Supporting Information

Effects of the number of cyclometalated ring and ancillary ligands on the rate of MeI oxidative addition to platinum(II)-pincer complexes

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XYZ Cartesian and energy of optimized structures

[(C^N^C)Pt(PPh$_2$Me)], 2a

Zero-point correction= 0.453232 (Hartree/Particle)
Thermal correction to Energy= 0.481223
Thermal correction to Enthalpy= 0.482167
Thermal correction to Gibbs Free Energy= 0.392551
Sum of electronic and zero-point Energies= -1672.522702
Sum of electronic and thermal Energies= -1672.494711
Sum of electronic and thermal Enthalpies= -1672.493767
Sum of electronic and thermal Free Energies= -1672.583382

Pt	0.59485700	-0.13296900	-0.03838800
P	-1.50287100	-1.02824900	-0.36191400
C	-1.28177900	2.42815400	0.55424400
H	-2.17855300	1.82891300	0.42904800
C	-1.44813100	3.78093400	0.87312600
H	-2.45008800	4.18877000	0.98926800
C	-0.33639400	4.60867700	1.04163900
H	-0.45902000	5.66008800	1.28704800
C	0.93872500	4.06783300	0.89360300
C	3.67512300	2.75671300	0.53943500
C	4.84337300	2.01589700	0.37047000
H	5.80863400	2.50802000	0.44780400
C	4.78454400	0.64944200	0.10316100
H	5.69479800	0.07701300	-0.02786200
C	3.53272400	0.02941600	0.00568000
C	2.43800300	2.10900300	0.43409300
C	1.10111200	2.70931300	0.57840200
C	-2.52423600	0.00627100	-1.50543000
C	-3.89184800	0.24620600	-1.31038800
H	-4.39530000	-0.13550600	-0.42777100
C	-4.61851500	0.99018300	-2.24419700
H	-5.67581500	1.17615100	-2.07610300
C	-3.99024900	1.49453800	-3.38419000
H	-4.55695200	2.07296000	-4.10859200
C	-2.62788000	1.25762400	-3.58713100
H	-2.13039000	1.65123300	-4.46923300
C	-1.89791100	0.52423100	-2.65105200
H	-0.83339600	0.36312600	-2.80173900
C	-2.47969000	-1.24387500	1.18508200
C	-2.07095600	-0.58177100	2.35428500
H	-1.19504600	0.05835300	2.32536300
C	-2.77947000	-0.74401700	3.54662500
H	-2.44881200	-0.22621000	4.44262100
C	-3.90239200	-1.57263100	3.58891000
H	-4.45131300	-1.70139700	4.51764100
C	-4.31481600	-2.24144500	2.43380900
H	-5.18436200	-2.89221800	2.45981800
C	-3.60814500	-2.08112400	1.24073600
H	-3.94306200	-2.61562800	0.35763200
C	-1.67879800	-2.67398800	-1.19649700
H	-1.41041100	-3.48241300	-0.51252900
H	-1.01831400	-2.70322200	-2.06680700
H	-2.70857300	-2.82025700	-1.53357200
C	1.88104100	-1.78283200	-0.32185100
C	1.65526800	-3.15414000	-0.52573600
C	3.25808100	-1.39355900	-0.25577600
C	2.69344400	-4.08251500	-0.67298400
H	0.64145600	-3.53220900	-0.57034400
C	4.30232200	-2.31882500	-0.40839300
C	4.02459800	-3.66719000	-0.62151400
H	2.45857900	-5.13338500	-0.82876500
H	5.33847100	-1.99479400	-0.35711000
H	4.83520400	-4.38115100	-0.73904500
C	-0.01785500	1.83758600	0.39153200
N	2.41739600	0.77928800	0.17293400
H	1.80430600	4.71063800	1.03090400
H	3.72465900	3.81877000	0.74656900

[(C^N^C)PtMeI(PPh$_2$Me)], 3a

Zero-point correction= 0.493139 (Hartree/Particle)
Thermal correction to Energy= 0.525104
Thermal correction to Enthalpy= 0.526048
Thermal correction to Gibbs Free Energy= 0.428746
Sum of electronic and zero-point Energies= -1723.783669
Sum of electronic and thermal Energies= -1723.751705
Sum of electronic and thermal Enthalpies= -1723.750760
Sum of electronic and thermal Free Energies= -1723.848063

Pt	0.41168500	0.14655300	-0.26667800
P	-1.81148700	0.52424500	0.50100600
C	-0.83087600	-2.57579800	-1.49281100
H	-1.83423200	-2.25659400	-1.23303300
C	-0.68243600	-3.80107200	-2.15435200
H	-1.56237300	-4.39553500	-2.38970500
C	0.58575900	-4.26231000	-2.51335400
H	0.70504100	-5.21467300	-3.02225600
C	1.70043400	-3.47896800	-2.22673500
C	4.04913400	-1.62874500	-1.57122000
C	4.99955800	-0.65456800	-1.27193900
H	6.05023600	-0.85356200	-1.46100700
C	4.61684900	0.57204700	-0.73226400
H	5.35970600	1.32579300	-0.50184500
C	3.26040100	0.81387900	-0.48581800
C	2.69860400	-1.36351100	-1.31629200
C	1.55022900	-2.24563100	-1.57086600
C	-2.93210000	-0.92449600	0.74673100
C	-4.29552700	-0.86430000	0.41594700
H	-4.70664800	0.01315100	-0.06981000
C	-5.14200700	-1.93512700	0.71372800
H	-6.19368400	-1.87433800	0.44816500
C	-4.64176800	-3.07184600	1.35014500
H	-5.30224500	-3.90294600	1.58126900
C	-3.28805300	-3.13512600	1.68958900
H	-2.88901500	-4.01537800	2.18560400
C	-2.43678000	-2.07194300	1.38868000
H	-1.38559400	-2.13418600	1.64920600
C	-2.77628000	1.67663200	-0.55373600
C	-3.17316400	1.27307000	-1.84158000
H	-2.93235200	0.27700700	-2.20108700
C	-3.89317700	2.13727400	-2.66503300
H	-4.19703900	1.80721700	-3.65420400
C	-4.21978000	3.42175700	-2.22054600
H	-4.77742600	4.09572200	-2.86446600
C	-3.83013400	3.83266900	-0.94568000
H	-4.08426200	4.82672800	-0.58933600
C	-3.11604300	2.96523300	-0.11434300
H	-2.83768900	3.30294000	0.87806900
C	-1.84130800	1.25505400	2.19423800
H	-1.19468200	2.13008000	2.26991900
H	-1.46334800	0.49356300	2.87909100
H	-2.86843800	1.51383800	2.46705700
C	1.24483500	2.03708000	0.25665000
C	0.66656900	3.24654800	0.65629500
C	2.65647200	2.04148500	0.05553900
C	1.43224300	4.39107800	0.91033000
H	-0.41058100	3.32911500	0.75953300
C	3.42744600	3.18626400	0.31644500
C	2.81928900	4.35932400	0.75567600
H	0.94129500	5.30914400	1.22468800
H	4.50337500	3.17209900	0.16630400
H	3.41909800	5.24233300	0.95688100
C	0.26782500	-1.77548100	-1.16149700
N	2.37038300	-0.16212300	-0.78426300
H	2.68461000	-3.82715600	-2.52809900
H	4.35194300	-2.58088000	-1.98940300
I	1.23483900	-1.01200500	2.35186900
C	0.05725300	0.97490400	-2.17558800
H	-0.57792600	0.29680000	-2.74375300
H	-0.41030900	1.95038300	-2.05551700
H	1.03344400	1.07337900	-2.65375000

[(C^N^C)PtMe(PPh$_2$Me)]$^+$, IMa

Zero-point correction= 0.492836 (Hartree/Particle)
Thermal correction to Energy= 0.521904
Thermal correction to Enthalpy= 0.522848
Thermal correction to Gibbs Free Energy= 0.433613
Sum of electronic and zero-point Energies= -1712.188915
Sum of electronic and thermal Energies= -1712.159847
Sum of electronic and thermal Enthalpies= -1712.158903
Sum of electronic and thermal Free Energies= -1712.248138

Pt	-0.59719300	-0.09650400	0.07780800
P	1.59119700	-0.97512700	0.49384100
C	1.21685600	2.54233600	-0.50920600
H	2.12804900	2.00734000	-0.26803200
C	1.33981000	3.88179700	-0.90182800
H	2.32649900	4.33191000	-0.97509800
C	0.20455100	4.63656500	-1.19396500
H	0.29311000	5.67441300	-1.50102600
C	-1.05282900	4.04722400	-1.08068400
C	-3.74633900	2.67342200	-0.68965500
C	-4.89476700	1.91570100	-0.46587600
H	-5.87149400	2.37613700	-0.57833100
C	-4.80387300	0.57550100	-0.09434600
H	-5.69996700	-0.00556800	0.08346400
C	-3.53959100	-0.00659700	0.04288900
C	-2.49347300	2.07039500	-0.53862900
C	-1.17438400	2.70487000	-0.69038200
C	2.57065800	0.21302200	1.49410800
C	3.93433300	0.43529400	1.25394400
H	4.43289500	-0.05506400	0.42412700
C	4.65756600	1.29741100	2.08191500
H	5.71191400	1.46916700	1.88611700
C	4.02915300	1.93504000	3.15316500
H	4.59399000	2.60626600	3.79343300
C	2.67214100	1.70926700	3.40158000
H	2.17950700	2.20228400	4.23441000
C	1.94356300	0.85412800	2.57538000
H	0.88659800	0.69315900	2.77419000
C	2.57545700	-1.39275900	-0.99207100
C	2.74952600	-0.43810500	-2.01041500
H	2.29915400	0.54459000	-1.92321600
C	3.50480700	-0.74349200	-3.14142500
H	3.63356400	0.00461700	-3.91790800
C	4.08833700	-2.00622300	-3.27700400
H	4.67276200	-2.24374800	-4.16097900
C	3.91719400	-2.96096900	-2.27420500
H	4.36751200	-3.94424500	-2.37146300
C	3.16672300	-2.65871700	-1.13576000
H	3.05503800	-3.41635900	-0.36897000
C	1.66536200	-2.46231100	1.58061300
H	1.33211100	-3.36562300	1.06929000
H	1.02589500	-2.28895000	2.44969000
H	2.69571800	-2.59987300	1.91989700
C	-1.85856700	-1.77607900	0.45977700
C	-1.58707600	-3.12240500	0.71825200
C	-3.23343800	-1.40003100	0.40471800
C	-2.60471900	-4.05382800	0.96271000
H	-0.56733800	-3.48309500	0.72477100
C	-4.25380500	-2.32986400	0.65597000
C	-3.94123300	-3.65674400	0.94341100
H	-2.34770500	-5.09045500	1.16473300

H	-5.29638800	-2.02788400	0.62348000
H	-4.73428900	-4.37273500	1.13729300
C	-0.02609700	1.90761300	-0.40234700
N	-2.44775400	0.76122600	-0.19008500
H	-1.93527800	4.64059900	-1.30065000
H	-3.82474700	3.71676700	-0.96820800
C	-0.62603700	-0.73594000	-1.90946800
H	-0.05852200	0.00333400	-2.46984100
H	-0.17708400	-1.72548300	-1.94716400
H	-1.67297800	-0.75902700	-2.20710300

TS

Zero-point correction= 0.490953 (Hartree/Particle)
Thermal correction to Energy= 0.523394
Thermal correction to Enthalpy= 0.524338
Thermal correction to Gibbs Free Energy= 0.423200
Sum of electronic and zero-point Energies= -1723.763405
Sum of electronic and thermal Energies= -1723.730964
Sum of electronic and thermal Enthalpies= -1723.730020
Sum of electronic and thermal Free Energies= -1723.831158

Pt	0.00016500	0.43921400	0.48151200
P	1.84952500	-0.30207800	-0.74134100
C	0.25269900	-2.36472500	2.07084500
H	1.05071300	-2.68610700	1.41275400
C	-0.15036400	-3.23931200	3.08832700
H	0.34125100	-4.20365300	3.19504100
C	-1.17768200	-2.88199900	3.96256600
H	-1.49254400	-3.55640500	4.75395900
C	-1.80330900	-1.64715400	3.80624500
C	-3.11640100	1.07008700	3.32345600
C	-3.61786700	2.32105100	2.96869000
H	-4.43966100	2.75044600	3.53404400
C	-3.07507700	3.02840500	1.89706800
H	-3.46701400	4.00180700	1.62908800
C	-2.01604000	2.46425500	1.17687500
C	-2.05967600	0.52716600	2.58293900
C	-1.40018900	-0.77365100	2.78423800
C	2.66188500	-1.90002600	-0.31322100
C	3.63759200	-1.94078800	0.69624900
H	3.93888700	-1.02768900	1.20048400
C	4.23274300	-3.14993200	1.05632300
H	4.98799600	-3.16513600	1.83696700
C	3.86204000	-4.33421300	0.41402200
H	4.32692000	-5.27512700	0.69427400
C	2.89316200	-4.30335500	-0.59074000
H	2.60034000	-5.21884800	-1.09670300
C	2.29404300	-3.09469300	-0.95286800
H	1.53962800	-3.09750400	-1.73283200
C	3.24305800	0.89727100	-0.65181800
C	3.37313300	1.73435200	0.46790500
H	2.63161100	1.70261400	1.26078100
C	4.45068700	2.61661500	0.57061700
H	4.53881700	3.25752200	1.44315300
C	5.40476700	2.67934300	-0.44680400
H	6.23897200	3.37089500	-0.36985800
C	5.28397500	1.84993500	-1.56450500
H	6.02293900	1.89284500	-2.35951400
C	4.21413100	0.95951600	-1.66508200
H	4.14607500	0.31708100	-2.53714200
C	1.46923500	-0.49411000	-2.53603900
H	1.13501000	0.46364200	-2.94009200
H	0.65886800	-1.21553400	-2.66344300
H	2.33968000	-0.84682100	-3.09463500
C	-0.21187700	2.30162300	-0.50980500
C	0.48754300	2.90586700	-1.56418600
C	-1.29593000	3.05662200	0.03653200
C	0.13877200	4.16115000	-2.07754600
H	1.34709000	2.40903200	-2.00264800
C	-1.64812300	4.31531600	-0.47542400
C	-0.93621800	4.86823100	-1.53756400
H	0.71075400	4.58572100	-2.89930100
H	-2.47855800	4.87184700	-0.05008000
H	-1.21453700	5.84096300	-1.93304200
C	-0.34185600	-1.11006400	1.88383500
N	-1.55915700	1.24305600	1.54708600
H	-2.60805500	-1.37294800	4.48290800
H	-3.54035300	0.52591800	4.15830900
C	-1.62419900	-0.65766900	-0.96557700
H	-1.38408000	-0.02156900	-1.80099300
H	-1.17298100	-1.63059700	-0.86277500
H	-2.46414600	-0.40608300	-0.33806400
I	-3.42798600	-1.88464000	-2.67549700