Supporting information

The Nature of the Bonding in Symmetrical Pincer Palladaycles

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CONTENT OF SUPPORTING INFORMATION

S1. Cartesian coordinates and calculated energies of $PdCl_2$ optimised at PBE

Pd	0.00000000	0.00000000	0.60390400
Cl	0.00000000	1.69348600	-0.81704600
Cl	0.00000000	-1.69348600	-0.81704600

Optimization using PBE/6-31+G(d,p)[SDD]

- Energy = -1047.9039066 au
- Zero-point energy correction = 0.001923 au
- Thermal correction to Gibbs free energy = -0.027367 au

Single point energy using ωB97XD/6-311++G(2df,2p)[SDD]

- Energy = -1048.3424475 au

S2. Cartesian coordinates and calculated energies of HCl optimised PBE

Cl	0.00000000	0.00000000	0.07185200
H	0.00000000	0.00000000	-1.22149200

Optimization using PBE/6-31+G(d,p)[SDD]

- Energy = -460.5940103 au
- Zero-point energy correction = 0.006599 au
- Thermal correction to Gibbs free energy = -0.011299 au

Single point energy using ωB97XD/6-311++G(2df,2p)[SDD]

- Energy = -460.8184718 au

S3. Cartesian coordinates and calculated energies of PdNCN pathway optimised at PBE

(1) Ligand

N	-3.14034600	-0.91474800	-0.05035200
N	3.45058400	-0.39650700	-0.02567400
C	-1.26877500	0.68460100	0.35343900
C	-1.02601100	2.06390100	0.24231700
H	-1.83590000	2.77336000	0.44713000
C	0.24640700	2.53467100	-0.12553000
H	0.42590700	3.61171600	-0.20647700
C	1.28165700	1.63172000	-0.39734600
H	2.27863900	1.98759200	-0.67601100
C	1.05507800	0.24286700	-0.30110400
C	-2.62271800	0.16252800	0.80109600
H	-2.53106800	-0.24915100	1.82430300
H	-3.34205600	1.01710100	0.86882000
C	-4.29683400	-1.56126300	0.56271200
H	-5.16310100	-0.86861900	0.70151100
H	-4.02023900	-1.96626000	1.55053600
H	-4.63090800	-2.39924000	-0.07122700
C	-3.45796900	-0.43696400	-1.39505500

H	-4.27329900	0.32750100	-1.39759500
H	-3.77975000	-1.28531000	-2.02105300
H	-2.56379600	0.01323600	-1.85376200
C	2.16287100	-0.74011200	-0.63925600
H	2.31710300	-0.74401000	-1.73525600
H	1.83487200	-1.77344600	-0.36348600
C	4.53577300	-1.19044500	-0.59426800
H	4.42125700	-2.28652900	-0.40740800
H	5.49605200	-0.87097300	-0.15646600
H	4.58501500	-1.03187400	-1.68454200
C	3.41027300	-0.52993300	1.42960300
H	3.23002100	-1.58241800	1.75945800
H	2.60791700	0.10165500	1.84193400
H	4.36957900	-0.19496700	1.85717100
C	-0.21722300	-0.21344300	0.07969000
H	-0.41309900	-1.28935700	0.15681100

Optimization using PBE/6-31+G(d,p)[SDD]

- Energy = -578.0689059 au
- Zero-point energy correction = 0.294541 au
- Thermal correction to Gibbs free energy = 0.251441 au

Single point energy using ωB97XD/6-311++G(2df,2p)[SDD]

- Energy = -578.7956829 au

(2) Int1

C	-0.73257000	0.86596400	-0.59331300
C	-1.31871400	1.83037600	1.97979000
C	0.20282900	1.71028400	0.08395700
C	-0.10969200	2.18807700	1.38330500
C	-2.23737100	0.99694100	1.30759800
C	-1.96529500	0.51338700	0.02509800
C	1.42791900	2.19371900	-0.68066700
C	3.10171500	0.83438800	-1.93056100
C	3.45682500	1.33450400	0.43084800
C	-2.91569800	-0.42785000	-0.68241300
C	-5.12129800	-1.41241600	-0.64846900
C	-4.87576400	0.97143100	-0.92609400
H	0.59039100	2.85491300	1.89737600
H	-1.55967300	2.20196800	2.98056000
H	-3.18918500	0.72199900	1.77168400
H	1.16960600	2.38373900	-1.73507300
H	1.84525900	3.12620600	-0.25987500
H	3.70937700	1.71005900	-2.23225100
H	2.33678000	0.63203300	-2.69401800
H	3.73973800	-0.05505000	-1.82726000
H	4.08265500	2.20698500	0.15709300
H	4.07642300	0.43299700	0.53726600

H	2.94835300	1.52607800	1.38669600
H	-2.60737300	-1.44896500	-0.38403400
H	-2.75362800	-0.36303400	-1.78793000
H	-5.15126300	-1.62843000	-1.74376300
H	-6.15741100	-1.25764000	-0.30468800
H	-4.71516700	-2.29765200	-0.13317800
H	-4.89117800	0.92328200	-2.04248800
H	-4.28290400	1.85189400	-0.62925300
H	-5.90995000	1.12038400	-0.57437000
H	-0.59912400	0.64846000	-1.66086900
Pd	1.13889600	-0.47031800	0.03714600
Cl	-0.25499200	-2.08460700	0.91678300
Cl	2.87751700	-1.98797500	0.00731100
N	2.44211300	1.09108100	-0.62773300
N	-4.31799700	-0.23601700	-0.32004100

Optimization using PBE/6-31+G(d,p)[SDD]

- Energy = -1626.0455495 au
- Zero-point energy correction = 0.299702 au
- Thermal correction to Gibbs free energy = 0.249572 au

Single point energy using ωB97XD/6-311++G(2df,2p)[SDD]

- Energy = -1627.2261216 au

(3) TS1

C	-0.39440200	0.85988800	-0.19544200
C	-1.88363100	3.25998500	-0.28759100
C	0.22609800	2.09580500	-0.53421400
C	-0.50892400	3.28722800	-0.57992000
C	-2.48277500	2.06618000	0.12592100
C	-1.75182100	0.85758100	0.21052400
C	1.71596100	2.05019400	-0.72320400
C	3.72101600	0.77701000	-0.12308700
C	2.24147600	1.53549900	1.64836600
C	-2.43153300	-0.34739300	0.84884200
C	-4.54199600	-1.37450300	1.42065600
C	-4.06362100	-0.85127000	-0.88283100
H	-0.01318900	4.23240900	-0.82805000
H	-2.47405700	4.17999400	-0.33967400
H	-3.53948500	2.03468600	0.41183500
H	1.98727000	1.69812100	-1.73400200
H	2.19702100	3.03586100	-0.56186900
H	4.29486500	1.72239800	-0.06392700
H	3.76437000	0.37226300	-1.14343700
H	4.13481100	0.02731300	0.56323300
H	2.88843400	2.42738500	1.76272700
H	2.59626700	0.73248100	2.30959700
H	1.20569200	1.79405900	1.90453100

H	-2.36739900	-0.20742400	1.94563100
H	-1.86989200	-1.28075300	0.62901800
H	-4.15894800	-2.42143100	1.36008700
H	-5.61797100	-1.39254400	1.17988500
H	-4.42890100	-1.02684200	2.46133700
H	-3.67489600	-1.87128300	-1.10704000
H	-3.55838700	-0.13771800	-1.55362100
H	-5.14235900	-0.83137700	-1.11044300
H	-0.33073900	-0.59838000	-1.19345400
N	2.30332400	1.04831000	0.24171900
N	-3.85614900	-0.45749900	0.51257400
Pd	1.03728900	-0.62563100	-0.02597700
Cl	-0.42485400	-2.08720200	-1.41322100
Cl	2.67114200	-2.21533200	0.55759800

Optimization using PBE/6-31+G(d,p)[SDD]

- Energy = -1626.0009458 au
- Zero-point energy correction = 0.293387 au
- Thermal correction to Gibbs free energy = 0.244363 au

Single point energy using ωB97XD/6-311++G(2df,2p)[SDD]

- Energy = -1627.174838 au

(4) Int2---HCl

C	-0.39722800	0.95321000	-0.09591800
C	-1.91622900	3.35095600	-0.33180800
C	0.20249300	2.18531200	-0.48447200
C	-0.53920100	3.36854100	-0.60776400
C	-2.50834700	2.16816700	0.12193800
C	-1.76602400	0.97112700	0.26782100
C	1.68678800	2.13783000	-0.70712400
C	3.67237900	0.79458200	-0.21546200
C	2.28250600	1.55449500	1.62196000
C	-2.47862400	-0.20829400	0.91131000
C	-4.53638100	-1.47546800	1.10246800
C	-3.72441300	-0.86256600	-1.08062900
H	-0.04619200	4.30072700	-0.90740400
H	-2.51264300	4.26288500	-0.43313700
H	-3.57163500	2.14719300	0.38551900
H	1.93227400	1.82262800	-1.73647500
H	2.18533000	3.11084700	-0.51910800
H	4.27067700	1.72499100	-0.15559400
H	3.67101400	0.41115900	-1.24475000
H	4.09278600	0.01918500	0.43738600
H	2.96170800	2.42408200	1.72495200
H	2.63630200	0.73113000	2.25797200
H	1.26560400	1.84101500	1.92010800
H	-2.65840300	0.03477900	1.97609500

H	-1.81621600	-1.10247100	0.92182000
H	-4.04009900	-2.47596500	1.12637600
H	-5.54578300	-1.60563500	0.67823500
H	-4.64169800	-1.12260500	2.14167100
H	-3.22489700	-1.86183700	-1.24983100
H	-3.17617700	-0.09822800	-1.65312500
H	-4.73891800	-0.95888900	-1.50174200
H	-1.49239900	-2.10481600	-1.12743500
N	2.27530600	1.09151000	0.20430000
N	-3.79661200	-0.49072800	0.31917700
Pd	0.97006300	-0.54037200	-0.01039800
Cl	-0.27822400	-2.49956700	-0.80855700
Cl	2.66700600	-2.23430800	0.26494000

Optimization using PBE/6-31+G(d,p)[SDD]

- Energy = -1626.0077763 au
- Zero-point energy correction = 0.296399 au
- Thermal correction to Gibbs free energy = 0.247384 au

Single point energy using ωB97XD/6-311++G(2df,2p)[SDD]

- Energy = -1627.1900992 au

(5) Int2

C	0.38528600	0.94569700	-0.07647800
C	1.84661900	3.32058900	-0.19956000
C	-0.25280700	2.16815600	0.22679000
C	0.48361900	3.36234500	0.15671000
C	2.48032500	2.09843600	-0.49000400
C	1.74359500	0.90098700	-0.43349600
C	-1.68072300	2.02154800	0.67867500
C	-3.34292400	0.21379600	0.98562000
C	-2.76086700	0.94742200	-1.26198500
C	2.27613500	-0.48338400	-0.73666400
C	3.82069700	-2.27161500	-0.26188700
C	2.96161200	-0.90477000	1.54789300
H	0.00925100	4.32492200	0.38104900
H	2.41711000	4.25278800	-0.25342700
H	3.54277800	2.07900200	-0.75685600
H	-1.72496400	1.93395600	1.77876900
H	-2.33937000	2.86252100	0.38393600
H	-4.16591300	0.95484700	1.03055300
H	-2.95290600	0.02776500	1.99593900
H	-3.70372900	-0.73652100	0.56847800
H	-3.63071100	1.63435600	-1.23065700
H	-3.06424400	-0.02007800	-1.68559100
H	-1.96494500	1.38545300	-1.87957000
H	2.61172400	-0.57336000	-1.78593900
H	1.35794900	-1.19305500	-0.66485400

H	3.04732900	-3.06482700	-0.14357900
H	4.69238800	-2.54092400	0.35572800
H	4.13619600	-2.24927200	-1.31757300
H	2.06283800	-1.53511000	1.75862500
H	2.73066000	0.12885800	1.84471800
H	3.80113500	-1.27223400	2.15839000
N	-2.24667400	0.73054300	0.12253500
N	3.32788100	-0.95302300	0.13480800
Pd	-0.69244100	-0.68153400	-0.05773600
Cl	-1.78483200	-2.78861300	-0.14690500

Optimization using PBE/6-31+G(d,p)[SDD]

- Energy = -1165.4097808 au
- Zero-point energy correction = 0.285928 au
- Thermal correction to Gibbs free energy = 0.238276 au

Single point energy using ωB97XD/6-311++G(2df,2p)[SDD]

- Energy = -1166.3584581 au

(6) TS2

C	1.90393400	3.17460000	-0.30665600
C	0.34952100	0.86817900	-0.04211700
C	1.71169700	0.74456800	-0.36891900
C	2.48820600	1.91202500	-0.50899600
Pd	-0.81884100	-0.69692700	0.00236900
C	0.54377200	3.29238800	0.04290100
C	-0.23670300	2.13391200	0.18511700
C	-1.67290100	2.07669700	0.63010800
C	-3.42829300	0.36688100	0.98246300
C	-2.78730700	0.99164200	-1.28270300
C	2.18465800	-0.67655700	-0.60123500
C	3.90959400	-0.37597100	1.22281800
C	3.99366400	-2.29422400	-0.31858500
N	3.22829800	-1.19784100	0.24256600
N	-2.30046400	0.79882700	0.11456800
H	2.44434300	-0.81252200	-1.67301300
H	1.23847700	-1.33166200	-0.48205500
H	3.54971600	1.84210100	-0.77404000
H	-1.72674600	2.02866000	1.73223300
H	-2.28398100	2.94103500	0.30204400
H	0.10473800	4.28489900	0.19808100
H	2.51064300	4.07731800	-0.42572500
H	4.50956300	-2.84367900	0.48679300
H	3.31888300	-3.00201200	-0.82879200
H	4.76227200	-1.95861600	-1.05408500
H	4.34211000	-1.02900000	2.00086400
H	4.74009700	0.23483600	0.79672800
H	3.20006900	0.31060600	1.70692500

H	-3.05676600	0.19576500	2.00231600
H	-4.21450100	1.14809400	0.99406700
H	-3.83263700	-0.57762800	0.59286300
H	-3.14067300	0.02763100	-1.67421600
H	-3.61676500	1.72766800	-1.28811500
H	-1.96058500	1.35970300	-1.90554600
Cl	-1.96914400	-2.76801800	-0.06596700

Optimization using PBE/6-31+G(d,p)[SDD]

- Energy = -1165.3968021 au
- Zero-point energy correction = 0.284798 au
- Thermal correction to Gibbs free energy = 0.237593 au

Single point energy using ωB97XD/6-311++G(2df,2p)[SDD]

- Energy = -1166.3440431 au

(7) Product

Pd	0.68754100	-0.00011800	-0.00004600
Cl	3.11142200	-0.00018900	-0.00007000
N	0.37409200	2.11717300	0.03083500
N	0.37359300	-2.11722100	-0.03083500
C	-1.24271500	0.00007300	0.00000000
C	-1.92563000	1.21349400	-0.20287800
C	-3.33152600	1.21344500	-0.19024200
H	-3.89524700	2.14209500	-0.33804700
C	-4.02372200	0.00043600	-0.00002700
H	-5.11793900	0.00057800	-0.00006400
C	-3.33185400	-1.21275600	0.19020000
H	-3.89581300	-2.14126000	0.33801300
C	-1.92596400	-1.21317000	0.20285400
C	-1.02123500	2.38439700	-0.50384900
H	-0.91742400	2.49898400	-1.59765200
H	-1.38944500	3.35134400	-0.10532300
C	1.38130900	2.87581200	-0.75457400
H	1.18447400	3.96433800	-0.68240700
H	1.33457600	2.55772300	-1.80601800
H	2.38190200	2.63672200	-0.36725800
C	0.45643600	2.52430400	1.46185900
H	0.31953600	3.62141600	1.55351300
H	1.44251300	2.23849500	1.85534400
H	-0.32705300	2.00595100	2.03243500
C	-1.02175900	-2.38423900	0.50382500
H	-1.39005800	-3.35116500	0.10531900
H	-0.91800200	-2.49884700	1.59764100
C	0.45602100	-2.52470200	-1.46174700
H	0.31922700	-3.62183500	-1.55312200
H	1.44206100	-2.23887700	-1.85529600
H	-0.32754100	-2.00657500	-2.03244600

C	1.38069300	-2.87571500	0.75489400
H	1.18338700	-3.96421300	0.68353900
H	1.33436900	-2.55679800	1.80609800
H	2.38129200	-2.63737600	0.36716200

Optimization using PBE/6-31+G(d,p)[SDD]

- Energy = -1165.4543999 au
- Zero-point energy correction = 0.288941 au
- Thermal correction to Gibbs free energy = 0.244536 au

Single point energy using ωB97XD/6-311++G(2df,2p)[SDD]

- Energy = -1166.4077768 au

S4. Cartesian coordinates and calculated energies of PdSCS pathway optimised at PBE

(1) Ligand

C	-0.00015800	-0.15328600	-0.00003300
C	0.00016800	2.64246800	-0.00011600
C	1.15695900	0.53477900	-0.40959000
C	1.14793700	1.94309500	-0.39974700
C	-1.14773900	1.94339900	0.39954300
C	-1.15708900	0.53506100	0.40947300
C	2.39077600	-0.22582100	-0.82684900
C	4.78794700	-1.51447700	-0.17580000
C	-2.39110000	-0.22520400	0.82684300
C	-4.78792500	-1.51442200	0.17606100
H	2.04602000	2.49022900	-0.70585600
H	0.00031100	3.73679700	-0.00017600
H	-2.04571200	2.49070300	0.70568100
H	2.11643400	-1.17845400	-1.31230600
H	2.99197000	0.36761200	-1.53730300
H	5.31414100	-0.87784900	-0.90586800
H	4.41720100	-2.42439100	-0.67575100
H	5.50038100	-1.81056500	0.60910000
H	-2.99236500	0.36873500	1.53681500
H	-2.11690400	-1.17751100	1.31304000
H	-5.31429900	-0.87744200	0.90569600
H	-4.41714800	-2.42400200	0.67659200
H	-5.50020600	-1.81103600	-0.60877300
H	-0.00024800	-1.24963000	-0.00001300
S	3.43597000	-0.60662900	0.65092400
S	-3.43585900	-0.60691800	-0.65089800

Optimization using PBE/6-31+G(d,p)[SDD]

- Energy = -1185.0063729 au
- Zero-point energy correction = 0.208627 au
- Thermal correction to Gibbs free energy = 0.164334 au

Single point energy using ωB97XD/6-311++G(2df,2p)[SDD]

- Energy = -1185.8931399 au

(2) Int1

C	0.81154000	1.11479800	0.38493900
C	1.24427600	3.14552900	-1.50754000
C	-0.09395800	2.21470800	0.28893400
C	0.11700900	3.21324200	-0.67030800
C	2.16549100	2.09793700	-1.38263700
C	1.98262700	1.08005800	-0.42561000
C	-1.29375000	2.24565700	1.19910800
C	-3.11668200	0.20579600	2.07119200
C	3.01104400	-0.00817600	-0.29004600
C	3.54965100	-2.27734400	1.28861600
H	-0.58630400	4.04745300	-0.75716800
H	1.41366400	3.93001200	-2.25162300
H	3.05579200	2.07809100	-2.01939200
H	-1.02935400	1.97528900	2.23464500
H	-1.80610900	3.21968200	1.19433000
H	-3.80669100	0.92108900	2.54426200
H	-2.30407300	-0.07663300	2.75592900
H	-3.65676100	-0.69597100	1.74832000
H	3.93526400	0.27775200	-0.81799000
H	2.59133800	-0.91773100	-0.77070900
H	4.42354700	-2.54669800	0.67532800
H	2.63350600	-2.71096100	0.85846400
H	3.69749700	-2.66975500	2.30627700
H	0.78231600	0.45355500	1.26595800
S	-2.44439000	0.94788200	0.53911500
S	3.38810400	-0.46323900	1.45568100
Pd	-0.87037900	-0.52964300	-0.31899400
Cl	-2.62538800	-2.00661800	-0.60897700
Cl	0.58602900	-2.04450600	-1.27040900

Optimization using PBE/6-31+G(d,p)[SDD]

- Energy = -2232.9752296 au
- Zero-point energy correction = 0.212403 au
- Thermal correction to Gibbs free energy = 0.160866 au

Single point energy using ωB97XD/6-311++G(2df,2p)[SDD]

- Energy = -2234.3164399 au

(3) TS1

C	0.35091000	0.98468200	0.11159500
C	1.72157400	3.46231100	0.06326000
C	-0.32819900	2.20778200	0.40654000
C	0.35404200	3.43179300	0.38397900

C	2.37758900	2.28370200	-0.30353700
C	1.70514100	1.04015400	-0.31435700
C	-1.82122200	2.15197400	0.59441800
C	-4.07940800	0.51948000	-0.09721500
C	2.43327300	-0.17848100	-0.83622400
C	4.56158900	-1.96615700	-0.81401600
H	-0.18256500	4.36300300	0.59528600
H	2.26184400	4.41367500	0.05855500
H	3.43036300	2.31175600	-0.60429400
H	-2.12052700	1.72185500	1.56592900
H	-2.30768600	3.13177300	0.45852300
H	-4.75094800	1.38231800	-0.22829300
H	-4.02343400	0.20363300	0.95366300
H	-4.41415900	-0.33286800	-0.70488100
H	2.70981400	-0.00368300	-1.89287300
H	1.78931600	-1.07164500	-0.80046900
H	4.74440400	-1.72642000	-1.87433500
H	3.84137500	-2.79643200	-0.73568600
H	5.51125000	-2.27796100	-0.35354500
H	0.45188100	-0.27229400	1.12498300
S	-2.42643300	0.97890500	-0.72333600
S	3.98202600	-0.50521900	0.11177800
Pd	-0.95690400	-0.65001000	-0.06056700
Cl	-2.44123700	-2.42502900	-0.41623900
Cl	0.59038000	-1.71312800	1.58340200

Optimization using PBE/6-31+G(d,p)[SDD]

- Energy = -2232.9368068 au
- Zero-point energy correction = 0.205639 au
- Thermal correction to Gibbs free energy = 0.155914 au

Single point energy using ωB97XD/6-311++G(2df,2p)[SDD]

- Energy = -2234.2710216 au

(4) Int2---HCl

C	0.25693900	1.14633800	-0.01254200
C	1.46803000	3.73417600	0.16453800
C	-0.49061000	2.30461000	0.35557000
C	0.10417700	3.57419600	0.44958900
C	2.20432000	2.62786600	-0.27032100
C	1.61233000	1.34908500	-0.38485600
C	-1.97067800	2.13347100	0.57903500
C	-4.03593200	0.21376200	0.12222200
C	2.45302000	0.24062100	-0.96706900
C	4.27560700	-1.90515100	-0.56016900
H	-0.50234600	4.44207900	0.73255300
H	1.93959400	4.71809000	0.24180000
H	3.25745400	2.75287500	-0.54993500

H	-2.21071000	1.75106600	1.58639600
H	-2.54663300	3.05509700	0.39157000
H	-4.81100000	0.98358700	-0.01764300
H	-3.88612900	-0.02291800	1.18482700
H	-4.29579300	-0.71139000	-0.41085000
H	3.12170700	0.61628700	-1.75864900
H	1.82393500	-0.57006300	-1.37081500
H	4.86698200	-1.53510300	-1.41084000
H	3.48892900	-2.59206600	-0.90916900
H	4.94087000	-2.43289200	0.13883200
H	2.11556200	-1.36858100	0.88579300
S	-2.48590700	0.82178400	-0.62836900
S	3.54286000	-0.49746500	0.34712900
Pd	-0.79692400	-0.60374300	-0.07366900
Cl	-2.18895800	-2.54570300	-0.22628900
Cl	0.84670000	-2.10234600	0.94974600

Optimization using PBE/6-31+G(d,p)[SDD]

- Energy = -2232.9653942 au
- Zero-point energy correction = 0.209021 au
- Thermal correction to Gibbs free energy = 0.160793 au

Single point energy using ωB97XD/6-311++G(2df,2p)[SDD]

- Energy = -2234.3012196 au

(5) Int2

C	-0.44046500	3.65539400	-0.06476900
C	0.17908800	0.90578200	0.05861200
C	-1.12583300	1.33256700	0.39209200
C	-1.40797100	2.71791300	0.31083100
Pd	0.73105200	-1.01674600	0.13668100
C	0.85962500	3.22511900	-0.35699300
C	1.17471000	1.85614400	-0.29614800
C	2.56757400	1.36779300	-0.57694300
C	3.99736100	-1.10085300	-0.38550800
C	-2.24770400	0.41789600	0.82010200
C	-4.48692100	-1.09469100	0.11102500
H	-2.74826100	0.83409700	1.71257900
H	-1.87618600	-0.59129800	1.05042500
H	-2.42370500	3.04848000	0.55417700
H	2.68179700	0.98927000	-1.60774500
H	3.34255600	2.12505100	-0.37564700
H	1.63879800	3.94831200	-0.62180200
H	-0.69325500	4.71872600	-0.10954100
H	-3.87220200	-2.00323300	0.21250100
H	-4.94944500	-0.83489000	1.07744300
H	-5.28565700	-1.28314600	-0.62267300
H	3.64053600	-1.29301300	-1.40768900

H	4.96770000	-0.57994500	-0.39974100
H	4.10679700	-2.05264100	0.15457200
Cl	-0.91056000	-2.53280700	-0.35404700
S	2.79156700	-0.08769100	0.54855100
S	-3.48501400	0.28168300	-0.54600100

Optimization using PBE/6-31+G(d,p)[SDD]

- Energy = -1772.3496229 au
- Zero-point energy correction = 0.200103 au
- Thermal correction to Gibbs free energy = 0.152977 au

Single point energy using ωB97XD/6-311++G(2df,2p)[SDD]

- Energy = -1773.4605087 au

(6) TS2

C	-0.24490600	3.84286800	-0.20435900
C	-0.32597100	1.02569300	-0.14713900
C	0.89385100	1.67791200	-0.44968300
C	0.90883800	3.08910700	-0.46056900
Pd	-0.36122000	-0.96638500	-0.20845100
C	-1.44708600	3.19059700	0.09433200
C	-1.49006900	1.78386400	0.13726400
C	-2.73943900	1.04391700	0.51618000
C	-3.32492200	-1.70850200	1.00563600
C	2.18430100	0.92873200	-0.67343700
C	4.16355700	-0.70701400	0.45946000
H	2.89699300	1.55139800	-1.24077100
H	2.02339300	-0.01477600	-1.22169000
H	1.85727500	3.59524400	-0.67318100
H	-2.80594300	0.87698100	1.60580300
H	-3.66796800	1.52662300	0.16947000
H	-2.35505000	3.76896000	0.29777400
H	-0.20467700	4.93553000	-0.23563800
H	4.70008500	-1.01436300	1.37018500
H	3.67740200	-1.58937600	0.01222200
H	4.88714400	-0.26422900	-0.24428700
H	-2.82880500	-1.56332300	1.97548200
H	-4.40209200	-1.48768500	1.07492400
H	-3.18405000	-2.74509400	0.66745600
Cl	1.14162500	-2.72075800	-0.40478000
S	-2.58726400	-0.62787300	-0.27525700
S	2.90888200	0.51085100	0.97813900

Optimization using PBE/6-31+G(d,p)[SDD]

- Energy = -1772.347369 au
- Zero-point energy correction = 0.199946 au
- Thermal correction to Gibbs free energy = 0.153997 au

Single point energy using ωB97XD/6-311++G(2df,2p)[SDD]

- Energy = -1773.4583413 au

(7) Product

C	4.10519700	-0.00012900	-0.00001300
C	1.27933700	-0.00003300	-0.00002100
C	1.99733700	-1.22282600	-0.02884600
C	3.40480300	-1.21686000	-0.00739600
Pd	-0.71390500	0.00002400	-0.00003400
C	3.40488600	1.21665000	0.00741600
C	1.99742000	1.22271100	0.02883700
C	1.21495200	2.50797400	0.13224700
C	-1.54704400	3.21550600	0.51328900
C	1.21478300	-2.50803900	-0.13227300
C	-1.54731500	-3.21546500	-0.51307100
H	1.69299200	-3.35107300	0.39375900
H	1.05732700	-2.79757600	-1.18660700
H	3.95802600	-2.16298600	-0.01032100
H	1.05755600	2.79755000	1.18658000
H	1.69319300	3.35097000	-0.39381800
H	3.95817400	2.16273800	0.01034500
H	5.19924700	-0.00016600	-0.00001600
H	-2.57527500	-2.88657000	-0.29802800
H	-1.31762300	-3.00674100	-1.56780500
H	-1.42427900	-4.28441300	-0.28174900
H	-1.31757900	3.00635900	1.56798500
H	-1.42360700	4.28448900	0.28232900
H	-2.57508800	2.88707600	0.29795700
Cl	-3.11635000	0.00007700	-0.00004100
S	-0.47843100	2.22382700	-0.58910700
S	-0.47854600	-2.22376500	0.58914700

Optimization using PBE/6-31+G(d,p)[SDD]

- Energy = -1772.3949618 au
- Zero-point energy correction = 0.200995 au
- Thermal correction to Gibbs free energy = 0.156628 au

Single point energy using ωB97XD/6-311++G(2df,2p)[SDD]

- Energy = -1773.5066915 au

S5. Cartesian coordinates and calculated energies of PdPCP pathway optimised at PBE

(1) Ligand

C	-0.01077400	-0.10703900	0.01144500
C	-0.01041700	2.65718200	0.39478300
C	-1.14067900	0.50241100	0.59718700

C	-1.12752700	1.89869100	0.77981800
C	1.10355000	2.03507300	-0.18259800
C	1.11469300	0.63822700	-0.38729000
C	-2.34701800	-0.31935500	0.98363000
C	-4.80104400	-1.63181100	0.36634500
C	-3.96988200	0.60510200	-1.19250400
C	2.31308600	-0.04340500	-1.00224500
C	4.92173900	-1.17884300	-0.88816100
C	3.19922500	-1.38756900	1.37103400
H	-1.99458200	2.39255300	1.23210100
H	-0.01061600	3.74126600	0.54718000
H	1.97503200	2.63036700	-0.47508900
H	-2.04426500	-1.20288300	1.57471400
H	-3.03761600	0.27721500	1.60816200
H	-5.25804900	-0.87286000	1.02677300
H	-4.53495100	-2.51521800	0.96972300
H	-5.54974200	-1.95032400	-0.37738100
H	-4.49340200	1.19887600	-0.42165400
H	-4.67401000	0.38237100	-2.01062300
H	-3.14786400	1.20935100	-1.60820900
H	2.65087100	0.50832900	-1.89827900
H	2.05496800	-1.06976800	-1.32275200
H	4.42151900	-2.10196600	-1.23231500
H	5.81381700	-1.45713500	-0.30345400
H	5.26497400	-0.61062200	-1.76828600
H	2.84542800	-2.30718400	0.87078400
H	2.37367100	-0.96623100	1.96683000
H	4.01590800	-1.65011500	2.06304400
H	-0.01728200	-1.19160700	-0.15127700
P	-3.28187600	-0.99465000	-0.51961800
P	3.80697500	-0.10244400	0.15970700

Optimization using PBE/6-31+G(d,p)[SDD]

- Energy = -1151.0872461 au
- Zero-point energy correction = 0.280704 au
- Thermal correction to Gibbs free energy = 0.233553 au

Single point energy using ωB97XD/6-311++G(2df,2p)[SDD]

- Energy = -1152.0670616 au

(2) Int1

C	0.63738400	1.06872900	0.14869100
C	1.23118000	3.49633900	-1.12421000
C	-0.19561500	2.20672900	0.36357500
C	0.10416800	3.40994100	-0.28581200
C	2.06316300	2.38963000	-1.30483600
C	1.80275200	1.15615200	-0.66274500
C	-1.42965700	2.08163800	1.22746400

C	-3.74150500	0.28692600	1.70303200
C	-3.37084400	1.51379500	-0.92678200
C	2.78013800	0.03179600	-0.79922700
C	4.92281700	-1.58750600	0.07681400
C	3.17970700	-0.47728600	2.02230400
H	-0.53880300	4.28344200	-0.13650100
H	1.46038700	4.43950200	-1.63010800
H	2.95070500	2.47184300	-1.94032600
H	-1.17303800	1.75075800	2.25082200
H	-1.98287400	3.03274600	1.30732700
H	-4.37206800	1.15881100	1.94438800
H	-3.25362000	-0.08523100	2.61671800
H	-4.35680400	-0.52286900	1.28317600
H	-4.07492600	2.28033200	-0.56258700
H	-3.91995900	0.72142300	-1.45838600
H	-2.64814700	1.96906300	-1.62108900
H	3.30909900	0.11493700	-1.76474300
H	2.27197600	-0.94880600	-0.76118800
H	4.17545100	-2.39773100	0.02180700
H	5.67986200	-1.84578100	0.83548900
H	5.43719600	-1.50659300	-0.89472900
H	2.52441200	-1.34195700	1.81577800
H	2.57463000	0.36430800	2.39671900
H	3.89113800	-0.74912000	2.81985700
H	0.54163900	0.18484900	0.84169100
Pd	-0.95875200	-0.83313200	-0.11666200
Cl	0.56231800	-2.56560000	-0.54829000
Cl	-2.78035800	-2.16747900	-0.59468700
P	-2.46104800	0.73877000	0.46733400
P	4.15510700	0.05797600	0.51955500

Optimization using PBE/6-31+G(d,p)[SDD]

- Energy = -2199.0783161 au
- Zero-point energy correction = 0.285002 au
- Thermal correction to Gibbs free energy = 0.230446 au

Single point energy using ωB97XD/6-311++G(2df,2p)[SDD]

- Energy = -2200.5162586 au

(3) TS1

C	0.17027300	0.96354100	0.25118700
C	1.32859200	3.53907700	0.16301200
C	-0.58183300	2.11880000	0.63658600
C	0.00217100	3.39298800	0.60224500
C	2.04794300	2.42689600	-0.28958500
C	1.48473500	1.13154700	-0.27444600
C	-2.05580000	1.93179000	0.92731100
C	-4.28172200	0.06791200	0.15309700

C	-2.74982700	1.45935700	-1.91569500
C	2.23530800	-0.03890500	-0.87651300
C	4.46374400	-1.66990500	-1.46225500
C	4.26512000	-0.49001500	1.13189800
H	-0.58041700	4.27251600	0.89689000
H	1.79057300	4.53116500	0.14258900
H	3.06403500	2.55372500	-0.67857600
H	-2.23686200	1.51843900	1.93741200
H	-2.63459300	2.86691800	0.82873600
H	-4.99573000	0.90613600	0.08835900
H	-4.27087900	-0.34514000	1.17255700
H	-4.57201900	-0.74026000	-0.53499100
H	-3.54796100	2.22053200	-1.88985000
H	-2.98597000	0.70296200	-2.67961800
H	-1.79018800	1.93335100	-2.17034300
H	2.06814200	-0.03081500	-1.97146400
H	1.82887600	-0.99783200	-0.50789000
H	3.84653000	-2.48149800	-1.03817000
H	5.52738100	-1.92152900	-1.32080600
H	4.27684100	-1.60775500	-2.54693500
H	3.68218800	-1.39042300	1.38744500
H	3.91256700	0.34338500	1.76086500
H	5.32897700	-0.66126900	1.36515200
H	0.33281800	-0.19063900	1.24172800
Pd	-0.94466400	-0.81549300	0.00920500
Cl	0.72509100	-1.54698800	1.93818200
Cl	-2.21903600	-2.69562900	-0.52173900
P	-2.59330100	0.62760200	-0.28522300
P	4.11563800	-0.01715400	-0.66591800

Optimization using PBE/6-31+G(d,p)[SDD]

- Energy = -2199.0454577 au
- Zero-point energy correction = 0.277989 au
- Thermal correction to Gibbs free energy = 0.224200 au

Single point energy using ωB97XD/6-311++G(2df,2p)[SDD]

- Energy = -2200.4740076 au

(4) Int2---HCl

C	0.17524900	1.20072800	-0.20313700
C	1.17153700	3.81218800	0.09198400
C	-0.67800300	2.24239000	0.24521600
C	-0.17454200	3.54717000	0.39186300
C	2.01185200	2.78472200	-0.36146100
C	1.52541400	1.47050800	-0.52513300
C	-2.11060000	1.86974200	0.55769600
C	-3.77345000	-0.63787000	0.35173700
C	-2.97936600	0.80200400	-2.07387900

C	2.41900800	0.36046200	-1.03476300
C	4.33520400	-1.71017400	-0.69776700
C	2.67187300	-0.94486600	1.48521800
H	-0.82872700	4.35340800	0.74157700
H	1.56508700	4.82687200	0.20609900
H	3.05923800	2.99997600	-0.60127300
H	-2.23764300	1.61830000	1.62771100
H	-2.84695700	2.65078700	0.29770200
H	-4.70098500	-0.04061100	0.33899100
H	-3.50507100	-0.89677300	1.38732500
H	-3.91531100	-1.56912600	-0.21750400
H	-3.95693200	1.30848800	-2.00471700
H	-3.07202600	-0.09524900	-2.70431800
H	-2.23884600	1.47975100	-2.52401300
H	2.93248100	0.67331800	-1.96253700
H	1.81520300	-0.53926800	-1.30380000
H	3.49995200	-2.38509900	-0.95576300
H	5.04360100	-2.25499300	-0.05249500
H	4.87096800	-1.43101700	-1.61982300
H	1.93352700	-1.64521800	1.04589300
H	2.13315200	-0.16226900	2.04194700
H	3.29140600	-1.50401700	2.20550600
H	-0.71120100	-0.85871100	1.63941000
Pd	-0.44719700	-0.70363200	-0.44618700
Cl	-0.98407100	-0.83692500	2.96810000
Cl	-0.75310300	-2.98936500	-0.80580800
P	-2.39913500	0.31016300	-0.40134800
P	3.75960500	-0.16993600	0.18896700

Optimization using PBE/6-31+G(d,p)[SDD]

- Energy = -2199.0631014 au
- Zero-point energy correction = 0.280035 au
- Thermal correction to Gibbs free energy = 0.224534 au

Single point energy using ωB97XD/6-311++G(2df,2p)[SDD]

- Energy = -2200.4972212 au

(5) Int2

C	0.99729200	3.80375300	-0.07602700
C	0.07277600	1.14232900	-0.07508800
C	1.39355000	1.42593900	-0.49819600
C	1.84418700	2.76226300	-0.48438800
Pd	-0.48619400	-0.78840900	-0.09974900
C	-0.31788100	3.52669200	0.33011100
C	-0.78367900	2.19907400	0.33305000
C	-2.18086400	1.81942500	0.77629200
C	-3.69293800	-0.75945500	1.08902200
C	-3.29788300	0.38774100	-1.56316000

C	2.29841600	0.29855300	-0.94543700
C	2.51876700	-0.84079300	1.65996000
C	4.19204900	-1.76429700	-0.45024600
H	2.82440800	0.56936900	-1.87920900
H	1.70134400	-0.61492400	-1.17838300
H	2.86775600	2.98480200	-0.80728100
H	-2.24659500	1.72327300	1.87676100
H	-2.96140400	2.53416700	0.45841500
H	-0.97803500	4.34256800	0.64544600
H	1.36074400	4.83599000	-0.08081500
H	3.35217400	-2.45065600	-0.65740600
H	4.72615300	-1.55388100	-1.39136600
H	4.89987500	-2.26531200	0.23016800
H	1.76400000	-1.55251900	1.26424100
H	3.12858100	-1.37014500	2.41085700
H	1.99710400	-0.01377600	2.16627300
H	-3.29581800	-0.87644200	2.10823300
H	-4.64898700	-0.20937500	1.11885600
H	-3.84690300	-1.76297300	0.66369500
H	-3.41764400	-0.58367300	-2.06614300
H	-4.28635000	0.85589000	-1.41730000
H	-2.66691600	1.03555300	-2.18977300
Cl	-0.79853200	-3.11261200	-0.17300500
P	-2.46395400	0.13008200	0.05580400
P	3.62420300	-0.16035300	0.32278900

Optimization using PBE/6-31+G(d,p)[SDD]

- Energy = -1738.4601217 au
- Zero-point energy correction = 0.271868 au
- Thermal correction to Gibbs free energy = 0.220168 au

Single point energy using ωB97XD/6-311++G(2df,2p)[SDD]

- Energy = -1739.6695216 au

(6) TS2

C	-4.12017800	0.87633400	-0.10146200
C	-1.34323400	0.28098800	0.00605900
C	-2.30904100	-0.74518900	0.17253300
C	-3.68370000	-0.44170700	0.09581000
Pd	0.61241600	-0.18090400	-0.01740800
C	-3.17755400	1.90437800	-0.24370100
C	-1.80056200	1.61348500	-0.20671700
C	-0.77413500	2.70567900	-0.43136700
C	2.15585500	2.80798000	-0.95826900
C	1.20130700	2.65164700	1.78362200
C	-1.88929900	-2.16018000	0.48969800
C	0.39532100	-2.46855700	-1.76572100
C	1.02319900	-2.83638500	1.37340300

H	-2.65175400	-2.87441200	0.13262200
H	-1.84446700	-2.30384100	1.58797900
H	-4.41985300	-1.24750300	0.20295700
H	-0.69224100	2.95714200	-1.50618000
H	-1.01100900	3.64416200	0.10290000
H	-3.51364900	2.93624700	-0.39862800
H	-5.19044800	1.10048700	-0.14691000
H	2.03276000	-2.78740300	0.93690600
H	0.91976300	-1.98439000	2.06107100
H	0.90202100	-3.78119300	1.92586800
H	1.49578800	-2.42246800	-1.73102500
H	0.08104700	-3.30352600	-2.41118100
H	0.02537500	-1.52222100	-2.18996500
H	1.96526500	2.56354400	-2.01409200
H	2.15494600	3.90260500	-0.82033200
H	3.13373800	2.38496600	-0.68182400
H	2.14851600	2.22042200	2.14237200
H	1.26926000	3.75291200	1.78421800
H	0.38940700	2.32806000	2.45198000
Cl	2.99248100	-0.57902500	-0.16368800
P	0.87014600	2.01624300	0.08800100
P	-0.22385700	-2.85153800	-0.02990700

Optimization using PBE/6-31+G(d,p)[SDD]

- Energy = -1738.4345589 au
- Zero-point energy correction = 0.272112 au
- Thermal correction to Gibbs free energy = 0.222278 au

Single point energy using ωB97XD/6-311++G(2df,2p)[SDD]

- Energy = -1739.6364842 au

(7) Product

Pd	-0.00017600	-0.69978800	-0.00018000
P	-2.27102100	-0.43061400	-0.02746100
P	2.27074200	-0.43201700	0.02775500
Cl	-0.00113700	-3.10173800	-0.00046800
C	0.00046300	1.33180700	-0.00002000
C	1.19575300	2.06426900	-0.26349700
C	1.18788900	3.47245900	-0.25030900
C	0.00130900	4.17703700	-0.00029400
C	-1.18569000	3.47319800	0.24992600
C	-1.19438100	2.06503800	0.26343200
C	-2.46838200	1.31016700	0.59876800
C	2.46938700	1.30865000	-0.59847100
H	-2.59392600	1.23428100	1.69617700
H	-3.37564900	1.80155600	0.20308700
H	2.59530000	1.23268000	-1.69584000
H	3.37681800	1.79946300	-0.20244900

H	2.11515500	4.02267900	-0.44848300
H	0.00161200	5.27151100	-0.00043700
H	-2.11261000	4.02402700	0.44802000
C	3.06033200	-0.45554900	1.69436000
H	2.55954200	0.28509200	2.33638400
H	2.92223300	-1.45318300	2.13938600
H	4.13720500	-0.22419900	1.63220600
C	3.35625800	-1.50796500	-0.99670100
H	4.41714400	-1.21928700	-0.91039500
H	3.21919000	-2.54861700	-0.66296200
H	3.03766500	-1.44714200	-2.04860500
C	-3.06137900	-0.45388600	-1.69369700
H	-2.92365600	-1.45154000	-2.13879400
H	-4.13817700	-0.22231900	-1.63109800
H	-2.56069900	0.28666800	-2.33591200
C	-3.35662000	-1.50589100	0.99760300
H	-4.41735900	-1.21647700	0.91194600
H	-3.22046200	-2.54661000	0.66369600
H	-3.03735000	-1.44536300	2.04931600

Optimization using PBE/6-31+G(d,p)[SDD]

- Energy = -1738.511456 au
- Zero-point energy correction = 0.273466 au
- Thermal correction to Gibbs free energy = 0.224647 au

Single point energy using ωB97XD/6-311++G(2df,2p)[SDD]

- Energy = -1739.7196009 au

S6. Cartesian coordinates and calculated Gibbs free energies optimised at ωB97XD for formation reaction

(1) $PdCl_2$

Pd	0.00000000	0.00000000	0.61284400
Cl	0.00000000	1.66139700	-0.82914200
Cl	0.00000000	-1.66139700	-0.82914200

Optimization using ωB97XD/6-31+G(d,p)[SDD]

- Energy = -1048.2719833 au
- Zero-point energy correction = 0.002065 au
- Thermal correction to Gibbs free energy = -0.027061 au

Single point energy using ωB97XD/6-311++G(2df,2p)[SDD]

- Energy = -1048.3428069 au

(2) HCl

Cl	0.00000000	0.00000000	0.07121100

H	0.00000000	0.00000000	-1.21058200

Optimization using ωB97XD/6-31+G(d,p)[SDD]

- Energy = -460.784617 au
- Zero-point energy correction = 0.006813 au
- Thermal correction to Gibbs free energy = -0.011068 au

Single point energy using ωB97XD/6-311++G(2df,2p)[SDD]

- Energy = -460.8185939 au

(3) Ligand of PdNCN

N	-3.09887800	-0.91345800	-0.07517800
N	3.41521500	-0.38651000	-0.01378100
C	-1.24140900	0.65375800	0.38703700
C	-1.02320700	2.02619800	0.30524000
H	-1.82890800	2.71542300	0.54536400
C	0.22374400	2.52077400	-0.08326700
H	0.38512800	3.59292200	-0.14337100
C	1.25408500	1.64570200	-0.40130600
H	2.23056000	2.02100400	-0.69285000
C	1.04906800	0.26263300	-0.33328200
C	-2.57523900	0.09807300	0.83385300
H	-2.45517900	-0.37329600	1.81705600
H	-3.29408000	0.93169700	0.96596200
C	-4.25976400	-1.57333300	0.49337600
H	-5.10114100	-0.87569400	0.67330300
H	-3.99484100	-2.04224600	1.44577800
H	-4.60777200	-2.35629700	-0.18649700
C	-3.40234600	-0.35608500	-1.38255100
H	-4.19144900	0.41978200	-1.33602500
H	-3.74274400	-1.15196000	-2.05091900
H	-2.50596900	0.09407300	-1.81574200
C	2.16695600	-0.68676700	-0.70320000
H	2.35811100	-0.60794500	-1.78040600
H	1.84043500	-1.72863900	-0.51277000
C	4.51165200	-1.16658700	-0.55728000
H	4.36512900	-2.25676000	-0.42696000
H	5.44461000	-0.88841400	-0.05855700
H	4.62321900	-0.96200000	-1.62629400
C	3.29622200	-0.58275200	1.42144600
H	3.06958400	-1.63499000	1.68313700
H	2.49979400	0.04934700	1.82150500
H	4.23413700	-0.30206200	1.90877500
C	-0.19477200	-0.21750000	0.06518200
H	-0.37293200	-1.28884900	0.12074300

Optimization using ωB97XD/6-31+G(d,p)[SDD]

- Energy = -578.6633177 au

- Zero-point energy correction = 0.306576 au
- Thermal correction to Gibbs free energy = 0.264023 au

Single point energy using ωB97XD/6-311++G(2df,2p)[SDD]

- Energy = -578.8000493 au

(4) Product of PdNCN

Pd	0.69653100	0.00000300	0.00000800
Cl	3.11519800	-0.00000100	-0.00002200
N	0.35915300	-2.11842900	-0.03315300
N	0.35914600	2.11843100	0.03316300
C	-1.23202100	0.00000000	0.00000500
C	-1.90948400	-1.19684600	0.22116500
C	-3.30425500	-1.19959300	0.21057000
H	-3.86038300	-2.11980000	0.37308100
C	-3.99138400	-0.00000800	-0.00001400
H	-5.07710600	-0.00001100	-0.00002100
C	-3.30425900	1.19958000	-0.21058900
H	-3.86038900	2.11978400	-0.37310800
C	-1.90948700	1.19684100	-0.22116500
C	-1.01103300	-2.36706000	0.52612500
H	-0.89793800	-2.46271300	1.61107400
H	-1.39691100	-3.32522200	0.14881700
C	1.36530600	-2.88863300	0.72246200
H	1.12975400	-3.96217300	0.68653000
H	1.37953700	-2.54731300	1.75880700
H	2.34950100	-2.70334500	0.29151700
C	0.40159500	-2.52363900	-1.45502000
H	0.25260300	-3.60973900	-1.54475500
H	1.37180400	-2.25220800	-1.87428800
H	-0.38530500	-2.00439000	-2.00474700
C	-1.01104000	2.36705900	-0.52612100
H	-1.39692000	3.32521900	-0.14881300
H	-0.89794000	2.46271200	-1.61107000
C	0.40158300	2.52365200	1.45502600
H	0.25259100	3.60975200	1.54475300
H	1.37179100	2.25222500	1.87430100
H	-0.38531800	2.00440600	2.00475500
C	1.36530200	2.88862800	-0.72245500
H	1.12975400	3.96216900	-0.68653100
H	1.37953500	2.54730000	-1.75879800
H	2.34949600	2.70333900	-0.29150700

Optimization using ωB97XD/6-31+G(d,p)[SDD]

- Energy = -1166.2379582 au
- Zero-point energy correction = 0.300958 au
- Thermal correction to Gibbs free energy = 0.257485 au

Single point energy using ωB97XD/6-311++G(2df,2p)[SDD]

- Energy = -1166.4124004 au

(5) Ligand of PdSCS

C	-0.00000400	-0.12442500	0.00001900
C	0.00000100	2.65021200	-0.00031200
C	1.14796500	0.55930800	-0.40283200
C	1.14039800	1.95585500	-0.39347300
C	-1.14039800	1.95595300	0.39301800
C	-1.14797000	0.55940900	0.40271100
C	2.37975000	-0.20162400	-0.81567200
C	4.71876500	-1.53113100	-0.17804400
C	-2.37975800	-0.20142300	0.81572400
C	-4.71875000	-1.53111400	0.17838800
H	2.03236200	2.49908300	-0.69348100
H	0.00000100	3.73572900	-0.00044800
H	-2.03236200	2.49925600	0.69289100
H	2.10398000	-1.12591100	-1.33326400
H	2.99302800	0.40161200	-1.49228900
H	5.25301900	-0.88436800	-0.87924800
H	4.33740600	-2.40982700	-0.70527700
H	5.41777300	-1.86202700	0.59264300
H	-2.99303800	0.40197200	1.49219800
H	-2.10399100	-1.12559000	1.33353500
H	-5.25299900	-0.88421600	0.87947200
H	-4.33738000	-2.40970300	0.70579100
H	-5.41776700	-1.86216600	-0.59222400
H	-0.00000700	-1.21241000	0.00014900
S	3.38093100	-0.63454100	0.65399000
S	-3.38093200	-0.63468100	-0.65384100

Optimization using ωB97XD/6-31+G(d,p)[SDD]

- Energy = -1185.743781 au
- Zero-point energy correction = 0.217166 au
- Thermal correction to Gibbs free energy = 0.174572 au

Single point energy using ωB97XD/6-311++G(2df,2p)[SDD]

- Energy = -1185.89687 au

(6) Product of PdSCS

C	-4.07642800	-0.00003400	0.00000100
C	-1.27205200	-0.00001100	-0.00000400
C	-1.98494400	1.21017100	-0.04127900
C	-3.38097700	1.20672600	-0.02559300
Pd	0.71773600	0.00000700	-0.00000400
C	-3.38095700	-1.20678100	0.02559300
C	-1.98492400	-1.21020400	0.04127600

C	-1.20555700	-2.49545100	0.14926100
C	1.52804300	-3.20983900	0.49420100
C	-1.20559800	2.49543100	-0.14926300
C	1.52798200	3.20989600	-0.49417100
H	-1.69562900	3.33331900	0.35367300
H	-1.04772500	2.76254400	-1.19940200
H	-3.92848700	2.14582700	-0.04319600
H	-1.04768400	-2.76256400	1.19940000
H	-1.69557300	-3.33334700	-0.35367800
H	-3.92845200	-2.14589100	0.04319900
H	-5.16187200	-0.00004200	0.00000200
H	2.55155700	2.92763800	-0.24112600
H	1.34226700	2.96242300	-1.54027900
H	1.36533400	4.27294500	-0.30670000
H	1.34221800	-2.96245100	1.54030900
H	1.36553200	-4.27289400	0.30665000
H	2.55160400	-2.92743800	0.24125400
Cl	3.11347000	0.00000500	-0.00000700
S	0.45797500	-2.22989200	-0.58982900
S	0.45793500	2.22989900	0.58983500

Optimization using ωB97XD/6-31+G(d,p)[SDD]

- Energy = -1773.311126 au
- Zero-point energy correction = 0.209679 au
- Thermal correction to Gibbs free energy = 0.166359 au

Single point energy using ωB97XD/6-311++G(2df,2p)[SDD]

- Energy = -1773.5106985 au

(7) Ligand of PdPCP

C	0.04745200	-0.11931600	-0.04308200
C	-0.04222700	2.60716900	0.43447000
C	-1.08499800	0.42636400	0.56994300
C	-1.11907600	1.80282100	0.80281800
C	1.07791200	2.04793900	-0.17014500
C	1.13399900	0.67196800	-0.41930000
C	-2.25719000	-0.44945700	0.92854100
C	-4.71482000	-1.69068400	0.28684000
C	-3.99636400	0.73275200	-0.97729700
C	2.35621700	0.04953700	-1.04137200
C	4.88110100	-1.19801700	-0.82012200
C	3.04205300	-1.37092300	1.32098500
H	-1.99148200	2.24681300	1.27498700
H	-0.07848100	3.67605600	0.62205700
H	1.91867600	2.67806600	-0.44739100
H	-1.90969900	-1.38397700	1.38360900
H	-2.90098700	0.05313500	1.66071400
H	-5.13523900	-1.03537500	1.05854000

H	-4.41088200	-2.63316100	0.75189800
H	-5.49652700	-1.91780600	-0.44392700
H	-4.46870300	1.19840200	-0.10409100
H	-4.74715200	0.61879400	-1.76463800
H	-3.21353200	1.39891400	-1.35023900
H	2.71975200	0.66928000	-1.86879900
H	2.11546500	-0.93844000	-1.45219000
H	4.36364000	-2.08844100	-1.19561100
H	5.72726200	-1.51820000	-0.20499200
H	5.28186100	-0.63911000	-1.67096900
H	2.66303500	-2.24802900	0.78309200
H	2.21978600	-0.92386500	1.88650100
H	3.80463200	-1.69700900	2.03413600
H	0.07825400	-1.18970700	-0.23696500
P	-3.26594800	-0.92111800	-0.57718000
P	3.76701300	-0.10470000	0.18055400

Optimization using ωB97XD/6-31+G(d,p)[SDD]

- Energy = -1151.9047895 au
- Zero-point energy correction = 0.291707 au
- Thermal correction to Gibbs free energy = 0.244710 au

Single point energy using ωB97XD/6-311++G(2df,2p)[SDD]

- Energy = -1152.0721151 au

(8) Product of PdPCP

Pd	0.00000600	-0.71509500	0.00001100
P	-2.26827700	-0.41773400	-0.02909000
P	2.26828300	-0.41769700	0.02911300
Cl	0.00003000	-3.10803900	-0.00004900
C	-0.00001100	1.31704800	-0.00000300
C	1.17807900	2.04481000	-0.28500200
C	1.17182500	3.44176400	-0.27381900
C	-0.00003600	4.14070900	-0.00002600
C	-1.17188500	3.44174800	0.27378100
C	-1.17811400	2.04479500	0.28498800
C	-2.44506800	1.29128100	0.63684900
C	2.44504800	1.29131400	-0.63684500
H	-2.54053700	1.20077500	1.72639500
H	-3.34886800	1.79094400	0.27014600
H	2.54052600	1.20079500	-1.72639000
H	3.34883800	1.79099700	-0.27014400
H	2.08789600	3.98657100	-0.48959800
H	-0.00004600	5.22654500	-0.00003600
H	-2.08796500	3.98654300	0.48955100
C	3.02925400	-0.36942300	1.69067400
H	2.51513600	0.38529800	2.29076300
H	2.89772200	-1.34261000	2.17000500

H	4.09554000	-0.12959600	1.63286000
C	3.36666100	-1.49987200	-0.94479000
H	4.41320800	-1.18930300	-0.86907700
H	3.25178700	-2.52193000	-0.57443800
H	3.05054000	-1.48631400	-1.99047800
C	-3.02924900	-0.36949000	-1.69065100
H	-2.89770300	-1.34267900	-2.16997100
H	-4.09553900	-0.12967700	-1.63284000
H	-2.51514300	0.38523300	-2.29074800
C	-3.36663800	-1.49991600	0.94482400
H	-4.41318900	-1.18935600	0.86911600
H	-3.25175800	-2.52197400	0.57447400
H	-3.05051200	-1.48635200	1.99051000

Optimization using ωB97XD/6-31+G(d,p)[SDD]

- Energy = -1739.5104236 au
- Zero-point energy correction = 0.283525 au
- Thermal correction to Gibbs free energy = 0.234836 au

Single point energy using ωB97XD/6-311++G(2df,2p)[SDD]

- Energy = -1739.7244846 au