.155916000	3.107125000
H	-1.111647000	-0.341486000	3.455642000
C	0.101227000	1.341786000	1.402032000
C	0.117895000	3.791606000	0.852329000
C	0.531209000	-3.327020000	3.466204000
H	0.704218000	-4.193834000	4.096623000
C	0.086166000	-1.051105000	1.819288000
C	-0.066545000	2.428277000	0.439469000
C	0.793019000	3.052103000	3.035968000
H	1.155504000	3.261649000	4.039931000
C	1.089162000	-3.262646000	2.195042000
H	1.699724000	-4.079146000	1.823718000
C	-0.270014000	-2.268701000	3.911598000
H	-0.736918000	-2.315629000	4.892418000
C	0.533225000	4.095155000	2.169614000
H	0.666634000	5.131041000	2.468168000
C	0.593597000	1.711502000	2.669007000
H	0.832016000	0.939190000	3.389755000
O	2.525858000	-2.953532000	-0.182040000
C	-0.506531000	3.085001000	-1.742357000
H	-0.709161000	2.769912000	-2.765717000
C	-0.423963000	4.457766000	-1.417449000
H	-0.587847000	5.212097000	-2.181479000
C	1.849272000	-1.889418000	-2.180107000
C	-0.102130000	4.799064000	-0.124624000
H	0.004871000	5.841490000	0.167030000
C	1.418402000	-2.193675000	0.002730000

C	2.575252000	-0.597784000	-2.638664000
H	3.144513000	-0.840729000	-3.545507000
H	1.799010000	0.122832000	-2.922680000
C	2.778629000	-2.984979000	-1.607826000
H	2.529585000	-3.987061000	-1.973558000
H	3.841428000	-2.788264000	-1.758109000
H	1.264490000	-2.267647000	-3.026122000
C	3.484375000	-0.002173000	-1.588295000
C	2.941316000	0.767992000	-0.550682000
C	4.865794000	-0.238362000	-1.597295000
C	3.751595000	1.274165000	0.465231000
H	1.877672000	0.960876000	-0.543082000
C	5.682517000	0.269396000	-0.583898000
H	5.308159000	-0.815384000	-2.407683000
C	5.126067000	1.022185000	0.452670000
H	3.300575000	1.860583000	1.261376000
H	6.752543000	0.078863000	-0.606620000
H	5.761582000	1.415239000	1.242010000
C	-2.633890000	-0.638878000	-2.774112000
H	-3.207209000	-1.173350000	-3.542161000
H	-2.042696000	0.132503000	-3.278977000
H	-1.946565000	-1.430672000	-2.381144000
C	-2.774368000	0.256024000	-0.382132000
C	-3.497000000	-0.573862000	0.691418000
C	-4.662525000	-1.023324000	-1.197214000
C	-3.566724000	-0.041631000	-1.689984000
C	-4.870666000	0.103615000	0.955577000
H	-5.354049000	-0.336117000	1.836334000
H	-4.767920000	1.178391000	1.140331000
C	-5.673725000	-0.212649000	-0.349202000
H	-6.560519000	-0.818242000	-0.130970000
H	-6.015043000	0.690416000	-0.867938000
H	-5.124690000	-1.603530000	-2.003671000
H	-2.908254000	-0.747546000	1.595221000
C	-3.934782000	-1.828408000	-0.097685000
H	-4.610771000	-2.480878000	0.467886000
H	-3.094124000	-2.429303000	-0.461163000
H	-4.028170000	0.859406000	-2.114646000
H	-2.692575000	1.315194000	-0.126621000