Supporting Information: Synthesis and Properties of NHC Supported Palladium(I) Dimers with Bridging Allyl, Cyclopentadienyl and Indenyl Ligands

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NMR Spectra of CpInd

Figure S1: ^{1}H NMR spectrum of **CpInd** at -50 °C.

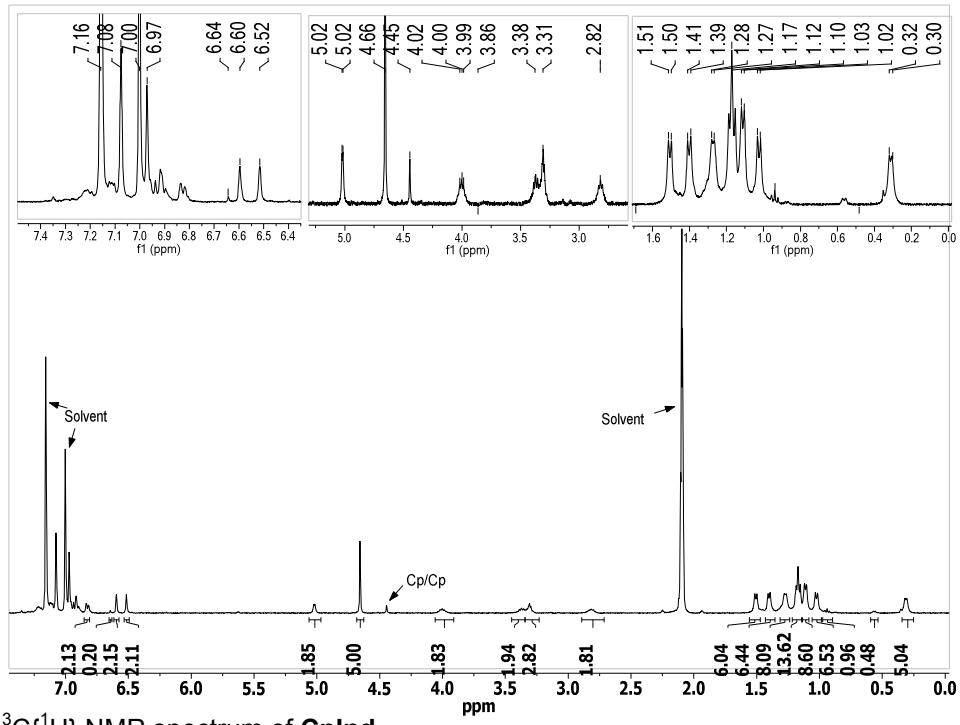
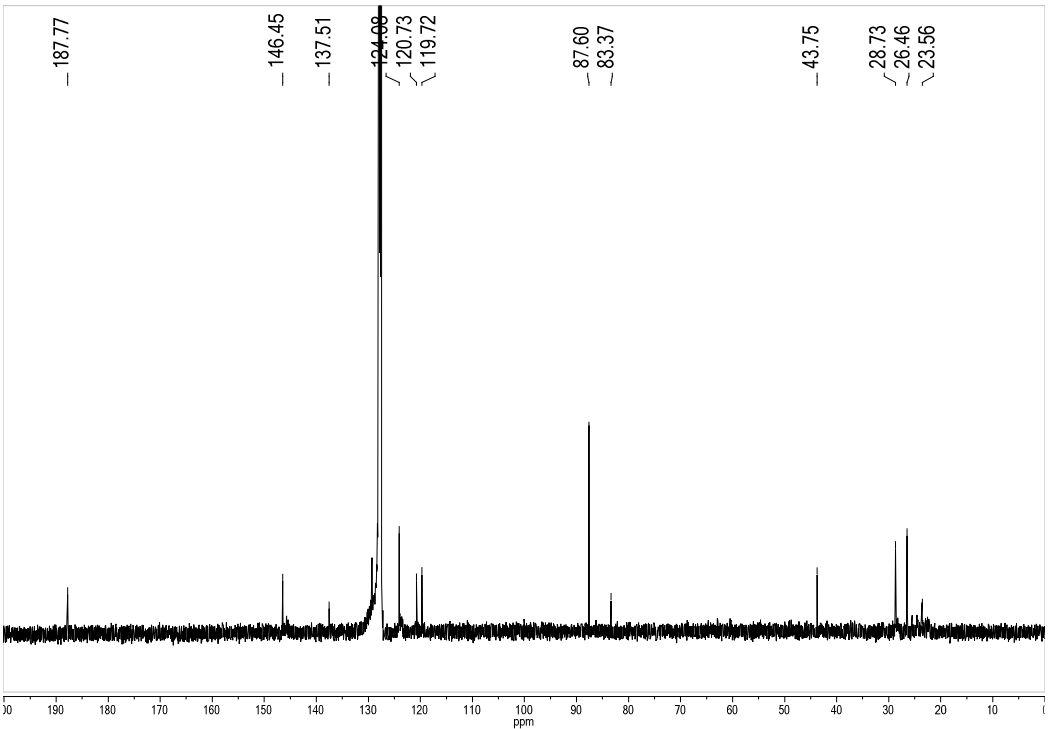


Figure S2: $^{13}C\{^{1}H\}$ NMR spectrum of **CpInd**.



*As was mentioned in the main text in some cases our synthesis of **CpInd** contained a **CpCp** impurity, in some cases it contained an **IndInd** impurity and in some cases it contained both. Here we show spectra which only contains a **CpCp** impurity.*

Ring Current Effect in AllInd, IndInd and CpInd

Figure S3: ORTEP of **AllInd** with methyl group located beneath the bridging indenyl ligand highlighted in red box. Hydrogen atoms are omitted for clarity.

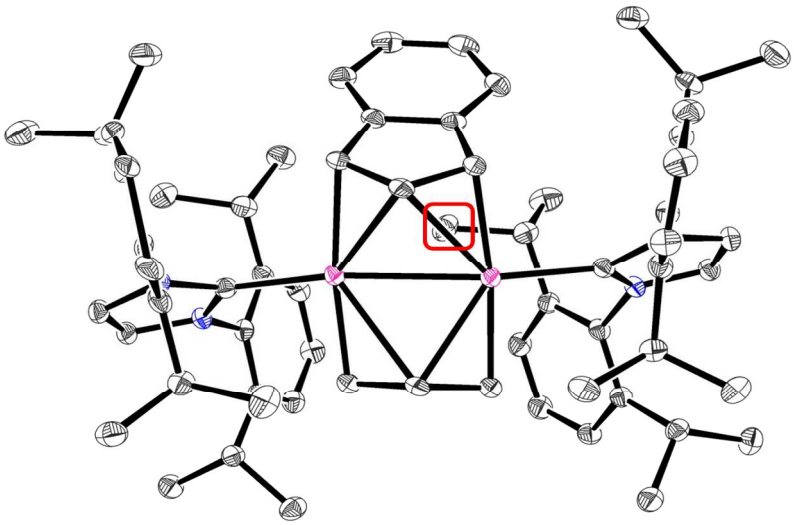


Figure S4: ORTEP of **IndInd** with methyl groups located above or below the bridging indenyl ligands highlighted in red box. Hydrogen atoms are omitted for clarity.

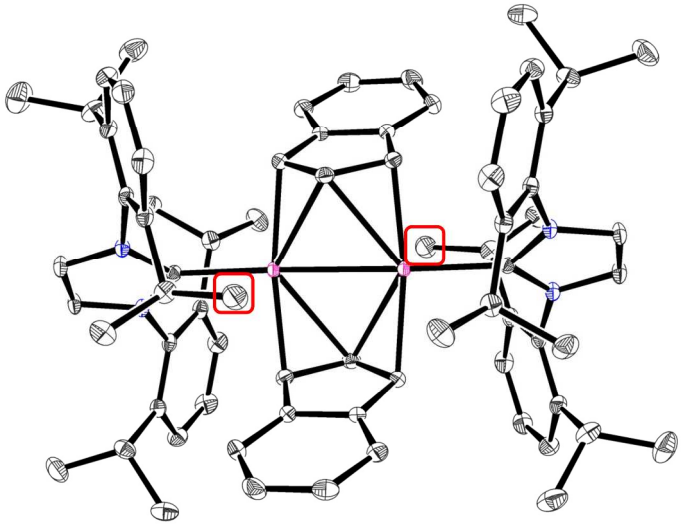
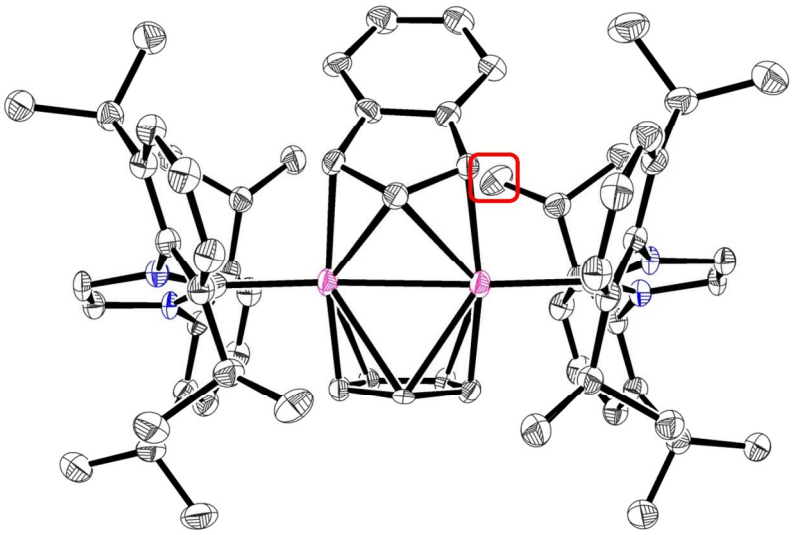


Figure S5: ORTEP of **CpInd** with methyl group located beneath the bridging indenyl ligand highlighted in red box. Hydrogen atoms are omitted for clarity.



Decomposition of AllAll^{+} and CpCp^{+} monitored by EPR Spectroscopy

Figure S6: EPR Spectra of **AllAll^{+}** with time.

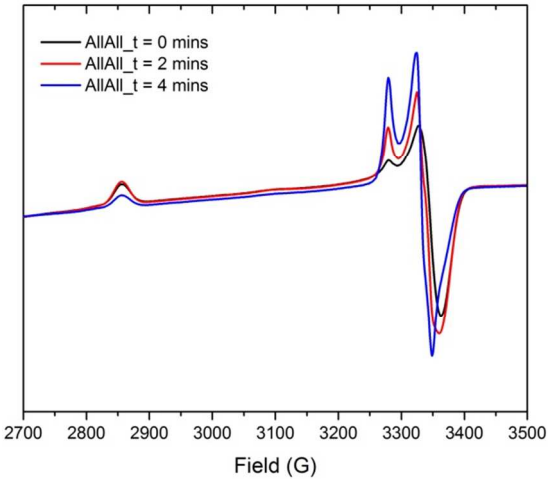
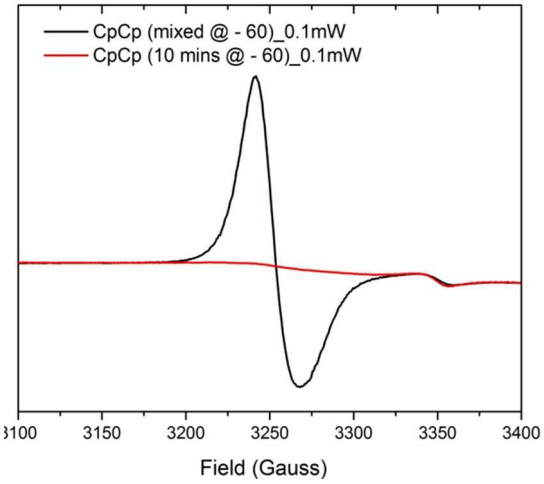


Figure S7: EPR Spectra of **CpCp^{+}** with time.



DFT Calculations

Figure S8: Optimized structure of **AllAll'**$^{+}$. (Hydrogen atoms omitted for clarity). Selected bond lengths (Å): Pd(1)-Pd(1A) 2.67, Pd(1)-C(1) 2.16, Pd(1)-C(2) 2.45, Pd(1)-C(1') 2.16, Pd(1)-C(2') 2.45, Pd(1A)-C(1A) 2.16, Pd(1A)-C(2) 2.45, Pd(1A)-C(1A') 2.16, Pd(1A)-C(2A') 2.45, Pd(1)-C(3) 2.08, Pd(1A)-C(3A) 2.08, C(1)-C(2) 1.44, C(1A)-C(2) 1.44, C(1')-C(2') 1.44, C(1A')-C(2') 1.44.

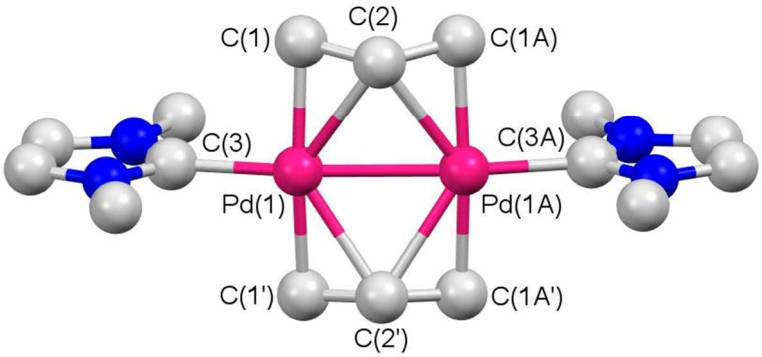


Figure S9: Optimized structure of **AllAll'**$^{+}$. (Hydrogen atoms omitted for clarity). Selected bond lengths (Å) and angles (°):Pd(1)-Pd(1A) 2.58, Pd(1)-C(1) 2.36, Pd(1)-C(2) 2.23, Pd(1)-C(3) 2.86, Pd(1)-C(1') 2.36, Pd(1)-C(2') 2.23, Pd(1)-C(3') 2.86, Pd(1A)-C(1A) 2.36, Pd(1A)-C(2) 2.23, Pd(1A)-C(1A') 2.36, Pd(1A)-C(2A') 2.23, Pd(1)-C(3) 2.86, Pd(1A)-C(3A) 2.86, Pd(1)-C(4) 2.12, Pd(1A)-C(4A) 2.12, C(1)-C(2) 1.44, C(1)-C(1A) 1.43, C(1A)-C(2A) 1.44, C(2)-C(3) 1.43, C(2A)-C(3) 1.43, C(1')-C(2') 1.44, C(1')-C(1A') 1.43, C(1A')-C(2A') 1.44, C(2')-C(3') 1.43, C(2A')-C(3') 1.43.

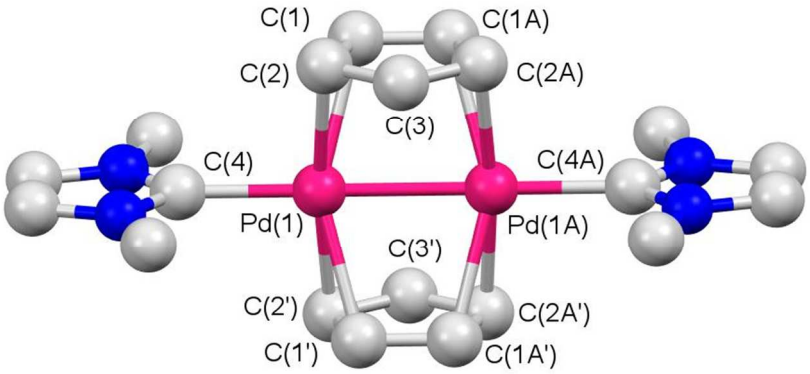


Figure S10: Calculated Mulliken spin population analysis of **AllAll'**$^{+}$. Color key population: *dark red* (-0.140)−*bright green* (+0.337).

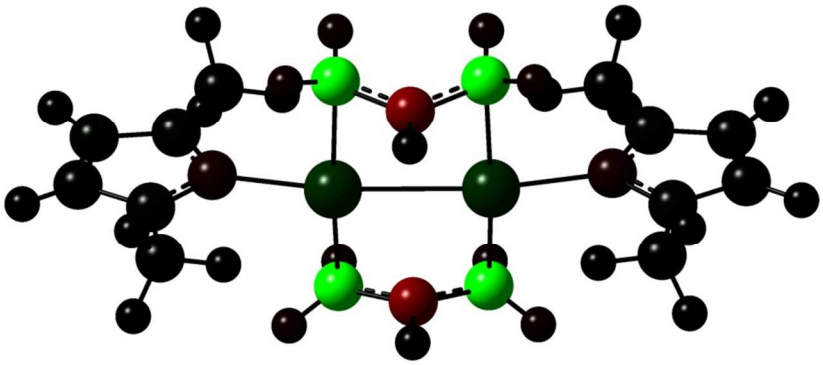
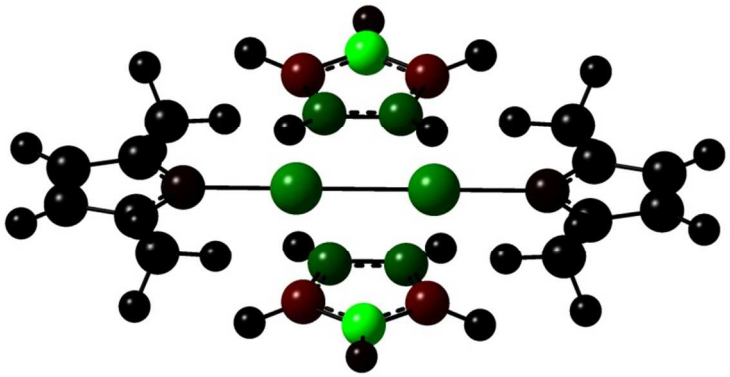


Figure S11: Calculated Mulliken spin population analysis of **CpCp'$^{+}$**. Color key population: *dark red* (-0.104)−*bright green* (+0.377).



Optimized coordinates and energies of structures are given below:

AllAll' ΔG = -29863.35443 eV

Pd	-1.37977000	-0.35010600	-0.07921400
N	-3.80047300	1.56427300	-0.14296200
N	-4.46349400	-0.45729800	0.16516800
C	-3.32624300	0.28527000	-0.01693200
C	-5.18535500	1.61413800	-0.04383700
C	-5.60532700	0.33474700	0.15010300
C	-1.21315400	-0.40931700	2.05445400
C	0.07174000	-1.05563400	2.04636400
C	1.33166200	-0.44572600	2.25952500
Pd	1.37973200	-0.34989300	0.07951300
N	3.80072000	1.56420300	0.14245900
N	4.46331700	-0.45752900	-0.16552800
C	3.32624000	0.28525900	0.01678500
C	5.18558100	1.61382400	0.04292000
C	5.60528200	0.33433400	-0.15094900
C	1.21310400	-0.40988800	-2.05410800
C	-0.07172100	-1.05637000	-2.04580200
C	-1.33169900	-0.44668800	-2.25920900
C	-4.44981800	-1.90464900	0.34006900
H	-4.99470600	-2.39154600	-0.47436600
H	-3.40266600	-2.21434500	0.32165800
H	-4.90249100	-2.17539700	1.29855900
C	-2.93187400	2.71523400	-0.35675400
H	-3.04204200	3.43176300	0.46282500
H	-1.90820200	2.33523200	-0.38307300
H	-3.17325400	3.20206700	-1.30644300
C	2.93237300	2.71533700	0.35634300
H	3.04240300	3.43172600	-0.46337700
H	1.90864900	2.33550500	0.38303800
H	3.17412500	3.20227400	1.30588500
C	4.44938400	-1.90492200	-0.34005600
H	4.99406400	-2.39172300	0.47457800
H	3.40217300	-2.21441800	-0.32170200
H	4.90214200	-2.17598900	-1.29841400
H	-6.59686000	-0.07156800	0.27616000
H	-5.74093100	2.53613300	-0.11699000
H	5.74132900	2.53574200	0.11574300

H	6.59670800	-0.07216500	-0.27725300
H	1.24112400	0.59646700	-2.47980100
H	2.04869600	-1.02977900	-2.38390500
H	-2.16706900	-1.07977100	-2.55040400
H	-1.35478400	0.55992800	-2.67850900
H	-1.24133900	0.59717100	2.47981700
H	-2.04869800	-1.02922500	2.38433700
H	1.35461600	0.56102000	2.67852800
H	2.16708100	-1.07862200	2.55098800
H	0.06192800	-2.14253100	1.95312300
H	-0.06177700	-2.14323500	-1.95221100

AllCp' ΔG = -31937.06814 eV

Pd	1.36618800	-0.06862000	0.12990800
N	4.36156200	0.69947800	0.49039500
N	4.18128900	-1.15300800	-0.58405300
C	3.42419600	-0.17182400	0.00086700
C	5.65568200	0.27344700	0.21870300
C	5.54147900	-0.89962100	-0.46146800
C	1.16211100	1.35487500	-1.61852000
C	-0.00161600	0.63493000	-2.04049200
C	-1.16328300	1.35803500	-1.61886500
Pd	-1.36618800	-0.06836600	0.12830100
N	-4.36115900	0.70000200	0.49013300
N	-4.18170800	-1.15358300	-0.58257500
C	-3.42416100	-0.17172700	0.00063300
C	-5.65548700	0.27357300	0.22006500
C	-5.54180600	-0.90016000	-0.45904200
C	-1.27859000	-1.39583000	1.77863100
C	0.00042400	-0.83598100	2.08649700
C	1.27932600	-1.39652000	1.78035300
C	3.59973200	-2.31173500	-1.25192100
H	3.91179600	-3.23412500	-0.75306300
H	2.51511400	-2.19974700	-1.18323300
H	3.90741600	-2.33852300	-2.30146800
C	4.01691600	1.92023100	1.21060300
H	4.39881300	2.79568800	0.67720600
H	2.92683300	1.96285500	1.25920100
H	4.43520300	1.89428700	2.22125800
C	-4.01599400	1.92144500	1.20892600
H	-4.43353000	1.89642900	2.21991600
H	-2.92587600	1.96415500	1.25668600
H	-4.39831600	2.79639200	0.67499700
C	-3.60069400	-2.31294200	-1.24981600
H	-3.90884100	-2.34047200	-2.29921000
H	-2.51602400	-2.20113500	-1.18168900
H	-3.91275100	-3.23487300	-0.75010900
H	6.29509100	-1.56006800	-0.86153300
H	6.52796100	0.82972700	0.52514400
H	-6.52753300	0.83006800	0.52677700
H	-6.29572400	-1.56106700	-0.85776700
H	-1.29483200	-2.43174700	1.43268900
H	-2.10178900	-1.14187000	2.44446300
H	1.29581700	-2.43232900	1.43418000
H	2.10235700	-1.14221900	2.44622300

H	2.14189100	1.24879600	-2.06988700
H	-2.14378500	1.25363600	-2.06902700
H	-0.00264400	-0.20893700	-2.72078900
H	0.00021000	0.04708500	2.72664800
C	0.69580000	2.54223000	-0.93559300
C	-0.69409900	2.54409600	-0.93577500
H	1.33203100	3.29827800	-0.48757400
H	-1.32842900	3.30169200	-0.48767800

AllInd' ΔG = -36117.66841 eV

C	0.00000500	0.06376700	-2.16381400
C	1.18093300	0.77601400	-1.75315000
C	0.71610800	2.02756500	-1.15940400
C	1.41547600	3.14144500	-0.66635900
C	0.70407000	4.24315100	-0.18270700
C	-0.70528700	4.24288600	-0.18258500
C	-1.41636200	3.14091200	-0.66611400
C	-0.71666400	2.02729900	-1.15928900
C	-1.18113600	0.77558100	-1.75295100
C	0.00038700	-2.83098400	0.51484700
C	1.27559900	-2.51536200	1.07737900
C	-1.27483400	-2.51565800	1.07759000
Pd	1.36230000	-0.81804300	-0.21364300
C	3.26079800	-0.29090100	0.34454300
N	3.61542600	0.56318900	1.35332000
C	4.99403800	0.69698200	1.45201200
C	5.53161700	-0.09054300	0.48135800
N	4.46330700	-0.68335900	-0.18092400
Pd	-1.36213200	-0.81835200	-0.21333000
C	-3.26068000	-0.29141000	0.34479200
N	-3.61554100	0.56197600	1.35408900
C	-4.99416000	0.69607400	1.45225700
C	-5.53151400	-0.09058800	0.48078100
N	-4.46306600	-0.68314800	-0.18150800
C	-2.64531300	1.22157900	2.22337900
H	-2.74648500	0.85265800	3.24876600
H	-1.65442600	0.98039600	1.83429500
H	-2.79238200	2.30388200	2.19901800
C	-4.58138900	-1.60865000	-1.30191800
H	-5.09470200	-1.12785100	-2.13989500
H	-3.56552100	-1.88126600	-1.59579500
H	-5.13271100	-2.50383500	-0.99901800
C	4.58185600	-1.60949000	-1.30079300
H	5.13226700	-2.50494700	-0.99703900
H	3.56603000	-1.88148800	-1.59538200
H	5.09621300	-1.12945600	-2.13856800
C	2.64499600	1.22329500	2.22201600
H	1.65428800	0.98522000	1.83057200
H	2.74326000	0.85216000	3.24689200
H	2.79474100	2.30527700	2.20004700
H	-5.46463000	1.33016500	2.18748900
H	-6.55898900	-0.27304800	0.20694400
H	-2.11329300	-3.14913200	0.79040300
H	-1.29626100	-2.20400500	2.12333200
H	0.00037900	-3.45682000	-0.37773000

H	1.29712200	-2.20351300	2.12305900
H	2.11419600	-3.14859800	0.79008800
H	0.00007400	-0.75992900	-2.86951600
H	-2.13204300	0.69017000	-2.26928400
H	2.13186200	0.69084000	-2.26947200
H	-2.50485000	3.15432200	-0.67714200
H	-1.24196000	5.11541000	0.18266900
H	1.24048200	5.11587700	0.18244700
H	2.50395700	3.15525300	-0.67755300
H	5.46435100	1.33146700	2.18700400
H	6.55916300	-0.27342000	0.20806700

CpInd' ΔG = -38191.29208 eV

C	0.00024700	0.45866300	-2.21138500
C	1.18409900	1.10564800	-1.70433700
C	0.71356500	2.27542700	-0.94689500
C	1.41372800	3.31197600	-0.31529600
C	0.70144700	4.34208800	0.31060600
C	-0.70479600	4.34121200	0.31090400
C	-1.41605800	3.31020400	-0.31469000
C	-0.71488500	2.27452200	-0.94657600
C	-1.18432700	1.10408700	-1.70373900
C	-0.00021300	-2.80019100	-0.12909400
C	1.16704600	-2.57066700	0.67582200
C	-1.16639700	-2.57185500	0.67748600
C	3.26536100	-0.26068300	0.20594300
N	3.65763600	0.42197000	1.32523600
C	5.04072600	0.49806000	1.42149600
C	5.54286400	-0.15163400	0.33646600
N	4.44956900	-0.60658200	-0.39049800
C	-3.26506200	-0.26163400	0.20612300
N	-3.65756800	0.42122400	1.32522700
C	-5.04066800	0.49793000	1.42083400
C	-5.54257800	-0.15133200	0.33544300
N	-4.44915200	-0.60684600	-0.39095700
C	-2.71933600	0.98192200	2.29412600
H	-2.86157400	0.50944000	3.27046300
H	-1.71422500	0.77321400	1.92410000
H	-2.86392000	2.06200700	2.37721700
C	-4.52697100	-1.36068300	-1.63676000
H	-5.01241700	-0.76334400	-2.41435900
H	-3.50078700	-1.59051900	-1.93209900
H	-5.08668100	-2.28819200	-1.48444800
C	4.52760200	-1.36009900	-1.63648400
H	5.08585600	-2.28846800	-1.48400700
H	3.50137100	-1.58839500	-1.93286600
H	5.01464800	-0.76312400	-2.41335900
C	2.71912400	0.98385500	2.29316300
H	1.71413200	0.77612300	1.92226300
H	2.85995200	0.51146200	3.26974000
H	2.86474400	2.06381200	2.37612000
H	-5.53891600	0.99824800	2.23661400
H	-6.56085800	-0.32465600	0.02392100
H	-2.13425700	-3.01812500	0.47304700
H	-0.00062600	-3.27414900	-1.10367300

H	2.13461900	-3.01711800	0.47029900
H	0.00047800	-0.24784400	-3.03369300
H	-2.12276200	1.11506700	-2.25059800
H	2.12259600	1.11737600	-2.25104400
H	-2.50423800	3.32304800	-0.32349000
H	-1.24258300	5.15627800	0.78925200
H	1.23841800	5.15782300	0.78873000
H	2.50188800	3.32620600	-0.32461300
H	5.53881900	0.99802400	2.23758500
H	6.56121200	-0.32567900	0.02557100
C	0.68951800	-2.25993100	2.01880800
C	-0.68732500	-2.26057600	2.01977500
H	1.32928800	-2.03301800	2.86517200
H	-1.32613500	-2.03421200	2.86701100
Pd	1.34859200	-0.63629700	-0.41277500
Pd	-1.34819400	-0.63756200	-0.41205800

CpCp' ΔG = -34010.74816 eV

Pd	-1.34083800	0.00002000	0.00004600
N	-4.25817000	-0.79956300	0.71819800
N	-4.25817500	0.79950900	-0.71820700
C	-3.40776600	-0.00002100	-0.00000100
C	-5.59002600	-0.50633000	0.45453700
C	-5.59002900	0.50619900	-0.45461700
C	-1.16646100	-1.65427700	-1.45366900
C	0.00110000	-0.97797700	-1.94637600
C	1.16725900	-1.65576200	-1.45248700
Pd	1.34074600	-0.00001700	-0.00012600
N	4.25815800	-0.79970200	0.71807300
N	4.25821500	0.79973700	-0.71791800
C	3.40778500	-0.00001900	0.00000400
C	5.59002500	-0.50642100	0.45451500
C	5.59006000	0.50634500	-0.45437500
C	1.16702300	1.65530800	1.45262000
C	0.00050000	0.97800000	1.94639900
C	-1.16670500	1.65474600	1.45350800
C	-3.79477600	1.82445000	-1.64728400
H	-4.15576700	2.80900400	-1.33568500
H	-2.70306200	1.80462400	-1.62106200
H	-4.14931500	1.60643500	-2.65912800
C	-3.79475400	-1.82442800	1.64735000
H	-4.15566800	-2.80901900	1.33578100
H	-2.70303900	-1.80452900	1.62117800
H	-4.14935600	-1.60638800	2.65916700
C	3.79469900	-1.82477100	1.64698000
H	4.14945300	-1.60707700	2.65881800
H	2.70298500	-1.80471200	1.62094000
H	4.15543200	-2.80932400	1.33508000
C	3.79482400	1.82491600	-1.64673900
H	4.14959900	1.60728600	-2.65858100
H	2.70310700	1.80489100	-1.62073200
H	4.15558300	2.80943300	-1.33475200
H	-6.40598600	1.03124700	-0.92656500
H	-6.40597900	-1.03140700	0.92645900
H	6.40596200	-1.03161100	0.92634100

H	6.40603500	1.03152000	-0.92615100
H	2.13077300	1.63295100	1.94961400
H	-2.13012700	1.63181600	1.95111500
H	-2.12969200	-1.63115800	-1.95164400
H	2.13113200	-1.63369100	-1.94924700
H	0.00196200	-0.23716400	-2.73753700
H	0.00098500	0.23722000	2.73758300
C	-0.69062100	-2.78526000	-0.66859700
C	0.68924600	-2.78613100	-0.66788400
H	-1.32829800	-3.49287500	-0.14946500
H	1.32550100	-3.49451000	-0.14804500
C	-0.69034900	2.78549900	0.66843900
C	0.68952800	2.78587300	0.66797200
H	-1.32766200	3.49338800	0.14923800
H	1.32609900	3.49400100	0.14818200

IndInd' ΔG = -42371.72939 eV

Pd	1.34934000	0.00019700	0.00040000
C	0.00061300	0.87033900	1.96476500
C	1.18194000	1.56374100	1.53169900
C	0.71573500	2.78248600	0.86511700
C	1.41539500	3.86859200	0.31683300
C	0.70310400	4.94224700	-0.22500800
C	-0.70498700	4.94161100	-0.22520900
C	-1.41647600	3.86730100	0.31638800
C	-0.71602400	2.78180000	0.86485200
C	-1.18138300	1.56255300	1.53119100
N	4.26975800	-0.72487700	0.79326100
C	3.42123200	0.00024400	-0.00003500
C	5.60152200	-0.45794700	0.50244000
C	5.60128300	0.45842400	-0.50354400
N	4.26938300	0.72537900	-0.79371100
Pd	-1.34933800	-0.00016100	-0.00041500
C	-0.00061800	-0.87028700	-1.96477700
C	-1.18194500	-1.56369300	-1.53171500
C	-0.71573600	-2.78244400	-0.86514500
C	-1.41539500	-3.86856100	-0.31688200
C	-0.70310500	-4.94222900	0.22493200
C	0.70498600	-4.94159400	0.22512800
C	1.41647400	-3.86727600	-0.31645400
C	0.71602300	-2.78176000	-0.86488900
C	1.18138300	-1.56250100	-1.53120900
N	-4.26979800	0.72489400	-0.79311900
C	-3.42123100	-0.00029000	0.00007600
C	-5.60154700	0.45781200	-0.50236900
C	-5.60125600	-0.45867100	0.50351400
N	-4.26934100	-0.72555600	0.79367500
C	-3.80691200	-1.64589400	1.82834600
H	-2.71954800	-1.69963700	1.74731800
H	-4.09102000	-1.27744300	2.81866600
H	-4.23749600	-2.63804500	1.66863200
C	-3.80796800	1.64540200	-1.82790000
H	-2.72052800	1.69887500	-1.74768400
H	-4.09291200	1.27725700	-2.81809300
H	-4.23821000	2.63760900	-1.66761100

C	3.80700400	1.64569300	-1.82842500
H	4.09109300	1.27717700	-2.81872600
H	2.71964200	1.69949000	-1.74740800
H	4.23764100	2.63782800	-1.66876000
C	3.80787300	-1.64517000	1.82820800
H	4.09270300	-1.27678900	2.81834700
H	2.72044500	-1.69871600	1.74790400
H	4.23818700	-2.63738800	1.66818200
H	6.41729900	-0.93330100	1.02459500
H	6.41681000	0.93377900	-1.02608900
H	-6.41735000	0.93317100	-1.02447800
H	-6.41675600	-0.93414300	1.02599400
H	0.00084200	0.05749600	2.68311800
H	1.23909200	5.79268900	-0.63902300
H	-1.24162000	5.79158100	-0.63936100
H	-2.50437200	3.88288300	0.32889500
H	-0.00084800	-0.05744200	-2.68312800
H	2.12451000	-1.51333000	-2.06494000
H	-2.12535300	-1.51484200	-2.06494400
H	-2.50327500	-3.88512800	-0.32974100
H	-1.23909200	-5.79268000	0.63892900
H	1.24162000	-5.79157500	0.63925700
H	2.50437000	-3.88286600	-0.32897500
H	2.50327500	3.88515700	0.32968400
H	2.12535000	1.51488600	2.06492300
H	-2.12452000	1.51337600	2.06490200

AllAll'$^{+}$ ΔG = -1097.288671 eV

Pd	1.33258700	-0.24809400	0.00017400
N	3.98867900	1.38257900	-0.00055900
N	4.40201300	-0.72889200	0.00006500
C	3.37242900	0.16606600	-0.00014800
C	5.37120500	1.24983500	-0.00059500
C	5.63235900	-0.08459700	-0.00017600
C	1.26696500	-0.09242300	-2.14751500
C	0.00003000	-0.74902700	-1.99496800
C	-1.26658000	-0.09161600	-2.14727700
Pd	-1.33264700	-0.24807900	0.00022600
N	-3.98877100	1.38253000	-0.00090700
N	-4.40203500	-0.72895600	0.00034200
C	-3.37247600	0.16603700	-0.00015100
C	-5.37129100	1.24973800	-0.00092900
C	-5.63240100	-0.08470200	-0.00010500
C	-1.26664500	-0.08863200	2.14766800
C	0.00010100	-0.74588000	1.99629500
C	1.26687000	-0.08853800	2.14745400
C	4.23151800	-2.18144200	0.00064700
H	4.68975100	-2.61264900	0.89412900
H	3.15999300	-2.38722500	-0.00013300
H	4.69125400	-2.61349300	-0.89164800
C	3.28104000	2.66148600	-0.00101400
H	3.54209300	3.23476400	-0.89412600
H	2.21217000	2.44306300	-0.00106200
H	3.54190600	3.23531600	0.89179900
C	-3.28118600	2.66146400	-0.00193200

H	-3.54264700	3.23596700	0.89027200
H	-2.21230700	2.44309000	-0.00113500
H	-3.54169300	3.23404800	-0.89565100
C	-4.23149600	-2.18150100	0.00138200
H	-4.69003800	-2.61374800	-0.89143700
H	-3.15996500	-2.38725100	0.00203000
H	-4.69089600	-2.61253900	0.89434200
H	6.56757800	-0.62205600	-0.00005200
H	6.03485200	2.10017100	-0.00094000
H	-6.03496900	2.10005100	-0.00147300
H	-6.56760300	-0.62219100	0.00023100
H	-1.27339900	0.96760900	2.41136400
H	-2.10050400	-0.66640100	2.53605900
H	2.10069500	-0.66621400	2.53606700
H	1.27354300	0.96771500	2.41112900
H	1.27403700	0.96331400	-2.41320700
H	2.10066700	-0.67118500	-2.53475900
H	-1.27295000	0.96422000	-2.41262000
H	-2.10050000	-0.66970800	-2.53506400
H	-0.00033800	-1.83619300	-2.03926400
H	0.00016900	-1.83297100	2.04231200

$CpCp'^{+}$ ΔG = -1249.711516 eV

Pd	1.29240100	-0.00027900	0.00009100
N	4.25476200	0.94352400	-0.51635600
N	4.25561700	-0.94239400	0.51589200
C	3.41434500	0.00019000	-0.00021500
C	5.58615400	0.59722200	-0.32737800
C	5.58669600	-0.59502500	0.32664600
C	1.16293700	-1.50056800	-1.64517900
C	-0.00234700	-2.22911200	-1.24381100
C	-1.16451300	-1.49682700	-1.64772200
Pd	-1.29243900	-0.00038200	0.00009900
N	-4.25471400	0.94389100	-0.51578500
N	-4.25575700	-0.94250800	0.51558100
C	-3.41439400	0.00030200	0.00004900
C	-5.58613900	0.59756300	-0.32710100
C	-5.58680200	-0.59500900	0.32633400
C	-1.16351900	1.49787900	1.64673200
C	0.00042600	2.22820700	1.24454700
C	1.16394600	1.49747400	1.64718700
C	3.81049900	-2.15707400	1.19774100
H	4.12884400	-2.13981200	2.24326400
H	2.72128900	-2.18433300	1.14328200
H	4.22833000	-3.03730000	0.70318300
C	3.80848900	2.15777800	-1.19820100
H	4.12438700	2.13958300	-2.24445900
H	2.71941200	2.18543000	-1.14125600
H	4.22778400	3.03823200	-0.70531200
C	-3.80830600	2.15833000	-1.19721300
H	-4.22761400	3.03865900	-0.70411100
H	-2.71923000	2.18590600	-1.14015100
H	-4.12408100	2.14045600	-2.24351400
C	-3.81070000	-2.15756300	1.19679500
H	-4.22884500	-3.03748700	0.70196800

H	-2.72151100	-2.18499900	1.14198700
H	-4.12873300	-2.14069600	2.24242100
H	6.40185900	-1.21353900	0.66813100
H	6.40075400	1.21644700	-0.66891500
H	-6.40067900	1.21697100	-0.66845100
H	-6.40202800	-1.21365800	0.66742300
H	-2.16023200	1.91301800	1.72082300
H	2.16080600	1.91220700	1.72156800
H	2.15922300	-1.91699700	-1.71773900
H	-2.16184700	-1.91021700	-1.72310000
H	-0.00443800	-3.19748200	-0.75941800
H	0.00067100	3.19663700	0.76027600
C	0.71800500	-0.28473300	-2.27166800
C	-0.71421600	-0.28238600	-2.27304000
H	1.33816500	0.40799700	-2.82645100
H	-1.33108900	0.41300300	-2.82816100
C	0.71598200	0.28223800	2.27270800
C	-0.71622400	0.28251200	2.27244700
H	1.33427700	-0.41209700	2.82756100
H	-1.33497200	-0.41153700	2.82715700

X-Ray Crystallography

X-Ray Data for AllCp

AllCp crystallizes in the monoclinic space group *C*2/*c* with half a molecule in the asymmetric unit along with two half molecules of toluene. One of the isopropyl groups was disordered over two positions. The cyclopentadienyl and allyl ligands are disordered about a crystallographic inversion center and were refined with the help of similarity restraints on the 1,2- and 1,3-distances and displacement parameters as well as rigid bond restraints for anisotropic displacement parameters. In addition, the 1,2-distance for three atoms of the cyclopentadienyl (C1-C2 and C1-C5) and the allyl (C6-C7 and C6-C8) ligands were restrained to be equivalent because the atoms overlap and when refined, the bond lengths in the cyclopentadienyl lengthen to approximately 1.5 Å and the bond lengths in the allyl shorten to 1.3 Å. The coordinates for the hydrogen atoms bound to C1, C2, C5, and C6 were taken from the difference Fourier synthesis and the hydrogen atoms were subsequently refined semi-freely with the help of a distance restraint. The hydrogen atoms bound to C7 and C8 were included into the model at geometrically calculated positions and refined using a riding model, based on the positions found on C7 (the hydrogen atoms on C8 could not be refined). One toluene is located near a crystallographic inversion center and the other near a two-fold rotation axis and each was disordered accordingly. The 1,2-distances in the aromatic ring of the toluene molecules were restrained to be 1.40 Å.

Table S1. Crystal data and structure refinement for **AllCp**

Empirical formula	C76 H98 N4 Pd2	
Formula weight	1280.38	
Temperature	150(2) K	
Wavelength	0.71075 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 26.4612(7) Å	α= 90°.
	b = 15.0518(4) Å	β= 94.665(7)°.
	c = 16.9005(12) Å	γ = 90°.
Volume	6709.0(5) Å^3	
Z	4	
Density (calculated)	1.268 Mg/m^3	
Absorption coefficient	0.580 mm^{-1}	
F(000)	2696	
Crystal size	0.15 x 0.10 x 0.10 mm^3	
Theta range for data collection	3.02 to 30.51°.	
Index ranges	-37<=h<=37, -21<=k<=21, -21<=l<=24	
Reflections collected	101885	
Independent reflections	10223 [R(int) = 0.0534]	
Completeness to theta = 30.51°	99.7 %	
Absorption correction	Semi-empirical from equivalents	

Max. and min. transmission	0.9442 and 0.9180
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	10223 / 399 / 508
Goodness-of-fit on F^2	1.116
Final R indices [I>2sigma(I)]	R1 = 0.0373, wR2 = 0.0723
R indices (all data)	R1 = 0.0455, wR2 = 0.0748
Largest diff. peak and hole	0.840 and -0.533 e.Å^{-3}

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for **AllCp**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Pd(1)	7355(1)	3059(1)	9397(1)	22(1)
N(1)	7425(1)	4392(1)	8001(1)	23(1)
N(2)	6676(1)	4373(1)	8391(1)	22(1)
C(1)	7506(8)	3628(9)	10934(11)	40(3)
C(2)	7101(7)	3917(10)	10386(9)	28(2)
C(3)	6677(2)	3357(3)	10612(3)	34(1)
C(4)	6831(2)	2818(3)	11232(3)	35(1)
C(5)	7368(6)	2953(11)	11471(11)	29(2)
C(6)	7546(9)	1523(10)	9156(12)	41(3)
C(7)	7676(6)	2196(10)	8628(10)	30(2)
C(8)	7926(7)	1218(10)	9719(9)	29(2)
C(9)	7142(1)	3982(1)	8539(1)	22(1)
C(10)	7144(1)	5014(1)	7541(1)	27(1)
C(11)	6674(1)	4997(1)	7783(1)	26(1)
C(21)	7948(1)	4202(1)	7868(1)	26(1)
C(22)	8336(1)	4547(1)	8389(1)	31(1)
C(23)	8834(1)	4401(2)	8206(2)	42(1)
C(24)	8940(1)	3941(2)	7534(2)	46(1)
C(25)	8552(1)	3598(2)	7035(1)	39(1)
C(26)	8046(1)	3711(1)	7191(1)	28(1)
C(27)	8251(1)	5065(1)	9136(1)	33(1)
C(28)	8466(1)	6005(2)	9090(2)	45(1)
C(29)	8489(1)	4572(2)	9864(2)	46(1)
C(30)	7635(1)	3303(1)	6625(1)	31(1)
C(31)	7570(1)	3832(2)	5855(1)	48(1)
C(32)	7749(1)	2331(2)	6432(2)	44(1)
C(41)	6220(1)	4122(1)	8750(1)	23(1)
C(42)	6015(1)	4711(1)	9282(1)	27(1)
C(47)	6246(1)	5604(1)	9521(1)	30(1)
C(48)	6252(1)	5770(2)	10415(1)	42(1)
C(49)	5957(1)	6362(2)	9074(1)	39(1)
C(43)	5564(1)	4457(2)	9594(1)	35(1)
C(44)	5333(1)	3663(2)	9394(2)	42(1)
C(45)	5542(1)	3094(2)	8868(1)	38(1)
C(46)	5989(1)	3313(1)	8529(1)	28(1)
C(50)	6188(1)	2702(1)	7911(1)	32(1)
C(51)	5820(5)	2753(10)	7119(6)	51(2)
C(52)	6235(6)	1747(8)	8199(8)	45(2)
C(51A)	5995(8)	2968(8)	7122(7)	50(3)
C(52A)	6093(6)	1718(9)	8061(9)	37(2)
C(7S)	10231(10)	6144(10)	4403(9)	123(5)
C(1S)	10073(2)	5385(5)	4862(4)	77(2)
C(2S)	9961(7)	5510(6)	5635(6)	73(3)

C(3S)	9777(3)	4819(4)	6068(4)	74(2)
C(4S)	9745(8)	3952(6)	5793(8)	74(3)
C(5S)	9893(3)	3833(6)	5031(5)	87(2)
C(6S)	10067(9)	4524(7)	4594(7)	94(3)
C(7T)	5675(3)	6752(5)	6594(4)	75(2)
C(1T)	5301(5)	6394(5)	7098(7)	56(2)
C(2T)	5003(13)	6983(3)	7490(20)	54(1)
C(3T)	4669(5)	6676(5)	8027(7)	63(2)
C(4T)	4615(4)	5765(5)	8109(5)	84(3)
C(5T)	4890(5)	5182(5)	7673(8)	93(4)
C(6T)	5235(5)	5481(5)	7166(8)	81(3)

Table S3. Anisotropic displacement parameters ($Å^2$x 10^3) for **AllCp**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Pd(1)	22(1)	23(1)	22(1)	6(1)	5(1)	5(1)
N(1)	21(1)	23(1)	26(1)	5(1)	7(1)	4(1)
N(2)	22(1)	22(1)	24(1)	5(1)	6(1)	4(1)
C(1)	55(5)	32(5)	32(6)	0(4)	10(4)	19(4)
C(2)	46(3)	11(4)	28(4)	-1(3)	6(3)	5(2)
C(3)	38(2)	31(2)	33(2)	10(2)	-1(2)	2(2)
C(4)	38(2)	32(2)	36(2)	12(2)	5(2)	2(2)
C(5)	37(3)	28(4)	21(5)	-6(3)	0(3)	9(3)
C(6)	67(6)	34(4)	22(3)	-7(3)	9(3)	16(4)
C(7)	44(4)	31(5)	15(4)	-2(3)	5(3)	11(3)
C(8)	40(3)	20(5)	29(4)	-7(3)	6(3)	8(3)
C(9)	20(1)	21(1)	26(1)	3(1)	5(1)	2(1)
C(10)	30(1)	24(1)	27(1)	9(1)	8(1)	6(1)
C(11)	28(1)	26(1)	26(1)	8(1)	5(1)	8(1)
C(21)	21(1)	26(1)	31(1)	7(1)	10(1)	3(1)
C(22)	26(1)	34(1)	34(1)	3(1)	8(1)	0(1)
C(23)	23(1)	54(1)	51(1)	-5(1)	7(1)	-2(1)
C(24)	23(1)	60(2)	57(2)	-6(1)	15(1)	1(1)
C(25)	31(1)	44(1)	45(1)	-6(1)	18(1)	3(1)
C(26)	26(1)	28(1)	32(1)	5(1)	10(1)	2(1)
C(27)	28(1)	38(1)	34(1)	0(1)	7(1)	-3(1)
C(28)	46(1)	39(1)	51(1)	0(1)	15(1)	-4(1)
C(29)	49(1)	48(1)	40(1)	4(1)	4(1)	-1(1)
C(30)	29(1)	35(1)	32(1)	0(1)	10(1)	0(1)
C(31)	55(2)	53(2)	37(1)	9(1)	3(1)	8(1)
C(32)	54(1)	36(1)	43(1)	-6(1)	12(1)	-4(1)
C(41)	18(1)	29(1)	23(1)	6(1)	4(1)	5(1)
C(42)	20(1)	33(1)	27(1)	2(1)	3(1)	7(1)
C(47)	24(1)	32(1)	33(1)	-4(1)	4(1)	6(1)
C(48)	39(1)	50(1)	36(1)	-10(1)	1(1)	10(1)
C(49)	38(1)	34(1)	44(1)	2(1)	5(1)	9(1)
C(43)	24(1)	46(1)	36(1)	0(1)	11(1)	7(1)
C(44)	24(1)	52(1)	52(1)	4(1)	16(1)	-2(1)
C(45)	27(1)	38(1)	51(1)	1(1)	9(1)	-5(1)
C(46)	24(1)	30(1)	31(1)	2(1)	5(1)	2(1)
C(50)	32(1)	30(1)	37(1)	-2(1)	8(1)	0(1)
C(51)	66(5)	49(6)	36(3)	-2(3)	-2(3)	18(4)
C(52)	54(6)	39(3)	38(5)	2(3)	-9(3)	17(4)
C(51A)	86(9)	32(4)	33(3)	1(3)	9(4)	5(4)

C(52A)	52(6)	32(3)	26(5)	6(3)	-4(4)	6(4)
C(7S)	67(8)	221(13)	84(9)	73(8)	14(8)	11(10)
C(1S)	38(3)	121(5)	72(4)	10(4)	4(3)	23(4)
C(2S)	58(5)	80(5)	83(6)	14(4)	10(6)	13(4)
C(3S)	68(4)	80(4)	78(4)	14(3)	22(3)	14(3)
C(4S)	60(6)	80(4)	85(6)	19(4)	25(6)	11(4)
C(5S)	78(5)	91(5)	92(5)	-25(4)	5(4)	24(4)
C(6S)	76(7)	138(6)	68(7)	-10(5)	4(6)	15(6)
C(7T)	85(5)	81(5)	59(4)	-12(3)	0(3)	14(4)
C(1T)	62(4)	39(3)	61(5)	3(3)	-32(3)	-2(3)
C(2T)	54(2)	45(2)	58(3)	14(8)	-14(2)	-8(8)
C(3T)	56(4)	71(5)	58(5)	12(5)	-19(3)	-20(5)
C(4T)	80(6)	85(6)	80(6)	41(5)	-44(4)	-41(5)
C(5T)	93(10)	68(5)	105(10)	20(6)	-65(5)	-30(6)
C(6T)	93(8)	40(4)	100(8)	11(4)	-55(5)	-9(4)

Table S4. Bond lengths (Å) for **AllCp**

Pd(1)-C(8)#1	2.037(13)
Pd(1)-C(9)	2.0539(17)
Pd(1)-C(7)	2.067(15)
Pd(1)-C(2)	2.258(14)
Pd(1)-C(5)#1	2.277(14)
Pd(1)-C(6)	2.407(16)
Pd(1)-C(6)#1	2.517(19)
Pd(1)-C(1)#1	2.631(14)
Pd(1)-Pd(1)#1	2.7050(3)
N(1)-C(9)	1.370(2)
N(1)-C(10)	1.392(2)
N(1)-C(21)	1.449(2)
N(2)-C(9)	1.370(2)
N(2)-C(11)	1.391(2)
N(2)-C(41)	1.446(2)
C(1)-C(2)	1.427(10)
C(1)-C(5)	1.430(10)
C(1)-Pd(1)#1	2.631(14)
C(1)-H(1)	0.970(19)
C(2)-C(3)	1.477(17)
C(2)-H(2)	0.940(19)
C(3)-C(4)	1.361(5)
C(3)-H(3)	0.9500
C(4)-C(5)	1.460(16)
C(4)-H(4)	0.9500
C(5)-Pd(1)#1	2.277(14)
C(5)-H(5)	0.944(19)
C(6)-C(8)	1.405(10)
C(6)-C(7)	1.411(10)
C(6)-Pd(1)#1	2.517(19)
C(6)-H(6)	0.976(19)
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(8)-Pd(1)#1	2.037(13)
C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900
C(10)-C(11)	1.341(2)
C(10)-H(10)	0.9500

C(11)-H(11)	0.9500
C(21)-C(22)	1.397(3)
C(21)-C(26)	1.403(3)
C(22)-C(23)	1.396(3)
C(22)-C(27)	1.517(3)
C(23)-C(24)	1.377(3)
C(23)-H(23)	0.9500
C(24)-C(25)	1.376(3)
C(24)-H(24)	0.9500
C(25)-C(26)	1.396(3)
C(25)-H(25)	0.9500
C(26)-C(30)	1.517(3)
C(27)-C(29)	1.528(3)
C(27)-C(28)	1.529(3)
C(27)-H(27)	1.0000
C(28)-H(28A)	0.9800
C(28)-H(28B)	0.9800
C(28)-H(28C)	0.9800
C(29)-H(29A)	0.9800
C(29)-H(29B)	0.9800
C(29)-H(29C)	0.9800
C(30)-C(31)	1.523(3)
C(30)-C(32)	1.535(3)
C(30)-H(30)	1.0000
C(31)-H(31A)	0.9800
C(31)-H(31B)	0.9800
C(31)-H(31C)	0.9800
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800
C(41)-C(46)	1.399(3)
C(41)-C(42)	1.402(3)
C(42)-C(43)	1.397(3)
C(42)-C(47)	1.517(3)
C(47)-C(48)	1.531(3)
C(47)-C(49)	1.538(3)
C(47)-H(47)	1.0000
C(48)-H(48A)	0.9800
C(48)-H(48B)	0.9800
C(48)-H(48C)	0.9800
C(49)-H(49A)	0.9800
C(49)-H(49B)	0.9800
C(49)-H(49C)	0.9800
C(43)-C(44)	1.373(3)
C(43)-H(43)	0.9500
C(44)-C(45)	1.382(3)
C(44)-H(44)	0.9500
C(45)-C(46)	1.395(3)
C(45)-H(45)	0.9500
C(46)-C(50)	1.517(3)
C(50)-C(51A)	1.445(13)
C(50)-C(52)	1.520(12)
C(50)-C(52A)	1.526(14)
C(50)-C(51)	1.590(9)
C(50)-H(50)	1.0000
C(50)-H(50A)	1.0000

C(51)-H(51A)	0.9800
C(51)-H(51B)	0.9800
C(51)-H(51C)	0.9800
C(52)-H(52A)	0.9800
C(52)-H(52B)	0.9800
C(52)-H(52C)	0.9800
C(51A)-H(51D)	0.9800
C(51A)-H(51E)	0.9800
C(51A)-H(51F)	0.9800
C(52A)-H(52D)	0.9800
C(52A)-H(52E)	0.9800
C(52A)-H(52F)	0.9800
C(7S)-C(1S)	1.460(13)
C(7S)-H(7S1)	0.9800
C(7S)-H(7S2)	0.9800
C(7S)-H(7S3)	0.9800
C(1S)-C(6S)	1.372(7)
C(1S)-C(2S)	1.377(7)
C(2S)-C(3S)	1.383(7)
C(2S)-H(2S)	0.9500
C(3S)-C(4S)	1.385(7)
C(3S)-H(3S)	0.9500
C(4S)-C(5S)	1.387(7)
C(4S)-H(4S)	0.9500
C(5S)-C(6S)	1.378(7)
C(5S)-H(5S)	0.9500
C(6S)-H(6S)	0.9500
C(7T)-C(1T)	1.459(12)
C(7T)-H(7T1)	0.9800
C(7T)-H(7T2)	0.9800
C(7T)-H(7T3)	0.9800
C(1T)-C(6T)	1.391(6)
C(1T)-C(2T)	1.392(7)
C(2T)-C(3T)	1.393(7)
C(2T)-H(2T)	0.9500
C(3T)-C(4T)	1.387(7)
C(3T)-H(3T)	0.9500
C(4T)-C(5T)	1.390(7)
C(4T)-H(4T)	0.9500
C(5T)-C(6T)	1.378(7)
C(5T)-H(5T)	0.9500
C(6T)-H(6T)	0.9500

Symmetry transformations used to generate equivalent atoms:
#1 -x+3/2,-y+1/2,-z+2

Table S5. Bond angles (°) for **AllCp**

C(8)#1-Pd(1)-C(9)	93.5(5)
C(8)#1-Pd(1)-C(7)	171.7(7)
C(9)-Pd(1)-C(7)	94.8(5)
C(8)#1-Pd(1)-C(2)	4.4(9)
C(9)-Pd(1)-C(2)	93.1(4)
C(7)-Pd(1)-C(2)	170.7(7)
C(8)#1-Pd(1)-C(5)#1	170.3(7)
C(9)-Pd(1)-C(5)#1	94.7(5)
C(7)-Pd(1)-C(5)#1	5.6(8)

C(2)-Pd(1)-C(5)#1	172.1(6)
C(8)#1-Pd(1)-C(6)	137.0(7)
C(9)-Pd(1)-C(6)	125.4(5)
C(7)-Pd(1)-C(6)	35.7(3)
C(2)-Pd(1)-C(6)	138.9(7)
C(5)#1-Pd(1)-C(6)	33.5(10)
C(8)#1-Pd(1)-C(6)#1	33.9(4)
C(9)-Pd(1)-C(6)#1	121.2(4)
C(7)-Pd(1)-C(6)#1	138.8(7)
C(2)-Pd(1)-C(6)#1	32.0(8)
C(5)#1-Pd(1)-C(6)#1	141.2(7)
C(6)-Pd(1)-C(6)#1	113.4(5)
C(8)#1-Pd(1)-C(1)#1	137.5(7)
C(9)-Pd(1)-C(1)#1	122.5(4)
C(7)-Pd(1)-C(1)#1	35.8(9)
C(2)-Pd(1)-C(1)#1	139.8(6)
C(5)#1-Pd(1)-C(1)#1	32.9(3)
C(6)-Pd(1)-C(1)#1	4.6(9)
C(6)#1-Pd(1)-C(1)#1	116.2(7)
C(8)#1-Pd(1)-Pd(1)#1	83.0(5)
C(9)-Pd(1)-Pd(1)#1	175.87(5)
C(7)-Pd(1)-Pd(1)#1	88.7(5)
C(2)-Pd(1)-Pd(1)#1	83.2(4)
C(5)#1-Pd(1)-Pd(1)#1	89.0(5)
C(6)-Pd(1)-Pd(1)#1	58.7(5)
C(6)#1-Pd(1)-Pd(1)#1	54.8(4)
C(1)#1-Pd(1)-Pd(1)#1	61.6(4)
C(9)-N(1)-C(10)	112.22(14)
C(9)-N(1)-C(21)	126.46(15)
C(10)-N(1)-C(21)	121.25(14)
C(9)-N(2)-C(11)	112.01(14)
C(9)-N(2)-C(41)	125.55(14)
C(11)-N(2)-C(41)	122.16(14)
C(2)-C(1)-C(5)	114.3(18)
C(2)-C(1)-Pd(1)#1	105.5(10)
C(5)-C(1)-Pd(1)#1	59.8(7)
C(2)-C(1)-H(1)	119(4)
C(5)-C(1)-H(1)	124(5)
Pd(1)#1-C(1)-H(1)	117(4)
C(1)-C(2)-C(3)	101.8(13)
C(1)-C(2)-Pd(1)	93.0(11)
C(3)-C(2)-Pd(1)	98.3(7)
C(1)-C(2)-H(2)	129(3)
C(3)-C(2)-H(2)	128(3)
Pd(1)-C(2)-H(2)	90(3)
C(4)-C(3)-C(2)	110.7(7)
C(4)-C(3)-H(3)	124.7
C(2)-C(3)-H(3)	124.7
C(3)-C(4)-C(5)	110.8(8)
C(3)-C(4)-H(4)	124.6
C(5)-C(4)-H(4)	124.6
C(1)-C(5)-C(4)	102.4(14)
C(1)-C(5)-Pd(1)#1	87.3(9)
C(4)-C(5)-Pd(1)#1	94.8(7)
C(1)-C(5)-H(5)	122(3)
C(4)-C(5)-H(5)	135(3)

Pd(1)#1-C(5)-H(5)	94(3)
C(8)-C(6)-C(7)	117.8(19)
C(8)-C(6)-Pd(1)	110.4(10)
C(7)-C(6)-Pd(1)	58.9(8)
C(8)-C(6)-Pd(1)#1	54.0(8)
C(7)-C(6)-Pd(1)#1	115.1(10)
Pd(1)-C(6)-Pd(1)#1	66.6(5)
C(8)-C(6)-H(6)	123(5)
C(7)-C(6)-H(6)	119(5)
Pd(1)-C(6)-H(6)	100(4)
Pd(1)#1-C(6)-H(6)	102(4)
C(6)-C(7)-Pd(1)	85.4(9)
C(6)-C(7)-H(7A)	114.4
Pd(1)-C(7)-H(7A)	114.4
C(6)-C(7)-H(7B)	114.4
Pd(1)-C(7)-H(7B)	114.4
H(7A)-C(7)-H(7B)	111.5
C(6)-C(8)-Pd(1)#1	92.2(11)
C(6)-C(8)-H(8A)	113.3
Pd(1)#1-C(8)-H(8A)	113.3
C(6)-C(8)-H(8B)	113.3
Pd(1)#1-C(8)-H(8B)	113.3
H(8A)-C(8)-H(8B)	110.6
N(1)-C(9)-N(2)	102.51(14)
N(1)-C(9)-Pd(1)	129.77(12)
N(2)-C(9)-Pd(1)	127.65(12)
C(11)-C(10)-N(1)	106.41(15)
C(11)-C(10)-H(10)	126.8
N(1)-C(10)-H(10)	126.8
C(10)-C(11)-N(2)	106.84(15)
C(10)-C(11)-H(11)	126.6
N(2)-C(11)-H(11)	126.6
C(22)-C(21)-C(26)	122.31(17)
C(22)-C(21)-N(1)	119.46(17)
C(26)-C(21)-N(1)	118.15(17)
C(23)-C(22)-C(21)	117.43(19)
C(23)-C(22)-C(27)	118.20(19)
C(21)-C(22)-C(27)	124.37(17)
C(24)-C(23)-C(22)	121.4(2)
C(24)-C(23)-H(23)	119.3
C(22)-C(23)-H(23)	119.3
C(25)-C(24)-C(23)	120.2(2)
C(25)-C(24)-H(24)	119.9
C(23)-C(24)-H(24)	119.9
C(24)-C(25)-C(26)	121.2(2)
C(24)-C(25)-H(25)	119.4
C(26)-C(25)-H(25)	119.4
C(25)-C(26)-C(21)	117.52(19)
C(25)-C(26)-C(30)	118.64(18)
C(21)-C(26)-C(30)	123.84(16)
C(22)-C(27)-C(29)	109.95(18)
C(22)-C(27)-C(28)	110.59(17)
C(29)-C(27)-C(28)	111.05(19)
C(22)-C(27)-H(27)	108.4
C(29)-C(27)-H(27)	108.4
C(28)-C(27)-H(27)	108.4

C(27)-C(28)-H(28A)	109.5
C(27)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
C(27)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
C(27)-C(29)-H(29A)	109.5
C(27)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5
C(27)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5
C(26)-C(30)-C(31)	110.71(18)
C(26)-C(30)-C(32)	112.21(18)
C(31)-C(30)-C(32)	109.08(19)
C(26)-C(30)-H(30)	108.2
C(31)-C(30)-H(30)	108.2
C(32)-C(30)-H(30)	108.2
C(30)-C(31)-H(31A)	109.5
C(30)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
C(30)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
C(30)-C(32)-H(32A)	109.5
C(30)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
C(30)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
C(46)-C(41)-C(42)	122.58(16)
C(46)-C(41)-N(2)	118.39(16)
C(42)-C(41)-N(2)	118.98(16)
C(43)-C(42)-C(41)	117.15(18)
C(43)-C(42)-C(47)	118.65(17)
C(41)-C(42)-C(47)	124.20(16)
C(42)-C(47)-C(48)	112.35(18)
C(42)-C(47)-C(49)	110.68(17)
C(48)-C(47)-C(49)	109.13(17)
C(42)-C(47)-H(47)	108.2
C(48)-C(47)-H(47)	108.2
C(49)-C(47)-H(47)	108.2
C(47)-C(48)-H(48A)	109.5
C(47)-C(48)-H(48B)	109.5
H(48A)-C(48)-H(48B)	109.5
C(47)-C(48)-H(48C)	109.5
H(48A)-C(48)-H(48C)	109.5
H(48B)-C(48)-H(48C)	109.5
C(47)-C(49)-H(49A)	109.5
C(47)-C(49)-H(49B)	109.5
H(49A)-C(49)-H(49B)	109.5
C(47)-C(49)-H(49C)	109.5
H(49A)-C(49)-H(49C)	109.5
H(49B)-C(49)-H(49C)	109.5
C(44)-C(43)-C(42)	121.47(19)
C(44)-C(43)-H(43)	119.3

C(42)-C(43)-H(43)	119.3
C(43)-C(44)-C(45)	120.25(19)
C(43)-C(44)-H(44)	119.9
C(45)-C(44)-H(44)	119.9
C(44)-C(45)-C(46)	121.0(2)
C(44)-C(45)-H(45)	119.5
C(46)-C(45)-H(45)	119.5
C(45)-C(46)-C(41)	117.50(18)
C(45)-C(46)-C(50)	119.41(18)
C(41)-C(46)-C(50)	122.99(17)
C(51A)-C(50)-C(46)	110.6(6)
C(51A)-C(50)-C(52)	124.9(6)
C(46)-C(50)-C(52)	112.1(6)
C(51A)-C(50)-C(52A)	111.9(6)
C(46)-C(50)-C(52A)	113.8(6)
C(52)-C(50)-C(52A)	16.1(5)
C(51A)-C(50)-C(51)	20.7(5)
C(46)-C(50)-C(51)	109.2(4)
C(52)-C(50)-C(51)	110.1(5)
C(52A)-C(50)-C(51)	95.1(5)
C(51A)-C(50)-H(50)	88.9
C(46)-C(50)-H(50)	108.4
C(52)-C(50)-H(50)	108.4
C(52A)-C(50)-H(50)	120.6
C(51)-C(50)-H(50)	108.4
C(51A)-C(50)-H(50A)	106.7
C(46)-C(50)-H(50A)	106.7
C(52)-C(50)-H(50A)	92.6
C(52A)-C(50)-H(50A)	106.7
C(51)-C(50)-H(50A)	125.1
H(50)-C(50)-H(50A)	18.9
C(50)-C(51)-H(51A)	109.5
C(50)-C(51)-H(51B)	109.5
H(51A)-C(51)-H(51B)	109.5
C(50)-C(51)-H(51C)	109.5
H(51A)-C(51)-H(51C)	109.5
H(51B)-C(51)-H(51C)	109.5
C(50)-C(52)-H(52A)	109.5
C(50)-C(52)-H(52B)	109.5
H(52A)-C(52)-H(52B)	109.5
C(50)-C(52)-H(52C)	109.5
H(52A)-C(52)-H(52C)	109.5
H(52B)-C(52)-H(52C)	109.5
C(50)-C(51A)-H(51D)	109.5
C(50)-C(51A)-H(51E)	109.5
H(51D)-C(51A)-H(51E)	109.5
C(50)-C(51A)-H(51F)	109.5
H(51D)-C(51A)-H(51F)	109.5
H(51E)-C(51A)-H(51F)	109.5
C(50)-C(52A)-H(52D)	109.5
C(50)-C(52A)-H(52E)	109.5
H(52D)-C(52A)-H(52E)	109.5
C(50)-C(52A)-H(52F)	109.5
H(52D)-C(52A)-H(52F)	109.5
H(52E)-C(52A)-H(52F)	109.5
C(6S)-C(1S)-C(2S)	116.4(8)

C(6S)-C(1S)-C(7S)	124.0(8)
C(2S)-C(1S)-C(7S)	119.4(8)
C(1S)-C(2S)-C(3S)	120.8(8)
C(1S)-C(2S)-H(2S)	119.6
C(3S)-C(2S)-H(2S)	119.6
C(2S)-C(3S)-C(4S)	123.1(7)
C(2S)-C(3S)-H(3S)	118.4
C(4S)-C(3S)-H(3S)	118.4
C(3S)-C(4S)-C(5S)	114.8(8)
C(3S)-C(4S)-H(4S)	122.6
C(5S)-C(4S)-H(4S)	122.6
C(6S)-C(5S)-C(4S)	122.2(9)
C(6S)-C(5S)-H(5S)	118.9
C(4S)-C(5S)-H(5S)	118.9
C(1S)-C(6S)-C(5S)	122.1(9)
C(1S)-C(6S)-H(6S)	118.9
C(5S)-C(6S)-H(6S)	118.9
C(6T)-C(1T)-C(2T)	120.6(8)
C(6T)-C(1T)-C(7T)	120.5(9)
C(2T)-C(1T)-C(7T)	118.8(7)
C(1T)-C(2T)-C(3T)	120.9(6)
C(1T)-C(2T)-H(2T)	119.6
C(3T)-C(2T)-H(2T)	119.6
C(4T)-C(3T)-C(2T)	118.0(7)
C(4T)-C(3T)-H(3T)	121.0
C(2T)-C(3T)-H(3T)	121.0
C(3T)-C(4T)-C(5T)	120.5(8)
C(3T)-C(4T)-H(4T)	119.7
C(5T)-C(4T)-H(4T)	119.7
C(6T)-C(5T)-C(4T)	121.7(8)
C(6T)-C(5T)-H(5T)	119.1
C(4T)-C(5T)-H(5T)	119.1
C(5T)-C(6T)-C(1T)	118.0(9)
C(5T)-C(6T)-H(6T)	121.0
C(1T)-C(6T)-H(6T)	121.0

Symmetry transformations used to generate equivalent atoms:
#1 -x+3/2,-y+1/2,-z+2

X-Ray Data for AllInd

AllInd crystallizes in the monoclinic space group $P2_1/c$ with one molecule in the asymmetric unit along with one molecule of toluene. One of the four aromatic groups was disordered over two positions. The toluene molecule was modeled as a three component disorder, all of which were restrained to be flat. The coordinates for the hydrogen atoms bound to C1, C2, C9, C11, C12, and C13 were taken from the difference Fourier synthesis and the hydrogen atoms were subsequently refined semi-freely with the help of a distance restraint.

Table S6. Crystal data and structure refinement for **AllInd**

Empirical formula	C73 H92 N4 Pd2

Formula weight	1238.31	
Temperature	93(2) K	
Wavelength	1.54187 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 19.0156(13) Å	α= 90°.
	b = 18.4373(4) Å	β= 97.804(7)°.
	c = 18.1286(3) Å	γ = 90°.
Volume	6297.0(5) $Å^3$	
Z	4	
Density (calculated)	1.306 Mg/m^3	
Absorption coefficient	4.937 mm^{-1}	
F(000)	2600	
Crystal size	0.05 x 0.05 x 0.03 mm^3	
Theta range for data collection	2.35 to 66.60°.	
Index ranges	-22<=h<=22, -21<=k<=21, -21<=l<=21	
Reflections collected	111730	
Independent reflections	11116 [R(int) = 0.0798]	
Completeness to theta = 66.60°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.8660 and 0.7904	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	11116 / 1139 / 986	
Goodness-of-fit on F^2	1.071	
Final R indices [I>2sigma(I)]	R1 = 0.0474, wR2 = 0.1257	
R indices (all data)	R1 = 0.0525, wR2 = 0.1314	
Largest diff. peak and hole	0.822 and -1.346 e.$Å^{-3}$	

Table S7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **AllInd**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	1630(2)	5618(2)	1314(2)	29(1)
C(2)	1588(2)	5676(2)	2092(2)	30(1)
C(3)	1367(2)	4965(2)	2328(2)	31(1)
C(4)	1186(2)	4720(2)	3002(2)	37(1)
C(5)	960(2)	4010(3)	3064(2)	43(1)
C(6)	917(2)	3539(2)	2461(2)	41(1)
C(7)	1096(2)	3769(2)	1786(2)	35(1)
C(8)	1315(2)	4491(2)	1707(2)	30(1)
C(9)	1490(2)	4891(2)	1062(2)	28(1)
C(11)	3584(2)	5705(2)	1068(2)	32(1)
C(12)	3786(2)	5894(2)	1823(2)	33(1)
C(13)	3684(2)	5022(2)	753(2)	33(1)
Pd(1)	2751(1)	5789(1)	2076(1)	26(1)
C(21)	3080(2)	6343(2)	3042(2)	28(1)
N(1)	3643(2)	6210(2)	3586(2)	27(1)
C(31)	4018(2)	5531(2)	3736(2)	28(1)
C(32)	3668(2)	4960(2)	4048(2)	32(1)
C(37)	2913(2)	5026(2)	4228(2)	38(1)
C(38)	2585(2)	4304(2)	4424(2)	45(1)
C(39)	2879(3)	5544(3)	4891(3)	54(1)
C(33)	4050(2)	4324(2)	4208(2)	37(1)
C(34)	4753(2)	4263(2)	4083(2)	40(1)
C(35)	5088(2)	4839(2)	3792(2)	37(1)

C(36)	4725(2)	5489(2)	3610(2)	29(1)
C(40)	5137(2)	6110(2)	3331(2)	32(1)
C(41)	5558(2)	5885(2)	2704(2)	41(1)
C(42)	5656(2)	6425(2)	3971(2)	38(1)
C(22)	3800(2)	6814(2)	4036(2)	31(1)
C(23)	3333(2)	7328(2)	3788(2)	32(1)
N(2)	2892(2)	7035(2)	3188(2)	27(1)
C(51)	2321(6)	7419(9)	2729(8)	26(2)
C(52)	1650(5)	7431(9)	2981(8)	34(2)
C(57)	1513(6)	7004(8)	3660(8)	40(2)
C(58)	745(7)	6713(9)	3604(11)	54(3)
C(59)	1677(14)	7472(12)	4366(9)	44(3)
C(53)	1119(6)	7848(8)	2574(9)	37(2)
C(54)	1254(7)	8267(8)	1981(8)	39(3)
C(55)	1924(8)	8286(7)	1775(7)	36(2)
C(56)	2486(7)	7881(8)	2160(8)	31(2)
C(60)	3210(7)	7901(9)	1902(9)	34(2)
C(61)	3174(11)	7627(15)	1096(10)	45(3)
C(62)	3518(11)	8675(10)	1971(15)	41(3)
C(51A)	2281(8)	7461(16)	2866(12)	29(3)
C(52A)	1642(8)	7384(15)	3168(13)	34(3)
C(57A)	1582(11)	6988(13)	3886(13)	44(4)
C(58A)	875(13)	6563(16)	3857(16)	57(5)
C(59A)	1660(20)	7510(20)	4555(14)	52(5)
C(53A)	1066(9)	7781(13)	2808(13)	33(3)
C(54A)	1112(9)	8156(12)	2158(12)	33(3)
C(55A)	1729(11)	8167(12)	1840(11)	32(3)
C(56A)	2332(9)	7785(13)	2170(11)	30(3)
C(60A)	3041(11)	7861(16)	1886(14)	35(3)
C(61A)	2987(18)	7640(30)	1060(16)	50(6)
C(62A)	3352(16)	8628(18)	2010(20)	39(4)
Pd(2)	2603(1)	4854(1)	896(1)	25(1)
C(26)	2515(2)	3936(2)	250(2)	27(1)
N(3)	2921(2)	3323(2)	359(2)	26(1)
C(71)	3584(2)	3279(2)	849(2)	28(1)
C(72)	3581(2)	3193(2)	1613(2)	30(1)
C(77)	2908(2)	3153(2)	1968(2)	35(1)
C(78)	2893(2)	3765(3)	2534(2)	48(1)
C(79)	2830(3)	2419(3)	2331(3)	54(1)
C(73)	4241(2)	3146(2)	2058(2)	37(1)
C(74)	4867(2)	3170(2)	1749(2)	41(1)
C(75)	4854(2)	3254(2)	992(2)	36(1)
C(76)	4214(2)	3318(2)	519(2)	30(1)
C(80)	4227(2)	3442(2)	-310(2)	33(1)
C(81)	4738(2)	4041(2)	-459(2)	42(1)
C(82)	4416(2)	2748(2)	-700(2)	42(1)
C(27)	2694(2)	2784(2)	-151(2)	30(1)
C(28)	2133(2)	3059(2)	-602(2)	30(1)
N(4)	2029(1)	3757(2)	-355(2)	25(1)
C(91)	1526(2)	4246(2)	-763(2)	28(1)
C(92)	1783(2)	4823(2)	-1150(2)	30(1)
C(97)	2572(2)	4946(2)	-1185(2)	32(1)
C(98)	2790(2)	5732(2)	-1036(2)	40(1)
C(99)	2768(2)	4689(3)	-1931(3)	49(1)
C(93)	1290(2)	5274(2)	-1561(2)	36(1)
C(94)	569(2)	5143(2)	-1600(2)	40(1)

C(95)	326(2)	4566(2)	-1226(2)	38(1)
C(96)	798(2)	4100(2)	-793(2)	30(1)
C(100)	510(2)	3480(2)	-381(2)	34(1)
C(101)	-44(2)	3732(2)	104(2)	42(1)
C(102)	184(2)	2889(2)	-929(3)	48(1)
C(7S)	991(5)	3548(6)	7343(5)	61(2)
C(1S)	970(5)	3868(9)	6544(8)	74(2)
C(2S)	1115(8)	3451(9)	5968(9)	78(3)
C(3S)	1042(10)	3730(8)	5249(8)	83(3)
C(4S)	858(10)	4463(8)	5131(9)	93(3)
C(5S)	737(9)	4893(9)	5739(10)	91(3)
C(6S)	762(9)	4573(10)	6419(10)	78(3)
C(7T)	630(20)	5589(16)	5480(20)	108(8)
C(1T)	810(13)	4782(17)	5710(20)	90(4)
C(2T)	835(19)	4570(20)	6430(20)	85(3)
C(3T)	1022(16)	3870(20)	6650(20)	78(3)
C(4T)	1162(18)	3350(20)	6130(20)	81(4)
C(5T)	1100(20)	3561(18)	5390(20)	84(4)
C(6T)	920(20)	4280(20)	5200(20)	91(4)
C(7U)	892(18)	5346(15)	5416(18)	93(7)
C(1U)	1008(12)	4603(14)	5850(13)	91(4)
C(2U)	1000(18)	4593(14)	6592(14)	90(3)
C(3U)	1063(17)	3940(14)	6972(14)	85(4)
C(4U)	1221(15)	3306(13)	6617(14)	82(4)
C(5U)	1230(20)	3300(15)	5855(16)	83(4)
C(6U)	1090(20)	3968(15)	5508(14)	92(4)

Table S8. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **AllInd**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	14(2)	39(2)	32(2)	0(2)	-4(1)	0(1)
C(2)	16(2)	38(2)	35(2)	-8(2)	0(1)	-3(2)
C(3)	22(2)	38(2)	32(2)	-2(2)	-1(1)	-2(2)
C(4)	30(2)	56(3)	26(2)	2(2)	4(2)	-1(2)
C(5)	30(2)	61(3)	38(2)	17(2)	3(2)	-1(2)
C(6)	28(2)	44(2)	48(2)	12(2)	-3(2)	-3(2)
C(7)	31(2)	34(2)	39(2)	1(2)	-4(2)	-1(2)
C(8)	19(2)	36(2)	34(2)	2(2)	0(1)	3(2)
C(9)	21(2)	36(2)	28(2)	-4(2)	0(1)	0(1)
C(11)	25(2)	33(2)	37(2)	-1(2)	4(2)	-8(2)
C(12)	25(2)	38(2)	35(2)	-9(2)	2(2)	-6(2)
C(13)	27(2)	38(2)	35(2)	-10(2)	4(2)	-4(2)
Pd(1)	25(1)	29(1)	25(1)	-4(1)	1(1)	-1(1)
C(21)	26(2)	30(2)	28(2)	0(1)	4(1)	1(2)
N(1)	27(2)	28(2)	24(1)	-3(1)	-1(1)	-2(1)
C(31)	32(2)	28(2)	25(2)	-3(1)	0(1)	2(2)
C(32)	35(2)	37(2)	23(2)	-2(2)	-4(2)	-5(2)
C(37)	34(2)	44(2)	35(2)	4(2)	3(2)	-5(2)
C(38)	46(2)	53(3)	35(2)	9(2)	4(2)	-8(2)
C(39)	56(3)	60(3)	49(3)	-6(2)	20(2)	-6(2)
C(33)	42(2)	35(2)	30(2)	4(2)	-4(2)	-2(2)
C(34)	40(2)	35(2)	42(2)	3(2)	-2(2)	7(2)
C(35)	37(2)	38(2)	34(2)	-2(2)	0(2)	2(2)
C(36)	32(2)	32(2)	22(2)	-2(1)	-1(1)	-1(2)

C(40)	28(2)	38(2)	28(2)	-1(2)	1(1)	-1(2)
C(41)	35(2)	57(3)	31(2)	-1(2)	6(2)	1(2)
C(42)	35(2)	42(2)	36(2)	0(2)	0(2)	0(2)
C(22)	29(2)	33(2)	28(2)	-7(2)	0(1)	-2(2)
C(23)	29(2)	35(2)	29(2)	-9(2)	0(1)	1(2)
N(2)	24(1)	29(2)	27(1)	-8(1)	1(1)	2(1)
C(51)	26(3)	27(3)	26(5)	-17(3)	1(2)	8(2)
C(52)	28(3)	36(4)	36(5)	-15(4)	3(3)	2(3)
C(57)	28(4)	49(4)	44(6)	-8(4)	8(4)	1(3)
C(58)	34(5)	51(7)	78(9)	-8(6)	17(5)	-4(4)
C(59)	40(5)	58(6)	37(6)	-9(5)	19(6)	3(4)
C(53)	24(3)	41(5)	44(7)	-16(4)	3(4)	1(3)
C(54)	27(5)	43(5)	45(5)	-6(3)	-1(4)	3(4)
C(55)	24(5)	37(5)	43(4)	-5(3)	-7(3)	-3(4)
C(56)	26(4)	30(4)	34(3)	-6(3)	-7(3)	-1(4)
C(60)	28(5)	37(4)	34(3)	0(3)	0(4)	5(4)
C(61)	53(9)	49(6)	33(4)	4(4)	3(5)	11(7)
C(62)	36(8)	37(5)	54(7)	4(4)	11(5)	2(4)
C(51A)	23(4)	39(6)	23(6)	-16(5)	-3(3)	5(4)
C(52A)	28(4)	39(5)	37(7)	-14(5)	5(4)	6(4)
C(57A)	34(6)	49(7)	51(8)	2(6)	13(6)	4(5)
C(58A)	42(9)	60(11)	73(13)	-5(8)	23(8)	1(7)
C(59A)	40(9)	80(12)	39(8)	-3(8)	11(10)	5(8)
C(53A)	24(4)	37(6)	38(8)	-13(6)	6(5)	0(4)
C(54A)	18(5)	39(7)	39(8)	-13(5)	-5(5)	-3(5)
C(55A)	22(6)	38(6)	33(5)	-2(4)	-4(5)	-4(6)
C(56A)	20(5)	39(6)	30(4)	-11(4)	-6(4)	-1(5)
C(60A)	29(6)	46(6)	30(5)	5(5)	-2(5)	11(6)
C(61A)	55(15)	60(9)	35(6)	-2(6)	6(8)	23(11)
C(62A)	27(10)	62(8)	30(7)	8(6)	12(7)	-5(7)
Pd(2)	23(1)	28(1)	25(1)	-3(1)	1(1)	0(1)
C(26)	25(2)	28(2)	27(2)	0(1)	2(1)	-1(1)
N(3)	26(2)	24(2)	27(1)	-1(1)	-1(1)	-1(1)
C(71)	24(2)	30(2)	29(2)	-2(1)	-4(1)	2(1)
C(72)	25(2)	35(2)	30(2)	-3(2)	1(1)	4(2)
C(77)	30(2)	47(2)	28(2)	5(2)	0(2)	5(2)
C(78)	38(2)	73(3)	33(2)	-10(2)	1(2)	12(2)
C(79)	48(3)	56(3)	61(3)	15(2)	17(2)	6(2)
C(73)	35(2)	46(2)	27(2)	-1(2)	-3(2)	5(2)
C(74)	29(2)	53(3)	38(2)	-6(2)	-6(2)	4(2)
C(75)	23(2)	41(2)	42(2)	-6(2)	2(2)	2(2)
C(76)	28(2)	30(2)	31(2)	0(2)	1(1)	2(2)
C(80)	31(2)	36(2)	32(2)	0(2)	5(2)	4(2)
C(81)	45(2)	39(2)	43(2)	-4(2)	13(2)	-2(2)
C(82)	55(3)	36(2)	36(2)	-2(2)	9(2)	3(2)
C(27)	29(2)	26(2)	33(2)	-4(2)	1(1)	3(1)
C(28)	32(2)	28(2)	27(2)	-5(1)	0(1)	0(2)
N(4)	20(1)	28(2)	25(1)	-2(1)	-3(1)	0(1)
C(91)	28(2)	30(2)	25(2)	0(1)	-2(1)	4(1)
C(92)	30(2)	32(2)	26(2)	0(1)	0(1)	1(2)
C(97)	29(2)	32(2)	35(2)	4(2)	6(2)	1(2)
C(98)	40(2)	35(2)	45(2)	5(2)	3(2)	-4(2)
C(99)	46(3)	55(3)	49(3)	-12(2)	19(2)	1(2)
C(93)	37(2)	33(2)	36(2)	6(2)	4(2)	2(2)
C(94)	35(2)	45(2)	38(2)	9(2)	-1(2)	8(2)
C(95)	26(2)	50(2)	37(2)	2(2)	0(2)	4(2)

C(96)	28(2)	34(2)	26(2)	0(2)	0(1)	0(2)
C(100)	24(2)	39(2)	36(2)	3(2)	-7(2)	-5(2)
C(101)	29(2)	55(3)	40(2)	6(2)	4(2)	-1(2)
C(102)	44(2)	46(3)	51(2)	-5(2)	2(2)	-12(2)
C(7S)	65(6)	64(6)	55(4)	-4(4)	5(4)	3(5)
C(1S)	82(6)	82(5)	54(4)	-1(4)	-1(5)	1(5)
C(2S)	84(6)	91(5)	61(5)	1(4)	22(5)	-5(5)
C(3S)	97(6)	94(6)	60(5)	-2(5)	19(6)	-6(6)
C(4S)	109(7)	105(7)	65(5)	7(5)	19(5)	18(6)
C(5S)	111(7)	99(6)	67(5)	13(4)	26(5)	23(6)
C(6S)	86(6)	89(5)	59(4)	6(4)	10(5)	11(5)
C(7T)	140(20)	104(10)	84(14)	14(8)	20(16)	31(16)
C(1T)	106(8)	98(6)	67(6)	7(5)	19(7)	17(7)
C(2T)	96(8)	95(6)	62(5)	1(5)	8(7)	9(7)
C(3T)	85(7)	90(6)	57(6)	0(5)	2(7)	-2(7)
C(4T)	87(8)	91(7)	65(8)	2(6)	16(8)	-3(7)
C(5T)	93(8)	96(7)	65(7)	1(7)	21(8)	3(8)
C(6T)	106(8)	103(8)	66(6)	6(6)	20(7)	16(8)
C(7U)	89(16)	106(9)	89(12)	20(10)	28(13)	8(14)
C(1U)	103(8)	104(6)	70(6)	9(5)	20(7)	17(7)
C(2U)	103(8)	98(6)	68(6)	3(5)	9(7)	8(7)
C(3U)	96(8)	94(7)	61(7)	-2(5)	0(8)	8(8)
C(4U)	88(8)	96(6)	61(7)	-6(6)	6(8)	2(7)
C(5U)	91(8)	98(6)	63(7)	1(6)	21(8)	-6(8)
C(6U)	103(7)	102(7)	72(6)	4(5)	19(7)	6(7)

Table S9. Bond lengths (Å) for **AllInd**

C(1)-C(9)	1.429(5)
C(1)-C(2)	1.430(5)
C(1)-Pd(1)	2.398(3)
C(1)-Pd(2)	2.522(4)
C(1)-H(1)	1.011(18)
C(2)-C(3)	1.459(5)
C(2)-Pd(1)	2.226(3)
C(2)-H(2)	0.987(18)
C(3)-C(4)	1.389(5)
C(3)-C(8)	1.418(5)
C(4)-C(5)	1.387(6)
C(4)-H(4)	0.9500
C(5)-C(6)	1.390(6)
C(5)-H(5)	0.9500
C(6)-C(7)	1.381(6)
C(6)-H(6)	0.9500
C(7)-C(8)	1.407(5)
C(7)-H(7)	0.9500
C(8)-C(9)	1.458(5)
C(9)-Pd(2)	2.180(4)
C(9)-H(9)	0.984(18)
C(11)-C(13)	1.407(5)
C(11)-C(12)	1.413(5)
C(11)-Pd(2)	2.424(4)
C(11)-Pd(1)	2.580(4)
C(11)-H(11)	0.966(18)
C(12)-Pd(1)	2.091(4)
C(12)-H(12A)	0.982(18)

C(12)-H(12B)	0.994(18)
C(13)-Pd(2)	2.128(4)
C(13)-H(13A)	0.989(18)
C(13)-H(13B)	0.998(18)
Pd(1)-C(21)	2.051(3)
Pd(1)-Pd(2)	2.7319(3)
C(21)-N(2)	1.361(5)
C(21)-N(1)	1.374(4)
N(1)-C(22)	1.389(4)
N(1)-C(31)	1.448(5)
C(31)-C(36)	1.396(5)
C(31)-C(32)	1.405(5)
C(32)-C(33)	1.388(6)
C(32)-C(37)	1.520(6)
C(37)-C(38)	1.533(6)
C(37)-C(39)	1.543(6)
C(37)-H(37)	1.0000
C(38)-H(38A)	0.9800
C(38)-H(38B)	0.9800
C(38)-H(38C)	0.9800
C(39)-H(39A)	0.9800
C(39)-H(39B)	0.9800
C(39)-H(39C)	0.9800
C(33)-C(34)	1.390(6)
C(33)-H(33)	0.9500
C(34)-C(35)	1.379(6)
C(34)-H(34)	0.9500
C(35)-C(36)	1.401(5)
C(35)-H(35)	0.9500
C(36)-C(40)	1.514(5)
C(40)-C(42)	1.531(5)
C(40)-C(41)	1.533(5)
C(40)-H(40)	1.0000
C(41)-H(41A)	0.9800
C(41)-H(41B)	0.9800
C(41)-H(41C)	0.9800
C(42)-H(42A)	0.9800
C(42)-H(42B)	0.9800
C(42)-H(42C)	0.9800
C(22)-C(23)	1.334(5)
C(22)-H(22)	0.9500
C(23)-N(2)	1.389(4)
C(23)-H(23)	0.9500
N(2)-C(51)	1.457(8)
N(2)-C(51A)	1.457(12)
C(51)-C(56)	1.406(9)
C(51)-C(52)	1.413(8)
C(52)-C(53)	1.398(9)
C(52)-C(57)	1.513(9)
C(57)-C(59)	1.541(9)
C(57)-C(58)	1.545(9)
C(57)-H(57)	1.0000
C(58)-H(58A)	0.9800
C(58)-H(58B)	0.9800
C(58)-H(58C)	0.9800
C(59)-H(59A)	0.9800

C(59)-H(59B)	0.9800
C(59)-H(59C)	0.9800
C(53)-C(54)	1.375(10)
C(53)-H(53)	0.9500
C(54)-C(55)	1.377(9)
C(54)-H(54)	0.9500
C(55)-C(56)	1.408(8)
C(55)-H(55)	0.9500
C(56)-C(60)	1.515(8)
C(60)-C(61)	1.540(9)
C(60)-C(62)	1.541(9)
C(60)-H(60)	1.0000
C(61)-H(61A)	0.9800
C(61)-H(61B)	0.9800
C(61)-H(61C)	0.9800
C(62)-H(62A)	0.9800
C(62)-H(62B)	0.9800
C(62)-H(62C)	0.9800
C(51A)-C(52A)	1.407(11)
C(51A)-C(56A)	1.410(11)
C(52A)-C(53A)	1.402(11)
C(52A)-C(57A)	1.510(12)
C(57A)-C(59A)	1.541(12)
C(57A)-C(58A)	1.550(12)
C(57A)-H(57A)	1.0000
C(58A)-H(58D)	0.9800
C(58A)-H(58E)	0.9800
C(58A)-H(58F)	0.9800
C(59A)-H(59D)	0.9800
C(59A)-H(59E)	0.9800
C(59A)-H(59F)	0.9800
C(53A)-C(54A)	1.378(12)
C(53A)-H(53A)	0.9500
C(54A)-C(55A)	1.376(12)
C(54A)-H(54A)	0.9500
C(55A)-C(56A)	1.408(11)
C(55A)-H(55A)	0.9500
C(56A)-C(60A)	1.513(11)
C(60A)-C(62A)	1.537(12)
C(60A)-C(61A)	1.542(12)
C(60A)-H(60A)	1.0000
C(61A)-H(61D)	0.9800
C(61A)-H(61E)	0.9800
C(61A)-H(61F)	0.9800
C(62A)-H(62D)	0.9800
C(62A)-H(62E)	0.9800
C(62A)-H(62F)	0.9800
Pd(2)-C(26)	2.052(4)
C(26)-N(3)	1.368(5)
C(26)-N(4)	1.375(4)
N(3)-C(27)	1.386(4)
N(3)-C(71)	1.443(4)
C(71)-C(72)	1.396(5)
C(71)-C(76)	1.411(5)
C(72)-C(73)	1.399(5)
C(72)-C(77)	1.510(5)

C(77)-C(79)	1.521(6)
C(77)-C(78)	1.528(6)
C(77)-H(77)	1.0000
C(78)-H(78A)	0.9800
C(78)-H(78B)	0.9800
C(78)-H(78C)	0.9800
C(79)-H(79A)	0.9800
C(79)-H(79B)	0.9800
C(79)-H(79C)	0.9800
C(73)-C(74)	1.385(6)
C(73)-H(73)	0.9500
C(74)-C(75)	1.378(6)
C(74)-H(74)	0.9500
C(75)-C(76)	1.394(5)
C(75)-H(75)	0.9500
C(76)-C(80)	1.524(5)
C(80)-C(81)	1.519(6)
C(80)-C(82)	1.529(5)
C(80)-H(80)	1.0000
C(81)-H(81A)	0.9800
C(81)-H(81B)	0.9800
C(81)-H(81C)	0.9800
C(82)-H(82A)	0.9800
C(82)-H(82B)	0.9800
C(82)-H(82C)	0.9800
C(27)-C(28)	1.351(5)
C(27)-H(27)	0.9500
C(28)-N(4)	1.385(5)
C(28)-H(28)	0.9500
N(4)-C(91)	1.444(4)
C(91)-C(92)	1.399(5)
C(91)-C(96)	1.403(5)
C(92)-C(93)	1.391(5)
C(92)-C(97)	1.527(5)
C(97)-C(98)	1.521(5)
C(97)-C(99)	1.528(5)
C(97)-H(97)	1.0000
C(98)-H(98A)	0.9800
C(98)-H(98B)	0.9800
C(98)-H(98C)	0.9800
C(99)-H(99A)	0.9800
C(99)-H(99B)	0.9800
C(99)-H(99C)	0.9800
C(93)-C(94)	1.385(6)
C(93)-H(93)	0.9500
C(94)-C(95)	1.375(6)
C(94)-H(94)	0.9500
C(95)-C(96)	1.403(5)
C(95)-H(95)	0.9500
C(96)-C(100)	1.510(5)
C(100)-C(101)	1.534(5)
C(100)-C(102)	1.546(6)
C(100)-H(100)	1.0000
C(101)-H(10C)	0.9800
C(101)-H(10D)	0.9800
C(101)-H(10E)	0.9800

C(102)-H(10F)	0.9800
C(102)-H(10G)	0.9800
C(102)-H(10H)	0.9800
C(7S)-C(1S)	1.559(18)
C(7S)-H(7S1)	0.9800
C(7S)-H(7S2)	0.9800
C(7S)-H(7S3)	0.9800
C(1S)-C(2S)	1.355(14)
C(1S)-C(6S)	1.369(14)
C(2S)-C(3S)	1.390(14)
C(2S)-H(2S)	0.9500
C(3S)-C(4S)	1.405(14)
C(3S)-H(3S)	0.9500
C(4S)-C(5S)	1.402(14)
C(4S)-H(4S)	0.9500
C(5S)-C(6S)	1.362(15)
C(5S)-H(5S)	0.9500
C(6S)-H(6S)	0.9500
C(7T)-C(1T)	1.57(2)
C(7T)-H(7T1)	0.9800
C(7T)-H(7T2)	0.9800
C(7T)-H(7T3)	0.9800
C(1T)-C(2T)	1.344(17)
C(1T)-C(6T)	1.356(17)
C(2T)-C(3T)	1.389(19)
C(2T)-H(2T)	0.9500
C(3T)-C(4T)	1.393(18)
C(3T)-H(3T)	0.9500
C(4T)-C(5T)	1.393(17)
C(4T)-H(4T)	0.9500
C(5T)-C(6T)	1.395(18)
C(5T)-H(5T)	0.9500
C(6T)-H(6T)	0.9500
C(7U)-C(1U)	1.58(2)
C(7U)-H(7U1)	0.9800
C(7U)-H(7U2)	0.9800
C(7U)-H(7U3)	0.9800
C(1U)-C(6U)	1.345(17)
C(1U)-C(2U)	1.347(17)
C(2U)-C(3U)	1.383(18)
C(2U)-H(2U)	0.9500
C(3U)-C(4U)	1.388(17)
C(3U)-H(3U)	0.9500
C(4U)-C(5U)	1.383(17)
C(4U)-H(4U)	0.9500
C(5U)-C(6U)	1.391(18)
C(5U)-H(5U)	0.9500
C(6U)-H(6U)	0.9500

Table S10. Bond angles (°) for **AllInd**

C(9)-C(1)-C(2)	110.7(3)
C(9)-C(1)-Pd(1)	114.8(2)
C(2)-C(1)-Pd(1)	65.53(18)
C(9)-C(1)-Pd(2)	59.56(19)
C(2)-C(1)-Pd(2)	118.8(2)

Pd(1)-C(1)-Pd(2)	67.41(9)
C(9)-C(1)-H(1)	124(2)
C(2)-C(1)-H(1)	123(2)
Pd(1)-C(1)-H(1)	103(2)
Pd(2)-C(1)-H(1)	104(2)
C(1)-C(2)-C(3)	106.2(3)
C(1)-C(2)-Pd(1)	78.7(2)
C(3)-C(2)-Pd(1)	114.5(2)
C(1)-C(2)-H(2)	126(2)
C(3)-C(2)-H(2)	122(2)
Pd(1)-C(2)-H(2)	101(2)
C(4)-C(3)-C(8)	120.0(4)
C(4)-C(3)-C(2)	131.7(4)
C(8)-C(3)-C(2)	108.3(3)
C(5)-C(4)-C(3)	119.6(4)
C(5)-C(4)-H(4)	120.2
C(3)-C(4)-H(4)	120.2
C(4)-C(5)-C(6)	120.8(4)
C(4)-C(5)-H(5)	119.6
C(6)-C(5)-H(5)	119.6
C(7)-C(6)-C(5)	120.6(4)
C(7)-C(6)-H(6)	119.7
C(5)-C(6)-H(6)	119.7
C(6)-C(7)-C(8)	119.5(4)
C(6)-C(7)-H(7)	120.2
C(8)-C(7)-H(7)	120.2
C(7)-C(8)-C(3)	119.4(3)
C(7)-C(8)-C(9)	131.4(3)
C(3)-C(8)-C(9)	109.1(3)
C(1)-C(9)-C(8)	105.7(3)
C(1)-C(9)-Pd(2)	86.0(2)
C(8)-C(9)-Pd(2)	115.3(2)
C(1)-C(9)-H(9)	125(2)
C(8)-C(9)-H(9)	119(2)
Pd(2)-C(9)-H(9)	100(2)
C(13)-C(11)-C(12)	125.4(4)
C(13)-C(11)-Pd(2)	60.8(2)
C(12)-C(11)-Pd(2)	112.8(3)
C(13)-C(11)-Pd(1)	118.1(3)
C(12)-C(11)-Pd(1)	54.1(2)
Pd(2)-C(11)-Pd(1)	66.09(9)
C(13)-C(11)-H(11)	116(3)
C(12)-C(11)-H(11)	118(3)
Pd(2)-C(11)-H(11)	104(3)
Pd(1)-C(11)-H(11)	105(3)
C(11)-C(12)-Pd(1)	92.8(2)
C(11)-C(12)-H(12A)	118(2)
Pd(1)-C(12)-H(12A)	111(2)
C(11)-C(12)-H(12B)	113(3)
Pd(1)-C(12)-H(12B)	104(2)
H(12A)-C(12)-H(12B)	115(4)
C(11)-C(13)-Pd(2)	83.9(2)
C(11)-C(13)-H(13A)	119(3)
Pd(2)-C(13)-H(13A)	104(3)
C(11)-C(13)-H(13B)	120(3)
Pd(2)-C(13)-H(13B)	102(3)

H(13A)-C(13)-H(13B)	117(4)
C(21)-Pd(1)-C(12)	87.35(14)
C(21)-Pd(1)-C(2)	102.97(13)
C(12)-Pd(1)-C(2)	168.18(14)
C(21)-Pd(1)-C(1)	134.65(13)
C(12)-Pd(1)-C(1)	132.45(14)
C(2)-Pd(1)-C(1)	35.77(13)
C(21)-Pd(1)-C(11)	119.25(13)
C(12)-Pd(1)-C(11)	33.15(13)
C(2)-Pd(1)-C(11)	135.29(13)
C(1)-Pd(1)-C(11)	99.61(12)
C(21)-Pd(1)-Pd(2)	165.90(10)
C(12)-Pd(1)-Pd(2)	83.43(10)
C(2)-Pd(1)-Pd(2)	87.43(10)
C(1)-Pd(1)-Pd(2)	58.46(9)
C(11)-Pd(1)-Pd(2)	54.20(8)
N(2)-C(21)-N(1)	103.1(3)
N(2)-C(21)-Pd(1)	125.0(2)
N(1)-C(21)-Pd(1)	129.9(3)
C(21)-N(1)-C(22)	111.3(3)
C(21)-N(1)-C(31)	127.1(3)
C(22)-N(1)-C(31)	121.5(3)
C(36)-C(31)-C(32)	122.9(3)
C(36)-C(31)-N(1)	118.5(3)
C(32)-C(31)-N(1)	118.5(3)
C(33)-C(32)-C(31)	117.0(4)
C(33)-C(32)-C(37)	120.4(4)
C(31)-C(32)-C(37)	122.5(3)
C(32)-C(37)-C(38)	113.9(4)
C(32)-C(37)-C(39)	110.9(3)
C(38)-C(37)-C(39)	107.2(3)
C(32)-C(37)-H(37)	108.2
C(38)-C(37)-H(37)	108.2
C(39)-C(37)-H(37)	108.2
C(37)-C(38)-H(38A)	109.5
C(37)-C(38)-H(38B)	109.5
H(38A)-C(38)-H(38B)	109.5
C(37)-C(38)-H(38C)	109.5
H(38A)-C(38)-H(38C)	109.5
H(38B)-C(38)-H(38C)	109.5
C(37)-C(39)-H(39A)	109.5
C(37)-C(39)-H(39B)	109.5
H(39A)-C(39)-H(39B)	109.5
C(37)-C(39)-H(39C)	109.5
H(39A)-C(39)-H(39C)	109.5
H(39B)-C(39)-H(39C)	109.5
C(32)-C(33)-C(34)	121.5(4)
C(32)-C(33)-H(33)	119.3
C(34)-C(33)-H(33)	119.3
C(35)-C(34)-C(33)	120.3(4)
C(35)-C(34)-H(34)	119.9
C(33)-C(34)-H(34)	119.9
C(34)-C(35)-C(36)	120.6(4)
C(34)-C(35)-H(35)	119.7
C(36)-C(35)-H(35)	119.7
C(31)-C(36)-C(35)	117.7(3)

C(31)-C(36)-C(40)	124.5(3)
C(35)-C(36)-C(40)	117.7(3)
C(36)-C(40)-C(42)	110.1(3)
C(36)-C(40)-C(41)	112.9(3)
C(42)-C(40)-C(41)	108.5(3)
C(36)-C(40)-H(40)	108.4
C(42)-C(40)-H(40)	108.4
C(41)-C(40)-H(40)	108.4
C(40)-C(41)-H(41A)	109.5
C(40)-C(41)-H(41B)	109.5
H(41A)-C(41)-H(41B)	109.5
C(40)-C(41)-H(41C)	109.5
H(41A)-C(41)-H(41C)	109.5
H(41B)-C(41)-H(41C)	109.5
C(40)-C(42)-H(42A)	109.5
C(40)-C(42)-H(42B)	109.5
H(42A)-C(42)-H(42B)	109.5
C(40)-C(42)-H(42C)	109.5
H(42A)-C(42)-H(42C)	109.5
H(42B)-C(42)-H(42C)	109.5
C(23)-C(22)-N(1)	106.9(3)
C(23)-C(22)-H(22)	126.6
N(1)-C(22)-H(22)	126.6
C(22)-C(23)-N(2)	106.9(3)
C(22)-C(23)-H(23)	126.5
N(2)-C(23)-H(23)	126.5
C(21)-N(2)-C(23)	111.7(3)
C(21)-N(2)-C(51)	122.7(8)
C(23)-N(2)-C(51)	125.5(8)
C(21)-N(2)-C(51A)	130.1(14)
C(23)-N(2)-C(51A)	117.9(13)
C(51)-N(2)-C(51A)	11.0(13)
C(56)-C(51)-C(52)	121.8(7)
C(56)-C(51)-N(2)	119.4(8)
C(52)-C(51)-N(2)	117.3(7)
C(53)-C(52)-C(51)	117.3(7)
C(53)-C(52)-C(57)	121.6(7)
C(51)-C(52)-C(57)	121.1(7)
C(52)-C(57)-C(59)	110.2(7)
C(52)-C(57)-C(58)	113.1(7)
C(59)-C(57)-C(58)	109.4(9)
C(52)-C(57)-H(57)	108.0
C(59)-C(57)-H(57)	108.0
C(58)-C(57)-H(57)	108.0
C(57)-C(58)-H(58A)	109.5
C(57)-C(58)-H(58B)	109.5
H(58A)-C(58)-H(58B)	109.5
C(57)-C(58)-H(58C)	109.5
H(58A)-C(58)-H(58C)	109.5
H(58B)-C(58)-H(58C)	109.5
C(57)-C(59)-H(59A)	109.5
C(57)-C(59)-H(59B)	109.5
H(59A)-C(59)-H(59B)	109.5
C(57)-C(59)-H(59C)	109.5
H(59A)-C(59)-H(59C)	109.5
H(59B)-C(59)-H(59C)	109.5

C(54)-C(53)-C(52)	121.5(7)
C(54)-C(53)-H(53)	119.2
C(52)-C(53)-H(53)	119.2
C(53)-C(54)-C(55)	120.3(7)
C(53)-C(54)-H(54)	119.9
C(55)-C(54)-H(54)	119.9
C(54)-C(55)-C(56)	121.3(8)
C(54)-C(55)-H(55)	119.3
C(56)-C(55)-H(55)	119.3
C(51)-C(56)-C(55)	117.2(7)
C(51)-C(56)-C(60)	122.9(7)
C(55)-C(56)-C(60)	119.6(7)
C(56)-C(60)-C(61)	111.1(8)
C(56)-C(60)-C(62)	110.4(7)
C(61)-C(60)-C(62)	110.4(10)
C(56)-C(60)-H(60)	108.3
C(61)-C(60)-H(60)	108.3
C(62)-C(60)-H(60)	108.3
C(60)-C(61)-H(61A)	109.5
C(60)-C(61)-H(61B)	109.5
H(61A)-C(61)-H(61B)	109.5
C(60)-C(61)-H(61C)	109.5
H(61A)-C(61)-H(61C)	109.5
H(61B)-C(61)-H(61C)	109.5
C(60)-C(62)-H(62A)	109.5
C(60)-C(62)-H(62B)	109.5
H(62A)-C(62)-H(62B)	109.5
C(60)-C(62)-H(62C)	109.5
H(62A)-C(62)-H(62C)	109.5
H(62B)-C(62)-H(62C)	109.5
C(52A)-C(51A)-C(56A)	124.0(10)
C(52A)-C(51A)-N(2)	118.3(11)
C(56A)-C(51A)-N(2)	116.0(11)
C(53A)-C(52A)-C(51A)	115.3(10)
C(53A)-C(52A)-C(57A)	120.6(10)
C(51A)-C(52A)-C(57A)	123.7(11)
C(52A)-C(57A)-C(59A)	111.5(12)
C(52A)-C(57A)-C(58A)	112.4(12)
C(59A)-C(57A)-C(58A)	109.3(14)
C(52A)-C(57A)-H(57A)	107.8
C(59A)-C(57A)-H(57A)	107.8
C(58A)-C(57A)-H(57A)	107.8
C(57A)-C(58A)-H(58D)	109.5
C(57A)-C(58A)-H(58E)	109.5
H(58D)-C(58A)-H(58E)	109.5
C(57A)-C(58A)-H(58F)	109.5
H(58D)-C(58A)-H(58F)	109.5
H(58E)-C(58A)-H(58F)	109.5
C(57A)-C(59A)-H(59D)	109.5
C(57A)-C(59A)-H(59E)	109.5
H(59D)-C(59A)-H(59E)	109.5
C(57A)-C(59A)-H(59F)	109.5
H(59D)-C(59A)-H(59F)	109.5
H(59E)-C(59A)-H(59F)	109.5
C(54A)-C(53A)-C(52A)	121.6(11)
C(54A)-C(53A)-H(53A)	119.2

C(52A)-C(53A)-H(53A)	119.2
C(55A)-C(54A)-C(53A)	121.4(11)
C(55A)-C(54A)-H(54A)	119.3
C(53A)-C(54A)-H(54A)	119.3
C(54A)-C(55A)-C(56A)	120.4(11)
C(54A)-C(55A)-H(55A)	119.8
C(56A)-C(55A)-H(55A)	119.8
C(55A)-C(56A)-C(51A)	116.2(10)
C(55A)-C(56A)-C(60A)	121.3(11)
C(51A)-C(56A)-C(60A)	121.1(11)
C(56A)-C(60A)-C(62A)	112.4(11)
C(56A)-C(60A)-C(61A)	111.2(13)
C(62A)-C(60A)-C(61A)	111.0(15)
C(56A)-C(60A)-H(60A)	107.3
C(62A)-C(60A)-H(60A)	107.3
C(61A)-C(60A)-H(60A)	107.3
C(60A)-C(61A)-H(61D)	109.5
C(60A)-C(61A)-H(61E)	109.5
H(61D)-C(61A)-H(61E)	109.5
C(60A)-C(61A)-H(61F)	109.5
H(61D)-C(61A)-H(61F)	109.5
H(61E)-C(61A)-H(61F)	109.5
C(60A)-C(62A)-H(62D)	109.5
C(60A)-C(62A)-H(62E)	109.5
H(62D)-C(62A)-H(62E)	109.5
C(60A)-C(62A)-H(62F)	109.5
H(62D)-C(62A)-H(62F)	109.5
H(62E)-C(62A)-H(62F)	109.5
C(26)-Pd(2)-C(13)	93.23(14)
C(26)-Pd(2)-C(9)	95.61(13)
C(13)-Pd(2)-C(9)	169.88(15)
C(26)-Pd(2)-C(11)	127.58(13)
C(13)-Pd(2)-C(11)	35.27(14)
C(9)-Pd(2)-C(11)	134.98(13)
C(26)-Pd(2)-C(1)	128.66(12)
C(13)-Pd(2)-C(1)	135.71(14)
C(9)-Pd(2)-C(1)	34.43(12)
C(11)-Pd(2)-C(1)	100.55(12)
C(26)-Pd(2)-Pd(1)	163.49(10)
C(13)-Pd(2)-Pd(1)	90.34(10)
C(9)-Pd(2)-Pd(1)	82.56(9)
C(11)-Pd(2)-Pd(1)	59.71(9)
C(1)-Pd(2)-Pd(1)	54.13(8)
N(3)-C(26)-N(4)	102.8(3)
N(3)-C(26)-Pd(2)	126.8(2)
N(4)-C(26)-Pd(2)	130.4(3)
C(26)-N(3)-C(27)	112.2(3)
C(26)-N(3)-C(71)	124.4(3)
C(27)-N(3)-C(71)	122.5(3)
C(72)-C(71)-C(76)	123.0(3)
C(72)-C(71)-N(3)	119.8(3)
C(76)-C(71)-N(3)	117.2(3)
C(71)-C(72)-C(73)	117.1(3)
C(71)-C(72)-C(77)	123.1(3)
C(73)-C(72)-C(77)	119.8(3)
C(72)-C(77)-C(79)	111.4(3)

C(72)-C(77)-C(78)	110.1(3)
C(79)-C(77)-C(78)	110.7(4)
C(72)-C(77)-H(77)	108.2
C(79)-C(77)-H(77)	108.2
C(78)-C(77)-H(77)	108.2
C(77)-C(78)-H(78A)	109.5
C(77)-C(78)-H(78B)	109.5
H(78A)-C(78)-H(78B)	109.5
C(77)-C(78)-H(78C)	109.5
H(78A)-C(78)-H(78C)	109.5
H(78B)-C(78)-H(78C)	109.5
C(77)-C(79)-H(79A)	109.5
C(77)-C(79)-H(79B)	109.5
H(79A)-C(79)-H(79B)	109.5
C(77)-C(79)-H(79C)	109.5
H(79A)-C(79)-H(79C)	109.5
H(79B)-C(79)-H(79C)	109.5
C(74)-C(73)-C(72)	121.2(3)
C(74)-C(73)-H(73)	119.4
C(72)-C(73)-H(73)	119.4
C(75)-C(74)-C(73)	120.5(4)
C(75)-C(74)-H(74)	119.8
C(73)-C(74)-H(74)	119.8
C(74)-C(75)-C(76)	121.2(4)
C(74)-C(75)-H(75)	119.4
C(76)-C(75)-H(75)	119.4
C(75)-C(76)-C(71)	117.1(3)
C(75)-C(76)-C(80)	119.3(3)
C(71)-C(76)-C(80)	123.6(3)
C(81)-C(80)-C(76)	112.4(3)
C(81)-C(80)-C(82)	109.2(3)
C(76)-C(80)-C(82)	111.6(3)
C(81)-C(80)-H(80)	107.8
C(76)-C(80)-H(80)	107.8
C(82)-C(80)-H(80)	107.8
C(80)-C(81)-H(81A)	109.5
C(80)-C(81)-H(81B)	109.5
H(81A)-C(81)-H(81B)	109.5
C(80)-C(81)-H(81C)	109.5
H(81A)-C(81)-H(81C)	109.5
H(81B)-C(81)-H(81C)	109.5
C(80)-C(82)-H(82A)	109.5
C(80)-C(82)-H(82B)	109.5
H(82A)-C(82)-H(82B)	109.5
C(80)-C(82)-H(82C)	109.5
H(82A)-C(82)-H(82C)	109.5
H(82B)-C(82)-H(82C)	109.5
C(28)-C(27)-N(3)	106.5(3)
C(28)-C(27)-H(27)	126.8
N(3)-C(27)-H(27)	126.8
C(27)-C(28)-N(4)	106.8(3)
C(27)-C(28)-H(28)	126.6
N(4)-C(28)-H(28)	126.6
C(26)-N(4)-C(28)	111.8(3)
C(26)-N(4)-C(91)	125.8(3)
C(28)-N(4)-C(91)	121.9(3)

C(92)-C(91)-C(96)	122.4(3)
C(92)-C(91)-N(4)	118.7(3)
C(96)-C(91)-N(4)	118.8(3)
C(93)-C(92)-C(91)	117.8(3)
C(93)-C(92)-C(97)	119.0(3)
C(91)-C(92)-C(97)	123.1(3)
C(98)-C(97)-C(92)	112.3(3)
C(98)-C(97)-C(99)	111.1(3)
C(92)-C(97)-C(99)	110.4(3)
C(98)-C(97)-H(97)	107.6
C(92)-C(97)-H(97)	107.6
C(99)-C(97)-H(97)	107.6
C(97)-C(98)-H(98A)	109.5
C(97)-C(98)-H(98B)	109.5
H(98A)-C(98)-H(98B)	109.5
C(97)-C(98)-H(98C)	109.5
H(98A)-C(98)-H(98C)	109.5
H(98B)-C(98)-H(98C)	109.5
C(97)-C(99)-H(99A)	109.5
C(97)-C(99)-H(99B)	109.5
H(99A)-C(99)-H(99B)	109.5
C(97)-C(99)-H(99C)	109.5
H(99A)-C(99)-H(99C)	109.5
H(99B)-C(99)-H(99C)	109.5
C(94)-C(93)-C(92)	121.0(4)
C(94)-C(93)-H(93)	119.5
C(92)-C(93)-H(93)	119.5
C(95)-C(94)-C(93)	120.4(4)
C(95)-C(94)-H(94)	119.8
C(93)-C(94)-H(94)	119.8
C(94)-C(95)-C(96)	121.1(4)
C(94)-C(95)-H(95)	119.4
C(96)-C(95)-H(95)	119.4
C(95)-C(96)-C(91)	117.2(3)
C(95)-C(96)-C(100)	119.5(3)
C(91)-C(96)-C(100)	123.2(3)
C(96)-C(100)-C(101)	112.2(3)
C(96)-C(100)-C(102)	111.0(3)
C(101)-C(100)-C(102)	109.6(3)
C(96)-C(100)-H(100)	108.0
C(101)-C(100)-H(100)	108.0
C(102)-C(100)-H(100)	108.0
C(100)-C(101)-H(10C)	109.5
C(100)-C(101)-H(10D)	109.5
H(10C)-C(101)-H(10D)	109.5
C(100)-C(101)-H(10E)	109.5
H(10C)-C(101)-H(10E)	109.5
H(10D)-C(101)-H(10E)	109.5
C(100)-C(102)-H(10F)	109.5
C(100)-C(102)-H(10G)	109.5
H(10F)-C(102)-H(10G)	109.5
C(100)-C(102)-H(10H)	109.5
H(10F)-C(102)-H(10H)	109.5
H(10G)-C(102)-H(10H)	109.5
C(1S)-C(7S)-H(7S1)	109.5
C(1S)-C(7S)-H(7S2)	109.5

H(7S1)-C(7S)-H(7S2)	109.5
C(1S)-C(7S)-H(7S3)	109.5
H(7S1)-C(7S)-H(7S3)	109.5
H(7S2)-C(7S)-H(7S3)	109.5
C(2S)-C(1S)-C(6S)	119.7(12)
C(2S)-C(1S)-C(7S)	121.3(11)
C(6S)-C(1S)-C(7S)	118.9(11)
C(1S)-C(2S)-C(3S)	120.5(12)
C(1S)-C(2S)-H(2S)	119.8
C(3S)-C(2S)-H(2S)	119.8
C(2S)-C(3S)-C(4S)	119.4(11)
C(2S)-C(3S)-H(3S)	120.3
C(4S)-C(3S)-H(3S)	120.3
C(5S)-C(4S)-C(3S)	119.2(13)
C(5S)-C(4S)-H(4S)	120.4
C(3S)-C(4S)-H(4S)	120.4
C(6S)-C(5S)-C(4S)	118.5(13)
C(6S)-C(5S)-H(5S)	120.7
C(4S)-C(5S)-H(5S)	120.7
C(5S)-C(6S)-C(1S)	122.4(11)
C(5S)-C(6S)-H(6S)	118.8
C(1S)-C(6S)-H(6S)	118.8
C(1T)-C(7T)-H(7T1)	109.5
C(1T)-C(7T)-H(7T2)	109.5
H(7T1)-C(7T)-H(7T2)	109.5
C(1T)-C(7T)-H(7T3)	109.5
H(7T1)-C(7T)-H(7T3)	109.5
H(7T2)-C(7T)-H(7T3)	109.5
C(2T)-C(1T)-C(6T)	118(2)
C(2T)-C(1T)-C(7T)	120.6(19)
C(6T)-C(1T)-C(7T)	120.9(19)
C(1T)-C(2T)-C(3T)	121.6(18)
C(1T)-C(2T)-H(2T)	119.2
C(3T)-C(2T)-H(2T)	119.2
C(2T)-C(3T)-C(4T)	120(2)
C(2T)-C(3T)-H(3T)	119.8
C(4T)-C(3T)-H(3T)	119.8
C(3T)-C(4T)-C(5T)	118(2)
C(3T)-C(4T)-H(4T)	121.0
C(5T)-C(4T)-H(4T)	121.0
C(4T)-C(5T)-C(6T)	118.8(18)
C(4T)-C(5T)-H(5T)	120.6
C(6T)-C(5T)-H(5T)	120.6
C(1T)-C(6T)-C(5T)	122.7(19)
C(1T)-C(6T)-H(6T)	118.6
C(5T)-C(6T)-H(6T)	118.6
C(1U)-C(7U)-H(7U1)	109.5
C(1U)-C(7U)-H(7U2)	109.5
H(7U1)-C(7U)-H(7U2)	109.5
C(1U)-C(7U)-H(7U3)	109.5
H(7U1)-C(7U)-H(7U3)	109.5
H(7U2)-C(7U)-H(7U3)	109.5
C(6U)-C(1U)-C(2U)	117.8(19)
C(6U)-C(1U)-C(7U)	123.0(17)
C(2U)-C(1U)-C(7U)	119.2(17)
C(1U)-C(2U)-C(3U)	119.8(18)

C(1U)-C(2U)-H(2U)	120.1
C(3U)-C(2U)-H(2U)	120.1
C(2U)-C(3U)-C(4U)	120.8(18)
C(2U)-C(3U)-H(3U)	119.6
C(4U)-C(3U)-H(3U)	119.6
C(5U)-C(4U)-C(3U)	120(2)
C(5U)-C(4U)-H(4U)	119.9
C(3U)-C(4U)-H(4U)	119.9
C(4U)-C(5U)-C(6U)	114.7(18)
C(4U)-C(5U)-H(5U)	122.7
C(6U)-C(5U)-H(5U)	122.7
C(1U)-C(6U)-C(5U)	126.1(18)
C(1U)-C(6U)-H(6U)	116.9
C(5U)-C(6U)-H(6U)	116.9

X-Ray Data for CpInd

CpInd crystallizes in the triclinic space group *P*-1 with half a molecule in the asymmetric unit along with two molecules of tetrahydrofuran. One of the tetrahydrofuran molecules and an isopropyl group were modeled as a two component disorders. The cyclopentadienyl and indenyl ligands are disordered about a crystallographic inversion center and were refined with the help of similarity restraints on the 1,2- and 1,3-distances and displacement parameters as well as rigid bond restraints for anisotropic displacement parameters. The anisotropic displacement parameters for the atom pairs C2/C19 and C5/C12 were constrained to be equivalent. The ellipsoid for the palladium atom is elongated, however, refinement of the palladium as a two component disorder did not lead to a better model. The coordinates for the hydrogen atoms bound to C1, C2, C5, C11, C12, and C19 were taken from the difference Fourier synthesis and the hydrogen atoms were subsequently refined semi-freely with the help of a distance restraint.

Table S11. Crystal data and structure refinement for **CpInd**

Empirical formula	C84 H116 N4 O4 Pd2	
Formula weight	1458.61	
Temperature	93(2) K	
Wavelength	1.54187 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 10.6789(2) Å	α= 106.710(7)°.
	b = 14.1144(3) Å	β= 103.424(7)°.
	c = 14.2052(10) Å	γ = 105.598(7)°.
Volume	1860.7(2) $Å^3$	
Z	1	
Density (calculated)	1.302 Mg/m^3	
Absorption coefficient	4.296 mm^{-1}	
F(000)	772	
Crystal size	0.15 x 0.10 x 0.10 mm^3	
Theta range for data collection	3.45 to 65.98°.	

Index ranges	-12<=h<=12, -16<=k<=16, -16<=l<=16
Reflections collected	61950
Independent reflections	6391 [R(int) = 0.1010]
Completeness to theta = 65.98°	98.6 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.6733 and 0.5651
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6391 / 385 / 564
Goodness-of-fit on F^2	1.123
Final R indices [I>2sigma(I)]	R1 = 0.0611, wR2 = 0.1587
R indices (all data)	R1 = 0.0677, wR2 = 0.1657
Largest diff. peak and hole	1.238 and -1.924 e.Å^{-3}

Table S12. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for **CpInd**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	2000(8)	74(7)	158(7)	30(2)
C(2)	1810(20)	-403(13)	915(11)	35(2)
C(3)	2004(11)	442(8)	1829(8)	37(2)
C(4)	2283(10)	1375(8)	1642(8)	36(2)
C(5)	2255(16)	1189(11)	603(8)	36(2)
C(11)	-1779(12)	-702(9)	-1463(9)	37(2)
C(12)	-2454(16)	-1355(11)	-989(9)	36(2)
C(13)	-3233(10)	-829(8)	-479(8)	40(2)
C(14)	-4174(10)	-1160(8)	1(8)	46(2)
C(15)	-4875(12)	-516(9)	358(10)	50(2)
C(16)	-4598(12)	476(9)	268(10)	50(2)
C(17)	-3659(10)	809(8)	-207(8)	44(2)
C(18)	-2995(9)	149(7)	-595(8)	39(2)
C(19)	-2060(20)	252(13)	-1178(12)	35(2)
Pd(1)	-263(1)	-927(1)	137(1)	40(1)
C(21)	-750(5)	-2336(4)	366(4)	38(1)
N(1)	-528(4)	-2460(3)	1311(3)	34(1)
C(31)	292(5)	-1663(4)	2324(3)	35(1)
C(32)	-235(5)	-918(4)	2804(4)	37(1)
C(37)	-1618(5)	-903(4)	2241(4)	45(1)
C(38)	-1770(10)	146(8)	2624(8)	62(3)
C(39)	-2780(9)	-1777(10)	2352(9)	67(3)
C(38A)	-1370(30)	340(20)	2200(30)	44(7)
C(39A)	-2740(30)	-1100(30)	2690(20)	49(7)
C(33)	578(6)	-187(4)	3804(4)	43(1)
C(34)	1838(6)	-196(4)	4298(4)	47(1)
C(35)	2344(6)	-938(4)	3811(4)	44(1)
C(36)	1577(5)	-1685(4)	2815(4)	37(1)
C(40)	2165(6)	-2491(4)	2293(4)	42(1)
C(41)	3650(6)	-1968(5)	2360(5)	55(1)
C(42)	2079(6)	-3336(4)	2774(5)	49(1)
C(22)	-1087(5)	-3528(4)	1185(4)	38(1)
C(23)	-1652(5)	-4076(4)	150(4)	37(1)
N(3)	-1458(4)	-3352(3)	-335(3)	32(1)
C(71)	-1963(5)	-3684(3)	-1459(3)	33(1)
C(72)	-1023(5)	-3601(4)	-2000(4)	37(1)
C(77)	524(5)	-3100(4)	-1423(4)	40(1)
C(78)	1062(6)	-3847(4)	-984(4)	45(1)

C(79)	1368(6)	-2765(5)	-2085(5)	55(1)
C(73)	-1575(6)	-3986(4)	-3085(4)	44(1)
C(74)	-2990(6)	-4469(4)	-3600(4)	50(1)
C(75)	-3879(6)	-4562(4)	-3046(4)	48(1)
C(76)	-3393(5)	-4164(4)	-1964(4)	39(1)
C(80)	-4432(6)	-4243(5)	-1378(5)	50(1)
C(81)	-5149(7)	-5393(5)	-1523(5)	62(2)
C(82)	-5508(7)	-3769(6)	-1739(6)	70(2)
O(1S)	4820(5)	8489(3)	5248(3)	64(1)
C(1S)	4635(8)	8972(5)	6204(5)	70(2)
C(2S)	4148(10)	8132(6)	6617(6)	84(2)
C(3S)	4420(10)	7199(6)	5966(7)	91(3)
C(4S)	5259(7)	7658(6)	5382(6)	72(2)
O(1T)	7660(6)	5995(4)	4302(4)	64(2)
C(1T)	8674(9)	5542(6)	4110(7)	64(2)
C(2T)	10071(9)	6392(7)	4690(7)	56(2)
C(3T)	9700(10)	7350(7)	4582(8)	68(2)
C(4T)	8323(9)	7128(6)	4727(7)	63(2)
O(1U)	8704(19)	6030(14)	3410(12)	69(4)
C(1U)	9640(30)	5870(20)	4190(20)	68(5)
C(2U)	10480(20)	6980(20)	4980(20)	68(5)
C(3U)	9450(30)	7530(20)	4910(20)	74(6)
C(4U)	8240(30)	6790(20)	3970(20)	79(5)

Table S13. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **CpInd**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	14(4)	34(4)	46(4)	19(3)	11(3)	9(3)
C(2)	35(6)	32(3)	41(6)	18(3)	9(5)	15(4)
C(3)	46(5)	29(5)	44(5)	21(4)	15(5)	16(4)
C(4)	35(5)	27(4)	43(5)	18(4)	10(4)	7(4)
C(5)	35(4)	30(3)	39(6)	17(4)	8(5)	7(3)
C(11)	39(5)	32(5)	40(5)	16(4)	12(4)	14(4)
C(12)	35(4)	30(3)	39(6)	17(4)	8(5)	7(3)
C(13)	39(5)	43(4)	43(5)	21(4)	13(3)	18(4)
C(14)	38(5)	47(5)	55(6)	23(4)	18(4)	12(4)
C(15)	44(6)	54(5)	50(6)	17(5)	20(4)	14(4)
C(16)	45(6)	50(4)	54(6)	11(5)	21(4)	19(4)
C(17)	37(5)	44(5)	54(5)	18(4)	14(4)	21(4)
C(18)	31(4)	31(4)	47(5)	9(3)	12(3)	4(3)
C(19)	35(6)	32(3)	41(6)	18(3)	9(5)	15(4)
Pd(1)	51(1)	32(1)	57(1)	25(1)	34(1)	24(1)
C(21)	41(3)	44(3)	30(2)	9(2)	16(2)	19(2)
N(1)	40(2)	28(2)	33(2)	12(2)	12(2)	11(2)
C(31)	43(3)	32(2)	31(2)	13(2)	14(2)	11(2)
C(32)	45(3)	31(2)	36(2)	11(2)	16(2)	15(2)
C(37)	43(3)	48(3)	50(3)	20(2)	19(2)	22(2)
C(38)	70(5)	64(4)	64(5)	21(4)	25(4)	43(4)
C(39)	49(4)	82(6)	84(6)	46(6)	31(4)	24(4)
C(38A)	38(14)	62(10)	53(16)	42(13)	16(12)	25(11)
C(39A)	69(14)	61(17)	35(12)	30(12)	32(11)	26(13)
C(33)	58(3)	38(3)	37(3)	11(2)	19(2)	22(2)
C(34)	58(3)	41(3)	39(3)	12(2)	14(2)	18(3)
C(35)	49(3)	41(3)	41(3)	16(2)	14(2)	16(2)

C(36)	42(3)	36(3)	36(2)	14(2)	15(2)	16(2)
C(40)	50(3)	36(3)	47(3)	17(2)	22(2)	18(2)
C(41)	56(3)	54(3)	66(4)	23(3)	32(3)	24(3)
C(42)	51(3)	41(3)	57(3)	18(3)	20(3)	20(2)
C(22)	49(3)	27(2)	44(3)	22(2)	20(2)	13(2)
C(23)	44(3)	25(2)	41(3)	13(2)	15(2)	12(2)
N(3)	44(2)	20(2)	34(2)	13(2)	15(2)	12(2)
C(71)	40(3)	28(2)	34(2)	12(2)	11(2)	16(2)
C(72)	48(3)	28(2)	39(2)	12(2)	16(2)	19(2)
C(77)	43(3)	32(2)	49(3)	16(2)	19(2)	16(2)
C(78)	46(3)	46(3)	52(3)	25(2)	23(2)	21(2)
C(79)	56(3)	54(3)	76(4)	37(3)	35(3)	25(3)
C(73)	59(3)	37(3)	39(3)	13(2)	21(2)	18(2)
C(74)	61(3)	43(3)	37(3)	12(2)	6(2)	16(3)
C(75)	50(3)	47(3)	46(3)	20(2)	10(2)	17(3)
C(76)	41(3)	35(3)	43(3)	15(2)	11(2)	18(2)
C(80)	41(3)	57(3)	58(3)	25(3)	20(3)	22(3)
C(81)	53(4)	66(4)	67(4)	27(3)	25(3)	15(3)
C(82)	53(4)	93(5)	83(5)	40(4)	30(3)	41(4)
O(1S)	70(3)	63(3)	57(2)	20(2)	16(2)	30(2)
C(1S)	88(5)	62(4)	62(4)	17(3)	24(4)	36(4)
C(2S)	101(6)	69(5)	83(5)	22(4)	43(5)	28(4)
C(3S)	127(7)	63(5)	101(6)	37(4)	47(6)	45(5)
C(4S)	68(4)	76(5)	70(4)	17(4)	16(3)	41(4)
O(1T)	61(3)	61(3)	62(3)	13(3)	19(3)	21(2)
C(1T)	73(5)	45(3)	66(5)	12(3)	17(4)	25(3)
C(2T)	65(4)	57(5)	47(5)	18(4)	30(4)	19(4)
C(3T)	91(5)	50(4)	68(5)	16(4)	45(4)	25(3)
C(4T)	81(5)	57(3)	60(4)	22(4)	31(4)	33(3)
O(1U)	76(9)	69(8)	54(7)	23(5)	24(6)	12(7)
C(1U)	83(9)	62(8)	62(9)	25(7)	30(8)	23(7)
C(2U)	75(8)	69(9)	56(8)	25(8)	26(7)	15(7)
C(3U)	82(9)	62(8)	74(9)	16(7)	42(8)	18(7)
C(4U)	86(8)	73(8)	77(8)	30(7)	24(7)	28(6)

Table S14. Bond lengths (Å) for **CpInd**

C(1)-C(5)	1.439(15)
C(1)-C(2)	1.449(18)
C(1)-Pd(1)	2.438(8)
C(1)-Pd(1)#1	2.490(8)
C(1)-H(1)	1.01(2)
C(2)-C(3)	1.414(16)
C(2)-Pd(1)	2.04(2)
C(2)-H(2)	1.00(2)
C(3)-C(4)	1.386(14)
C(3)-H(3)	0.9500
C(4)-C(5)	1.414(14)
C(4)-H(4)	0.9500
C(5)-Pd(1)#1	2.021(15)
C(5)-H(5)	0.99(2)
C(11)-C(19)	1.423(18)
C(11)-C(12)	1.430(17)
C(11)-Pd(1)#1	2.548(12)
C(11)-Pd(1)	2.621(12)
C(11)-H(11)	1.00(2)

C(12)-C(13)	1.439(17)
C(12)-Pd(1)	2.312(15)
C(12)-H(12)	1.00(2)
C(13)-C(14)	1.394(12)
C(13)-C(18)	1.399(14)
C(14)-C(15)	1.386(14)
C(14)-H(14)	0.9500
C(15)-C(16)	1.400(18)
C(15)-H(15)	0.9500
C(16)-C(17)	1.387(14)
C(16)-H(16)	0.9500
C(17)-C(18)	1.384(12)
C(17)-H(17)	0.9500
C(18)-C(19)	1.442(19)
C(19)-Pd(1)#1	2.336(19)
C(19)-H(19)	1.00(2)
Pd(1)-C(5)#1	2.021(15)
Pd(1)-C(21)	2.055(5)
Pd(1)-C(19)#1	2.336(19)
Pd(1)-C(1)#1	2.490(8)
Pd(1)-C(11)#1	2.548(12)
Pd(1)-Pd(1)#1	2.6861(6)
C(21)-N(3)	1.366(6)
C(21)-N(1)	1.377(6)
N(1)-C(22)	1.404(6)
N(1)-C(31)	1.435(6)
C(31)-C(36)	1.401(7)
C(31)-C(32)	1.404(7)
C(32)-C(33)	1.393(7)
C(32)-C(37)	1.516(7)
C(37)-C(39A)	1.48(3)
C(37)-C(38)	1.490(9)
C(37)-C(39)	1.571(10)
C(37)-C(38A)	1.72(3)
C(37)-H(37)	1.0000
C(37)-H(37A)	1.0000
C(38)-H(38A)	0.9800
C(38)-H(38B)	0.9800
C(38)-H(38C)	0.9800
C(39)-H(39A)	0.9800
C(39)-H(39B)	0.9800
C(39)-H(39C)	0.9800
C(38A)-H(38D)	0.9800
C(38A)-H(38E)	0.9800
C(38A)-H(38F)	0.9800
C(39A)-H(39D)	0.9800
C(39A)-H(39E)	0.9800
C(39A)-H(39F)	0.9800
C(33)-C(34)	1.371(8)
C(33)-H(33)	0.9500
C(34)-C(35)	1.389(7)
C(34)-H(34)	0.9500
C(35)-C(36)	1.388(7)
C(35)-H(35)	0.9500
C(36)-C(40)	1.534(7)
C(40)-C(41)	1.526(8)

C(40)-C(42)	1.529(7)
C(40)-H(40)	1.0000
C(41)-H(41A)	0.9800
C(41)-H(41B)	0.9800
C(41)-H(41C)	0.9800
C(42)-H(42A)	0.9800
C(42)-H(42B)	0.9800
C(42)-H(42C)	0.9800
C(22)-C(23)	1.345(7)
C(22)-H(22)	0.9500
C(23)-N(3)	1.386(6)
C(23)-H(23)	0.9500
N(3)-C(71)	1.447(6)
C(71)-C(72)	1.400(7)
C(71)-C(76)	1.400(7)
C(72)-C(73)	1.393(7)
C(72)-C(77)	1.520(7)
C(77)-C(79)	1.529(7)
C(77)-C(78)	1.539(7)
C(77)-H(77)	1.0000
C(78)-H(78A)	0.9800
C(78)-H(78B)	0.9800
C(78)-H(78C)	0.9800
C(79)-H(79A)	0.9800
C(79)-H(79B)	0.9800
C(79)-H(79C)	0.9800
C(73)-C(74)	1.389(8)
C(73)-H(73)	0.9500
C(74)-C(75)	1.370(8)
C(74)-H(74)	0.9500
C(75)-C(76)	1.387(7)
C(75)-H(75)	0.9500
C(76)-C(80)	1.533(7)
C(80)-C(81)	1.526(9)
C(80)-C(82)	1.539(8)
C(80)-H(80)	1.0000
C(81)-H(81A)	0.9800
C(81)-H(81B)	0.9800
C(81)-H(81C)	0.9800
C(82)-H(82A)	0.9800
C(82)-H(82B)	0.9800
C(82)-H(82C)	0.9800
O(1S)-C(4S)	1.419(7)
O(1S)-C(1S)	1.419(7)
C(1S)-C(2S)	1.494(9)
C(1S)-H(1S1)	0.9900
C(1S)-H(1S2)	0.9900
C(2S)-C(3S)	1.518(10)
C(2S)-H(2S1)	0.9900
C(2S)-H(2S2)	0.9900
C(3S)-C(4S)	1.502(10)
C(3S)-H(3S1)	0.9900
C(3S)-H(3S2)	0.9900
C(4S)-H(4S1)	0.9900
C(4S)-H(4S2)	0.9900
O(1T)-C(4T)	1.435(9)

O(1T)-C(1T)	1.437(9)
C(1T)-C(2T)	1.497(11)
C(1T)-H(1T1)	0.9900
C(1T)-H(1T2)	0.9900
C(2T)-C(3T)	1.546(11)
C(2T)-H(2T1)	0.9900
C(2T)-H(2T2)	0.9900
C(3T)-C(4T)	1.494(10)
C(3T)-H(3T1)	0.9900
C(3T)-H(3T2)	0.9900
C(4T)-H(4T1)	0.9900
C(4T)-H(4T2)	0.9900
O(1U)-C(4U)	1.408(15)
O(1U)-C(1U)	1.428(15)
C(1U)-C(2U)	1.510(16)
C(1U)-H(1U1)	0.9900
C(1U)-H(1U2)	0.9900
C(2U)-C(3U)	1.510(17)
C(2U)-H(2U1)	0.9900
C(2U)-H(2U2)	0.9900
C(3U)-C(4U)	1.491(15)
C(3U)-H(3U1)	0.9900
C(3U)-H(3U2)	0.9900
C(4U)-H(4U1)	0.9900
C(4U)-H(4U2)	0.9900

Symmetry transformations used to generate equivalent atoms:
#1 -x,-y,-z

Table S15. Bond angles (°) for **CpInd**

C(5)-C(1)-C(2)	109.7(11)
C(5)-C(1)-Pd(1)	109.1(8)
C(2)-C(1)-Pd(1)	56.7(8)
C(5)-C(1)-Pd(1)#1	54.3(7)
C(2)-C(1)-Pd(1)#1	108.7(9)
Pd(1)-C(1)-Pd(1)#1	66.1(2)
C(5)-C(1)-H(1)	116(6)
C(2)-C(1)-H(1)	128(6)
Pd(1)-C(1)-H(1)	124(6)
Pd(1)#1-C(1)-H(1)	118(6)
C(3)-C(2)-C(1)	105.5(12)
C(3)-C(2)-Pd(1)	103.1(12)
C(1)-C(2)-Pd(1)	86.9(9)
C(3)-C(2)-H(2)	124(7)
C(1)-C(2)-H(2)	125(7)
Pd(1)-C(2)-H(2)	102(7)
C(4)-C(3)-C(2)	109.1(11)
C(4)-C(3)-H(3)	125.5
C(2)-C(3)-H(3)	125.5
C(3)-C(4)-C(5)	111.2(10)
C(3)-C(4)-H(4)	124.4
C(5)-C(4)-H(4)	124.4
C(4)-C(5)-C(1)	104.5(10)
C(4)-C(5)-Pd(1)#1	101.9(10)
C(1)-C(5)-Pd(1)#1	90.4(7)

C(4)-C(5)-H(5)	118(6)
C(1)-C(5)-H(5)	128(6)
Pd(1)#1-C(5)-H(5)	108(6)
C(19)-C(11)-C(12)	107.3(13)
C(19)-C(11)-Pd(1)#1	65.0(9)
C(12)-C(11)-Pd(1)#1	112.8(8)
C(19)-C(11)-Pd(1)	112.7(9)
C(12)-C(11)-Pd(1)	61.6(7)
Pd(1)#1-C(11)-Pd(1)	62.6(3)
C(19)-C(11)-H(11)	124(7)
C(12)-C(11)-H(11)	118(7)
Pd(1)#1-C(11)-H(11)	119(6)
Pd(1)-C(11)-H(11)	117(6)
C(11)-C(12)-C(13)	108.1(10)
C(11)-C(12)-Pd(1)	85.5(8)
C(13)-C(12)-Pd(1)	111.6(8)
C(11)-C(12)-H(12)	121(7)
C(13)-C(12)-H(12)	119(6)
Pd(1)-C(12)-H(12)	106(6)
C(14)-C(13)-C(18)	120.1(8)
C(14)-C(13)-C(12)	131.6(10)
C(18)-C(13)-C(12)	108.1(8)
C(15)-C(14)-C(13)	119.5(9)
C(15)-C(14)-H(14)	120.2
C(13)-C(14)-H(14)	120.2
C(14)-C(15)-C(16)	119.9(9)
C(14)-C(15)-H(15)	120.0
C(16)-C(15)-H(15)	120.0
C(17)-C(16)-C(15)	120.7(9)
C(17)-C(16)-H(16)	119.7
C(15)-C(16)-H(16)	119.7
C(18)-C(17)-C(16)	119.3(9)
C(18)-C(17)-H(17)	120.3
C(16)-C(17)-H(17)	120.3
C(17)-C(18)-C(13)	120.4(8)
C(17)-C(18)-C(19)	131.3(11)
C(13)-C(18)-C(19)	108.3(9)
C(11)-C(19)-C(18)	108.0(12)
C(11)-C(19)-Pd(1)#1	81.4(11)
C(18)-C(19)-Pd(1)#1	113.4(10)
C(11)-C(19)-H(19)	131(7)
C(18)-C(19)-H(19)	119(7)
Pd(1)#1-C(19)-H(19)	91(7)
C(5)#1-Pd(1)-C(2)	170.4(7)
C(5)#1-Pd(1)-C(21)	93.0(4)
C(2)-Pd(1)-C(21)	96.1(5)
C(5)#1-Pd(1)-C(12)	10.6(6)
C(2)-Pd(1)-C(12)	167.5(6)
C(21)-Pd(1)-C(12)	93.8(4)
C(5)#1-Pd(1)-C(19)#1	167.5(5)
C(2)-Pd(1)-C(19)#1	5.7(8)
C(21)-Pd(1)-C(19)#1	96.0(5)
C(12)-Pd(1)-C(19)#1	170.1(7)
C(5)#1-Pd(1)-C(1)	137.1(4)
C(2)-Pd(1)-C(1)	36.4(5)
C(21)-Pd(1)-C(1)	124.8(2)

C(12)-Pd(1)-C(1)	131.1(4)
C(19)#1-Pd(1)-C(1)	40.0(5)
C(5)#1-Pd(1)-C(1)#1	35.3(4)
C(2)-Pd(1)-C(1)#1	135.4(5)
C(21)-Pd(1)-C(1)#1	121.2(2)
C(12)-Pd(1)-C(1)#1	41.6(4)
C(19)#1-Pd(1)-C(1)#1	132.4(5)
C(1)-Pd(1)-C(1)#1	113.9(2)
C(5)#1-Pd(1)-C(11)#1	134.0(5)
C(2)-Pd(1)-C(11)#1	37.2(5)
C(21)-Pd(1)-C(11)#1	120.8(3)
C(12)-Pd(1)-C(11)#1	139.6(4)
C(19)#1-Pd(1)-C(11)#1	33.5(4)
C(1)-Pd(1)-C(11)#1	45.0(3)
C(1)#1-Pd(1)-C(11)#1	98.9(3)
C(5)#1-Pd(1)-C(11)	39.7(4)
C(2)-Pd(1)-C(11)	134.6(6)
C(21)-Pd(1)-C(11)	121.7(3)
C(12)-Pd(1)-C(11)	33.0(4)
C(19)#1-Pd(1)-C(11)	137.5(5)
C(1)-Pd(1)-C(11)	98.2(3)
C(1)#1-Pd(1)-C(11)	43.8(3)
C(11)#1-Pd(1)-C(11)	117.4(3)
C(5)#1-Pd(1)-Pd(1)#1	84.8(4)
C(2)-Pd(1)-Pd(1)#1	86.0(5)
C(21)-Pd(1)-Pd(1)#1	177.09(13)
C(12)-Pd(1)-Pd(1)#1	84.4(3)
C(19)#1-Pd(1)-Pd(1)#1	85.9(4)
C(1)-Pd(1)-Pd(1)#1	57.90(19)
C(1)#1-Pd(1)-Pd(1)#1	56.05(18)
C(11)#1-Pd(1)-Pd(1)#1	60.0(3)
C(11)-Pd(1)-Pd(1)#1	57.4(3)
N(3)-C(21)-N(1)	102.8(4)
N(3)-C(21)-Pd(1)	130.3(3)
N(1)-C(21)-Pd(1)	126.7(3)
C(21)-N(1)-C(22)	111.8(4)
C(21)-N(1)-C(31)	127.3(4)
C(22)-N(1)-C(31)	120.5(4)
C(36)-C(31)-C(32)	122.4(4)
C(36)-C(31)-N(1)	118.2(4)
C(32)-C(31)-N(1)	119.4(4)
C(33)-C(32)-C(31)	117.1(5)
C(33)-C(32)-C(37)	121.9(4)
C(31)-C(32)-C(37)	121.0(4)
C(39A)-C(37)-C(38)	75.9(16)
C(39A)-C(37)-C(32)	118.5(13)
C(38)-C(37)-C(32)	114.0(5)
C(39A)-C(37)-C(39)	35.0(14)
C(38)-C(37)-C(39)	110.3(6)
C(32)-C(37)-C(39)	108.1(5)
C(39A)-C(37)-C(38A)	104.5(17)
C(38)-C(37)-C(38A)	30.6(11)
C(32)-C(37)-C(38A)	108.3(10)
C(39)-C(37)-C(38A)	136.2(11)
C(39A)-C(37)-H(37)	126.7
C(38)-C(37)-H(37)	108.1

C(32)-C(37)-H(37)	108.1
C(39)-C(37)-H(37)	108.1
C(38A)-C(37)-H(37)	82.5
C(39A)-C(37)-H(37A)	108.4
C(38)-C(37)-H(37A)	128.4
C(32)-C(37)-H(37A)	108.4
C(39)-C(37)-H(37A)	82.0
C(38A)-C(37)-H(37A)	108.4
H(37)-C(37)-H(37A)	27.9
C(37)-C(38)-H(38A)	109.5
C(37)-C(38)-H(38B)	109.5
H(38A)-C(38)-H(38B)	109.5
C(37)-C(38)-H(38C)	109.5
H(38A)-C(38)-H(38C)	109.5
H(38B)-C(38)-H(38C)	109.5
C(37)-C(39)-H(39A)	109.5
C(37)-C(39)-H(39B)	109.5
H(39A)-C(39)-H(39B)	109.5
C(37)-C(39)-H(39C)	109.5
H(39A)-C(39)-H(39C)	109.5
H(39B)-C(39)-H(39C)	109.5
C(37)-C(38A)-H(38D)	109.5
C(37)-C(38A)-H(38E)	109.5
H(38D)-C(38A)-H(38E)	109.5
C(37)-C(38A)-H(38F)	109.5
H(38D)-C(38A)-H(38F)	109.5
H(38E)-C(38A)-H(38F)	109.5
C(37)-C(39A)-H(39D)	109.5
C(37)-C(39A)-H(39E)	109.5
H(39D)-C(39A)-H(39E)	109.5
C(37)-C(39A)-H(39F)	109.5
H(39D)-C(39A)-H(39F)	109.5
H(39E)-C(39A)-H(39F)	109.5
C(34)-C(33)-C(32)	121.4(5)
C(34)-C(33)-H(33)	119.3
C(32)-C(33)-H(33)	119.3
C(33)-C(34)-C(35)	120.7(5)
C(33)-C(34)-H(34)	119.6
C(35)-C(34)-H(34)	119.6
C(36)-C(35)-C(34)	120.3(5)
C(36)-C(35)-H(35)	119.8
C(34)-C(35)-H(35)	119.8
C(35)-C(36)-C(31)	118.1(4)
C(35)-C(36)-C(40)	119.2(5)
C(31)-C(36)-C(40)	122.7(4)
C(41)-C(40)-C(42)	109.9(5)
C(41)-C(40)-C(36)	112.4(4)
C(42)-C(40)-C(36)	110.5(4)
C(41)-C(40)-H(40)	108.0
C(42)-C(40)-H(40)	108.0
C(36)-C(40)-H(40)	108.0
C(40)-C(41)-H(41A)	109.5
C(40)-C(41)-H(41B)	109.5
H(41A)-C(41)-H(41B)	109.5
C(40)-C(41)-H(41C)	109.5
H(41A)-C(41)-H(41C)	109.5

H(41B)-C(41)-H(41C)	109.5
C(40)-C(42)-H(42A)	109.5
C(40)-C(42)-H(42B)	109.5
H(42A)-C(42)-H(42B)	109.5
C(40)-C(42)-H(42C)	109.5
H(42A)-C(42)-H(42C)	109.5
H(42B)-C(42)-H(42C)	109.5
C(23)-C(22)-N(1)	105.8(4)
C(23)-C(22)-H(22)	127.1
N(1)-C(22)-H(22)	127.1
C(22)-C(23)-N(3)	107.5(4)
C(22)-C(23)-H(23)	126.2
N(3)-C(23)-H(23)	126.2
C(21)-N(3)-C(23)	112.1(4)
C(21)-N(3)-C(71)	126.3(4)
C(23)-N(3)-C(71)	121.6(4)
C(72)-C(71)-C(76)	122.8(4)
C(72)-C(71)-N(3)	119.6(4)
C(76)-C(71)-N(3)	117.4(4)
C(73)-C(72)-C(71)	116.8(5)
C(73)-C(72)-C(77)	122.0(5)
C(71)-C(72)-C(77)	121.2(4)
C(72)-C(77)-C(79)	113.9(5)
C(72)-C(77)-C(78)	111.2(4)
C(79)-C(77)-C(78)	108.8(4)
C(72)-C(77)-H(77)	107.6
C(79)-C(77)-H(77)	107.6
C(78)-C(77)-H(77)	107.6
C(77)-C(78)-H(78A)	109.5
C(77)-C(78)-H(78B)	109.5
H(78A)-C(78)-H(78B)	109.5
C(77)-C(78)-H(78C)	109.5
H(78A)-C(78)-H(78C)	109.5
H(78B)-C(78)-H(78C)	109.5
C(77)-C(79)-H(79A)	109.5
C(77)-C(79)-H(79B)	109.5
H(79A)-C(79)-H(79B)	109.5
C(77)-C(79)-H(79C)	109.5
H(79A)-C(79)-H(79C)	109.5
H(79B)-C(79)-H(79C)	109.5
C(74)-C(73)-C(72)	121.3(5)
C(74)-C(73)-H(73)	119.4
C(72)-C(73)-H(73)	119.4
C(75)-C(74)-C(73)	120.3(5)
C(75)-C(74)-H(74)	119.8
C(73)-C(74)-H(74)	119.8
C(74)-C(75)-C(76)	121.0(5)
C(74)-C(75)-H(75)	119.5
C(76)-C(75)-H(75)	119.5
C(75)-C(76)-C(71)	117.7(5)
C(75)-C(76)-C(80)	119.1(5)
C(71)-C(76)-C(80)	123.1(5)
C(81)-C(80)-C(76)	110.8(5)
C(81)-C(80)-C(82)	110.1(5)
C(76)-C(80)-C(82)	111.1(5)
C(81)-C(80)-H(80)	108.2

C(76)-C(80)-H(80)	108.2
C(82)-C(80)-H(80)	108.2
C(80)-C(81)-H(81A)	109.5
C(80)-C(81)-H(81B)	109.5
H(81A)-C(81)-H(81B)	109.5
C(80)-C(81)-H(81C)	109.5
H(81A)-C(81)-H(81C)	109.5
H(81B)-C(81)-H(81C)	109.5
C(80)-C(82)-H(82A)	109.5
C(80)-C(82)-H(82B)	109.5
H(82A)-C(82)-H(82B)	109.5
C(80)-C(82)-H(82C)	109.5
H(82A)-C(82)-H(82C)	109.5
H(82B)-C(82)-H(82C)	109.5
C(4S)-O(1S)-C(1S)	104.3(5)
O(1S)-C(1S)-C(2S)	108.2(5)
O(1S)-C(1S)-H(1S1)	110.0
C(2S)-C(1S)-H(1S1)	110.0
O(1S)-C(1S)-H(1S2)	110.1
C(2S)-C(1S)-H(1S2)	110.1
H(1S1)-C(1S)-H(1S2)	108.4
C(1S)-C(2S)-C(3S)	103.6(6)
C(1S)-C(2S)-H(2S1)	111.0
C(3S)-C(2S)-H(2S1)	111.0
C(1S)-C(2S)-H(2S2)	111.0
C(3S)-C(2S)-H(2S2)	111.0
H(2S1)-C(2S)-H(2S2)	109.0
C(4S)-C(3S)-C(2S)	103.9(6)
C(4S)-C(3S)-H(3S1)	111.0
C(2S)-C(3S)-H(3S1)	111.0
C(4S)-C(3S)-H(3S2)	111.0
C(2S)-C(3S)-H(3S2)	111.0
H(3S1)-C(3S)-H(3S2)	109.0
O(1S)-C(4S)-C(3S)	105.3(5)
O(1S)-C(4S)-H(4S1)	110.7
C(3S)-C(4S)-H(4S1)	110.7
O(1S)-C(4S)-H(4S2)	110.7
C(3S)-C(4S)-H(4S2)	110.7
H(4S1)-C(4S)-H(4S2)	108.8
C(4T)-O(1T)-C(1T)	107.9(6)
O(1T)-C(1T)-C(2T)	108.0(6)
O(1T)-C(1T)-H(1T1)	110.1
C(2T)-C(1T)-H(1T1)	110.1
O(1T)-C(1T)-H(1T2)	110.1
C(2T)-C(1T)-H(1T2)	110.1
H(1T1)-C(1T)-H(1T2)	108.4
C(1T)-C(2T)-C(3T)	98.7(6)
C(1T)-C(2T)-H(2T1)	112.0
C(3T)-C(2T)-H(2T1)	112.0
C(1T)-C(2T)-H(2T2)	112.0
C(3T)-C(2T)-H(2T2)	112.0
H(2T1)-C(2T)-H(2T2)	109.7
C(4T)-C(3T)-C(2T)	102.5(7)
C(4T)-C(3T)-H(3T1)	111.3
C(2T)-C(3T)-H(3T1)	111.3
C(4T)-C(3T)-H(3T2)	111.3

C(2T)-C(3T)-H(3T2)	111.3
H(3T1)-C(3T)-H(3T2)	109.2
O(1T)-C(4T)-C(3T)	106.1(6)
O(1T)-C(4T)-H(4T1)	110.5
C(3T)-C(4T)-H(4T1)	110.5
O(1T)-C(4T)-H(4T2)	110.5
C(3T)-C(4T)-H(4T2)	110.5
H(4T1)-C(4T)-H(4T2)	108.7
C(4U)-O(1U)-C(1U)	105.1(15)
O(1U)-C(1U)-C(2U)	103.3(14)
O(1U)-C(1U)-H(1U1)	111.1
C(2U)-C(1U)-H(1U1)	111.1
O(1U)-C(1U)-H(1U2)	111.1
C(2U)-C(1U)-H(1U2)	111.1
H(1U1)-C(1U)-H(1U2)	109.1
C(3U)-C(2U)-C(1U)	102.5(13)
C(3U)-C(2U)-H(2U1)	111.3
C(1U)-C(2U)-H(2U1)	111.3
C(3U)-C(2U)-H(2U2)	111.3
C(1U)-C(2U)-H(2U2)	111.3
H(2U1)-C(2U)-H(2U2)	109.2
C(4U)-C(3U)-C(2U)	105.4(12)
C(4U)-C(3U)-H(3U1)	110.7
C(2U)-C(3U)-H(3U1)	110.7
C(4U)-C(3U)-H(3U2)	110.7
C(2U)-C(3U)-H(3U2)	110.7
H(3U1)-C(3U)-H(3U2)	108.8
O(1U)-C(4U)-C(3U)	105.9(14)
O(1U)-C(4U)-H(4U1)	110.6
C(3U)-C(4U)-H(4U1)	110.6
O(1U)-C(4U)-H(4U2)	110.6
C(3U)-C(4U)-H(4U2)	110.6
H(4U1)-C(4U)-H(4U2)	108.7

Symmetry transformations used to generate equivalent atoms:
#1 -x,-y,-z

X-Ray Data for CpCp

CpCp crystallizes in the triclinic space group *P*-1 with two half molecules in the asymmetric unit along with one molecule of toluene. Some of the ellipsoids for the isopropyl groups are elongated, however, refinement of these atoms as disordered did not lead to a better model. The toluene molecule is disordered over two positions which were each restrained to be flat. The coordinates for the hydrogen atoms bound to C1, C2, C5, C6, C7 and C10 were taken from the difference Fourier synthesis and the hydrogen atoms were subsequently refined semi-freely with the help of a distance restraint.

Table S16. Crystal data and structure refinement for **CpCp**

Empirical formula	C71 H90 N4 Pd2
Formula weight	1212.27

Temperature	150(2) K	
Wavelength	0.71075 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 12.2057(3) Å	α= 70.805(5)°.
	b = 15.0286(4) Å	β= 88.840(6)°.
	c = 19.8101(14) Å	γ = 66.416(5)°.
Volume	3119.1(2) $Å^3$	
Z	2	
Density (calculated)	1.291 Mg/m^3	
Absorption coefficient	0.620 mm^{-1}	
F(000)	1272	
Crystal size	0.35 x 0.30 x 0.20 mm^3	
Theta range for data collection	3.04 to 30.51°.	
Index ranges	-17<=h<=17, -21<=k<=21, -27<=l<=28	
Reflections collected	94538	
Independent reflections	18367 [R(int) = 0.0281]	
Completeness to theta = 30.51°	96.3 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.8860 and 0.8122	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	18367 / 275 / 794	
Goodness-of-fit on F^2	1.070	
Final R indices [I>2sigma(I)]	R1 = 0.0309, wR2 = 0.0662	
R indices (all data)	R1 = 0.0380, wR2 = 0.0690	
Largest diff. peak and hole	0.630 and -0.678 e.$Å^{-3}$	

Table S17. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **CpCp**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Pd(1)	5083(1)	5681(1)	4386(1)	19(1)
C(1)	6347(2)	3811(1)	4672(1)	30(1)
C(2)	5772(2)	4422(1)	3952(1)	28(1)
C(3)	4728(2)	4236(2)	3870(1)	32(1)
C(4)	4650(2)	3553(2)	4508(1)	31(1)
C(5)	5644(2)	3270(1)	5032(1)	30(1)
C(11)	5025(1)	6833(1)	3453(1)	18(1)
N(1)	4352(1)	7178(1)	2800(1)	18(1)
C(21)	3703(2)	6674(1)	2584(1)	20(1)
C(22)	4206(2)	6147(1)	2110(1)	24(1)
C(27)	5428(2)	6020(2)	1860(1)	30(1)
C(28)	6243(2)	4888(2)	1958(1)	44(1)
C(29)	5288(2)	6699(2)	1066(1)	41(1)
C(23)	3532(2)	5721(2)	1867(1)	32(1)
C(24)	2433(2)	5806(2)	2091(1)	36(1)
C(25)	1974(2)	6306(2)	2572(1)	33(1)
C(26)	2594(2)	6757(1)	2832(1)	24(1)
C(30)	2083(2)	7329(2)	3351(1)	30(1)
C(31)	1235(2)	6953(2)	3814(1)	44(1)
C(32)	1458(3)	8497(2)	2947(2)	54(1)
C(12)	4456(2)	8042(1)	2314(1)	22(1)
C(13)	5208(2)	8252(1)	2653(1)	22(1)
N(2)	5546(1)	7517(1)	3346(1)	18(1)
C(41)	6419(2)	7465(1)	3855(1)	20(1)

C(42)	7590(2)	6674(1)	3987(1)	24(1)
C(47)	7955(2)	5890(2)	3606(1)	30(1)
C(48)	8913(3)	4841(2)	4063(2)	66(1)
C(49)	8353(3)	6313(3)	2886(2)	64(1)
C(43)	8426(2)	6667(2)	4459(1)	31(1)
C(44)	8115(2)	7419(2)	4773(1)	34(1)
C(45)	6964(2)	8193(2)	4627(1)	30(1)
C(46)	6082(2)	8234(1)	4166(1)	23(1)
C(50)	4825(2)	9103(1)	4010(1)	27(1)
C(51)	4297(2)	9213(2)	4701(1)	37(1)
C(52)	4827(2)	10132(2)	3523(1)	37(1)
Pd(2)	9533(1)	6019(1)	9617(1)	17(1)
C(6)	8541(2)	5257(1)	10629(1)	26(1)
C(7)	8625(2)	6210(1)	10544(1)	25(1)
C(8)	9573(2)	5962(1)	11090(1)	28(1)
C(9)	10046(2)	4921(1)	11478(1)	27(1)
C(10)	9425(2)	4444(1)	11202(1)	24(1)
C(61)	8785(1)	7580(1)	9032(1)	18(1)
N(3)	8082(1)	8085(1)	8375(1)	20(1)
C(71)	7773(2)	7621(1)	7920(1)	20(1)
C(72)	6870(2)	7257(1)	8093(1)	23(1)
C(77)	6320(2)	7236(2)	8790(1)	29(1)
C(78)	5889(2)	6378(2)	9068(1)	48(1)
C(79)	5317(3)	8283(2)	8721(2)	67(1)
C(73)	6509(2)	6918(1)	7598(1)	30(1)
C(74)	7027(2)	6930(2)	6969(1)	34(1)
C(75)	7934(2)	7264(2)	6824(1)	31(1)
C(76)	8333(2)	7618(1)	7298(1)	24(1)
C(80)	9339(2)	7980(2)	7126(1)	31(1)
C(81)	10417(2)	7210(2)	6908(1)	43(1)
C(82)	8881(2)	9048(2)	6525(1)	45(1)
C(62)	7700(2)	9155(1)	8152(1)	27(1)
C(63)	8173(2)	9339(1)	8668(1)	27(1)
N(4)	8820(1)	8384(1)	9204(1)	21(1)
C(91)	9473(2)	8320(1)	9830(1)	22(1)
C(92)	8809(2)	8710(1)	10333(1)	28(1)
C(97)	7446(2)	9087(2)	10290(1)	33(1)
C(98)	7049(2)	8608(2)	11004(1)	47(1)
C(99)	6820(2)	10275(2)	10046(1)	47(1)
C(93)	9454(2)	8747(2)	10891(1)	38(1)
C(94)	10685(2)	8405(2)	10945(1)	41(1)
C(95)	11321(2)	8004(2)	10448(1)	36(1)
C(96)	10729(2)	7956(1)	9876(1)	27(1)
C(100)	11421(2)	7558(2)	9316(1)	35(1)
C(101)	12668(2)	6699(3)	9622(2)	68(1)
C(102)	11479(3)	8446(3)	8684(2)	75(1)
C(7S)	2065(17)	10482(13)	7173(9)	83(4)
C(1S)	2202(10)	9763(8)	6746(6)	58(2)
C(2S)	3037(10)	8738(7)	7018(6)	63(2)
C(3S)	3211(8)	8068(6)	6652(6)	67(2)
C(4S)	2518(11)	8427(8)	5985(6)	68(2)
C(5S)	1688(10)	9440(9)	5706(5)	74(2)
C(6S)	1551(15)	10098(9)	6093(8)	65(2)
C(7T)	2211(17)	10324(12)	7167(8)	70(3)
C(1T)	2178(12)	9726(10)	6682(7)	72(3)
C(2T)	2885(13)	8698(10)	6775(7)	81(3)

C(3T)	2777(13)	8286(9)	6277(8)	82(3)
C(4T)	1921(11)	8879(9)	5660(7)	85(2)
C(5T)	1203(10)	9929(9)	5572(6)	82(2)
C(6T)	1342(17)	10326(11)	6080(9)	74(2)

Table S18. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **CpCp**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Pd(1)	28(1)	17(1)	14(1)	-3(1)	1(1)	-13(1)
C(1)	33(1)	25(1)	33(1)	-11(1)	4(1)	-12(1)
C(2)	43(1)	24(1)	22(1)	-9(1)	9(1)	-17(1)
C(3)	48(1)	28(1)	23(1)	-8(1)	0(1)	-18(1)
C(4)	45(1)	27(1)	28(1)	-9(1)	4(1)	-20(1)
C(5)	48(1)	21(1)	20(1)	-6(1)	2(1)	-17(1)
C(11)	21(1)	18(1)	17(1)	-6(1)	3(1)	-10(1)
N(1)	21(1)	17(1)	16(1)	-3(1)	1(1)	-10(1)
C(21)	24(1)	19(1)	17(1)	-3(1)	-2(1)	-11(1)
C(22)	28(1)	22(1)	19(1)	-6(1)	-2(1)	-10(1)
C(27)	30(1)	33(1)	25(1)	-14(1)	4(1)	-10(1)
C(28)	44(1)	39(1)	37(1)	-17(1)	7(1)	-2(1)
C(29)	42(1)	44(1)	32(1)	-11(1)	13(1)	-16(1)
C(23)	42(1)	27(1)	28(1)	-13(1)	-4(1)	-14(1)
C(24)	42(1)	33(1)	38(1)	-9(1)	-9(1)	-23(1)
C(25)	29(1)	35(1)	35(1)	-5(1)	-3(1)	-20(1)
C(26)	23(1)	24(1)	23(1)	-4(1)	0(1)	-12(1)
C(30)	26(1)	39(1)	27(1)	-11(1)	7(1)	-15(1)
C(31)	38(1)	56(1)	39(1)	-13(1)	16(1)	-24(1)
C(32)	66(2)	37(1)	58(2)	-21(1)	31(1)	-18(1)
C(12)	27(1)	19(1)	17(1)	-1(1)	1(1)	-10(1)
C(13)	28(1)	19(1)	19(1)	-2(1)	3(1)	-13(1)
N(2)	22(1)	18(1)	16(1)	-3(1)	2(1)	-11(1)
C(41)	24(1)	21(1)	18(1)	-4(1)	2(1)	-14(1)
C(42)	25(1)	25(1)	22(1)	-6(1)	1(1)	-12(1)
C(47)	26(1)	29(1)	34(1)	-15(1)	2(1)	-8(1)
C(48)	79(2)	36(1)	59(2)	-22(1)	-14(2)	6(1)
C(49)	85(2)	73(2)	43(1)	-33(1)	29(1)	-32(2)
C(43)	27(1)	35(1)	28(1)	-7(1)	-2(1)	-14(1)
C(44)	36(1)	43(1)	29(1)	-12(1)	-4(1)	-23(1)
C(45)	39(1)	33(1)	29(1)	-14(1)	4(1)	-22(1)
C(46)	29(1)	22(1)	23(1)	-7(1)	4(1)	-16(1)
C(50)	31(1)	23(1)	32(1)	-12(1)	5(1)	-14(1)
C(51)	47(1)	33(1)	45(1)	-23(1)	17(1)	-23(1)
C(52)	42(1)	24(1)	41(1)	-8(1)	6(1)	-13(1)
Pd(2)	20(1)	13(1)	17(1)	-4(1)	1(1)	-7(1)
C(6)	24(1)	28(1)	26(1)	-10(1)	8(1)	-12(1)
C(7)	28(1)	19(1)	24(1)	-6(1)	7(1)	-6(1)
C(8)	38(1)	21(1)	25(1)	-10(1)	4(1)	-12(1)
C(9)	34(1)	22(1)	23(1)	-7(1)	1(1)	-8(1)
C(10)	31(1)	19(1)	22(1)	-6(1)	8(1)	-10(1)
C(61)	22(1)	16(1)	17(1)	-5(1)	3(1)	-8(1)
N(3)	25(1)	14(1)	18(1)	-4(1)	-2(1)	-6(1)
C(71)	25(1)	16(1)	18(1)	-6(1)	-2(1)	-6(1)
C(72)	24(1)	20(1)	23(1)	-6(1)	-1(1)	-8(1)
C(77)	29(1)	35(1)	28(1)	-14(1)	7(1)	-16(1)

C(78)	60(2)	69(2)	40(1)	-22(1)	20(1)	-48(1)
C(79)	61(2)	56(2)	67(2)	-28(1)	30(2)	-4(1)
C(73)	36(1)	27(1)	30(1)	-9(1)	-2(1)	-17(1)
C(74)	51(1)	32(1)	26(1)	-12(1)	-2(1)	-21(1)
C(75)	48(1)	29(1)	19(1)	-10(1)	4(1)	-17(1)
C(76)	32(1)	18(1)	19(1)	-5(1)	2(1)	-10(1)
C(80)	37(1)	31(1)	26(1)	-9(1)	8(1)	-18(1)
C(81)	43(1)	44(1)	38(1)	-13(1)	15(1)	-16(1)
C(82)	55(1)	33(1)	43(1)	-5(1)	16(1)	-23(1)
C(62)	37(1)	15(1)	23(1)	-3(1)	-4(1)	-7(1)
C(63)	40(1)	14(1)	24(1)	-5(1)	-2(1)	-10(1)
N(4)	28(1)	15(1)	19(1)	-5(1)	0(1)	-9(1)
C(91)	33(1)	16(1)	19(1)	-5(1)	-2(1)	-12(1)
C(92)	41(1)	20(1)	23(1)	-8(1)	1(1)	-12(1)
C(97)	40(1)	29(1)	32(1)	-16(1)	8(1)	-12(1)
C(98)	60(2)	45(1)	41(1)	-22(1)	21(1)	-24(1)
C(99)	48(1)	30(1)	53(1)	-16(1)	8(1)	-5(1)
C(93)	59(1)	32(1)	26(1)	-14(1)	1(1)	-19(1)
C(94)	59(1)	37(1)	31(1)	-11(1)	-11(1)	-22(1)
C(95)	39(1)	34(1)	38(1)	-10(1)	-8(1)	-19(1)
C(96)	34(1)	23(1)	28(1)	-8(1)	0(1)	-16(1)
C(100)	32(1)	42(1)	44(1)	-23(1)	9(1)	-22(1)
C(101)	40(1)	76(2)	85(2)	-47(2)	3(1)	-7(1)
C(102)	99(3)	75(2)	57(2)	-23(2)	42(2)	-45(2)
C(7S)	61(6)	80(6)	111(8)	-52(6)	13(5)	-19(5)
C(1S)	51(4)	55(3)	85(4)	-30(3)	32(3)	-37(3)
C(2S)	57(3)	57(3)	85(5)	-26(3)	24(3)	-34(2)
C(3S)	65(4)	53(3)	98(5)	-33(3)	37(3)	-34(3)
C(4S)	76(6)	76(5)	88(6)	-48(5)	54(4)	-53(4)
C(5S)	76(5)	89(6)	73(4)	-31(4)	38(3)	-49(4)
C(6S)	62(6)	61(4)	79(4)	-23(3)	32(3)	-34(3)
C(7T)	59(6)	56(5)	88(5)	-14(4)	36(4)	-26(5)
C(1T)	61(5)	66(4)	89(5)	-25(4)	44(4)	-28(4)
C(2T)	64(5)	68(4)	110(6)	-33(4)	40(4)	-28(3)
C(3T)	76(7)	71(5)	112(9)	-36(5)	51(5)	-42(4)
C(4T)	82(6)	87(6)	100(5)	-35(5)	56(4)	-50(5)
C(5T)	74(6)	86(5)	96(5)	-28(4)	43(4)	-48(4)
C(6T)	61(5)	72(5)	96(5)	-23(4)	41(4)	-40(4)

Table S19. Bond lengths (Å) for **CpCp**

Pd(1)-C(11)	2.0550(15)
Pd(1)-C(5)#1	2.1532(18)
Pd(1)-C(2)	2.1882(18)
Pd(1)-C(1)	2.4734(19)
Pd(1)-C(1)#1	2.618(2)
Pd(1)-Pd(1)#1	2.6808(3)
C(1)-C(2)	1.425(3)
C(1)-C(5)	1.434(3)
C(1)-Pd(1)#1	2.618(2)
C(1)-H(1)	0.990(15)
C(2)-C(3)	1.434(3)
C(2)-H(2)	0.979(15)
C(3)-C(4)	1.371(3)
C(3)-H(3)	0.9500
C(4)-C(5)	1.442(3)

C(4)-H(4)	0.9500
C(5)-Pd(1)#1	2.1532(18)
C(5)-H(5)	0.982(15)
C(11)-N(1)	1.371(2)
C(11)-N(2)	1.3706(19)
N(1)-C(12)	1.391(2)
N(1)-C(21)	1.446(2)
C(21)-C(22)	1.401(2)
C(21)-C(26)	1.402(2)
C(22)-C(23)	1.399(3)
C(22)-C(27)	1.521(3)
C(27)-C(28)	1.536(3)
C(27)-C(29)	1.536(3)
C(27)-H(27)	1.0000
C(28)-H(28A)	0.9800
C(28)-H(28B)	0.9800
C(28)-H(28C)	0.9800
C(29)-H(29A)	0.9800
C(29)-H(29B)	0.9800
C(29)-H(29C)	0.9800
C(23)-C(24)	1.375(3)
C(23)-H(23)	0.9500
C(24)-C(25)	1.379(3)
C(24)-H(24)	0.9500
C(25)-C(26)	1.398(2)
C(25)-H(25)	0.9500
C(26)-C(30)	1.521(3)
C(30)-C(31)	1.524(3)
C(30)-C(32)	1.527(3)
C(30)-H(30)	1.0000
C(31)-H(31A)	0.9800
C(31)-H(31B)	0.9800
C(31)-H(31C)	0.9800
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800
C(12)-C(13)	1.338(2)
C(12)-H(12)	0.9500
C(13)-N(2)	1.391(2)
C(13)-H(13)	0.9500
N(2)-C(41)	1.445(2)
C(41)-C(46)	1.400(2)
C(41)-C(42)	1.405(2)
C(42)-C(43)	1.394(2)
C(42)-C(47)	1.520(3)
C(47)-C(49)	1.515(3)
C(47)-C(48)	1.516(3)
C(47)-H(47)	1.0000
C(48)-H(48A)	0.9800
C(48)-H(48B)	0.9800
C(48)-H(48C)	0.9800
C(49)-H(49A)	0.9800
C(49)-H(49B)	0.9800
C(49)-H(49C)	0.9800
C(43)-C(44)	1.385(3)
C(43)-H(43)	0.9500

C(44)-C(45)	1.378(3)
C(44)-H(44)	0.9500
C(45)-C(46)	1.395(2)
C(45)-H(45)	0.9500
C(46)-C(50)	1.519(3)
C(50)-C(52)	1.530(3)
C(50)-C(51)	1.531(3)
C(50)-H(50)	1.0000
C(51)-H(51A)	0.9800
C(51)-H(51B)	0.9800
C(51)-H(51C)	0.9800
C(52)-H(52A)	0.9800
C(52)-H(52B)	0.9800
C(52)-H(52C)	0.9800
Pd(2)-C(61)	2.0549(15)
Pd(2)-C(10)#2	2.1651(17)
Pd(2)-C(7)	2.1651(17)
Pd(2)-C(6)	2.5086(17)
Pd(2)-C(6)#2	2.5304(18)
Pd(2)-Pd(2)#2	2.6839(3)
C(6)-C(10)	1.425(3)
C(6)-C(7)	1.430(2)
C(6)-Pd(2)#2	2.5305(18)
C(6)-H(6)	0.975(15)
C(7)-C(8)	1.446(3)
C(7)-H(7)	0.963(15)
C(8)-C(9)	1.370(2)
C(8)-H(8)	0.9500
C(9)-C(10)	1.448(3)
C(9)-H(9)	0.9500
C(10)-Pd(2)#2	2.1651(17)
C(10)-H(10)	0.962(15)
C(61)-N(3)	1.372(2)
C(61)-N(4)	1.374(2)
N(3)-C(62)	1.393(2)
N(3)-C(71)	1.443(2)
C(71)-C(76)	1.397(2)
C(71)-C(72)	1.405(2)
C(72)-C(73)	1.394(2)
C(72)-C(77)	1.519(3)
C(77)-C(78)	1.518(3)
C(77)-C(79)	1.523(3)
C(77)-H(77)	1.0000
C(78)-H(78A)	0.9800
C(78)-H(78B)	0.9800
C(78)-H(78C)	0.9800
C(79)-H(79A)	0.9800
C(79)-H(79B)	0.9800
C(79)-H(79C)	0.9800
C(73)-C(74)	1.384(3)
C(73)-H(73)	0.9500
C(74)-C(75)	1.377(3)
C(74)-H(74)	0.9500
C(75)-C(76)	1.398(3)
C(75)-H(75)	0.9500
C(76)-C(80)	1.521(3)

C(80)-C(81)	1.531(3)
C(80)-C(82)	1.536(3)
C(80)-H(80)	1.0000
C(81)-H(81A)	0.9800
C(81)-H(81B)	0.9800
C(81)-H(81C)	0.9800
C(82)-H(82A)	0.9800
C(82)-H(82B)	0.9800
C(82)-H(82C)	0.9800
C(62)-C(63)	1.338(3)
C(62)-H(62)	0.9500
C(63)-N(4)	1.390(2)
C(63)-H(63)	0.9500
N(4)-C(91)	1.443(2)
C(91)-C(96)	1.399(3)
C(91)-C(92)	1.402(2)
C(92)-C(93)	1.398(3)
C(92)-C(97)	1.521(3)
C(97)-C(98)	1.530(3)
C(97)-C(99)	1.536(3)
C(97)-H(97)	1.0000
C(98)-H(98A)	0.9800
C(98)-H(98B)	0.9800
C(98)-H(98C)	0.9800
C(99)-H(99A)	0.9800
C(99)-H(99B)	0.9800
C(99)-H(99C)	0.9800
C(93)-C(94)	1.373(3)
C(93)-H(93)	0.9500
C(94)-C(95)	1.385(3)
C(94)-H(94)	0.9500
C(95)-C(96)	1.394(3)
C(95)-H(95)	0.9500
C(96)-C(100)	1.515(3)
C(100)-C(101)	1.517(3)
C(100)-C(102)	1.525(4)
C(100)-H(100)	1.0000
C(101)-H(10A)	0.9800
C(101)-H(10B)	0.9800
C(101)-H(10C)	0.9800
C(102)-H(10D)	0.9800
C(102)-H(10E)	0.9800
C(102)-H(10F)	0.9800
C(7S)-C(1S)	1.536(9)
C(7S)-H(7S1)	0.9800
C(7S)-H(7S2)	0.9800
C(7S)-H(7S3)	0.9800
C(1S)-C(6S)	1.362(9)
C(1S)-C(2S)	1.387(9)
C(2S)-C(3S)	1.374(9)
C(2S)-H(2S)	0.9500
C(3S)-C(4S)	1.401(10)
C(3S)-H(3S)	0.9500
C(4S)-C(5S)	1.373(10)
C(4S)-H(4S)	0.9500
C(5S)-C(6S)	1.398(9)

C(5S)-H(5S)	0.9500
C(6S)-H(6S)	0.9500
C(7T)-C(1T)	1.527(11)
C(7T)-H(7T1)	0.9800
C(7T)-H(7T2)	0.9800
C(7T)-H(7T3)	0.9800
C(1T)-C(6T)	1.371(11)
C(1T)-C(2T)	1.385(10)
C(2T)-C(3T)	1.359(11)
C(2T)-H(2T)	0.9500
C(3T)-C(4T)	1.404(11)
C(3T)-H(3T)	0.9500
C(4T)-C(5T)	1.417(10)
C(4T)-H(4T)	0.9500
C(5T)-C(6T)	1.371(11)
C(5T)-H(5T)	0.9500
C(6T)-H(6T)	0.9500

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+1,-z+1 #2 -x+2,-y+1,-z+2

Table S20. Bond angles (°) for **CpCp**

C(11)-Pd(1)-C(5)#1	93.46(6)
C(11)-Pd(1)-C(2)	96.14(6)
C(5)#1-Pd(1)-C(2)	170.24(7)
C(11)-Pd(1)-C(1)	124.82(6)
C(5)#1-Pd(1)-C(1)	137.43(7)
C(2)-Pd(1)-C(1)	34.93(7)
C(11)-Pd(1)-C(1)#1	118.59(6)
C(5)#1-Pd(1)-C(1)#1	33.20(6)
C(2)-Pd(1)-C(1)#1	137.95(6)
C(1)-Pd(1)-C(1)#1	116.53(5)
C(11)-Pd(1)-Pd(1)#1	173.77(4)
C(5)#1-Pd(1)-Pd(1)#1	82.09(5)
C(2)-Pd(1)-Pd(1)#1	88.21(5)
C(1)-Pd(1)-Pd(1)#1	60.89(5)
C(1)#1-Pd(1)-Pd(1)#1	55.64(4)
C(2)-C(1)-C(5)	108.25(17)
C(2)-C(1)-Pd(1)	61.53(10)
C(5)-C(1)-Pd(1)	106.87(13)
C(2)-C(1)-Pd(1)#1	111.41(13)
C(5)-C(1)-Pd(1)#1	55.31(10)
Pd(1)-C(1)-Pd(1)#1	63.47(5)
C(2)-C(1)-H(1)	124.6(14)
C(5)-C(1)-H(1)	125.5(14)
Pd(1)-C(1)-H(1)	109.0(13)
Pd(1)#1-C(1)-H(1)	109.6(14)
C(1)-C(2)-C(3)	107.04(16)
C(1)-C(2)-Pd(1)	83.54(11)
C(3)-C(2)-Pd(1)	102.27(13)
C(1)-C(2)-H(2)	123.8(14)
C(3)-C(2)-H(2)	125.1(13)
Pd(1)-C(2)-H(2)	102.7(13)
C(4)-C(3)-C(2)	109.09(18)
C(4)-C(3)-H(3)	125.5
C(2)-C(3)-H(3)	125.5

C(3)-C(4)-C(5)	109.33(18)
C(3)-C(4)-H(4)	125.3
C(5)-C(4)-H(4)	125.3
C(1)-C(5)-C(4)	106.27(16)
C(1)-C(5)-Pd(1)#1	91.49(11)
C(4)-C(5)-Pd(1)#1	104.04(13)
C(1)-C(5)-H(5)	120.7(14)
C(4)-C(5)-H(5)	124.1(14)
Pd(1)#1-C(5)-H(5)	103.3(13)
N(1)-C(11)-N(2)	102.53(13)
N(1)-C(11)-Pd(1)	128.22(11)
N(2)-C(11)-Pd(1)	128.94(11)
C(11)-N(1)-C(12)	111.88(13)
C(11)-N(1)-C(21)	126.33(13)
C(12)-N(1)-C(21)	121.47(13)
C(22)-C(21)-C(26)	122.85(15)
C(22)-C(21)-N(1)	117.47(14)
C(26)-C(21)-N(1)	119.64(15)
C(23)-C(22)-C(21)	117.04(17)
C(23)-C(22)-C(27)	119.77(16)
C(21)-C(22)-C(27)	123.19(15)
C(22)-C(27)-C(28)	112.16(17)
C(22)-C(27)-C(29)	111.02(16)
C(28)-C(27)-C(29)	109.24(16)
C(22)-C(27)-H(27)	108.1
C(28)-C(27)-H(27)	108.1
C(29)-C(27)-H(27)	108.1
C(27)-C(28)-H(28A)	109.5
C(27)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
C(27)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
C(27)-C(29)-H(29A)	109.5
C(27)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5
C(27)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5
C(24)-C(23)-C(22)	121.41(18)
C(24)-C(23)-H(23)	119.3
C(22)-C(23)-H(23)	119.3
C(23)-C(24)-C(25)	120.28(17)
C(23)-C(24)-H(24)	119.9
C(25)-C(24)-H(24)	119.9
C(24)-C(25)-C(26)	121.27(18)
C(24)-C(25)-H(25)	119.4
C(26)-C(25)-H(25)	119.4
C(25)-C(26)-C(21)	117.12(17)
C(25)-C(26)-C(30)	121.61(17)
C(21)-C(26)-C(30)	121.27(15)
C(26)-C(30)-C(31)	113.51(17)
C(26)-C(30)-C(32)	110.72(17)
C(31)-C(30)-C(32)	110.41(18)
C(26)-C(30)-H(30)	107.3
C(31)-C(30)-H(30)	107.3

C(32)-C(30)-H(30)	107.3
C(30)-C(31)-H(31A)	109.5
C(30)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
C(30)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
C(30)-C(32)-H(32A)	109.5
C(30)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
C(30)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
C(13)-C(12)-N(1)	106.96(14)
C(13)-C(12)-H(12)	126.5
N(1)-C(12)-H(12)	126.5
C(12)-C(13)-N(2)	106.46(14)
C(12)-C(13)-H(13)	126.8
N(2)-C(13)-H(13)	126.8
C(11)-N(2)-C(13)	112.17(13)
C(11)-N(2)-C(41)	125.74(13)
C(13)-N(2)-C(41)	121.93(13)
C(46)-C(41)-C(42)	122.97(16)
C(46)-C(41)-N(2)	118.71(15)
C(42)-C(41)-N(2)	118.23(14)
C(43)-C(42)-C(41)	117.03(16)
C(43)-C(42)-C(47)	120.93(16)
C(41)-C(42)-C(47)	121.98(15)
C(49)-C(47)-C(48)	111.2(2)
C(49)-C(47)-C(42)	110.36(18)
C(48)-C(47)-C(42)	112.82(18)
C(49)-C(47)-H(47)	107.4
C(48)-C(47)-H(47)	107.4
C(42)-C(47)-H(47)	107.4
C(47)-C(48)-H(48A)	109.5
C(47)-C(48)-H(48B)	109.5
H(48A)-C(48)-H(48B)	109.5
C(47)-C(48)-H(48C)	109.5
H(48A)-C(48)-H(48C)	109.5
H(48B)-C(48)-H(48C)	109.5
C(47)-C(49)-H(49A)	109.5
C(47)-C(49)-H(49B)	109.5
H(49A)-C(49)-H(49B)	109.5
C(47)-C(49)-H(49C)	109.5
H(49A)-C(49)-H(49C)	109.5
H(49B)-C(49)-H(49C)	109.5
C(44)-C(43)-C(42)	121.08(18)
C(44)-C(43)-H(43)	119.5
C(42)-C(43)-H(43)	119.5
C(45)-C(44)-C(43)	120.60(18)
C(45)-C(44)-H(44)	119.7
C(43)-C(44)-H(44)	119.7
C(44)-C(45)-C(46)	121.01(18)
C(44)-C(45)-H(45)	119.5
C(46)-C(45)-H(45)	119.5
C(45)-C(46)-C(41)	117.30(17)

C(45)-C(46)-C(50)	119.74(16)
C(41)-C(46)-C(50)	122.95(15)
C(46)-C(50)-C(52)	110.73(15)
C(46)-C(50)-C(51)	112.15(16)
C(52)-C(50)-C(51)	110.22(16)
C(46)-C(50)-H(50)	107.9
C(52)-C(50)-H(50)	107.9
C(51)-C(50)-H(50)	107.9
C(50)-C(51)-H(51A)	109.5
C(50)-C(51)-H(51B)	109.5
H(51A)-C(51)-H(51B)	109.5
C(50)-C(51)-H(51C)	109.5
H(51A)-C(51)-H(51C)	109.5
H(51B)-C(51)-H(51C)	109.5
C(50)-C(52)-H(52A)	109.5
C(50)-C(52)-H(52B)	109.5
H(52A)-C(52)-H(52B)	109.5
C(50)-C(52)-H(52C)	109.5
H(52A)-C(52)-H(52C)	109.5
H(52B)-C(52)-H(52C)	109.5
C(61)-Pd(2)-C(10)#2	95.83(6)
C(61)-Pd(2)-C(7)	93.71(6)
C(10)#2-Pd(2)-C(7)	170.46(6)
C(61)-Pd(2)-C(6)	120.92(6)
C(10)#2-Pd(2)-C(6)	137.41(6)
C(7)-Pd(2)-C(6)	34.66(6)
C(61)-Pd(2)-C(6)#2	123.45(6)
C(10)#2-Pd(2)-C(6)#2	34.23(6)
C(7)-Pd(2)-C(6)#2	137.41(6)
C(6)-Pd(2)-C(6)#2	115.64(4)
C(61)-Pd(2)-Pd(2)#2	178.94(4)
C(10)#2-Pd(2)-Pd(2)#2	84.75(4)
C(7)-Pd(2)-Pd(2)#2	85.71(5)
C(6)-Pd(2)-Pd(2)#2	58.21(4)
C(6)#2-Pd(2)-Pd(2)#2	57.42(4)
C(10)-C(6)-C(7)	108.97(16)
C(10)-C(6)-Pd(2)	110.50(11)
C(7)-C(6)-Pd(2)	59.42(9)
C(10)-C(6)-Pd(2)#2	58.70(9)
C(7)-C(6)-Pd(2)#2	110.83(11)
Pd(2)-C(6)-Pd(2)#2	64.37(4)
C(10)-C(6)-H(6)	125.6(13)
C(7)-C(6)-H(6)	123.9(13)
Pd(2)-C(6)-H(6)	106.8(13)
Pd(2)#2-C(6)-H(6)	108.0(13)
C(6)-C(7)-C(8)	106.28(15)
C(6)-C(7)-Pd(2)	85.92(11)
C(8)-C(7)-Pd(2)	104.64(12)
C(6)-C(7)-H(7)	124.1(13)
C(8)-C(7)-H(7)	123.8(13)
Pd(2)-C(7)-H(7)	102.3(13)
C(9)-C(8)-C(7)	109.17(16)
C(9)-C(8)-H(8)	125.4
C(7)-C(8)-H(8)	125.4
C(8)-C(9)-C(10)	109.31(17)
C(8)-C(9)-H(9)	125.3

C(10)-C(9)-H(9)	125.3
C(6)-C(10)-C(9)	106.27(15)
C(6)-C(10)-Pd(2)#2	87.07(11)
C(9)-C(10)-Pd(2)#2	104.54(12)
C(6)-C(10)-H(10)	123.7(13)
C(9)-C(10)-H(10)	123.5(13)
Pd(2)#2-C(10)-H(10)	102.7(13)
N(3)-C(61)-N(4)	102.37(13)
N(3)-C(61)-Pd(2)	128.07(11)
N(4)-C(61)-Pd(2)	129.53(11)
C(61)-N(3)-C(62)	112.23(14)
C(61)-N(3)-C(71)	127.14(13)
C(62)-N(3)-C(71)	120.58(14)
C(76)-C(71)-C(72)	122.98(15)
C(76)-C(71)-N(3)	118.05(15)
C(72)-C(71)-N(3)	118.83(15)
C(73)-C(72)-C(71)	116.93(16)
C(73)-C(72)-C(77)	121.86(16)
C(71)-C(72)-C(77)	121.21(15)
C(78)-C(77)-C(72)	112.83(17)
C(78)-C(77)-C(79)	111.0(2)
C(72)-C(77)-C(79)	111.86(18)
C(78)-C(77)-H(77)	106.9
C(72)-C(77)-H(77)	106.9
C(79)-C(77)-H(77)	106.9
C(77)-C(78)-H(78A)	109.5
C(77)-C(78)-H(78B)	109.5
H(78A)-C(78)-H(78B)	109.5
C(77)-C(78)-H(78C)	109.5
H(78A)-C(78)-H(78C)	109.5
H(78B)-C(78)-H(78C)	109.5
C(77)-C(79)-H(79A)	109.5
C(77)-C(79)-H(79B)	109.5
H(79A)-C(79)-H(79B)	109.5
C(77)-C(79)-H(79C)	109.5
H(79A)-C(79)-H(79C)	109.5
H(79B)-C(79)-H(79C)	109.5
C(74)-C(73)-C(72)	121.31(18)
C(74)-C(73)-H(73)	119.3
C(72)-C(73)-H(73)	119.3
C(75)-C(74)-C(73)	120.31(17)
C(75)-C(74)-H(74)	119.8
C(73)-C(74)-H(74)	119.8
C(74)-C(75)-C(76)	121.13(17)
C(74)-C(75)-H(75)	119.4
C(76)-C(75)-H(75)	119.4
C(71)-C(76)-C(75)	117.28(17)
C(71)-C(76)-C(80)	122.65(16)
C(75)-C(76)-C(80)	120.07(16)
C(76)-C(80)-C(81)	112.24(17)
C(76)-C(80)-C(82)	111.06(17)
C(81)-C(80)-C(82)	109.26(17)
C(76)-C(80)-H(80)	108.0
C(81)-C(80)-H(80)	108.0
C(82)-C(80)-H(80)	108.0
C(80)-C(81)-H(81A)	109.5

C(80)-C(81)-H(81B)	109.5
H(81A)-C(81)-H(81B)	109.5
C(80)-C(81)-H(81C)	109.5
H(81A)-C(81)-H(81C)	109.5
H(81B)-C(81)-H(81C)	109.5
C(80)-C(82)-H(82A)	109.5
C(80)-C(82)-H(82B)	109.5
H(82A)-C(82)-H(82B)	109.5
C(80)-C(82)-H(82C)	109.5
H(82A)-C(82)-H(82C)	109.5
H(82B)-C(82)-H(82C)	109.5
C(63)-C(62)-N(3)	106.45(15)
C(63)-C(62)-H(62)	126.8
N(3)-C(62)-H(62)	126.8
C(62)-C(63)-N(4)	107.00(15)
C(62)-C(63)-H(63)	126.5
N(4)-C(63)-H(63)	126.5
C(61)-N(4)-C(63)	111.94(14)
C(61)-N(4)-C(91)	127.61(13)
C(63)-N(4)-C(91)	120.38(13)
C(96)-C(91)-C(92)	123.02(16)
C(96)-C(91)-N(4)	118.60(16)
C(92)-C(91)-N(4)	118.14(16)
C(93)-C(92)-C(91)	117.01(19)
C(93)-C(92)-C(97)	120.06(18)
C(91)-C(92)-C(97)	122.92(16)
C(92)-C(97)-C(98)	112.30(18)
C(92)-C(97)-C(99)	111.12(18)
C(98)-C(97)-C(99)	109.74(18)
C(92)-C(97)-H(97)	107.8
C(98)-C(97)-H(97)	107.8
C(99)-C(97)-H(97)	107.8
C(97)-C(98)-H(98A)	109.5
C(97)-C(98)-H(98B)	109.5
H(98A)-C(98)-H(98B)	109.5
C(97)-C(98)-H(98C)	109.5
H(98A)-C(98)-H(98C)	109.5
H(98B)-C(98)-H(98C)	109.5
C(97)-C(99)-H(99A)	109.5
C(97)-C(99)-H(99B)	109.5
H(99A)-C(99)-H(99B)	109.5
C(97)-C(99)-H(99C)	109.5
H(99A)-C(99)-H(99C)	109.5
H(99B)-C(99)-H(99C)	109.5
C(94)-C(93)-C(92)	121.3(2)
C(94)-C(93)-H(93)	119.4
C(92)-C(93)-H(93)	119.4
C(93)-C(94)-C(95)	120.47(19)
C(93)-C(94)-H(94)	119.8
C(95)-C(94)-H(94)	119.8
C(94)-C(95)-C(96)	121.0(2)
C(94)-C(95)-H(95)	119.5
C(96)-C(95)-H(95)	119.5
C(95)-C(96)-C(91)	117.20(18)
C(95)-C(96)-C(100)	120.92(18)
C(91)-C(96)-C(100)	121.85(16)

C(96)-C(100)-C(101)	113.4(2)
C(96)-C(100)-C(102)	110.77(19)
C(101)-C(100)-C(102)	111.2(2)
C(96)-C(100)-H(100)	107.0
C(101)-C(100)-H(100)	107.0
C(102)-C(100)-H(100)	107.0
C(100)-C(101)-H(10A)	109.5
C(100)-C(101)-H(10B)	109.5
H(10A)-C(101)-H(10B)	109.5
C(100)-C(101)-H(10C)	109.5
H(10A)-C(101)-H(10C)	109.5
H(10B)-C(101)-H(10C)	109.5
C(100)-C(102)-H(10D)	109.5
C(100)-C(102)-H(10E)	109.5
H(10D)-C(102)-H(10E)	109.5
C(100)-C(102)-H(10F)	109.5
H(10D)-C(102)-H(10F)	109.5
H(10E)-C(102)-H(10F)	109.5
C(6S)-C(1S)-C(2S)	117.7(8)
C(6S)-C(1S)-C(7S)	122.5(10)
C(2S)-C(1S)-C(7S)	119.8(9)
C(3S)-C(2S)-C(1S)	122.1(8)
C(3S)-C(2S)-H(2S)	118.9
C(1S)-C(2S)-H(2S)	118.9
C(2S)-C(3S)-C(4S)	119.1(7)
C(2S)-C(3S)-H(3S)	120.4
C(4S)-C(3S)-H(3S)	120.4
C(5S)-C(4S)-C(3S)	119.6(8)
C(5S)-C(4S)-H(4S)	120.2
C(3S)-C(4S)-H(4S)	120.2
C(4S)-C(5S)-C(6S)	119.3(8)
C(4S)-C(5S)-H(5S)	120.4
C(6S)-C(5S)-H(5S)	120.4
C(1S)-C(6S)-C(5S)	122.1(8)
C(1S)-C(6S)-H(6S)	118.9
C(5S)-C(6S)-H(6S)	118.9
C(1T)-C(7T)-H(7T1)	109.5
C(1T)-C(7T)-H(7T2)	109.5
H(7T1)-C(7T)-H(7T2)	109.5
C(1T)-C(7T)-H(7T3)	109.5
H(7T1)-C(7T)-H(7T3)	109.5
H(7T2)-C(7T)-H(7T3)	109.5
C(6T)-C(1T)-C(2T)	118.9(10)
C(6T)-C(1T)-C(7T)	113.0(11)
C(2T)-C(1T)-C(7T)	128.1(11)
C(3T)-C(2T)-C(1T)	121.2(11)
C(3T)-C(2T)-H(2T)	119.4
C(1T)-C(2T)-H(2T)	119.4
C(2T)-C(3T)-C(4T)	121.2(11)
C(2T)-C(3T)-H(3T)	119.4
C(4T)-C(3T)-H(3T)	119.4
C(3T)-C(4T)-C(5T)	117.0(10)
C(3T)-C(4T)-H(4T)	121.5
C(5T)-C(4T)-H(4T)	121.5
C(6T)-C(5T)-C(4T)	120.5(10)
C(6T)-C(5T)-H(5T)	119.7

C(4T)-C(5T)-H(5T)	119.7
C(5T)-C(6T)-C(1T)	121.3(10)
C(5T)-C(6T)-H(6T)	119.4
C(1T)-C(6T)-H(6T)	119.4

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+1,-z+1 #2 -x+2,-y+1,-z+2

X-Ray Data for IndInd

IndInd crystallizes in the monoclinic space group $P2_1/c$ with half a molecule in the asymmetric unit along with 1.5 molecules of toluene. One of the toluene molecules was modeled as a two component disorder. The second toluene is located near a crystallographic inversion center and disordered over four positions, two of which are pairwise related to the other two by the inversion center. The coordinates for the hydrogen atoms bound to C1, C2, and C9 were taken from the difference Fourier synthesis and the hydrogen atoms were subsequently refined semi-freely with the help of a distance restraint.

Table S21. Crystal data and structure refinement for **IndInd**

Empirical formula	C93 H110 N4 Pd2	
Formula weight	1496.65	
Temperature	150(2) K	
Wavelength	0.71075 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 13.0237(3) Å	α= 90°.
	b = 14.3884(3) Å	β= 98.096(7)°.
	c = 21.0780(15) Å	γ = 90°.
Volume	3910.4(3) Å^3	
Z	2	
Density (calculated)	1.271 Mg/m^3	
Absorption coefficient	0.508 mm^{-1}	
F(000)	1576	
Crystal size	0.15 x 0.15 x 0.15 mm^3	
Theta range for data collection	3.00 to 30.51°.	
Index ranges	-18<=h<=18, -20<=k<=20, -30<=l<=30	
Reflections collected	118556	
Independent reflections	11920 [R(int) = 0.0648]	
Completeness to theta = 30.51°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9277 and 0.9277	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	11920 / 639 / 625	
Goodness-of-fit on F^2	1.058	
Final R indices [I>2sigma(I)]	R1 = 0.0353, wR2 = 0.0669	
R indices (all data)	R1 = 0.0489, wR2 = 0.0712	
Largest diff. peak and hole	0.503 and -0.615 e.Å^{-3}	

Table S22. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x

10^3) for **IndInd**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Pd(1)	5079(1)	9088(1)	137(1)	16(1)
C(1)	6524(1)	10003(1)	-154(1)	22(1)
C(2)	6360(1)	9099(1)	-425(1)	22(1)
C(3)	6043(1)	9240(1)	-1113(1)	21(1)
C(4)	5873(2)	8610(1)	-1620(1)	28(1)
C(5)	5649(2)	8941(2)	-2243(1)	33(1)
C(6)	5606(2)	9892(2)	-2363(1)	34(1)
C(7)	5771(2)	10529(1)	-1868(1)	29(1)
C(8)	5992(1)	10211(1)	-1235(1)	22(1)
C(9)	6255(1)	10704(1)	-628(1)	22(1)
N(1)	6166(1)	7356(1)	768(1)	19(1)
C(21)	7202(1)	7740(1)	829(1)	20(1)
C(22)	7492(1)	8443(1)	1277(1)	23(1)
C(27)	6748(2)	8866(1)	1689(1)	26(1)
C(28)	6805(2)	9926(2)	1702(1)	43(1)
C(29)	6942(2)	8488(2)	2370(1)	50(1)
C(23)	8526(2)	8737(1)	1348(1)	30(1)
C(24)	9221(2)	8356(2)	988(1)	34(1)
C(25)	8906(2)	7677(2)	539(1)	32(1)
C(26)	7890(1)	7354(1)	446(1)	25(1)
C(30)	7563(2)	6625(2)	-65(1)	36(1)
C(31)	7896(2)	6885(2)	-713(1)	49(1)
C(32)	7988(2)	5660(2)	140(1)	56(1)
C(11)	5276(1)	7731(1)	442(1)	18(1)
C(12)	6005(1)	6461(1)	984(1)	25(1)
C(13)	5009(1)	6256(1)	791(1)	24(1)
N(2)	4567(1)	7032(1)	464(1)	18(1)
C(41)	3487(1)	7016(1)	185(1)	20(1)
C(42)	2741(1)	6933(1)	600(1)	22(1)
C(47)	2999(2)	6972(1)	1325(1)	29(1)
C(48)	2300(2)	7671(2)	1611(1)	38(1)
C(49)	2892(2)	6015(2)	1630(1)	47(1)
C(43)	1709(1)	6815(1)	328(1)	30(1)
C(44)	1432(2)	6794(2)	-328(1)	36(1)
C(45)	2180(2)	6898(2)	-728(1)	32(1)
C(46)	3224(1)	7009(1)	-487(1)	23(1)
C(50)	4040(2)	7076(1)	-934(1)	26(1)
C(51)	3584(2)	7319(2)	-1623(1)	38(1)
C(52)	4643(2)	6161(2)	-932(1)	37(1)
C(7S)	203(5)	8211(4)	2827(3)	71(2)
C(1S)	508(4)	9233(4)	2883(2)	50(1)
C(2S)	7(6)	9840(5)	3230(4)	65(2)
C(3S)	285(8)	10771(5)	3265(6)	73(2)
C(4S)	1084(4)	11105(4)	2997(3)	65(2)
C(5S)	1606(4)	10505(5)	2643(3)	67(1)
C(6S)	1335(7)	9568(7)	2601(5)	53(2)
C(7T)	1520(7)	11238(6)	2629(4)	78(2)
C(1T)	952(5)	10391(4)	2812(3)	51(1)
C(2T)	268(10)	10427(6)	3260(6)	58(2)
C(3T)	-267(7)	9625(6)	3396(5)	61(2)
C(4T)	-116(5)	8808(5)	3125(3)	54(2)
C(5T)	589(5)	8757(6)	2694(3)	56(2)

C(6T)	1085(8)	9548(8)	2522(7)	48(2)
C(7U)	10137(9)	1027(9)	976(5)	73(3)
C(1U)	10046(6)	425(6)	382(4)	54(2)
C(2U)	10877(8)	-121(9)	253(7)	54(3)
C(3U)	10767(8)	-701(7)	-293(6)	65(3)
C(4U)	9848(9)	-734(8)	-698(6)	65(3)
C(5U)	9029(10)	-183(13)	-572(8)	66(3)
C(6U)	9123(9)	375(13)	-35(7)	55(3)
C(7V)	10500(40)	550(30)	880(18)	69(8)
C(1V)	10210(30)	150(30)	214(18)	60(4)
C(2V)	10800(40)	-540(60)	-20(30)	60(5)
C(3V)	10440(30)	-950(20)	-620(20)	62(5)
C(4V)	9440(30)	-850(30)	-890(20)	62(5)
C(5V)	8870(40)	-140(50)	-680(30)	62(5)
C(6V)	9250(40)	350(50)	-130(30)	59(5)

Table S23. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **CpCp**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Pd(1)	20(1)	13(1)	16(1)	1(1)	3(1)	2(1)
C(1)	19(1)	28(1)	21(1)	1(1)	5(1)	2(1)
C(2)	24(1)	22(1)	21(1)	5(1)	7(1)	5(1)
C(3)	21(1)	21(1)	22(1)	2(1)	8(1)	3(1)
C(4)	32(1)	25(1)	28(1)	-3(1)	9(1)	2(1)
C(5)	39(1)	41(1)	22(1)	-9(1)	9(1)	-1(1)
C(6)	40(1)	45(1)	19(1)	6(1)	6(1)	1(1)
C(7)	32(1)	29(1)	26(1)	9(1)	7(1)	3(1)
C(8)	23(1)	20(1)	23(1)	2(1)	7(1)	2(1)
C(9)	22(1)	20(1)	26(1)	-1(1)	8(1)	2(1)
N(1)	20(1)	16(1)	22(1)	2(1)	1(1)	0(1)
C(21)	18(1)	19(1)	22(1)	4(1)	-2(1)	1(1)
C(22)	22(1)	22(1)	24(1)	3(1)	-2(1)	1(1)
C(27)	27(1)	27(1)	25(1)	-6(1)	0(1)	-1(1)
C(28)	66(2)	30(1)	37(1)	-5(1)	21(1)	2(1)
C(29)	55(2)	56(2)	42(1)	15(1)	20(1)	10(1)
C(23)	26(1)	26(1)	35(1)	0(1)	-4(1)	-4(1)
C(24)	20(1)	35(1)	45(1)	9(1)	0(1)	-3(1)
C(25)	24(1)	36(1)	37(1)	6(1)	7(1)	7(1)
C(26)	24(1)	24(1)	26(1)	3(1)	2(1)	5(1)
C(30)	31(1)	38(1)	37(1)	-10(1)	4(1)	7(1)
C(31)	46(1)	65(2)	35(1)	-10(1)	8(1)	17(1)
C(32)	71(2)	32(1)	66(2)	-14(1)	10(1)	10(1)
C(11)	20(1)	15(1)	18(1)	-1(1)	3(1)	1(1)
C(12)	26(1)	18(1)	30(1)	7(1)	-2(1)	2(1)
C(13)	27(1)	16(1)	28(1)	8(1)	0(1)	0(1)
N(2)	20(1)	14(1)	19(1)	2(1)	0(1)	1(1)
C(41)	21(1)	15(1)	22(1)	0(1)	-2(1)	0(1)
C(42)	24(1)	20(1)	23(1)	1(1)	1(1)	-1(1)
C(47)	25(1)	38(1)	22(1)	2(1)	2(1)	-5(1)
C(48)	34(1)	54(1)	28(1)	-9(1)	10(1)	-5(1)
C(49)	44(1)	56(2)	42(1)	23(1)	8(1)	-3(1)
C(43)	21(1)	33(1)	34(1)	-1(1)	3(1)	-1(1)
C(44)	22(1)	48(1)	36(1)	-4(1)	-5(1)	0(1)
C(45)	32(1)	38(1)	24(1)	-3(1)	-6(1)	2(1)

C(46)	27(1)	19(1)	22(1)	-1(1)	0(1)	1(1)
C(50)	33(1)	25(1)	19(1)	-3(1)	1(1)	-2(1)
C(51)	46(1)	44(1)	22(1)	3(1)	0(1)	-8(1)
C(52)	45(1)	36(1)	31(1)	-10(1)	8(1)	6(1)
C(7S)	75(4)	61(3)	66(4)	-1(3)	-23(3)	9(3)
C(1S)	42(2)	60(3)	43(3)	-12(2)	-11(2)	9(2)
C(2S)	48(4)	74(4)	73(5)	-17(4)	9(3)	4(3)
C(3S)	52(3)	72(4)	95(5)	-37(5)	9(3)	8(4)
C(4S)	47(3)	64(3)	79(4)	-23(3)	-7(2)	0(2)
C(5S)	46(3)	80(3)	75(4)	3(3)	10(2)	5(3)
C(6S)	49(4)	65(3)	44(3)	-7(3)	1(3)	27(2)
C(7T)	67(5)	73(4)	92(6)	3(5)	-1(4)	-22(4)
C(1T)	36(3)	65(3)	50(3)	-5(3)	-2(2)	1(2)
C(2T)	56(4)	58(4)	63(4)	-1(4)	14(3)	18(4)
C(3T)	50(4)	75(4)	58(4)	10(3)	14(3)	17(3)
C(4T)	47(3)	64(3)	50(3)	14(3)	-1(2)	-1(3)
C(5T)	58(4)	59(3)	47(4)	-1(3)	-2(3)	7(3)
C(6T)	36(5)	66(3)	43(4)	-6(3)	6(4)	4(3)
C(7U)	68(6)	72(7)	84(6)	16(5)	24(5)	-3(5)
C(1U)	34(3)	46(6)	84(6)	31(4)	16(3)	5(3)
C(2U)	30(3)	43(7)	93(9)	29(5)	15(4)	2(4)
C(3U)	46(4)	45(5)	108(9)	18(5)	23(5)	-6(3)
C(4U)	50(5)	51(7)	97(9)	14(5)	21(5)	-11(4)
C(5U)	40(5)	61(6)	98(8)	21(5)	15(4)	-12(4)
C(6U)	24(3)	50(8)	94(7)	28(5)	17(4)	-1(4)
C(7V)	75(18)	42(15)	87(13)	35(11)	4(11)	-6(15)
C(1V)	42(7)	50(10)	89(9)	31(7)	12(7)	-7(7)
C(2V)	41(9)	47(11)	92(11)	36(9)	12(8)	-4(8)
C(3V)	42(8)	54(10)	94(11)	29(8)	19(9)	-8(8)
C(4V)	43(9)	56(10)	90(11)	25(8)	17(8)	-11(9)
C(5V)	38(8)	54(9)	94(10)	27(8)	13(7)	-10(7)
C(6V)	39(8)	51(10)	90(10)	29(7)	15(8)	-5(8)

Table S24. Bond lengths (Å) for **IndInd**

Pd(1)-C(11)	2.0609(16)
Pd(1)-C(9)#1	2.1637(17)
Pd(1)-C(2)	2.1785(16)
Pd(1)-C(1)	2.4451(17)
Pd(1)-C(1)#1	2.4681(17)
Pd(1)-Pd(1)#1	2.6889(2)
C(1)-C(2)	1.426(3)
C(1)-C(9)	1.429(2)
C(1)-Pd(1)#1	2.4681(17)
C(1)-H(1)	0.978(15)
C(2)-C(3)	1.465(2)
C(2)-H(2)	0.964(15)
C(3)-C(4)	1.395(2)
C(3)-C(8)	1.420(2)
C(4)-C(5)	1.388(3)
C(4)-H(4)	0.9500
C(5)-C(6)	1.391(3)
C(5)-H(5)	0.9500
C(6)-C(7)	1.383(3)
C(6)-H(6)	0.9500
C(7)-C(8)	1.401(2)

C(7)-H(7)	0.9500
C(8)-C(9)	1.462(2)
C(9)-Pd(1)#1	2.1637(17)
C(9)-H(9)	0.986(15)
N(1)-C(11)	1.372(2)
N(1)-C(12)	1.392(2)
N(1)-C(21)	1.447(2)
C(21)-C(22)	1.398(2)
C(21)-C(26)	1.402(2)
C(22)-C(23)	1.399(3)
C(22)-C(27)	1.517(3)
C(27)-C(29)	1.523(3)
C(27)-C(28)	1.526(3)
C(27)-H(27)	1.0000
C(28)-H(28A)	0.9800
C(28)-H(28B)	0.9800
C(28)-H(28C)	0.9800
C(29)-H(29A)	0.9800
C(29)-H(29B)	0.9800
C(29)-H(29C)	0.9800
C(23)-C(24)	1.374(3)
C(23)-H(23)	0.9500
C(24)-C(25)	1.382(3)
C(24)-H(24)	0.9500
C(25)-C(26)	1.391(3)
C(25)-H(25)	0.9500
C(26)-C(30)	1.521(3)
C(30)-C(32)	1.533(3)
C(30)-C(31)	1.537(3)
C(30)-H(30)	1.0000
C(31)-H(31A)	0.9800
C(31)-H(31B)	0.9800
C(31)-H(31C)	0.9800
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800
C(11)-N(2)	1.370(2)
C(12)-C(13)	1.337(2)
C(12)-H(12)	0.9500
C(13)-N(2)	1.394(2)
C(13)-H(13)	0.9500
N(2)-C(41)	1.446(2)
C(41)-C(42)	1.402(2)
C(41)-C(46)	1.410(2)
C(42)-C(43)	1.395(2)
C(42)-C(47)	1.519(2)
C(47)-C(48)	1.534(3)
C(47)-C(49)	1.534(3)
C(47)-H(47)	1.0000
C(48)-H(48A)	0.9800
C(48)-H(48B)	0.9800
C(48)-H(48C)	0.9800
C(49)-H(49A)	0.9800
C(49)-H(49B)	0.9800
C(49)-H(49C)	0.9800
C(43)-C(44)	1.378(3)

C(43)-H(43)	0.9500
C(44)-C(45)	1.382(3)
C(44)-H(44)	0.9500
C(45)-C(46)	1.392(3)
C(45)-H(45)	0.9500
C(46)-C(50)	1.520(3)
C(50)-C(51)	1.528(3)
C(50)-C(52)	1.533(3)
C(50)-H(50)	1.0000
C(51)-H(51A)	0.9800
C(51)-H(51B)	0.9800
C(51)-H(51C)	0.9800
C(52)-H(52A)	0.9800
C(52)-H(52B)	0.9800
C(52)-H(52C)	0.9800
C(7S)-C(1S)	1.524(7)
C(7S)-H(7S1)	0.9800
C(7S)-H(7S2)	0.9800
C(7S)-H(7S3)	0.9800
C(1S)-C(2S)	1.362(8)
C(1S)-C(6S)	1.387(9)
C(2S)-C(3S)	1.387(8)
C(2S)-H(2S)	0.9500
C(3S)-C(4S)	1.342(9)
C(3S)-H(3S)	0.9500
C(4S)-C(5S)	1.381(8)
C(4S)-H(4S)	0.9500
C(5S)-C(6S)	1.394(10)
C(5S)-H(5S)	0.9500
C(6S)-H(6S)	0.9500
C(7T)-C(1T)	1.505(9)
C(7T)-H(7T1)	0.9800
C(7T)-H(7T2)	0.9800
C(7T)-H(7T3)	0.9800
C(1T)-C(6T)	1.380(11)
C(1T)-C(2T)	1.387(9)
C(2T)-C(3T)	1.398(10)
C(2T)-H(2T)	0.9500
C(3T)-C(4T)	1.334(9)
C(3T)-H(3T)	0.9500
C(4T)-C(5T)	1.382(8)
C(4T)-H(4T)	0.9500
C(5T)-C(6T)	1.382(11)
C(5T)-H(5T)	0.9500
C(6T)-H(6T)	0.9500
C(7U)-C(1U)	1.512(10)
C(7U)-H(7U1)	0.9800
C(7U)-H(7U2)	0.9800
C(7U)-H(7U3)	0.9800
C(1U)-C(6U)	1.388(10)
C(1U)-C(2U)	1.394(10)
C(2U)-C(3U)	1.413(11)
C(2U)-H(2U)	0.9500
C(3U)-C(4U)	1.371(11)
C(3U)-H(3U)	0.9500
C(4U)-C(5U)	1.384(11)

C(4U)-H(4U)	0.9500
C(5U)-C(6U)	1.380(11)
C(5U)-H(5U)	0.9500
C(6U)-H(6U)	0.9500
C(7V)-C(1V)	1.517(16)
C(7V)-H(7V1)	0.9800
C(7V)-H(7V2)	0.9800
C(7V)-H(7V3)	0.9800
C(1V)-C(2V)	1.381(14)
C(1V)-C(6V)	1.388(14)
C(2V)-C(3V)	1.400(15)
C(2V)-H(2V)	0.9500
C(3V)-C(4V)	1.365(15)
C(3V)-H(3V)	0.9500
C(4V)-C(5V)	1.372(15)
C(4V)-H(4V)	0.9500
C(5V)-C(6V)	1.389(15)
C(5V)-H(5V)	0.9500
C(6V)-H(6V)	0.9500

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+2,-z

Table S25. Bond angles (°) for **IndInd**

C(11)-Pd(1)-C(9)#1	93.14(6)
C(11)-Pd(1)-C(2)	96.03(6)
C(9)#1-Pd(1)-C(2)	170.74(7)
C(11)-Pd(1)-C(1)	121.47(6)
C(9)#1-Pd(1)-C(1)	138.06(6)
C(2)-Pd(1)-C(1)	35.32(6)
C(11)-Pd(1)-C(1)#1	124.48(6)
C(9)#1-Pd(1)-C(1)#1	35.16(6)
C(2)-Pd(1)-C(1)#1	135.91(6)
C(1)-Pd(1)-C(1)#1	113.64(4)
C(11)-Pd(1)-Pd(1)#1	173.93(5)
C(9)#1-Pd(1)-Pd(1)#1	85.76(5)
C(2)-Pd(1)-Pd(1)#1	85.26(5)
C(1)-Pd(1)-Pd(1)#1	57.23(4)
C(1)#1-Pd(1)-Pd(1)#1	56.41(4)
C(2)-C(1)-C(9)	110.85(16)
C(2)-C(1)-Pd(1)	62.07(9)
C(9)-C(1)-Pd(1)	115.70(12)
C(2)-C(1)-Pd(1)#1	114.19(12)
C(9)-C(1)-Pd(1)#1	60.70(9)
Pd(1)-C(1)-Pd(1)#1	66.36(4)
C(2)-C(1)-H(1)	122.7(12)
C(9)-C(1)-H(1)	124.4(12)
Pd(1)-C(1)-H(1)	102.1(12)
Pd(1)#1-C(1)-H(1)	105.3(12)
C(1)-C(2)-C(3)	106.01(15)
C(1)-C(2)-Pd(1)	82.60(10)
C(3)-C(2)-Pd(1)	114.15(11)
C(1)-C(2)-H(2)	122.9(12)
C(3)-C(2)-H(2)	121.5(12)
Pd(1)-C(2)-H(2)	102.9(12)

C(4)-C(3)-C(8)	120.15(16)
C(4)-C(3)-C(2)	131.31(16)
C(8)-C(3)-C(2)	108.38(15)
C(5)-C(4)-C(3)	119.43(18)
C(5)-C(4)-H(4)	120.3
C(3)-C(4)-H(4)	120.3
C(4)-C(5)-C(6)	120.45(18)
C(4)-C(5)-H(5)	119.8
C(6)-C(5)-H(5)	119.8
C(7)-C(6)-C(5)	121.10(18)
C(7)-C(6)-H(6)	119.5
C(5)-C(6)-H(6)	119.5
C(6)-C(7)-C(8)	119.44(18)
C(6)-C(7)-H(7)	120.3
C(8)-C(7)-H(7)	120.3
C(7)-C(8)-C(3)	119.43(16)
C(7)-C(8)-C(9)	131.80(17)
C(3)-C(8)-C(9)	108.67(15)
C(1)-C(9)-C(8)	105.88(15)
C(1)-C(9)-Pd(1)#1	84.14(10)
C(8)-C(9)-Pd(1)#1	112.38(12)
C(1)-C(9)-H(9)	122.4(12)
C(8)-C(9)-H(9)	121.4(12)
Pd(1)#1-C(9)-H(9)	104.2(12)
C(11)-N(1)-C(12)	111.79(14)
C(11)-N(1)-C(21)	127.32(14)
C(12)-N(1)-C(21)	120.42(14)
C(22)-C(21)-C(26)	122.86(16)
C(22)-C(21)-N(1)	119.71(15)
C(26)-C(21)-N(1)	117.37(15)
C(21)-C(22)-C(23)	117.00(17)
C(21)-C(22)-C(27)	122.99(16)
C(23)-C(22)-C(27)	119.99(17)
C(22)-C(27)-C(29)	111.20(17)
C(22)-C(27)-C(28)	112.28(16)
C(29)-C(27)-C(28)	109.84(18)
C(22)-C(27)-H(27)	107.8
C(29)-C(27)-H(27)	107.8
C(28)-C(27)-H(27)	107.8
C(27)-C(28)-H(28A)	109.5
C(27)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
C(27)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
C(27)-C(29)-H(29A)	109.5
C(27)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5
C(27)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5
C(24)-C(23)-C(22)	121.31(18)
C(24)-C(23)-H(23)	119.3
C(22)-C(23)-H(23)	119.3
C(23)-C(24)-C(25)	120.33(18)
C(23)-C(24)-H(24)	119.8

C(25)-C(24)-H(24)	119.8
C(24)-C(25)-C(26)	121.16(18)
C(24)-C(25)-H(25)	119.4
C(26)-C(25)-H(25)	119.4
C(25)-C(26)-C(21)	117.30(17)
C(25)-C(26)-C(30)	119.73(17)
C(21)-C(26)-C(30)	122.96(17)
C(26)-C(30)-C(32)	111.74(18)
C(26)-C(30)-C(31)	112.11(19)
C(32)-C(30)-C(31)	109.59(19)
C(26)-C(30)-H(30)	107.7
C(32)-C(30)-H(30)	107.7
C(31)-C(30)-H(30)	107.7
C(30)-C(31)-H(31A)	109.5
C(30)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
C(30)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
C(30)-C(32)-H(32A)	109.5
C(30)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
C(30)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
N(2)-C(11)-N(1)	102.83(13)
N(2)-C(11)-Pd(1)	130.54(12)
N(1)-C(11)-Pd(1)	126.01(12)
C(13)-C(12)-N(1)	106.82(15)
C(13)-C(12)-H(12)	126.6
N(1)-C(12)-H(12)	126.6
C(12)-C(13)-N(2)	106.84(15)
C(12)-C(13)-H(13)	126.6
N(2)-C(13)-H(13)	126.6
C(11)-N(2)-C(13)	111.71(14)
C(11)-N(2)-C(41)	128.33(14)
C(13)-N(2)-C(41)	119.94(14)
C(42)-C(41)-C(46)	122.37(16)
C(42)-C(41)-N(2)	117.87(15)
C(46)-C(41)-N(2)	119.57(15)
C(43)-C(42)-C(41)	117.73(16)
C(43)-C(42)-C(47)	118.85(16)
C(41)-C(42)-C(47)	123.42(16)
C(42)-C(47)-C(48)	111.06(16)
C(42)-C(47)-C(49)	111.54(17)
C(48)-C(47)-C(49)	109.34(17)
C(42)-C(47)-H(47)	108.3
C(48)-C(47)-H(47)	108.3
C(49)-C(47)-H(47)	108.3
C(47)-C(48)-H(48A)	109.5
C(47)-C(48)-H(48B)	109.5
H(48A)-C(48)-H(48B)	109.5
C(47)-C(48)-H(48C)	109.5
H(48A)-C(48)-H(48C)	109.5
H(48B)-C(48)-H(48C)	109.5
C(47)-C(49)-H(49A)	109.5

C(47)-C(49)-H(49B)	109.5
H(49A)-C(49)-H(49B)	109.5
C(47)-C(49)-H(49C)	109.5
H(49A)-C(49)-H(49C)	109.5
H(49B)-C(49)-H(49C)	109.5
C(44)-C(43)-C(42)	121.11(18)
C(44)-C(43)-H(43)	119.4
C(42)-C(43)-H(43)	119.4
C(43)-C(44)-C(45)	120.08(18)
C(43)-C(44)-H(44)	120.0
C(45)-C(44)-H(44)	120.0
C(44)-C(45)-C(46)	121.76(18)
C(44)-C(45)-H(45)	119.1
C(46)-C(45)-H(45)	119.1
C(45)-C(46)-C(41)	116.94(17)
C(45)-C(46)-C(50)	120.94(16)
C(41)-C(46)-C(50)	122.06(16)
C(46)-C(50)-C(51)	113.04(16)
C(46)-C(50)-C(52)	110.22(16)
C(51)-C(50)-C(52)	109.28(16)
C(46)-C(50)-H(50)	108.1
C(51)-C(50)-H(50)	108.1
C(52)-C(50)-H(50)	108.1
C(50)-C(51)-H(51A)	109.5
C(50)-C(51)-H(51B)	109.5
H(51A)-C(51)-H(51B)	109.5
C(50)-C(51)-H(51C)	109.5
H(51A)-C(51)-H(51C)	109.5
H(51B)-C(51)-H(51C)	109.5
C(50)-C(52)-H(52A)	109.5
C(50)-C(52)-H(52B)	109.5
H(52A)-C(52)-H(52B)	109.5
C(50)-C(52)-H(52C)	109.5
H(52A)-C(52)-H(52C)	109.5
H(52B)-C(52)-H(52C)	109.5
C(2S)-C(1S)-C(6S)	117.8(6)
C(2S)-C(1S)-C(7S)	121.3(6)
C(6S)-C(1S)-C(7S)	120.8(6)
C(1S)-C(2S)-C(3S)	120.4(7)
C(1S)-C(2S)-H(2S)	119.8
C(3S)-C(2S)-H(2S)	119.8
C(4S)-C(3S)-C(2S)	122.4(7)
C(4S)-C(3S)-H(3S)	118.8
C(2S)-C(3S)-H(3S)	118.8
C(3S)-C(4S)-C(5S)	118.3(6)
C(3S)-C(4S)-H(4S)	120.9
C(5S)-C(4S)-H(4S)	120.9
C(4S)-C(5S)-C(6S)	120.0(7)
C(4S)-C(5S)-H(5S)	120.0
C(6S)-C(5S)-H(5S)	120.0
C(1S)-C(6S)-C(5S)	120.9(7)
C(1S)-C(6S)-H(6S)	119.5
C(5S)-C(6S)-H(6S)	119.5
C(1T)-C(7T)-H(7T1)	109.5
C(1T)-C(7T)-H(7T2)	109.5
H(7T1)-C(7T)-H(7T2)	109.5

C(1T)-C(7T)-H(7T3)	109.5
H(7T1)-C(7T)-H(7T3)	109.5
H(7T2)-C(7T)-H(7T3)	109.5
C(6T)-C(1T)-C(2T)	117.8(7)
C(6T)-C(1T)-C(7T)	120.0(7)
C(2T)-C(1T)-C(7T)	122.1(7)
C(1T)-C(2T)-C(3T)	119.7(8)
C(1T)-C(2T)-H(2T)	120.2
C(3T)-C(2T)-H(2T)	120.2
C(4T)-C(3T)-C(2T)	122.1(7)
C(4T)-C(3T)-H(3T)	118.9
C(2T)-C(3T)-H(3T)	118.9
C(3T)-C(4T)-C(5T)	118.7(7)
C(3T)-C(4T)-H(4T)	120.6
C(5T)-C(4T)-H(4T)	120.6
C(4T)-C(5T)-C(6T)	120.4(8)
C(4T)-C(5T)-H(5T)	119.8
C(6T)-C(5T)-H(5T)	119.8
C(1T)-C(6T)-C(5T)	121.0(9)
C(1T)-C(6T)-H(6T)	119.5
C(5T)-C(6T)-H(6T)	119.5
C(1U)-C(7U)-H(7U1)	109.5
C(1U)-C(7U)-H(7U2)	109.5
H(7U1)-C(7U)-H(7U2)	109.5
C(1U)-C(7U)-H(7U3)	109.5
H(7U1)-C(7U)-H(7U3)	109.5
H(7U2)-C(7U)-H(7U3)	109.5
C(6U)-C(1U)-C(2U)	118.3(8)
C(6U)-C(1U)-C(7U)	120.9(8)
C(2U)-C(1U)-C(7U)	120.7(8)
C(1U)-C(2U)-C(3U)	120.0(9)
C(1U)-C(2U)-H(2U)	120.0
C(3U)-C(2U)-H(2U)	120.0
C(4U)-C(3U)-C(2U)	120.4(9)
C(4U)-C(3U)-H(3U)	119.8
C(2U)-C(3U)-H(3U)	119.8
C(3U)-C(4U)-C(5U)	119.4(10)
C(3U)-C(4U)-H(4U)	120.3
C(5U)-C(4U)-H(4U)	120.3
C(6U)-C(5U)-C(4U)	120.6(10)
C(6U)-C(5U)-H(5U)	119.7
C(4U)-C(5U)-H(5U)	119.7
C(5U)-C(6U)-C(1U)	121.3(9)
C(5U)-C(6U)-H(6U)	119.4
C(1U)-C(6U)-H(6U)	119.4
C(1V)-C(7V)-H(7V1)	109.5
C(1V)-C(7V)-H(7V2)	109.5
H(7V1)-C(7V)-H(7V2)	109.5
C(1V)-C(7V)-H(7V3)	109.5
H(7V1)-C(7V)-H(7V3)	109.5
H(7V2)-C(7V)-H(7V3)	109.5
C(2V)-C(1V)-C(6V)	117.6(17)
C(2V)-C(1V)-C(7V)	122.6(19)
C(6V)-C(1V)-C(7V)	118.8(19)
C(1V)-C(2V)-C(3V)	119.8(18)
C(1V)-C(2V)-H(2V)	120.1

C(3V)-C(2V)-H(2V)	120.1
C(4V)-C(3V)-C(2V)	121(2)
C(4V)-C(3V)-H(3V)	119.6
C(2V)-C(3V)-H(3V)	119.6
C(3V)-C(4V)-C(5V)	118(2)
C(3V)-C(4V)-H(4V)	121.0
C(5V)-C(4V)-H(4V)	121.0
C(4V)-C(5V)-C(6V)	120.2(19)
C(4V)-C(5V)-H(5V)	119.9
C(6V)-C(5V)-H(5V)	119.9
C(1V)-C(6V)-C(5V)	121.4(18)
C(1V)-C(6V)-H(6V)	119.3
C(5V)-C(6V)-H(6V)	119.3

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+2,-z