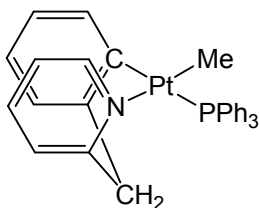


## Supporting Information

### Reactivity comparison of five- and six-membered cycloplatinated(II) complexes in oxidative addition reactions

The Cartesian coordinates (in angstroms) for all optimized species discussed in the present work

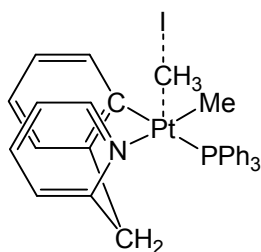
2



Pt	0.88563400	-0.71135600	-0.02981500
C	0.35926000	-2.69632800	-0.26977900
H	1.23752300	-3.34732700	-0.29056700
H	-0.29857200	-3.02525100	0.54692600
H	-0.19181200	-2.83641000	-1.20868700
C	2.86436400	-1.25180600	0.00658600
C	3.78968800	-0.48561800	-0.73943100
C	3.38516600	-2.31503000	0.76729800
C	5.15648900	-0.79186500	-0.73083600
C	4.75187100	-2.61687800	0.78553100
H	2.71157200	-2.92932300	1.36000500
C	5.64439200	-1.86030700	0.02547100
H	5.84543300	-0.18986600	-1.32141200
H	5.11582700	-3.44502000	1.39042200
H	6.70667400	-2.09204200	0.02364700
C	1.19045100	2.26019600	1.10218500
C	2.72666100	1.76296100	-0.57191500
C	1.70712100	3.53909400	1.27786800
H	0.35932200	1.90658200	1.70005500
C	3.28722700	3.03879900	-0.45327200
C	2.77478300	3.94045400	0.47589600
H	1.27620800	4.19673200	2.02513500
H	4.12455400	3.31037800	-1.08786600
H	3.20438900	4.93286400	0.57591700
N	1.67509100	1.39073900	0.19494000
C	3.29930800	0.72927400	-1.51578900
P	-1.46308000	-0.08247200	-0.04225700
C	-2.68256500	-1.44786100	-0.31445400
C	-3.44737100	-1.99798000	0.72329900
C	-2.80022800	-1.99404000	-1.60460600
C	-4.31432600	-3.06697500	0.47634100
H	-3.37600900	-1.59417900	1.72782700
C	-3.66906800	-3.05661000	-1.85022900
H	-2.21608200	-1.58302100	-2.42350800
C	-4.42870400	-3.59805600	-0.80868600

H	-4.90209300	-3.47892400	1.29223100
H	-3.75086200	-3.46327300	-2.85451500
H	-5.10412700	-4.42740300	-0.99958900
C	-1.97600100	0.63031200	1.58860400
C	-1.41513900	0.06206900	2.74768900
C	-2.87066400	1.70230400	1.72815700
C	-1.75702500	0.54226600	4.01326400
H	-0.69918900	-0.75045300	2.65363200
C	-3.20301100	2.18812000	2.99527200
H	-3.30676600	2.16765800	0.85072100
C	-2.65139500	1.60831700	4.13962900
H	-1.31720100	0.08943400	4.89751900
H	-3.89324900	3.02250100	3.08537000
H	-2.91131600	1.98870100	5.12359800
C	-2.00287000	1.15542800	-1.30494100
C	-1.03568100	1.92022200	-1.97458600
C	-3.35866100	1.34735800	-1.62797000
C	-1.41291200	2.86427100	-2.93334500
H	0.01455900	1.76975200	-1.75081600
C	-3.73427600	2.29178400	-2.58388400
H	-4.12362900	0.75037200	-1.14078500
C	-2.76170800	3.05369600	-3.23782600
H	-0.65062200	3.44520700	-3.44514300
H	-4.78572500	2.42795200	-2.82153100
H	-3.05516900	3.78517700	-3.98572600
H	2.52011900	0.43129500	-2.22974600
H	4.11631200	1.18016100	-2.08753400

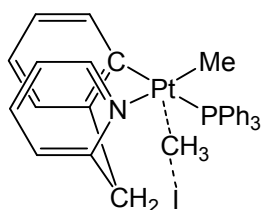
### TS1



Pt	-0.32231000	-0.76545900	-0.71565400
C	-0.18590700	-0.09297700	-2.66604300
H	-1.13193000	-0.20941700	-3.19959000
H	0.11785000	0.95857100	-2.70341900
H	0.57563100	-0.68308900	-3.19253600
C	-1.93014600	-1.93650400	-1.24369600
C	-1.94841700	-3.26937500	-0.77307700
C	-3.01744000	-1.51907100	-2.03075700
C	-3.00318100	-4.13079300	-1.10311100
C	-4.07318500	-2.37797500	-2.35461300
H	-3.05571800	-0.50036800	-2.40601600
C	-4.06581500	-3.69473700	-1.89644000
H	-2.99119000	-5.15458300	-0.73361800
H	-4.89706800	-2.01414500	-2.96426300
H	-4.87703400	-4.37384300	-2.14551300
C	-0.57923300	-0.93564500	2.48321700

C	-0.79602600	-3.00042000	1.43438500
C	-0.79257200	-1.48691500	3.74158500
H	-0.39759700	0.12621600	2.36964400
C	-1.00981100	-3.62005400	2.66916200
C	-1.00804800	-2.86094100	3.83669600
H	-0.78672500	-0.84777000	4.61762400
H	-1.18044100	-4.69103400	2.70265700
H	-1.17557900	-3.33241300	4.80040900
N	-0.57496800	-1.66791900	1.35365100
C	-0.84082200	-3.77849400	0.13845400
P	1.81976100	0.39289000	-0.14452600
C	2.60589300	1.39120200	-1.49254500
C	2.75272200	2.78433400	-1.44358400
C	3.06540400	0.70350800	-2.63059200
C	3.33791400	3.47439800	-2.50988800
H	2.42485700	3.34215900	-0.57388600
C	3.65377600	1.39280000	-3.68955000
H	2.97297200	-0.37708400	-2.68856500
C	3.78843100	2.78320700	-3.63435300
H	3.44452000	4.55408300	-2.45226700
H	4.00543100	0.84346800	-4.55839500
H	4.24420200	3.32100600	-4.46092800
C	1.73676000	1.53567500	1.30634100
C	0.84042700	2.62130800	1.27198300
C	2.47657300	1.31324400	2.47854300
C	0.69964300	3.46643000	2.37369800
H	0.25192200	2.82059900	0.38136300
C	2.32776400	2.15681900	3.58277100
H	3.17026600	0.48186900	2.53692500
C	1.44179800	3.23403500	3.53461200
H	0.00458300	4.29939700	2.32324000
H	2.90864100	1.96773300	4.48128400
H	1.32748700	3.88714800	4.39498900
C	3.18888000	-0.77375300	0.28096600
C	2.90497300	-2.10035900	0.63517900
C	4.52993900	-0.34905200	0.26623600
C	3.93491600	-2.98538000	0.96596000
H	1.87822300	-2.44488100	0.65432700
C	5.55670300	-1.23233800	0.59836300
H	4.77347800	0.67241400	-0.00886100
C	5.26155000	-2.55372800	0.94723800
H	3.69695000	-4.01094200	1.23391700
H	6.58740200	-0.88933300	0.58158300
H	6.06310800	-3.24188600	1.20070500
H	0.13249400	-3.69476900	-0.36386200
H	-0.99249200	-4.83783400	0.36505600
C	-1.98360600	1.10057200	-0.19762100
H	-2.79158500	0.39060400	-0.16436800
H	-1.41982200	1.31493200	0.69345700
H	-1.71447600	1.56724400	-1.13038300
I	-3.63243400	3.10735300	0.37067000

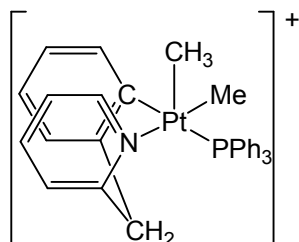
TS2



Pt	0.35997700	-0.80675900	-0.69360200
C	0.33310900	0.07145700	-2.57298600
H	1.34487300	0.14928200	-2.97868000
H	-0.25995700	-0.57503400	-3.23529900
H	-0.12362900	1.06403800	-2.57090300
C	2.04148200	-1.85595100	-1.24781100
C	3.04230200	-2.14890100	-0.29289300
C	2.22061000	-2.36928900	-2.54545700
C	4.17181700	-2.89902800	-0.65030900
C	3.34209400	-3.12788600	-2.89576300
H	1.47276500	-2.17639300	-3.30891300
C	4.33218800	-3.38585000	-1.94804700
H	4.93264600	-3.10635900	0.09988700
H	3.44043700	-3.51044700	-3.90925000
H	5.21395000	-3.96500900	-2.20974900
C	-0.63959900	-2.65762700	1.71195700
C	1.66000400	-2.32579300	1.78618400
C	-0.61088400	-3.51896900	2.80190100
H	-1.57281200	-2.43102100	1.21136200
C	1.75784000	-3.17432200	2.89407300
C	0.61543300	-3.77602900	3.41348900
H	-1.53153300	-3.96985800	3.15598700
H	2.73232200	-3.35919300	3.33371600
H	0.68239800	-4.43730500	4.27218800
N	0.46256000	-2.05957300	1.21594900
C	2.88812200	-1.71354100	1.15700700
P	-1.77430500	0.31736900	-0.10801500
C	-2.32068200	1.65567000	-1.25988700
C	-3.28659700	1.44062900	-2.25286400
C	-1.69009100	2.91095100	-1.18678800
C	-3.61762300	2.45897200	-3.15129300
H	-3.78982500	0.48249400	-2.32836300
C	-2.02351300	3.92539900	-2.08400700
H	-0.94551700	3.10740000	-0.42030300
C	-2.98799400	3.70154500	-3.07081900
H	-4.37216600	2.27699900	-3.91159400
H	-1.52927000	4.88993900	-2.01064700
H	-3.24680400	4.49176100	-3.76983800
C	-3.14957500	-0.91651400	-0.16596100
C	-3.10820900	-1.89393000	-1.17781900
C	-4.20924500	-0.93930100	0.75441600
C	-4.11300500	-2.85766200	-1.27657200
H	-2.28432300	-1.90344200	-1.88638500
C	-5.20747900	-1.91192200	0.65897100

H	-4.25721400	-0.20537700	1.55177600
C	-5.16424300	-2.86962000	-0.35638600
H	-4.06853100	-3.60226000	-2.06630400
H	-6.01875200	-1.91922500	1.38158300
H	-5.94201900	-3.62475800	-0.42700800
C	-1.91424100	1.13924500	1.53858900
C	-0.98056800	0.84767000	2.54495200
C	-2.93633400	2.06678700	1.81178300
C	-1.06748600	1.46267700	3.79653600
H	-0.18179100	0.14073000	2.35148400
C	-3.02360400	2.67694200	3.06321900
H	-3.65906700	2.32231600	1.04319200
C	-2.08885200	2.37678600	4.05811100
H	-0.33200400	1.23055900	4.56142300
H	-3.81808600	3.39174100	3.25815500
H	-2.15392000	2.85892000	5.02940300
H	2.81671100	-0.62331800	1.23252800
H	3.76766200	-2.01142600	1.73464400
C	1.74140100	1.27766400	-0.17011200
H	1.16546800	1.87805400	-0.85229300
H	2.62737600	0.77945600	-0.52411600
H	1.43118700	1.19078400	0.85772600
I	3.20223400	3.42883200	0.49870900

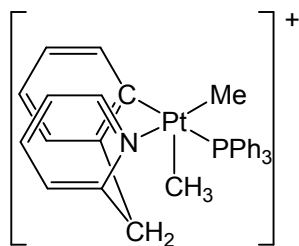
**IM1**



Pt	-0.92641600	-0.73137200	-0.18297000
C	-0.45374300	-2.73670600	-0.02204000
H	-0.32716600	-2.92163800	1.05294400
H	-1.25800500	-3.36872100	-0.39847400
H	0.47757100	-2.96613700	-0.54175800
C	-2.92900300	-1.20138800	-0.12487400
C	-3.73004800	-0.44651700	0.75593100
C	-3.52942200	-2.22488500	-0.86968900
C	-5.09313800	-0.74742300	0.88367300
C	-4.89099600	-2.51426900	-0.73950200
H	-2.94330500	-2.81545400	-1.56682800
C	-5.67656500	-1.77744800	0.14558400
H	-5.70227900	-0.16320800	1.56966200
H	-5.33027500	-3.31416700	-1.32962500
H	-6.73495800	-1.99500000	0.25743600
C	-1.15088700	2.38319200	-1.07339500
C	-2.62012800	1.80170400	0.63662200
C	-1.63162200	3.68669300	-1.11877200
H	-0.35393100	2.06397600	-1.73376900
C	-3.14347200	3.09673900	0.64829000

C	-2.64731800	4.05161100	-0.23659000
H	-1.21229800	4.39053300	-1.82894500
H	-3.93698000	3.34354500	1.34554700
H	-3.04889400	5.06021800	-0.23848000
N	-1.62868100	1.46132200	-0.21795200
C	-3.15571700	0.71931500	1.54815800
P	1.59325400	-0.09443100	0.04152200
C	2.81623400	-1.46512900	-0.13468300
C	3.77151000	-1.51376300	-1.16049700
C	2.77907700	-2.50962400	0.80815100
C	4.66305300	-2.58675400	-1.24606600
H	3.83929700	-0.71435400	-1.88908800
C	3.67381300	-3.57509700	0.72226800
H	2.06106800	-2.48680300	1.62232000
C	4.61623600	-3.61906100	-0.30902000
H	5.39881800	-2.60629200	-2.04487000
H	3.63427100	-4.36966700	1.46171900
H	5.31191200	-4.45038200	-0.37681100
C	2.15703800	1.22941300	-1.10901500
C	2.08384900	1.02022300	-2.49973200
C	2.59722100	2.47473900	-0.63413000
C	2.45367600	2.02996100	-3.38934200
H	1.74978000	0.06650600	-2.89632300
C	2.95890700	3.48499800	-1.52873800
H	2.65944800	2.66158000	0.43216400
C	2.88849600	3.26684200	-2.90537700
H	2.39948800	1.84899100	-4.45882000
H	3.29815000	4.44261800	-1.14444800
H	3.17119700	4.05391000	-3.59823100
C	1.93832900	0.55699400	1.73015700
C	0.91115800	1.16419700	2.47008600
C	3.22539400	0.47967600	2.29131100
C	1.16120800	1.67845100	3.74420800
H	-0.08525600	1.25086700	2.05211200
C	3.47221300	0.99443800	3.56414200
H	4.03476800	0.01442100	1.73846600
C	2.44112000	1.59204500	4.29409400
H	0.35488600	2.14268900	4.30451600
H	4.47094900	0.92691700	3.98558500
H	2.63551200	1.98783800	5.28670400
H	-2.35055100	0.37453800	2.21353700
H	-3.92602400	1.14637800	2.19501200
C	-0.92036600	-0.89755200	-2.23903000
H	-0.55616000	0.05813900	-2.61678800
H	-0.25018700	-1.71402500	-2.51028200
H	-1.93505400	-1.08731500	-2.58275200

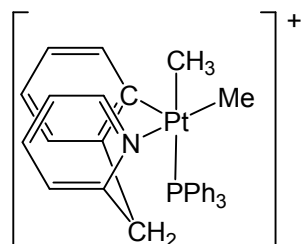
**IM2**



Pt	0.91336600	-0.68847000	-0.05768700
C	0.40787600	-2.69792200	0.04042200
H	1.18935100	-3.31147300	-0.40918000
H	0.32514600	-2.92360300	1.11153000
H	-0.54668300	-2.89843100	-0.44572900
C	2.91214600	-1.17268500	0.01975000
C	3.86742700	-0.36884200	-0.63691000
C	3.36186000	-2.25242300	0.79463900
C	5.22992300	-0.67754500	-0.51932800
C	4.72470500	-2.54251200	0.91595600
H	2.65284500	-2.88312600	1.32036000
C	5.66349600	-1.76109300	0.24502100
H	5.96001600	-0.05379500	-1.03006200
H	5.04368700	-3.38199100	1.52814100
H	6.72408100	-1.98374100	0.32108200
C	1.05988300	2.35044100	0.97035000
C	2.76978400	1.88404800	-0.54036000
C	1.52654600	3.63994400	1.19130800
H	0.18251500	1.98368400	1.48891100
C	3.28157700	3.17435600	-0.37445200
C	2.65689000	4.06488300	0.49456400
H	1.00997300	4.28693600	1.89148100
H	4.17244700	3.46466900	-0.92095300
H	3.05111400	5.06702000	0.63203000
N	1.65352200	1.49221600	0.11555600
C	3.46886400	0.87246900	-1.41880300
P	-1.58693700	-0.05475800	-0.00634500
C	-2.73249400	-1.46821500	-0.29850400
C	-3.37120000	-2.13558100	0.75680600
C	-2.91258100	-1.93857200	-1.61242700
C	-4.17677800	-3.24866800	0.50281100
H	-3.25172200	-1.78875000	1.77776500
C	-3.71832800	-3.04975300	-1.86070700
H	-2.44168100	-1.42881200	-2.44815400
C	-4.35127500	-3.70884100	-0.80306200
H	-4.67038200	-3.75115700	1.32967500
H	-3.85331000	-3.39742300	-2.88079500
H	-4.97910900	-4.57342600	-0.99771500
C	-2.00383800	0.56396200	1.67967500
C	-1.40039500	-0.05941400	2.78843700
C	-2.87864700	1.64014400	1.89795400
C	-1.68074700	0.37399700	4.08515700
H	-0.71211900	-0.88846100	2.64627600
C	-3.14975300	2.07546700	3.19688800

H	-3.34764900	2.14309900	1.05912000
C	-2.55507700	1.44388000	4.29122800
H	-1.21164400	-0.12068800	4.93059600
H	-3.82714900	2.91037700	3.35103400
H	-2.76811500	1.78592900	5.29979100
C	-2.17836200	1.22659200	-1.18588400
C	-1.26709800	2.11495700	-1.77815300
C	-3.54612600	1.34771600	-1.49374300
C	-1.71226500	3.10596700	-2.65592900
H	-0.20932500	2.03849100	-1.55505600
C	-3.98705000	2.34062100	-2.36857400
H	-4.26700000	0.66451700	-1.05628300
C	-3.07136000	3.22088100	-2.95165700
H	-0.99485600	3.78371800	-3.10928200
H	-5.04575200	2.42359000	-2.59624400
H	-3.41693600	3.99026200	-3.63598800
H	2.81839800	0.61580700	-2.26189200
H	4.35868900	1.33909700	-1.84890700
C	0.85107400	-1.00564000	-2.10609000
H	0.70575300	-0.02335700	-2.55798400
H	1.79016200	-1.46254100	-2.41579600
H	0.01407000	-1.66565100	-2.33024600

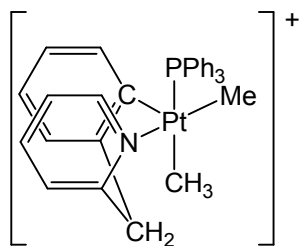
**IM1'**



Pt	-0.86038700	-0.27745700	-1.19201300
C	0.11077700	-1.81262900	-2.19449100
H	0.52181200	-2.54525200	-1.49593800
H	-0.55970300	-2.31148000	-2.89748800
H	0.92563100	-1.34075000	-2.75530100
C	-2.01111800	-1.53526700	-0.09194500
C	-2.46831700	-1.11108500	1.16934200
C	-2.35931600	-2.79804400	-0.58264300
C	-3.26471500	-1.99769000	1.91426300
C	-3.14708200	-3.66158100	0.18322100
H	-2.02031500	-3.12590300	-1.55594400
C	-3.60277200	-3.26190800	1.43786200
H	-3.61751900	-1.67885600	2.89184100
H	-3.40075700	-4.64096200	-0.21260100
H	-4.21860100	-3.92328800	2.03999600
C	-2.20695100	2.54474100	-1.08456200
C	-2.46852200	1.42896000	0.94507300
C	-2.96416600	3.62607500	-0.65345000
H	-1.77787100	2.52030600	-2.08083000
C	-3.25242900	2.47727800	1.43617200
C	-3.50316200	3.58695300	0.63358500



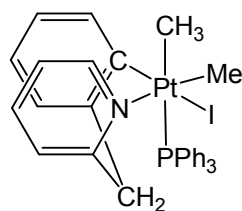
H	-3.13012300	4.46854400	-1.31550100
H	-3.65531800	2.41509300	2.44133800
H	-4.10955900	4.40718900	1.00497300
N	-1.96378200	1.47422500	-0.30311100
C	-2.12226400	0.22861100	1.78993800
H	-1.04624300	0.27345200	2.00641900
H	-2.62959500	0.31823500	2.75345900
C	-2.35014200	-0.33126400	-2.64970600
H	-1.93976000	0.27225900	-3.47044400
H	-2.55193600	-1.34384200	-2.99934000
H	-3.26685600	0.12134200	-2.26648500
P	1.35192100	0.05640700	0.21155200
C	2.60735000	0.61768500	-1.02842500
C	3.25727000	-0.33157300	-1.83895900
C	2.86050700	1.98044900	-1.25326000
C	4.13573800	0.07494400	-2.84401600
H	3.09578000	-1.39206000	-1.67795600
C	3.73772300	2.38287400	-2.26298900
H	2.39089600	2.73735300	-0.63533700
C	4.37564200	1.43354000	-3.06284300
H	4.63439700	-0.67357200	-3.45308200
H	3.92489000	3.44183000	-2.41654500
H	5.05854000	1.74851700	-3.84645100
C	2.08563000	-1.44625200	0.97004500
C	3.47103100	-1.55853600	1.18766800
C	1.24250500	-2.49040200	1.38238100
C	3.99728700	-2.69406900	1.80329200
H	4.13985200	-0.76326600	0.87394900
C	1.77427400	-3.62498300	2.00003900
H	0.17165600	-2.42391500	1.22100800
C	3.15023500	-3.72901800	2.20989400
H	5.06874400	-2.76966800	1.96434800
H	1.11152400	-4.42683800	2.31190400
H	3.56324200	-4.61331600	2.68656600
C	1.38767000	1.33881800	1.54022700
C	2.01128100	1.10853300	2.77749100
C	0.76638000	2.58134000	1.31642500
C	2.02318000	2.10195600	3.75899800
H	2.49014300	0.15738900	2.98052200
C	0.79037600	3.57488400	2.29598200
H	0.26031100	2.77962700	0.37756900
C	1.41796200	3.33703700	3.52089500
H	2.51024100	1.90686700	4.71007700
H	0.31186800	4.53047100	2.10211400
H	1.43129900	4.10817000	4.28563000

**IM2'**

Pt	-0.75425000	0.20252800	-1.39091100
C	0.19711200	1.64366800	-2.54525500
H	-0.52193100	2.37515000	-2.91996900
H	0.98846700	2.14964600	-1.99070300
H	0.63809700	1.10177400	-3.39221100
C	-1.72221600	1.57649100	-0.26615800
C	-2.99104700	1.28206800	0.26164500
C	-1.08333000	2.78148000	0.04249500
C	-3.57175100	2.22157400	1.13184100
C	-1.69058200	3.70114300	0.90241600
H	-0.10742400	3.01162000	-0.36193800
C	-2.93920100	3.42055400	1.45279900
H	-4.54823700	1.99941200	1.55493600
H	-1.17639800	4.62932700	1.13497400
H	-3.41977600	4.12663000	2.12337000
C	-1.28183400	-2.68863000	-0.21836800
C	-3.10793700	-1.29414500	0.14734800
C	-1.90675700	-3.76966500	0.38880800
H	-0.28059300	-2.78573100	-0.62189100
C	-3.78609800	-2.33613500	0.78870100
C	-3.18621500	-3.58577200	0.91178800
H	-1.39366600	-4.72253600	0.45458900
H	-4.78251200	-2.15877900	1.17907800
H	-3.70721200	-4.39975900	1.40617400
N	-1.86244800	-1.47837300	-0.33737900
C	-3.78994700	0.03771500	-0.07171400
H	-4.10403400	0.08066200	-1.12235100
H	-4.71231000	0.04576100	0.51411100
P	1.28050900	-0.07829700	0.21124200
C	2.55168300	-1.20110600	-0.50949300
C	2.25111400	-2.00735300	-1.61998600
C	3.84302400	-1.27178300	0.04633100
C	3.21022900	-2.87383100	-2.15135800
H	1.27457700	-1.96824600	-2.09390400
C	4.79770100	-2.13867400	-0.48461900
H	4.10564300	-0.64477200	0.89278900
C	4.48246700	-2.94342400	-1.58316700
H	2.96047700	-3.48810400	-3.01143500
H	5.78824600	-2.18303600	-0.04145600
H	5.22785200	-3.61632700	-1.99689200
C	0.83093400	-0.79293600	1.84906000
C	1.51236500	-1.87933700	2.41953800
C	-0.25637500	-0.23084800	2.54325500
C	1.12395200	-2.38080700	3.66419600

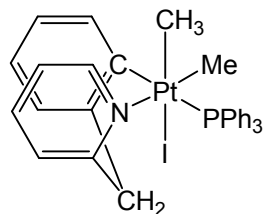
H	2.34398800	-2.34083600	1.89898800
C	-0.63263500	-0.72793700	3.79146000
H	-0.81324600	0.59420300	2.11101500
C	0.05641600	-1.80473300	4.35488500
H	1.66045800	-3.22273200	4.09229400
H	-1.46839600	-0.27686200	4.31863000
H	-0.24054600	-2.19492600	5.32411900
C	2.23974700	1.45114800	0.58619300
C	2.10618000	2.13861200	1.80185000
C	3.08901300	1.97827000	-0.40456900
C	2.80702200	3.32698700	2.02141600
H	1.46761500	1.74699900	2.58598800
C	3.78669800	3.16548000	-0.18017400
H	3.22610600	1.45307600	-1.34503200
C	3.64585500	3.84428500	1.03291100
H	2.69882400	3.84320600	2.97098500
H	4.44379400	3.55509900	-0.95231400
H	4.19120800	4.76718900	1.20755700
C	-2.21083000	0.26633100	-2.89378000
H	-2.84163700	-0.62188400	-2.80837000
H	-2.81528200	1.17488000	-2.84354800
H	-1.66972900	0.24364600	-3.84525200

#### 4-cis-anti



Pt	0.84375000	-0.36995600	-0.96807400
C	-0.13261600	0.12134500	-2.73833700
H	-0.29045600	1.20172600	-2.79552800
H	0.46645900	-0.20343400	-3.59319400
H	-1.09000600	-0.40018400	-2.75713400
C	2.02909700	1.31671100	-1.09320800
C	2.56528300	1.90256700	0.07163200
C	2.38505800	1.86012300	-2.33634700
C	3.42902000	3.00388400	-0.04280300
C	3.23815000	2.96252700	-2.43660900
H	1.99783400	1.42560400	-3.25055100
C	3.76724500	3.54066100	-1.28373300
H	3.83409500	3.44831800	0.86379800
H	3.48806600	3.35957900	-3.41740900
H	4.43506300	4.39546000	-1.34633100
C	2.36589700	-2.26040600	1.11114600
C	2.57332900	-0.02876000	1.72102200
C	3.19889500	-2.67896200	2.14214100
H	1.91700800	-2.97095500	0.42762700
C	3.42088300	-0.38045800	2.77684700
C	3.73808500	-1.71779800	2.99564900

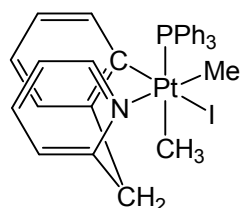
H	3.41493000	-3.73504100	2.26274800
H	3.82335700	0.39890400	3.41537200
H	4.39467500	-2.00229400	3.81251800
N	2.05105900	-0.96747100	0.90423600
C	2.21432400	1.41328600	1.46352300
H	1.13885400	1.53474400	1.64246900
H	2.71809400	2.03719000	2.20683600
I	-0.57660900	-2.97530300	-1.02590400
C	2.40710800	-1.27128500	-2.04550100
H	2.20926500	-2.34361000	-2.07728200
H	2.44651800	-0.86599000	-3.05792700
H	3.34968600	-1.06957100	-1.53208400
P	-1.23933500	0.61793300	0.34177100
C	-2.88789700	-0.04617100	-0.18551500
C	-3.40523300	0.37073200	-1.42450300
C	-3.64026700	-0.93337500	0.59574300
C	-4.63947200	-0.09893400	-1.87335800
H	-2.85418600	1.07657000	-2.03776000
C	-4.87867100	-1.39886500	0.14558800
H	-3.27010100	-1.26357600	1.55970700
C	-5.38026700	-0.98755100	-1.08972700
H	-5.02338200	0.23465100	-2.83350900
H	-5.44966600	-2.08356900	0.76670500
H	-6.34277000	-1.35163500	-1.43816700
C	-1.59432700	2.43365600	0.24096500
C	-2.81332700	2.94733700	0.72532000
C	-0.67762000	3.31650900	-0.34603600
C	-3.09378800	4.30995300	0.64007000
H	-3.54757200	2.27914200	1.16483100
C	-0.96405700	4.68273000	-0.43638800
H	0.25752700	2.94229900	-0.74269700
C	-2.16808300	5.18232100	0.05808700
H	-4.03741100	4.68975400	1.02189200
H	-0.24271200	5.35079700	-0.89859100
H	-2.39042700	6.24342800	-0.01355500
C	-1.15539700	0.25351300	2.15474100
C	-1.31114900	1.24059700	3.14126400
C	-0.87797600	-1.06619700	2.55761300
C	-1.20400800	0.91394700	4.49565700
H	-1.51178400	2.26846600	2.86122100
C	-0.78630600	-1.39029900	3.91192700
H	-0.73560300	-1.84156000	1.81044700
C	-0.94700700	-0.40112100	4.88559400
H	-1.32511000	1.69231900	5.24406800
H	-0.58097000	-2.41653100	4.20374300
H	-0.86833200	-0.65338200	5.93945500

**4-trans-anti**

Pt	-0.86786700	-0.19249000	-0.63535900
C	-0.47927500	-1.88454300	-1.78253700
H	-1.32218200	-2.56954900	-1.68981600
H	-0.34177900	-1.60607800	-2.83205200
H	0.42161200	-2.37560900	-1.41671800
C	-2.88895500	-0.39539300	-1.02522500
C	-3.84459300	0.03855900	-0.08392200
C	-3.34809900	-0.90396400	-2.24948900
C	-5.21214900	-0.07853100	-0.38205700
C	-4.71119300	-1.01903500	-2.53422400
H	-2.63812400	-1.21759300	-3.00673300
C	-5.65378400	-0.60899800	-1.59274300
H	-5.93935700	0.25369400	0.35595500
H	-5.02839100	-1.42392800	-3.49231000
H	-6.71776700	-0.69121400	-1.79822000
C	-0.64121100	2.85126500	0.39393900
C	-2.59501500	1.85693500	1.16206400
C	-0.97567100	4.08179700	0.94357900
H	0.28453300	2.73267000	-0.15542200
C	-2.99379100	3.06872600	1.74052700
C	-2.18118400	4.19231400	1.63647300
H	-0.30414200	4.92514400	0.82507200
H	-3.94237800	3.11538600	2.26488800
H	-2.48357800	5.13528200	2.08209900
N	-1.42000300	1.75663600	0.50285000
C	-3.45943500	0.62844200	1.26026100
P	1.72599000	0.05821500	-0.19269500
C	2.78601000	-1.40427700	-0.62097300
C	3.84214900	-1.35163600	-1.54328300
C	2.53484700	-2.61596400	0.04873200
C	4.61942600	-2.48539600	-1.79854600
H	4.07576600	-0.42991700	-2.06280400
C	3.31529600	-3.74340700	-0.20665900
H	1.72416800	-2.68009100	0.76828100
C	4.35872400	-3.68379100	-1.13405200
H	5.43336000	-2.42319400	-2.51569300
H	3.10406400	-4.66964700	0.32054000
H	4.96457200	-4.56328600	-1.33368200
C	2.48069000	1.44366100	-1.16094100
C	2.43725100	1.40191900	-2.56774200
C	3.04659100	2.57011800	-0.54185900
C	2.96520500	2.44460700	-3.32950300
H	1.99666300	0.54807300	-3.07392800
C	3.56217100	3.61984000	-1.30749600
H	3.09344000	2.63138300	0.53983500

C	3.52744100	3.55897800	-2.70090100
H	2.93114600	2.38741800	-4.41375500
H	3.99678100	4.48164400	-0.80874100
H	3.93348800	4.37317500	-3.29439500
C	2.26063200	0.40438500	1.54253700
C	1.33079300	0.81396800	2.50805500
C	3.61193500	0.27414500	1.91004700
C	1.74386100	1.09978200	3.81234500
H	0.28196400	0.88684800	2.24976100
C	4.02127000	0.55742900	3.21271100
H	4.34555400	-0.05238500	1.17933100
C	3.08728200	0.97259000	4.16675900
H	1.01053100	1.41078600	4.55104700
H	5.06808600	0.45018800	3.48303200
H	3.40650800	1.18898100	5.18255200
H	-2.91161800	-0.12555000	1.84034100
H	-4.36266800	0.87928400	1.82314500
C	-0.84594900	1.04605400	-2.32257000
H	-0.65182600	0.44990800	-3.21628200
H	-1.81794800	1.53322700	-2.40681900
H	-0.06212200	1.79295500	-2.19765700
I	-1.01909800	-2.13220700	1.66901500

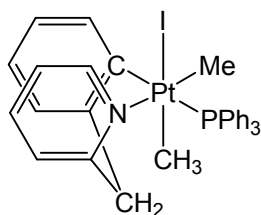
#### 4-*cis-syn*



Pt	-0.94513300	-0.18813100	-0.99343200
C	-0.01251300	-0.41021700	-2.83970500
H	-0.47482700	0.25433700	-3.57350100
H	1.05046600	-0.17302500	-2.76185600
H	-0.13244400	-1.44883800	-3.15346200
C	-1.00908700	1.85980600	-1.21536600
C	-2.05610900	2.60404900	-0.62881800
C	-0.03086700	2.54763100	-1.94654000
C	-2.05381000	4.00411000	-0.75163600
C	-0.05256000	3.93950100	-2.07449400
H	0.77440600	2.00476100	-2.42325000
C	-1.06468700	4.67764300	-1.46586000
H	-2.85928300	4.57032900	-0.28889200
H	0.72859200	4.43596700	-2.64442700
H	-1.09263200	5.76066000	-1.54996700
C	-1.85155500	-0.86530300	1.98920500
C	-2.95844800	1.01564200	1.19927200
C	-2.50453200	-0.81036700	3.21410000
H	-1.13723700	-1.64870000	1.77410000
C	-3.64512400	1.13532400	2.41325800
C	-3.42399900	0.21392600	3.43169300

H	-2.28753000	-1.55472500	3.97228300
H	-4.35224500	1.94808400	2.54280700
H	-3.95607200	0.29575500	4.37487800
N	-2.07253900	0.01929500	0.99717100
C	-3.24802200	1.97679900	0.07238700
H	-3.85700900	1.44262200	-0.66741100
H	-3.88675400	2.77278500	0.46452700
P	1.42247600	0.02929100	0.33674000
C	2.64002300	-1.36252600	0.43438200
C	2.39627500	-2.57915100	-0.21285900
C	3.87249900	-1.17680700	1.09213000
C	3.35366000	-3.59950900	-0.18916400
H	1.45795300	-2.73817600	-0.73045900
C	4.82033200	-2.19738900	1.12152300
H	4.09489400	-0.23083300	1.57703000
C	4.56217900	-3.41399900	0.47992300
H	3.14678900	-4.53751600	-0.69691400
H	5.76365000	-2.04086800	1.63750000
H	5.30459200	-4.20718400	0.49885100
C	1.13763500	0.53507000	2.09087600
C	1.56761300	-0.23464600	3.18302200
C	0.39160900	1.70200500	2.34326900
C	1.28646700	0.16769400	4.49152400
H	2.12220800	-1.15185000	3.02146500
C	0.12390500	2.10768400	3.65060900
H	0.00479700	2.29072000	1.51708800
C	0.57291800	1.34250700	4.73029500
H	1.62976800	-0.44194600	5.32283600
H	-0.44497500	3.01693400	3.82364200
H	0.36025300	1.65630900	5.74845100
C	2.56426200	1.33113400	-0.34334600
C	2.76047600	2.58941000	0.24120200
C	3.26605900	1.02297000	-1.52373300
C	3.62648800	3.51853700	-0.34285100
H	2.25295400	2.85429100	1.16126200
C	4.12355200	1.95393300	-2.10956300
H	3.16358900	0.04252900	-1.97943000
C	4.30484300	3.20890000	-1.52181800
H	3.76923100	4.48559700	0.13170600
H	4.65567900	1.69395100	-3.02043200
H	4.97598100	3.93338500	-1.97449700
C	-2.70959200	-0.31730100	-2.11981500
H	-3.51660200	-0.62747300	-1.45275200
H	-2.92884200	0.64749000	-2.58271200
H	-2.55926600	-1.07553200	-2.88805100
I	-1.30902700	-3.15193200	-0.77514300

#### 4-trans-syn



Pt	0.84421400	-0.36832100	-0.55087300
C	0.53695300	-2.25360700	-1.37668200
H	1.21902300	-2.40415800	-2.21591500
H	0.73155600	-2.99254200	-0.59697900
H	-0.49115900	-2.34948100	-1.72621100
C	2.86224500	-0.52402300	-0.95738800
C	3.61311700	0.62848300	-1.26724400
C	3.52596500	-1.75851300	-0.91181600
C	4.99122300	0.51043200	-1.51578500
C	4.89483200	-1.86377100	-1.16923800
H	2.97860500	-2.65562600	-0.65081900
C	5.63621700	-0.72345600	-1.47695400
H	5.56112100	1.40769800	-1.74826900
H	5.37621600	-2.83754600	-1.12037500
H	6.70215400	-0.79033300	-1.67772100
C	0.74200500	2.01854600	1.58963900
C	2.32477700	2.44848900	-0.05673800
C	1.07278500	3.16997900	2.29299300
H	-0.01813800	1.34275400	1.95936100
C	2.71305100	3.61891800	0.60568900
C	2.08144300	3.98990300	1.78876500
H	0.55306700	3.40435600	3.21557200
H	3.50968700	4.22488000	0.18697200
H	2.37524200	4.89624900	2.30979800
N	1.34028400	1.66656500	0.43411300
C	3.00235000	2.01921800	-1.33543500
P	-1.79089800	-0.01177900	-0.20445600
C	-2.80744900	-1.38256700	-0.92883500
C	-3.47041500	-2.33053700	-0.13599200
C	-2.86669400	-1.52015000	-2.32870400
C	-4.17097500	-3.38680700	-0.72500000
H	-3.45766600	-2.24784600	0.94448300
C	-3.57057800	-2.57241600	-2.91426900
H	-2.37946600	-0.79324200	-2.97074500
C	-4.22289200	-3.51305200	-2.11327300
H	-4.68067100	-4.10710200	-0.09122400
H	-3.60815200	-2.65455600	-3.99688400
H	-4.76959000	-4.33385400	-2.56870600
C	-2.48076000	0.21611600	1.49954600
C	-2.19579800	-0.73828900	2.49230900
C	-3.27954000	1.32191600	1.83776800
C	-2.71477600	-0.60053300	3.78102200
H	-1.55124500	-1.58014200	2.26828300
C	-3.78747400	1.46107400	3.13114600



H	-3.51275400	2.07720200	1.09630700
C	-3.51130500	0.49949400	4.10491900
H	-2.48444400	-1.35077300	4.53215700
H	-4.40270000	2.32330000	3.37329700
H	-3.90968200	0.60900700	5.10975800
C	-2.43241100	1.48163000	-1.09424400
C	-1.63444400	2.63449400	-1.17350100
C	-3.73165400	1.52618300	-1.62936300
C	-2.11554600	3.79623200	-1.78135800
H	-0.63433200	2.63018200	-0.75692600
C	-4.20970400	2.68670600	-2.24045600
H	-4.37593600	0.65588700	-1.56939700
C	-3.40267100	3.82398100	-2.32072700
H	-1.48069400	4.67618600	-1.83449800
H	-5.21561500	2.70059700	-2.65066100
H	-3.77584200	4.72568300	-2.79814200
H	2.27354100	2.07603300	-2.15119500
H	3.78421700	2.74606400	-1.57168000
I	1.39924000	-1.56780400	2.12147200
C	0.55130300	0.28041700	-2.52714600
H	0.24264400	1.32688600	-2.52971000
H	1.48048500	0.15157400	-3.08478200
H	-0.22546700	-0.33093600	-2.98896800