SUPPORTING INFORMATION

Carbonium vs. Carbenium Ion-like Transition State Geometries for Carbocation Cyclization–How Strain Associated with Bridging Affects 5-*exo* vs. 6-*endo* Selectivity

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All structures were optimized using density functional theory (M06-2X for organic structures and M06) [1] for organometallic systems with 6-31G(d) basis for main group atoms and SDD basis for Pt and Pd in gas phase or in dichloromethane (as indicated) using CPCM[2] solvation model with UFF radii.

Figure S1. Relative free energy barriers (energies of respective intermediates are in parenthesis) of 6-*endo* and 5-*exo* ring closures (M=Pt$(PH_3)_3$ and $PdCl_2MeCN$) . All structures were calculated using M06 using 6-31G(d) (and SDD for Pt) basis set in gas phase. Free energies are in kcal/mol.

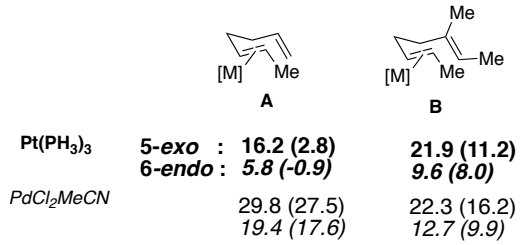
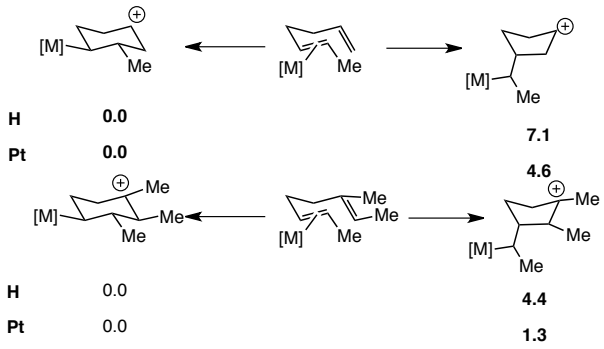


Figure S2. Relative energetics of 6-*endo* and 5-*exo* intermediates (M=Pt$(PH_3)_3$ and H) . All structures were calculated using M06-2X for M=H and M06 using 6-31G(d) (and SDD for Pt) basis set in gas phase for M=Pt. Free energies are in kcal/mol.

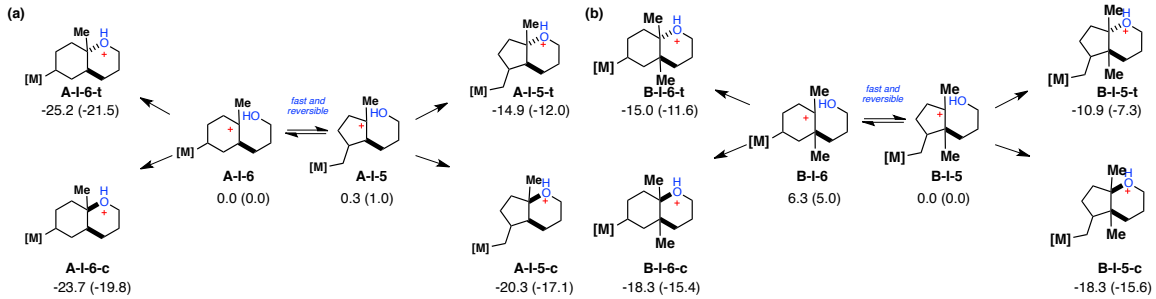


As shown in Figure S3, once the cyclization occurs i.e., to generate intermediates **A-I-6** or **A-I-5** then trapping of these intermediates with an appended nucleophile is downhill in energy and fast (finding the transition states for nucleophile attack was not found for

[1] (a) Zhao, Y.; Truhlar, D. G. *Theor. Chem. Acc.* **2008**, 120, 215– 241. (b) Zhao, Y.; Truhlar, D. G. *Acc. Chem. Res.* **2008**, 41, 157– 167
[2] Barone, V.; Cossi, M. *J. Phys. Chem. A* **1998**, *102*, 1995.

any structures indicative of spontaneous and barrierless OH attack once the cyclic intermediates are formed).

Figure S3. Relative energetics of 6-*endo* and 5-*exo* intermediates (M=Pt(PH$_3$)$_3$). All structures were calculated using M06 using 6-31G(d) (and SDD for Pt) basis set in gas phase. Enthalpies and free energies (parenthesis) are in kcal/mol.



Molecular and atomic electron populations can be split into two electronic contributions, based on the integration of the exchange density: electron localization and delocalization,[3] as shown in equations 1-3. In these definitions, η_i and η_j denote the occupation numbers of natural orbitals ϕ_i and ϕ_j, and $S_{ij}(A)$ is the overlap integral of ϕ_i and ϕ_j, which corresponds to the exchange density at DFT level, over the basin of atom A. $\lambda(A)$ provides a measure of the number of electrons located on that atom, whereas $\delta(A)$ accounts for the number of electrons shared by two different atoms, A and B, not necessarily bonded, in the molecule.

$$\lambda(A) = \sum_{i,j} \eta_i^{1/2} \eta_j^{1/2} S_{ij}(A)^2 \qquad \text{eq. 1}$$

$$\delta(A,B) = 2 \sum_{i,j} \eta_i^{1/2} \eta_j^{1/2} S_{ij}(A) S_{ij}(B) \qquad \text{eq.2}$$

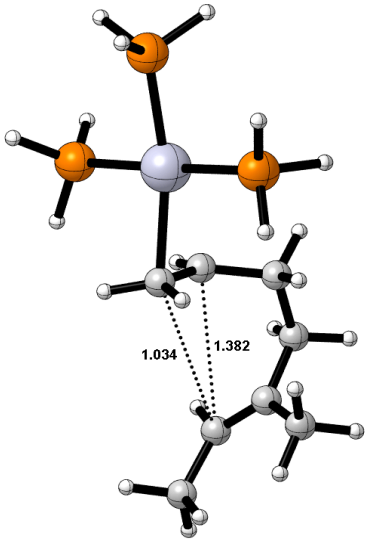
$$N(A) = \lambda(A) + \frac{1}{2} \sum_{A \neq B} \delta(A,B) \qquad \text{eq. 3}$$

Electron delocalization, calculated by the integration of exchange density between nuclephilic and electrophilic atoms of Pt-complexed reactant for R1=CH$_3$/R2=CH$_3$/R3=H and R1=CH$_3$/R2=H/R3=CH$_3$ systems (Table 1, entries 5 and 6) were obtained to understand the regioselectivity in these molecules (Figure S4).[4] The former case (trans isomer) shows a larger 5-exo delocalization whereas the latter (cis isomer) presents greater delocalization at 6-endo. The electron delocalization between two atoms controls the ring formation explaining the experimental results. This behavior

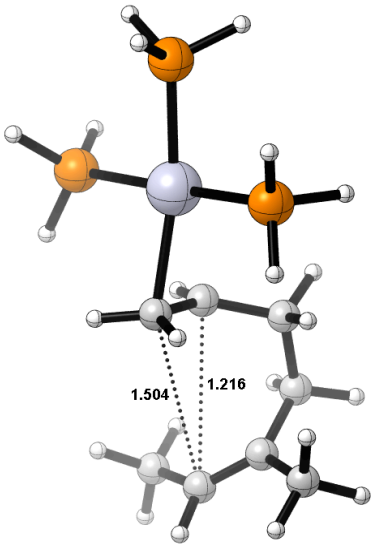
[3] (a) Fradera, X. ; Austen, M. A.; Bader, R. F. W. *J. Phys. Chem. A* **1999**, 103, 304–314. (b) Bader, R. F. W.; Streitwieser, A.; Neuhaus, A.; Laidig, K. E.; Speers, P. *J. Am. Chem. Soc.*, **1996**, 118 (21), 4959–4965.
[4] Electron delocalization was calculated using the *AIMAll* program (Version 12.09.23), Todd A. Keith, TK Gristmill Software, Overland Park KS, USA, 2012 (aim.tkgristmill.com).

agrees with the rule developed by Matín-Pendás *et al.*: a bond between two atoms is found when the exchange between them is the largest.[5] In this case, the ring formation process follow the maximum exchange path.

Figure S4. Electron delocalization (x 10^{-2}) between nuclephilic and electrophilic atoms of Pt-complexed reactant for R1=CH_3/R2=CH_3/R3=H and R1=CH_3/R2=H/R3=CH systems.



δ(5-*exo*) = 1.382 x 10^{-2} e
δ(6-*endo*) = 1.034 x 10^{-2} e



δ(5-*exo*) = 1.216 x 10^{-2} e
δ(6-*endo*) = 1.504 x 10^{-2} e

[5] Martín Pendás, A.; Francisco, E.; Blanco, M. A.; Gatti, C. *Chem. Eur. J.* **2007**, 13, 9362 – 9371

Energies and XYZ coordinates:

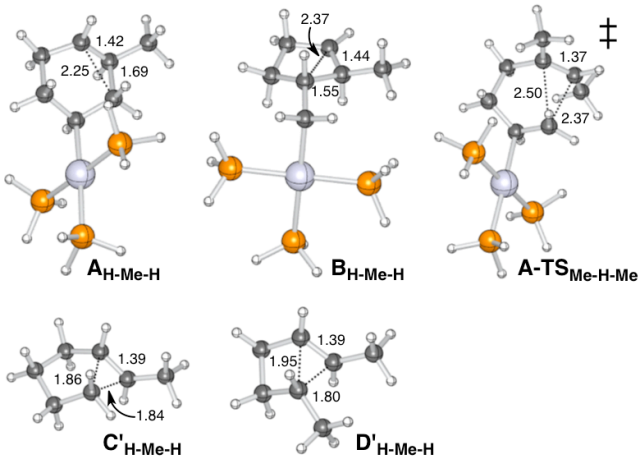


Figure 2. Representative structures of computed minima and a transition structure.

Figure 2, $A_{H\text{-}Me\text{-}H}$
HF: -1421.89739649

C	-3.217692000	-1.033927000	0.597816000
C	-1.848369000	-0.957878000	-0.006890000
C	-1.350876000	0.639382000	-0.256588000
C	-1.404472000	0.934471000	1.130670000
C	-2.653492000	1.101456000	1.838145000
C	-3.217876000	-0.397137000	1.966056000
H	-1.061944000	-1.451471000	0.583825000
H	-1.772700000	-1.326423000	-1.039596000
H	-3.886922000	-0.453938000	-0.059297000
H	-2.530879000	1.513534000	2.844824000
H	-3.387171000	1.683866000	1.268335000
H	-2.584794000	-0.941342000	2.680654000
H	-4.211842000	-0.305666000	2.422423000
H	-2.173910000	1.075706000	-0.835931000
Pt	-4.042744000	-3.040024000	0.705106000
C	-0.013934000	0.651968000	-0.961911000
H	-0.079939000	0.150135000	-1.933177000
H	0.309142000	1.682255000	-1.147161000
H	0.763220000	0.154452000	-0.367456000
P	-2.007602000	-3.947783000	1.475679000
H	-1.007616000	-4.113736000	0.502944000
H	-1.313152000	-3.235996000	2.468932000
H	-2.039020000	-5.231294000	2.047310000
P	-5.052889000	-5.216931000	0.839986000
H	-5.188438000	-5.751948000	2.132555000
H	-6.355801000	-5.386149000	0.342106000
H	-4.382787000	-6.265177000	0.186113000
P	-6.011726000	-2.044674000	-0.090694000
H	-5.937346000	-1.577851000	-1.412754000
H	-7.206263000	-2.782394000	-0.112447000
H	-6.403460000	-0.883659000	0.596974000
H	-0.485507000	0.783683000	1.711787000

Figure 2, $B_{H\text{-}Me\text{-}H}$

HF: -1421.88522044

C	-3.057684000	-0.976557000	0.828363000
C	-1.814933000	-0.206247000	0.311248000
C	-1.139225000	0.252810000	1.496184000
C	-1.958953000	0.110788000	2.673991000
C	-3.351152000	-0.263172000	2.152992000
H	-2.681378000	-1.990433000	1.069130000
H	-1.467486000	-0.785451000	3.138712000
H	-1.848152000	0.891035000	3.438833000
H	-3.912430000	-0.871533000	2.869721000
H	-3.913604000	0.666771000	1.967951000
H	-2.201745000	0.836429000	0.056008000
C	-1.006483000	-0.751291000	-0.850926000
H	-1.621676000	-0.832517000	-1.753244000
H	-0.138739000	-0.125745000	-1.089054000
H	-0.647182000	-1.759899000	-0.612830000
C	-4.194101000	-1.160778000	-0.169882000
H	-3.788233000	-1.654130000	-1.064681000
H	-4.895987000	-1.898535000	0.243202000
P	-6.721440000	0.165984000	1.126035000
H	-6.648692000	1.101879000	2.173207000
H	-8.105543000	0.148024000	0.884741000
H	-6.546983000	-1.042969000	1.820713000
P	-6.803319000	2.353625000	-1.501572000
H	-7.175630000	2.363647000	-2.857791000
H	-8.066080000	2.510854000	-0.902228000
H	-6.300893000	3.659755000	-1.367401000
P	-4.127725000	0.592700000	-2.750761000
H	-4.670293000	1.275172000	-3.853061000
H	-2.843254000	1.166044000	-2.709155000
H	-3.842573000	-0.659819000	-3.319862000
Pt	-5.379318000	0.519165000	-0.769640000
H	-0.122701000	0.662547000	1.500139000

Figure 2, $A\text{-}TS_{Me\text{-}H\text{-}Me}$

HF: -1461.40135362

C	-2.742862000	-1.242866000	0.647307000
C	-1.842645000	-1.099822000	-0.437440000
C	-1.408466000	1.233578000	-0.462134000
C	-0.935379000	0.885176000	0.771781000
C	-1.821906000	0.641649000	1.946031000
C	-2.184495000	-0.876481000	1.994592000
H	-0.805261000	-1.422632000	-0.349829000
H	-2.191864000	-0.968293000	-1.461845000
H	-3.714742000	-0.761874000	0.478189000
H	-1.304518000	0.901071000	2.878663000
H	-2.745214000	1.230469000	1.904952000
H	-1.264613000	-1.433434000	2.226402000
H	-2.896360000	-1.067948000	2.805467000
C	0.518537000	0.610747000	0.976905000
H	0.687803000	-0.332360000	1.517242000

H	1.075584000	0.582044000	0.033571000
H	0.955062000	1.400577000	1.604764000
Pt	-3.083329000	-3.376288000	0.185832000
P	-1.214830000	-4.063547000	1.456685000
H	-0.002563000	-3.395846000	1.223901000
H	-1.360883000	-3.928474000	2.844871000
H	-0.817683000	-5.404365000	1.344192000
P	-4.960318000	-2.652218000	-1.026926000
H	-6.091674000	-2.397049000	-0.239894000
H	-4.798177000	-1.431351000	-1.701570000
H	-5.477333000	-3.480272000	-2.032498000
P	-3.564094000	-5.645054000	-0.262527000
H	-2.539066000	-6.350550000	-0.909842000
H	-3.797329000	-6.449406000	0.862109000
H	-4.672389000	-5.950909000	-1.064572000
H	-0.666169000	1.309329000	-1.261793000
C	-2.763975000	1.753256000	-0.808304000
H	-2.701258000	2.836144000	-0.983742000
H	-3.136860000	1.311295000	-1.741883000
H	-3.513357000	1.590390000	-0.027166000

Figure 2, C'$_{H\text{-}Me\text{-}H}$

HF: -274.13380407

C	-2.974975000	-1.047280000	0.775023000
C	-1.748322000	-0.938099000	-0.117147000
C	-1.308838000	0.740216000	-0.722361000
C	-0.984725000	0.588506000	0.620467000
C	-1.921099000	0.900950000	1.757083000
C	-2.618427000	-0.425206000	2.122711000
H	-0.902569000	-1.572037000	0.159751000
H	-1.952981000	-1.146524000	-1.172938000
H	-3.817614000	-0.523666000	0.311187000
H	-1.355526000	1.317689000	2.593691000
H	-2.661314000	1.639480000	1.434556000
H	-1.928530000	-1.075278000	2.670929000
H	-3.490851000	-0.254030000	2.755816000
H	-2.289850000	1.159269000	-0.951481000
C	-0.306267000	0.682818000	-1.834012000
H	-0.739566000	0.270625000	-2.747843000
H	0.006723000	1.710181000	-2.050586000
H	0.580384000	0.108664000	-1.553892000
H	-3.251184000	-2.103227000	0.855231000
H	0.043377000	0.316174000	0.857880000

Figure 2, D'$_{H\text{-}Me\text{-}H}$

HF: -274.11184901

C	-2.937117000	-1.131398000	0.795993000
C	-2.350232000	-0.588212000	-0.528016000
C	-1.703252000	0.630253000	0.078983000
C	-0.982725000	0.499290000	1.259893000
C	-2.692996000	0.107111000	1.672475000
H	-1.627549000	-1.246378000	-1.017933000
H	-3.114539000	-0.305922000	-1.252074000

H	-3.993511000	-1.400289000	0.741691000
H	-3.399858000	0.911447000	1.440786000
H	-2.382999000	-1.992752000	1.178117000
C	-2.614533000	-0.053539000	3.185184000
H	-3.602679000	-0.417033000	3.491857000
H	-1.865984000	-0.791443000	3.481716000
H	-2.433113000	0.891307000	3.699471000
H	-0.551013000	-0.479461000	1.473820000
C	-0.378156000	1.677441000	1.968213000
H	-0.258119000	1.478130000	3.034712000
H	0.618114000	1.861300000	1.554326000
H	-0.977720000	2.582332000	1.834815000
H	-1.938740000	1.634671000	-0.277412000

Table 1. Free energies (kcal/mol; gas phase) of intermediates formed via activation with $[Pt(PH_3)_3]^{2+}$ or H^+ relative to lowest energy intermediate for each system. R^1, R^2 and R^3 correspond to labels in Scheme 1.

Entry	X	R^1	R^2	R^3	***6-endo***		***5-exo***	
					A	**C**	**D**	**B**
1	H	H	H	H	0.0			3.8
	Pt				0.0			5.3
2	H	Me	H	H	0.0			2.0
	Pt				1.3			0.0
3	H	H	Me	H		0.0	12.6	
	Pt				0.0			5.5
4	H	H	H	Me		0.0	14.0	
	Pt				0.4			0.0
5	H	Me	Me	H	0.0			1.4
	Pt				0.0			2.4
6	H	Me	H	Me	0.0			1.6
	Pt				2.0			0.0
7	H	H	Me	Me		0.0	14.4	
	Pt				0.0*			12.2*
8	H	Me	Me	Me	0.8			0.0
	Pt				5.5			0.0

*These structures resemble 4- and 5- membered carbocycles with exocyclic 3° carbocation groups; structural data is available in the Supporting Information.

Table 1, Entry 1, H, A

HF: -234.83249371

C	-2.972452000	-1.014515000	0.698638000
C	-1.866762000	-1.011032000	-0.343010000
C	-1.325294000	0.502842000	-0.572742000
C	-0.953129000	0.796034000	0.780578000
C	-1.936702000	1.077145000	1.785016000
C	-2.474152000	-0.438706000	2.013191000
H	-1.032938000	-1.655332000	-0.049470000

H	-2.199235000	-1.321395000	-1.336871000
H	-3.841901000	-0.453609000	0.339017000
H	-1.535449000	1.442677000	2.730116000
H	-2.783325000	1.666211000	1.427541000
H	-1.674993000	-1.048330000	2.444944000
H	-3.256526000	-0.325082000	2.767818000
H	-2.167322000	1.092136000	-0.940650000
H	-3.301932000	-2.046972000	0.864595000
H	0.061131000	0.550035000	1.103375000
H	-0.495196000	0.464049000	-1.278050000

Table 1, Entry 1, H, B

HF: -234.82269995

C	-2.918011000	-1.073429000	0.862695000
C	-2.389282000	-0.556239000	-0.487423000
C	-1.392136000	0.436116000	-0.155730000
C	-1.420627000	0.760042000	1.248295000
C	-2.712790000	0.120911000	1.812909000
H	-2.132965000	-1.251977000	-1.291988000
H	-3.149212000	0.136239000	-0.940636000
H	-3.955641000	-1.403198000	0.803737000
H	-3.522214000	0.846484000	1.659227000
H	-2.308014000	-1.926171000	1.183362000
C	-2.625439000	-0.242427000	3.288401000
H	-3.563275000	-0.691280000	3.624169000
H	-1.821065000	-0.963931000	3.466865000
H	-2.439738000	0.641756000	3.903525000
H	-0.552617000	0.114074000	1.563028000
H	-0.707686000	0.881802000	-0.878817000
H	-1.132097000	1.777605000	1.527502000

Table 1, Entry 1, Pt, A

HF: -1382.61051696

C	-3.197196000	-1.039766000	0.574168000
C	-1.831476000	-0.979036000	-0.052197000
C	-1.358708000	0.580354000	-0.193892000
C	-1.431024000	0.985390000	1.177706000
C	-2.693785000	1.158294000	1.824678000
C	-3.185252000	-0.405978000	1.937428000
H	-1.059352000	-1.498975000	0.532921000
H	-1.785560000	-1.357752000	-1.081250000
H	-3.873815000	-0.460971000	-0.076362000
H	-2.645154000	1.571342000	2.835777000
H	-3.445118000	1.667706000	1.211258000
H	-2.520835000	-0.920261000	2.644562000
H	-4.169410000	-0.323419000	2.417083000
H	-2.090061000	1.067903000	-0.847755000
Pt	-4.041066000	-3.039885000	0.710015000
P	-2.000017000	-3.966157000	1.446021000
H	-1.019591000	-4.132710000	0.453911000
H	-1.283086000	-3.267996000	2.432629000
H	-2.034305000	-5.253470000	2.008698000
P	-5.060080000	-5.210491000	0.852906000

H	-5.189238000	-5.744001000	2.146610000
H	-6.366404000	-5.372878000	0.362098000
H	-4.396561000	-6.259679000	0.194075000
P	-6.015955000	-2.037818000	-0.066027000
H	-5.953354000	-1.577409000	-1.390925000
H	-7.213512000	-2.770847000	-0.070799000
H	-6.395624000	-0.872283000	0.620794000
H	-0.530688000	0.901845000	1.796759000
H	-0.355597000	0.593940000	-0.628693000

Table 1, Entry 1, Pt, B

HF: -1382.59900677

C	-3.023381000	-0.929980000	0.811136000
C	-1.870483000	-0.009808000	0.350335000
C	-1.174792000	0.370055000	1.554189000
C	-1.953808000	0.057484000	2.724235000
C	-3.334697000	-0.348911000	2.196336000
H	-2.568202000	-1.925609000	0.970386000
H	-1.394034000	-0.847367000	3.088304000
H	-1.861012000	0.759471000	3.564881000
H	-3.847249000	-1.049180000	2.863734000
H	-3.949453000	0.561393000	2.104599000
H	-2.323157000	0.984941000	0.075116000
C	-4.159181000	-1.129490000	-0.185176000
H	-3.732402000	-1.607936000	-1.079931000
H	-4.843989000	-1.886784000	0.221903000
P	-6.678743000	0.212705000	1.139353000
H	-6.591243000	1.146390000	2.187367000
H	-8.065937000	0.198861000	0.915550000
H	-6.501075000	-0.997260000	1.831971000
P	-6.781412000	2.366581000	-1.526882000
H	-6.938076000	2.551333000	-2.912332000
H	-8.129531000	2.377073000	-1.126145000
H	-6.393994000	3.662430000	-1.144066000
P	-4.203471000	0.456825000	-2.817418000
H	-4.375322000	1.477322000	-3.768212000
H	-2.802374000	0.347731000	-2.793046000
H	-4.539298000	-0.683234000	-3.565734000
Pt	-5.369405000	0.530106000	-0.786405000
H	-0.179681000	0.826311000	1.583929000
H	-1.238813000	-0.294537000	-0.501311000

Table 1, Entry 2, H, A

HF: -274.15067209

C	-3.075989000	-0.989194000	0.683075000
C	-1.998993000	-1.057736000	-0.390660000
C	-1.326695000	0.376143000	-0.592652000
C	-0.844494000	0.655249000	0.749902000
C	-1.829167000	0.960564000	1.775301000
C	-2.505779000	-0.468542000	1.995401000
H	-1.223671000	-1.785624000	-0.127809000
H	-2.394954000	-1.335033000	-1.370696000

H	-3.901114000	-0.349245000	0.350194000
H	-1.390962000	1.305614000	2.713372000
H	-2.609449000	1.639336000	1.422126000
H	-1.762335000	-1.160312000	2.405691000
H	-3.272017000	-0.314725000	2.758958000
H	-2.115188000	1.063135000	-0.910181000
H	-3.492028000	-1.989833000	0.841836000
C	0.557455000	0.410481000	1.107547000
H	1.050929000	1.391517000	0.970145000
H	0.691840000	0.138684000	2.157455000
H	1.057398000	-0.287529000	0.431480000
H	-0.532158000	0.304234000	-1.337310000

Table 1, Entry 2, H, B

HF: -274.14319640

C	-2.928489000	-1.059901000	0.906851000
C	-2.838037000	-0.204313000	-0.366634000
C	-1.993851000	0.939097000	-0.016363000
C	-1.802410000	0.985813000	1.433931000
C	-2.808315000	-0.021742000	2.036123000
H	-2.592895000	-0.679597000	-1.322348000
H	-3.813972000	0.307452000	-0.535442000
H	-3.850251000	-1.641049000	0.953342000
H	-3.770401000	0.494893000	2.147472000
H	-2.084338000	-1.758600000	0.942583000
C	-2.375799000	-0.589165000	3.380421000
H	-3.113792000	-1.306556000	3.747231000
H	-1.414254000	-1.106610000	3.292969000
H	-2.275075000	0.199363000	4.130652000
H	-0.778379000	0.555379000	1.537538000
H	-1.740829000	1.993276000	1.857678000
C	-1.402470000	1.861218000	-0.983387000
H	-0.416329000	1.422747000	-1.228069000
H	-1.961015000	1.899521000	-1.921973000
H	-1.216058000	2.854791000	-0.570882000

Table 1, Entry 2, Pt, A

HF: -1421.91807534

C	-3.258394000	-1.152879000	0.557383000
C	-1.856158000	-1.092271000	-0.005598000
C	-1.402654000	0.431969000	-0.202597000
C	-1.519611000	0.965407000	1.142383000
C	-2.855347000	1.109568000	1.688604000
C	-3.330244000	-0.412127000	1.874505000
H	-1.112822000	-1.567037000	0.654657000
H	-1.760126000	-1.556093000	-0.995590000
H	-3.903955000	-0.625445000	-0.165895000
H	-2.883292000	1.617601000	2.658483000
H	-3.553851000	1.578195000	0.985005000
H	-2.698517000	-0.877434000	2.646627000
H	-4.342828000	-0.346297000	2.293513000
Pt	-4.086192000	-3.140883000	0.776283000
P	-2.061091000	-3.972769000	1.639805000

H	-1.037030000	-4.175823000	0.699442000
H	-1.394040000	-3.199333000	2.605925000
H	-2.083474000	-5.222029000	2.283418000
P	-5.090842000	-5.321436000	1.009568000
H	-4.942651000	-5.951687000	2.257391000
H	-6.477177000	-5.448919000	0.817958000
H	-4.615037000	-6.326171000	0.149647000
P	-6.034431000	-2.210104000	-0.137400000
H	-5.941985000	-1.882804000	-1.499707000
H	-7.236956000	-2.934514000	-0.100993000
H	-6.429408000	-0.980041000	0.415463000
C	-0.343412000	1.116692000	1.993038000
H	-0.026988000	2.174154000	1.877115000
H	-0.557662000	0.991634000	3.061665000
H	0.514836000	0.515942000	1.668247000
H	-0.382704000	0.457349000	-0.600693000
H	-2.105099000	0.889089000	-0.909639000

Table 1, Entry 2, Pt, B

HF: -1421.91779995

C	-2.120274000	0.685393000	0.292990000
C	-3.557446000	0.919947000	-0.230101000
C	-4.431188000	0.886260000	0.939423000
C	-3.705390000	0.324182000	2.079133000
C	-2.384098000	-0.205689000	1.514128000
H	-1.748238000	1.662736000	0.651760000
H	-3.531492000	1.210877000	2.731150000
H	-4.314606000	-0.344820000	2.703868000
H	-1.569860000	-0.192554000	2.246524000
H	-2.523162000	-1.249302000	1.190088000
C	-1.183585000	0.108034000	-0.758442000
H	-1.635733000	-0.824498000	-1.136767000
H	-1.123193000	0.778689000	-1.629123000
P	3.129249000	-0.627890000	0.514148000
H	4.075382000	0.395244000	0.323803000
H	3.368848000	-0.943331000	1.862946000
H	3.795153000	-1.695242000	-0.114671000
Pt	0.831636000	-0.224635000	-0.137826000
P	1.063887000	2.101536000	0.040780000
H	2.318986000	2.657947000	-0.258250000
H	0.223068000	2.871706000	-0.781235000
H	0.816623000	2.683031000	1.297002000
P	0.430574000	-2.486632000	-0.574856000
H	1.450233000	-3.434296000	-0.382325000
H	-0.632909000	-3.089229000	0.117343000
H	0.062711000	-2.739805000	-1.906120000
H	-3.743588000	1.749547000	-0.926282000
H	-3.881365000	0.005905000	-0.785744000
C	-5.797434000	1.376173000	0.972848000
H	-6.395481000	0.972839000	1.796003000
H	-5.724660000	2.472451000	1.126881000
H	-6.304678000	1.268598000	0.004625000

Table 1, Entry 3, H, C

HF: -274.13380407

C	-2.974975000	-1.047280000	0.775023000
C	-1.748322000	-0.938099000	-0.117147000
C	-1.308838000	0.740216000	-0.722361000
C	-0.984725000	0.588506000	0.620467000
C	-1.921099000	0.900950000	1.757083000
C	-2.618427000	-0.425206000	2.122711000
H	-0.902569000	-1.572037000	0.159751000
H	-1.952981000	-1.146524000	-1.172938000
H	-3.817614000	-0.523666000	0.311187000
H	-1.355526000	1.317689000	2.593691000
H	-2.661314000	1.639480000	1.434556000
H	-1.928530000	-1.075278000	2.670929000
H	-3.490851000	-0.254030000	2.755816000
H	-2.289850000	1.159269000	-0.951481000
C	-0.306267000	0.682818000	-1.834012000
H	-0.739566000	0.270625000	-2.747843000
H	0.006723000	1.710181000	-2.050586000
H	0.580384000	0.108664000	-1.553892000
H	-3.251184000	-2.103227000	0.855231000
H	0.043377000	0.316174000	0.857880000

Table 1, Entry 3, H, D

HF: -274.11184901

C	-2.937117000	-1.131398000	0.795993000
C	-2.350232000	-0.588212000	-0.528016000
C	-1.703252000	0.630253000	0.078983000
C	-0.982725000	0.499290000	1.259893000
C	-2.692996000	0.107111000	1.672475000
H	-1.627549000	-1.246378000	-1.017933000
H	-3.114539000	-0.305922000	-1.252074000
H	-3.993511000	-1.400289000	0.741691000
H	-3.399858000	0.911447000	1.440786000
H	-2.382999000	-1.992752000	1.178117000
C	-2.614533000	-0.053539000	3.185184000
H	-3.602679000	-0.417033000	3.491857000
H	-1.865984000	-0.791443000	3.481716000
H	-2.433113000	0.891307000	3.699471000
H	-0.551013000	-0.479461000	1.473820000
C	-0.378156000	1.677441000	1.968213000
H	-0.258119000	1.478130000	3.034712000
H	0.618114000	1.861300000	1.554326000
H	-0.977720000	2.582332000	1.834815000
H	-1.938740000	1.634671000	-0.277412000

Table 1, Entry 3, Pt, A

HF: -1421.89739649

C	-3.217692000	-1.033927000	0.597816000
C	-1.848369000	-0.957878000	-0.006890000
C	-1.350876000	0.639382000	-0.256588000
C	-1.404472000	0.934471000	1.130670000
C	-2.653492000	1.101456000	1.838145000

C	-3.217876000	-0.397137000	1.966056000
H	-1.061944000	-1.451471000	0.583825000
H	-1.772700000	-1.326423000	-1.039596000
H	-3.886922000	-0.453938000	-0.059297000
H	-2.530879000	1.513534000	2.844824000
H	-3.387171000	1.683866000	1.268335000
H	-2.584794000	-0.941342000	2.680654000
H	-4.211842000	-0.305666000	2.422423000
H	-2.173910000	1.075706000	-0.835931000
Pt	-4.042744000	-3.040024000	0.705106000
C	-0.013934000	0.651968000	-0.961911000
H	-0.079939000	0.150135000	-1.933177000
H	0.309142000	1.682255000	-1.147161000
H	0.763220000	0.154452000	-0.367456000
P	-2.007602000	-3.947783000	1.475679000
H	-1.007616000	-4.113736000	0.502944000
H	-1.313152000	-3.235996000	2.468932000
H	-2.039020000	-5.231294000	2.047310000
P	-5.052889000	-5.216931000	0.839986000
H	-5.188438000	-5.751948000	2.132555000
H	-6.355801000	-5.386149000	0.342106000
H	-4.382787000	-6.265177000	0.186113000
P	-6.011726000	-2.044674000	-0.090694000
H	-5.937346000	-1.577851000	-1.412754000
H	-7.206263000	-2.782394000	-0.112447000
H	-6.403460000	-0.883659000	0.596974000
H	-0.485507000	0.783683000	1.711787000

Table 1, Entry 3, Pt, B

HF: -1421.88522044

C	-3.057684000	-0.976557000	0.828363000
C	-1.814933000	-0.206247000	0.311248000
C	-1.139225000	0.252810000	1.496184000
C	-1.958953000	0.110788000	2.673991000
C	-3.351152000	-0.263172000	2.152992000
H	-2.681378000	-1.990433000	1.069130000
H	-1.467486000	-0.785451000	3.138712000
H	-1.848152000	0.891035000	3.438833000
H	-3.912430000	-0.871533000	2.869721000
H	-3.913604000	0.666771000	1.967951000
H	-2.201745000	0.836429000	0.056008000
C	-1.006483000	-0.751291000	-0.850926000
H	-1.621676000	-0.832517000	-1.753244000
H	-0.138739000	-0.125745000	-1.089054000
H	-0.647182000	-1.759899000	-0.612830000
C	-4.194101000	-1.160778000	-0.169882000
H	-3.788233000	-1.654130000	-1.064681000
H	-4.895987000	-1.898535000	0.243202000
P	-6.721440000	0.165984000	1.126035000
H	-6.648692000	1.101879000	2.173207000
H	-8.105543000	0.148024000	0.884741000
H	-6.546983000	-1.042969000	1.820713000
P	-6.803319000	2.353625000	-1.501572000

H	-7.175630000	2.363647000	-2.857791000
H	-8.066080000	2.510854000	-0.902228000
H	-6.300893000	3.659755000	-1.367401000
P	-4.127725000	0.592700000	-2.750761000
H	-4.670293000	1.275172000	-3.853061000
H	-2.843254000	1.166044000	-2.709155000
H	-3.842573000	-0.659819000	-3.319862000
Pt	-5.379318000	0.519165000	-0.769640000
H	-0.122701000	0.662547000	1.500139000

Table 1, Entry 4, H, C

HF: -274.13173807

C	-2.970007000	-1.090998000	0.903153000
C	-1.797593000	-0.970127000	-0.059115000
C	-1.437131000	0.730441000	-0.737655000
C	-1.046886000	0.581239000	0.590904000
C	-1.897531000	0.901447000	1.792400000
C	-2.552972000	-0.429784000	2.215975000
H	-0.932620000	-1.592455000	0.176404000
H	-2.057371000	-1.188528000	-1.100946000
H	-3.858581000	-0.612187000	0.480004000
H	-1.264987000	1.317140000	2.579953000
H	-2.659762000	1.643666000	1.541941000
H	-1.820397000	-1.056441000	2.735487000
H	-3.391511000	-0.266268000	2.895150000
H	-3.203628000	-2.153832000	1.020947000
H	-0.005411000	0.323540000	0.770616000
H	-0.672223000	0.548039000	-1.492016000
C	-2.685460000	1.394341000	-1.226914000
H	-2.408382000	2.419262000	-1.501771000
H	-3.065059000	0.908922000	-2.128976000
H	-3.474723000	1.447135000	-0.477702000

Table 1, Entry 4, H, D

HF: -274.10892460

C	-3.137409000	-1.026042000	0.684304000
C	-2.312013000	-0.610671000	-0.560733000
C	-1.693206000	0.579651000	0.119747000
C	-0.986866000	0.425974000	1.308577000
C	-2.741615000	0.112368000	1.652776000
H	-1.575604000	-1.352938000	-0.877375000
H	-2.917380000	-0.320715000	-1.417763000
H	-4.214767000	-1.038222000	0.511168000
H	-3.352701000	1.007852000	1.516999000
H	-2.842411000	-2.000983000	1.078722000
C	-2.702334000	-0.218094000	3.142392000
H	-3.746278000	-0.401806000	3.422664000
H	-2.131206000	-1.124965000	3.343538000
H	-2.327496000	0.605893000	3.752417000
H	-1.965227000	1.586915000	-0.192968000
C	-0.152073000	-0.777076000	1.656007000
H	-0.566561000	-1.713275000	1.277595000
H	0.832611000	-0.632730000	1.199300000

H	-0.004356000	-0.855215000	2.733966000
H	-0.724647000	1.350434000	1.821335000

Table 1, Entry 4, Pt, A

HF: -1421.89455313

C	-3.238919000	-1.025777000	0.960581000
C	-2.140120000	-0.913041000	-0.051827000
C	-1.614786000	0.702469000	-0.268609000
C	-1.221157000	0.785914000	1.091063000
C	-2.160510000	0.909717000	2.185460000
C	-2.739269000	-0.581921000	2.313434000
H	-1.268615000	-1.538440000	0.182344000
H	-2.423869000	-1.123870000	-1.092884000
H	-4.061416000	-0.349931000	0.680276000
H	-1.679849000	1.172514000	3.133302000
H	-2.995609000	1.587822000	1.982211000
H	-1.917429000	-1.209454000	2.689094000
H	-3.515311000	-0.546876000	3.087865000
Pt	-4.062217000	-3.029743000	0.840571000
P	-2.409751000	-3.895276000	2.281371000
H	-1.075551000	-3.520744000	2.046723000
H	-2.557933000	-3.563777000	3.638350000
H	-2.278625000	-5.292509000	2.357067000
P	-5.018020000	-5.226571000	0.627436000
H	-5.276152000	-5.924663000	1.819586000
H	-6.251271000	-5.367556000	-0.031009000
H	-4.236600000	-6.165533000	-0.067536000
P	-5.702350000	-2.059206000	-0.527548000
H	-5.231218000	-1.088222000	-1.428979000
H	-6.486077000	-2.871072000	-1.363163000
H	-6.682838000	-1.336841000	0.171395000
H	-0.767485000	0.604471000	-0.956079000
C	-2.727380000	1.554896000	-0.838265000
H	-2.344965000	2.562527000	-1.038411000
H	-3.067168000	1.144952000	-1.796872000
H	-3.593090000	1.656223000	-0.176301000
H	-0.200393000	0.472521000	1.336334000

Table 1, Entry 4, Pt, B

HF: -1421.89334852

C	-2.108810000	0.603721000	0.327170000
C	-3.478949000	1.122225000	-0.133214000
C	-4.412955000	0.874316000	0.891488000
C	-3.821902000	0.042434000	1.967794000
C	-2.487859000	-0.444433000	1.387498000
H	-1.673477000	1.474128000	0.851051000
H	-3.666999000	0.766367000	2.790773000
H	-4.486836000	-0.727942000	2.374754000
H	-1.715441000	-0.568160000	2.154402000
H	-2.630179000	-1.428121000	0.913036000
C	-1.164637000	0.139058000	-0.774042000
H	-1.567083000	-0.772928000	-1.244126000
H	-1.118000000	0.887167000	-1.580103000

P	3.143482000	-0.532419000	0.558403000
H	4.115975000	0.379117000	0.109362000
H	3.395343000	-0.508621000	1.941059000
H	3.765741000	-1.743914000	0.208679000
Pt	0.850554000	-0.186539000	-0.140564000
P	1.152200000	2.141455000	-0.168231000
H	2.110295000	2.608126000	-1.083534000
H	0.041084000	2.930468000	-0.515038000
H	1.580758000	2.776222000	1.010087000
P	0.414520000	-2.473690000	-0.344633000
H	1.447452000	-3.405880000	-0.148283000
H	-0.579482000	-2.996482000	0.500992000
H	-0.070461000	-2.861478000	-1.604341000
H	-3.547709000	2.008315000	-0.764931000
C	-4.457527000	-0.021459000	-0.803434000
H	-5.064319000	0.478780000	-1.559225000
H	-3.747880000	-0.747354000	-1.212816000
H	-5.145891000	-0.626256000	-0.184919000
H	-5.399625000	1.338801000	0.948506000

Table 1, Entry 5, H, A

HF: -313.44790541

C	-2.985668000	-0.932642000	0.730581000
C	-1.906488000	-0.930357000	-0.341828000
C	-1.307656000	0.541625000	-0.585490000
C	-0.841580000	0.819956000	0.764577000
C	-1.843949000	1.076143000	1.793274000
C	-2.448099000	-0.372831000	2.040852000
H	-1.084191000	-1.608186000	-0.083517000
H	-2.284240000	-1.231480000	-1.323565000
H	-3.849815000	-0.347189000	0.397094000
H	-1.416820000	1.457886000	2.722485000
H	-2.654698000	1.716847000	1.437511000
H	-1.671038000	-1.022884000	2.457773000
H	-3.223220000	-0.253425000	2.801397000
H	-2.177021000	1.165341000	-0.819896000
C	0.566257000	0.643745000	1.143286000
H	1.040405000	1.617189000	0.914469000
H	0.702136000	0.460032000	2.210719000
H	1.090478000	-0.094408000	0.531487000
C	-0.288841000	0.536280000	-1.718477000
H	-0.804999000	0.336237000	-2.659966000
H	0.211596000	1.503931000	-1.810579000
H	0.470302000	-0.239994000	-1.588093000
H	-3.335479000	-1.958537000	0.888089000

Table 1, Entry 5, H, B

HF: -313.44219454

C	-2.979046000	-1.094666000	0.939955000
C	-2.820490000	-0.303999000	-0.367283000
C	-1.853648000	0.759158000	-0.075267000
C	-1.561249000	0.800941000	1.355978000
C	-2.676069000	-0.047270000	2.022294000

H	-2.621416000	-0.847258000	-1.297186000
H	-3.743766000	0.284409000	-0.566912000
H	-3.967888000	-1.543637000	1.039774000
H	-3.550420000	0.608254000	2.144544000
C	-1.298091000	1.679807000	-1.066106000
H	-1.461000000	1.365672000	-2.097007000
H	-1.801230000	2.648999000	-0.898661000
H	-0.237970000	1.878524000	-0.869040000
H	-2.236315000	-1.900538000	0.978097000
C	-2.282444000	-0.625969000	3.373183000
H	-3.091061000	-1.244745000	3.770485000
H	-1.388903000	-1.253715000	3.283684000
H	-2.080785000	0.160801000	4.104915000
H	-0.665309000	0.122059000	1.322326000
C	-1.157121000	2.126477000	1.988902000
H	-0.840589000	1.959197000	3.020010000
H	-0.329063000	2.606307000	1.461025000
H	-2.010575000	2.811038000	2.002776000

Table 1, Entry 5, Pt, A

HF: -1461.20306262

C	-3.209106000	-1.032562000	0.861412000
C	-2.085042000	-0.923418000	-0.140013000
C	-1.508487000	0.589360000	-0.253429000
C	-1.129575000	0.826130000	1.129055000
C	-2.203347000	0.933799000	2.109161000
C	-2.748756000	-0.558898000	2.221388000
H	-1.236245000	-1.582286000	0.104734000
H	-2.379815000	-1.162577000	-1.172055000
H	-4.011956000	-0.343319000	0.548272000
H	-1.856757000	1.267820000	3.093293000
H	-3.032490000	1.563619000	1.765389000
H	-1.931001000	-1.174161000	2.629523000
H	-3.548313000	-0.536781000	2.972403000
H	-2.388746000	1.197066000	-0.509165000
Pt	-4.061795000	-3.020076000	0.807793000
C	0.258248000	0.737740000	1.574709000
H	0.690967000	1.747569000	1.418088000
H	0.361226000	0.520830000	2.643664000
H	0.878617000	0.072750000	0.961189000
C	-0.439954000	0.669884000	-1.327037000
H	-0.892548000	0.502820000	-2.310478000
H	0.035885000	1.657230000	-1.351436000
H	0.344735000	-0.086300000	-1.196936000
P	-2.368551000	-3.868710000	2.205417000
H	-1.046882000	-3.458886000	1.956362000
H	-2.494051000	-3.563008000	3.571179000
H	-2.198206000	-5.262815000	2.258815000
P	-5.069293000	-5.210285000	0.670128000
H	-5.665622000	-5.710268000	1.840789000
H	-6.106925000	-5.411128000	-0.256490000
H	-4.218194000	-6.278086000	0.334547000
P	-5.713825000	-2.050709000	-0.542400000

H	-5.234061000	-1.194504000	-1.548113000
H	-6.594249000	-2.870105000	-1.267412000
H	-6.605284000	-1.205116000	0.137291000

Table 1, Entry 5, Pt, B

HF: -1461.19661504

C	-3.180707000	-1.055420000	0.705847000
C	-1.971016000	-0.116135000	0.467454000
C	-1.480649000	0.202684000	1.812725000
C	-2.487940000	-0.141608000	2.812450000
C	-3.742366000	-0.524041000	2.027430000
H	-2.745274000	-2.054409000	0.906452000
H	-2.045325000	-1.037314000	3.307271000
H	-2.577431000	0.591017000	3.627442000
H	-4.364047000	-1.247857000	2.565403000
H	-4.342396000	0.383157000	1.847415000
H	-2.419150000	0.883936000	0.212382000
C	-0.161699000	0.727641000	2.119192000
H	-0.051975000	1.092165000	3.144386000
H	0.554543000	-0.104592000	1.964726000
H	0.158637000	1.486328000	1.389834000
C	-0.942027000	-0.507596000	-0.579047000
H	-1.426164000	-0.718078000	-1.538848000
H	-0.191602000	0.272042000	-0.753959000
H	-0.420344000	-1.426483000	-0.281385000
C	-4.139417000	-1.234400000	-0.466826000
H	-3.564355000	-1.574729000	-1.340085000
H	-4.801547000	-2.082109000	-0.240269000
P	-6.935049000	-0.323023000	0.605568000
H	-7.191839000	0.549592000	1.677970000
H	-8.241262000	-0.567768000	0.149191000
H	-6.652392000	-1.520072000	1.284538000
P	-6.952637000	2.126963000	-1.776639000
H	-7.144711000	2.272722000	-3.162322000
H	-8.293089000	2.075902000	-1.352649000
H	-6.635625000	3.451163000	-1.426642000
P	-3.955027000	0.779797000	-2.828382000
H	-4.389038000	1.587093000	-3.893872000
H	-2.716886000	1.385722000	-2.546395000
H	-3.535735000	-0.372960000	-3.513539000
Pt	-5.426613000	0.374279000	-1.052273000

Table 1, Entry 6, H, A

HF: -313.44584884

C	-3.043761000	-1.123340000	0.693141000
C	-1.985451000	-1.029224000	-0.398447000
C	-1.432440000	0.471110000	-0.570436000
C	-0.961766000	0.683175000	0.791783000
C	-1.931868000	0.861383000	1.862593000
C	-2.495395000	-0.621836000	2.022702000
H	-1.148445000	-1.703102000	-0.184770000
H	-2.373129000	-1.289897000	-1.388120000
H	-3.942239000	-0.563597000	0.415572000

H	-1.477674000	1.178091000	2.803330000
H	-2.766701000	1.509201000	1.589313000
H	-1.690957000	-1.271323000	2.384855000
H	-3.257214000	-0.569690000	2.804206000
H	-3.348648000	-2.170051000	0.800008000
C	-2.517349000	1.406237000	-1.109357000
H	-2.787116000	1.083973000	-2.117817000
H	-3.424505000	1.402921000	-0.503274000
H	-2.146278000	2.431961000	-1.172747000
C	0.456625000	0.484248000	1.121900000
H	0.897726000	1.496966000	1.061211000
H	0.615374000	0.134616000	2.145054000
H	0.985566000	-0.130740000	0.389822000
H	-0.587784000	0.414500000	-1.263545000

Table 1, Entry 6, H, B

HF: -313.44033510

C	-3.223640000	-1.057100000	0.984812000
C	-2.984821000	-0.270322000	-0.312400000
C	-1.933038000	0.707384000	-0.002997000
C	-1.657244000	0.722531000	1.427199000
C	-2.825880000	-0.053870000	2.083015000
H	-2.841857000	-0.817501000	-1.250103000
H	-3.849103000	0.405944000	-0.496722000
H	-4.255753000	-1.397958000	1.077363000
H	-3.645734000	0.666456000	2.206159000
H	-2.579783000	-1.942694000	1.012701000
C	-2.521617000	-0.681287000	3.436487000
H	-3.429986000	-1.123252000	3.853157000
H	-1.774968000	-1.477091000	3.355596000
H	-2.159835000	0.064898000	4.150165000
H	-1.450391000	1.720305000	1.827000000
C	-1.231573000	1.506962000	-1.011389000
H	-0.527872000	0.829787000	-1.524332000
H	-1.924498000	1.842677000	-1.791231000
H	-0.674215000	2.344021000	-0.589169000
C	-0.292784000	-0.075614000	1.462970000
H	0.504735000	0.482283000	0.969676000
H	-0.041426000	-0.190136000	2.519657000
H	-0.374406000	-1.070426000	1.017628000

Table 1, Entry 6, Pt, A

HF: -1461.20044734

C	-3.241815000	-1.085555000	0.917161000
C	-2.160965000	-0.969632000	-0.132608000
C	-1.581800000	0.540092000	-0.248779000
C	-1.147159000	0.741497000	1.124825000
C	-2.149971000	0.847098000	2.172440000
C	-2.706490000	-0.650833000	2.262307000
H	-1.319264000	-1.647642000	0.077156000
H	-2.500532000	-1.195469000	-1.153852000
H	-4.059657000	-0.391306000	0.667883000
H	-1.730848000	1.130803000	3.143932000

H	-2.991135000	1.500157000	1.917384000
H	-1.870961000	-1.280417000	2.608514000
H	-3.464388000	-0.641365000	3.055737000
Pt	-4.116741000	-3.062691000	0.834276000
P	-2.433853000	-3.955046000	2.215832000
H	-1.101571000	-3.609074000	1.929258000
H	-2.517615000	-3.618965000	3.577517000
H	-2.325236000	-5.354298000	2.294274000
P	-5.132897000	-5.243928000	0.653852000
H	-5.395942000	-5.927034000	1.854049000
H	-6.378115000	-5.363557000	0.013137000
H	-4.390146000	-6.214914000	-0.040041000
P	-5.769652000	-2.053490000	-0.486811000
H	-5.302236000	-1.113268000	-1.422156000
H	-6.610758000	-2.849494000	-1.281378000
H	-6.701176000	-1.287214000	0.232395000
H	-0.715061000	0.477630000	-0.920851000
C	-2.625359000	1.490364000	-0.825422000
H	-2.221090000	2.505004000	-0.911434000
H	-2.889592000	1.161479000	-1.837534000
H	-3.545627000	1.546450000	-0.234349000
C	0.260756000	0.580366000	1.483083000
H	0.693283000	1.601504000	1.454992000
H	0.415612000	0.222749000	2.508468000
H	0.834845000	-0.001228000	0.751420000

Table 1, Entry 6, Pt, B

HF: -1461.20142681

C	-2.000978000	0.520041000	0.293041000
C	-3.419407000	0.947962000	-0.180640000
C	-4.268431000	0.828608000	1.000640000
C	-3.589751000	0.051058000	2.039676000
C	-2.314785000	-0.498247000	1.398180000
H	-1.573689000	1.414236000	0.782323000
H	-3.337404000	0.837454000	2.787730000
H	-4.243497000	-0.638902000	2.592260000
H	-1.498391000	-0.612222000	2.120051000
H	-2.512566000	-1.491050000	0.965724000
C	-1.062357000	0.038648000	-0.804205000
H	-1.457363000	-0.893663000	-1.236312000
H	-1.039206000	0.760803000	-1.635479000
P	3.274409000	-0.526683000	0.485885000
H	4.233820000	0.386422000	0.012189000
H	3.545409000	-0.479299000	1.864544000
H	3.907201000	-1.736706000	0.149426000
Pt	0.965903000	-0.225247000	-0.190873000
P	1.211630000	2.105485000	-0.284168000
H	2.180990000	2.574555000	-1.186493000
H	0.088291000	2.851319000	-0.683854000
H	1.588710000	2.789859000	0.884121000
P	0.556236000	-2.520185000	-0.347603000
H	1.590371000	-3.441398000	-0.109200000
H	-0.453634000	-3.030840000	0.486350000

H	0.100456000	-2.937645000	-1.608525000
H	-3.479322000	1.937319000	-0.656442000
C	-4.095681000	-0.065269000	-1.168629000
H	-5.094774000	0.273249000	-1.460614000
H	-3.473665000	-0.098973000	-2.069963000
H	-4.168548000	-1.080314000	-0.760021000
C	-5.618600000	1.356912000	1.126121000
H	-6.311676000	0.514785000	0.932032000
H	-5.845287000	1.660647000	2.157498000
H	-5.850896000	2.153589000	0.412433000

Table 1, Entry 7, H, C

HF: -313.43981190

C	-2.961337000	-1.186065000	1.014838000
C	-1.801031000	-1.031382000	0.026310000
C	-1.367130000	0.838258000	-0.838438000
C	-1.128999000	0.440572000	0.500796000
C	-1.961488000	0.884320000	1.701670000
C	-2.551619000	-0.414852000	2.268050000
H	-0.973981000	-1.730610000	0.163820000
H	-2.129678000	-1.138033000	-1.015302000
H	-3.879243000	-0.767448000	0.588172000
H	-1.325382000	1.416337000	2.412426000
H	-2.760313000	1.567649000	1.398622000
H	-1.783610000	-0.968489000	2.818769000
H	-3.385224000	-0.233500000	2.948927000
C	-0.300346000	0.674133000	-1.860886000
H	-0.694149000	0.297850000	-2.808436000
H	0.088294000	1.684737000	-2.059446000
H	0.530294000	0.057429000	-1.513562000
H	-3.143056000	-2.250711000	1.189014000
C	-2.639166000	1.481419000	-1.262770000
H	-2.487794000	2.564731000	-1.138202000
H	-2.861115000	1.297091000	-2.315215000
H	-3.490139000	1.204971000	-0.638737000
H	-0.080618000	0.244150000	0.723149000

Table 1, Entry 7, H, D

HF: -313.41445622

C	-3.175079000	-1.132909000	0.691047000
C	-2.320928000	-0.597378000	-0.476418000
C	-1.765269000	0.578679000	0.322632000
C	-0.766540000	0.454023000	1.286954000
C	-2.960622000	0.095869000	1.576715000
H	-1.563689000	-1.279763000	-0.866637000
H	-2.923850000	-0.237560000	-1.310100000
H	-4.227442000	-1.311286000	0.459257000
H	-3.659183000	0.908186000	1.364804000
H	-2.770724000	-2.037712000	1.151591000
C	-2.793200000	-0.070202000	3.068706000
H	-3.773438000	-0.393101000	3.440457000
H	-2.074536000	-0.847596000	3.339096000
H	-2.547313000	0.864318000	3.578323000

C	-0.311735000	1.654141000	2.041492000
H	-0.230093000	1.440878000	3.111815000
H	0.702235000	1.896654000	1.693764000
H	-0.947666000	2.525576000	1.875190000
H	-1.996059000	1.594126000	0.005761000
C	-0.069215000	-0.828652000	1.570944000
H	-0.584289000	-1.710828000	1.190947000
H	0.898005000	-0.765263000	1.049303000
H	0.155179000	-0.943364000	2.634521000

Table 1, Entry 7, Pt, A

HF: -1461.19754067

C	-3.474524000	-1.211960000	0.607539000
C	-2.068307000	-1.022795000	0.027681000
C	-1.097738000	1.049932000	-0.495723000
C	-1.583428000	0.397456000	0.694096000
C	-2.797275000	0.909946000	1.465944000
C	-3.527132000	-0.370354000	1.878894000
H	-1.304789000	-1.754623000	0.317277000
H	-2.082500000	-1.024973000	-1.071750000
H	-4.155960000	-0.729070000	-0.114530000
H	-2.487235000	1.533208000	2.312750000
H	-3.452613000	1.523831000	0.833772000
H	-2.993901000	-0.849357000	2.714624000
H	-4.550372000	-0.180415000	2.226184000
Pt	-4.136739000	-3.235470000	0.875306000
C	0.296775000	0.867709000	-0.906596000
H	0.388706000	0.664800000	-1.982208000
H	0.796557000	1.846007000	-0.766100000
H	0.843701000	0.128651000	-0.313407000
P	-2.177874000	-3.769009000	2.053387000
H	-1.134152000	-4.349153000	1.311430000
H	-1.498673000	-2.713481000	2.689033000
H	-2.288457000	-4.686122000	3.112163000
P	-5.010597000	-5.472306000	1.184309000
H	-4.554640000	-6.232928000	2.275791000
H	-6.399906000	-5.590591000	1.365555000
H	-4.810410000	-6.385773000	0.135061000
P	-6.075309000	-2.527499000	-0.229726000
H	-5.919327000	-2.196009000	-1.585247000
H	-7.204633000	-3.361989000	-0.273281000
H	-6.621411000	-1.339743000	0.285216000
H	-0.754907000	0.145171000	1.368822000
C	-1.971364000	1.883127000	-1.332036000
H	-1.994766000	2.885472000	-0.863454000
H	-1.599870000	2.009964000	-2.353232000
H	-3.014462000	1.543167000	-1.334670000

Table 1, Entry 7, Pt, B

HF: -1461.17600643

C	-1.659506000	0.537640000	0.701852000
C	-3.768615000	0.519435000	-0.684023000
C	-3.397672000	0.893705000	0.625660000

C	-3.482859000	-0.066195000	1.813131000
C	-2.065068000	-0.617134000	1.608272000
H	-1.374430000	1.420190000	1.290034000
H	-3.574572000	0.499840000	2.745130000
H	-4.301776000	-0.791927000	1.780646000
H	-1.449157000	-0.733512000	2.508705000
H	-2.065765000	-1.573315000	1.064165000
C	-3.756130000	1.520313000	-1.761963000
H	-3.109655000	1.185047000	-2.588502000
H	-4.763886000	1.578845000	-2.207440000
H	-3.463944000	2.521651000	-1.432125000
C	-0.787351000	0.342191000	-0.488263000
H	-1.104076000	-0.513496000	-1.102183000
H	-0.783633000	1.225163000	-1.144374000
P	3.507690000	-0.343969000	0.900793000
H	4.428766000	0.698024000	0.695224000
H	3.708727000	-0.597681000	2.268252000
H	4.209260000	-1.418469000	0.326656000
Pt	1.231577000	0.002301000	0.180789000
C	-4.148566000	-0.857386000	-1.039746000
H	-3.929810000	-1.102535000	-2.085468000
H	-3.747111000	-1.620582000	-0.365199000
H	-5.248621000	-0.914957000	-0.933646000
P	1.513870000	2.327238000	0.038684000
H	1.746953000	2.786316000	-1.267936000
H	0.416090000	3.120663000	0.413865000
H	2.558863000	2.949312000	0.741570000
P	0.832296000	-2.311551000	0.125127000
H	0.460194000	-2.919851000	1.336238000
H	-0.188157000	-2.757226000	-0.732017000
H	1.899621000	-3.135179000	-0.270662000
H	-3.515311000	1.965103000	0.814703000

Table 1, Entry 8, H, A

HF: -352.74173027

C	-3.033273000	-1.065853000	0.757557000
C	-2.003664000	-1.009423000	-0.361647000
C	-1.428582000	0.479899000	-0.641409000
C	-0.930595000	0.721022000	0.711496000
C	-1.876494000	0.944587000	1.803882000
C	-2.448548000	-0.515959000	2.052131000
H	-1.162111000	-1.679672000	-0.150253000
H	-2.416921000	-1.300559000	-1.333744000
H	-3.939074000	-0.517328000	0.482262000
H	-1.385216000	1.297124000	2.712735000
H	-2.709139000	1.596377000	1.538285000
H	-1.640566000	-1.158724000	2.419065000
H	-3.189453000	-0.426777000	2.850088000
C	-0.363411000	0.389724000	-1.736178000
H	-0.851480000	0.155388000	-2.685388000
H	0.155451000	1.345692000	-1.858045000
H	0.378928000	-0.390517000	-1.551467000
H	-3.332502000	-2.108897000	0.908033000

C	0.488599000	0.527943000	1.053811000
H	0.981245000	1.475500000	0.766544000
H	0.652938000	0.377364000	2.121717000
H	0.977973000	-0.247336000	0.460137000
C	-2.576713000	1.394913000	-1.098152000
H	-2.204940000	2.411069000	-1.258012000
H	-2.957058000	1.024154000	-2.053326000
H	-3.414798000	1.438938000	-0.403120000

Table 1, Entry 8, H, B

HF: -352.73994379

C	-3.235012000	-0.962977000	1.046724000
C	-2.914481000	-0.261089000	-0.279934000
C	-1.779223000	0.636348000	-0.004933000
C	-1.452194000	0.648352000	1.412983000
C	-2.687296000	0.007064000	2.107378000
H	-2.786981000	-0.877563000	-1.176367000
H	-3.718908000	0.459400000	-0.537371000
H	-4.302310000	-1.155381000	1.165171000
H	-3.412004000	0.823672000	2.238359000
H	-2.720477000	-1.928183000	1.099590000
C	-2.425358000	-0.629868000	3.465242000
H	-3.369860000	-0.956443000	3.907896000
H	-1.780981000	-1.510409000	3.382495000
H	-1.965152000	0.076462000	4.162777000
C	-0.941929000	1.952146000	2.015723000
H	-0.639161000	1.776435000	3.051303000
H	-0.073609000	2.346524000	1.480569000
H	-1.730099000	2.710682000	2.016307000
C	-1.114547000	1.443058000	-1.033438000
H	-0.088188000	1.707156000	-0.768325000
H	-1.173147000	0.999937000	-2.029289000
H	-1.677703000	2.393651000	-1.060023000
C	-0.254463000	-0.397400000	1.325883000
H	0.604674000	0.028790000	0.805112000
H	0.021810000	-0.580218000	2.368584000
H	-0.523002000	-1.353671000	0.870320000

Table 1, Entry 8, Pt, A

HF: -1500.48179479

C	-3.287440000	-1.130640000	0.554804000
C	-1.890895000	-1.057056000	-0.011322000
C	-1.355498000	0.470835000	-0.263643000
C	-1.504029000	0.941047000	1.112454000
C	-2.842349000	1.109725000	1.669326000
C	-3.359731000	-0.384420000	1.868914000
H	-1.144930000	-1.542718000	0.638958000
H	-1.795466000	-1.510013000	-1.009817000
H	-3.952990000	-0.627061000	-0.164062000
H	-2.830340000	1.612479000	2.642618000
H	-3.539475000	1.620235000	0.998122000
H	-2.741721000	-0.857644000	2.647618000
H	-4.375442000	-0.304805000	2.278290000

Pt	-4.063723000	-3.138841000	0.779151000
C	0.072018000	0.379939000	-0.790558000
H	0.057232000	-0.015189000	-1.813081000
H	0.542458000	1.370565000	-0.835009000
H	0.718662000	-0.279634000	-0.199504000
P	-2.058277000	-3.882494000	1.748700000
H	-1.014874000	-4.173813000	0.853257000
H	-1.406415000	-3.019338000	2.647715000
H	-2.097625000	-5.064815000	2.506988000
P	-5.059442000	-5.329112000	0.986365000
H	-4.457056000	-6.273327000	1.836672000
H	-6.384301000	-5.373794000	1.454637000
H	-5.174856000	-6.080509000	-0.195807000
P	-6.015142000	-2.271370000	-0.191829000
H	-5.893948000	-1.900127000	-1.540625000
H	-7.189380000	-3.042290000	-0.214924000
H	-6.476212000	-1.076183000	0.385542000
C	-2.238809000	1.160373000	-1.308587000
H	-1.843264000	2.159384000	-1.529126000
H	-2.203800000	0.585276000	-2.241937000
H	-3.287921000	1.272823000	-1.022238000
C	-0.364898000	1.025501000	2.028829000
H	0.069124000	2.034536000	1.872652000
H	-0.652134000	0.972031000	3.084723000
H	0.452744000	0.333745000	1.797855000

Table 1, Entry 8, Pt, B

HF: -1500.48718631

C	-1.782401000	0.385616000	0.242007000
C	-3.228596000	0.662494000	-0.287782000
C	-4.044868000	0.711126000	0.924274000
C	-3.340260000	0.107417000	2.059627000
C	-2.020804000	-0.436461000	1.513657000
H	-1.407847000	1.380125000	0.553255000
H	-3.172486000	0.970734000	2.740558000
H	-3.969982000	-0.571080000	2.654194000
H	-1.200717000	-0.351795000	2.235598000
H	-2.129948000	-1.503746000	1.269272000
C	-3.355206000	1.831198000	-1.251322000
H	-2.756635000	1.637762000	-2.150263000
H	-4.386333000	1.991585000	-1.588456000
H	-2.995998000	2.763095000	-0.794128000
C	-0.820385000	-0.234407000	-0.760974000
H	-1.150836000	-1.257805000	-0.996559000
H	-0.841216000	0.310594000	-1.717469000
P	1.269833000	2.060194000	-0.592520000
H	1.471791000	2.940744000	0.484517000
H	2.267200000	2.499863000	-1.479306000
H	0.118058000	2.613835000	-1.182230000
P	3.559956000	-0.263409000	0.508861000
H	4.323225000	-1.381189000	0.126397000
H	4.403455000	0.768732000	0.059126000
H	3.839196000	-0.228852000	1.886220000

P	1.009153000	-2.559735000	0.047282000
H	2.113137000	-3.340440000	0.430596000
H	0.028484000	-3.026924000	0.938830000
H	0.618355000	-3.198070000	-1.141100000
Pt	1.225528000	-0.240609000	-0.149789000
C	-3.860033000	-0.626618000	-0.938796000
H	-3.257070000	-0.834590000	-1.832277000
H	-3.841823000	-1.515769000	-0.297985000
H	-4.889989000	-0.444310000	-1.262505000
C	-5.364914000	1.317487000	1.029917000
H	-5.939622000	1.266893000	0.096750000
H	-5.950811000	0.951537000	1.879150000
H	-5.187542000	2.399569000	1.194494000

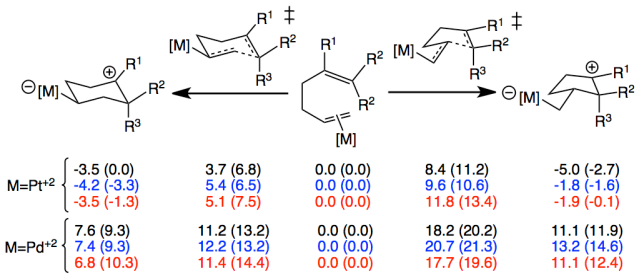


Figure 3. Computed reaction enthalpies (free energies in parentheses; kcal/mol; in DCE) and barriers for $[Pt(PH_3)_3]^{2+}$ and $[PdCl_2(NCMe)]$ promoted 6-*endo* and 5-*exo* cyclizations. Black are for $R^1=R^2=R^3=CH_3$; Blue are for $R^1=R^3=CH_3/R^2=H$; Red are for $R^1=R^2=CH_3/R^3=H$. Preferences for 6-*endo* cyclization with $[Pt(PH_3)_3]^{2+}$ are also predicted for systems with a methyl group added to the terminal carbon of the Pt-complexed C=C π-bond (and $R^1=R^2=R^3=H$ or $R^1=R^2=R^3=CH_3$); see Supporting Information for details.

Figure 3, Pt, 6-endo Int, Black

HF: -1500.69772037

C	-3.334125000	-1.088263000	0.538734000
C	-1.967222000	-1.035172000	-0.088141000
C	-1.383430000	0.482511000	-0.271117000
C	-1.503084000	0.908918000	1.119851000
C	-2.820942000	1.125708000	1.683091000
C	-3.360592000	-0.373943000	1.866342000
H	-1.206688000	-1.584230000	0.485404000
H	-1.950475000	-1.431300000	-1.114140000
H	-4.028729000	-0.572549000	-0.141365000
H	-2.789252000	1.603571000	2.666690000
H	-3.518322000	1.648096000	1.023496000
H	-2.738423000	-0.864594000	2.627770000
H	-4.369205000	-0.274009000	2.286842000
Pt	-4.069157000	-3.101745000	0.775779000
C	0.037132000	0.368283000	-0.807869000
H	0.006165000	-0.062966000	-1.815306000
H	0.505528000	1.358116000	-0.882930000
H	0.682723000	-0.272328000	-0.196617000
P	-2.047306000	-3.796978000	1.763751000
H	-1.033794000	-4.186430000	0.873526000
H	-1.352161000	-2.873081000	2.563986000
H	-2.086225000	-4.908334000	2.620759000

P	-4.969600000	-5.311407000	0.999574000
H	-4.810881000	-5.953286000	2.239194000
H	-6.347922000	-5.488629000	0.796398000
H	-4.456613000	-6.293434000	0.136628000
P	-6.027555000	-2.265966000	-0.180784000
H	-5.924396000	-1.886933000	-1.527581000
H	-7.185830000	-3.057576000	-0.197461000
H	-6.503620000	-1.079877000	0.399946000
C	-2.251938000	1.240341000	-1.277604000
H	-1.895442000	2.272740000	-1.377869000
H	-2.157285000	0.756665000	-2.257287000
H	-3.314550000	1.270073000	-1.023869000
C	-0.353139000	0.851976000	2.029725000
H	0.312068000	1.694902000	1.771701000
H	-0.634812000	0.940522000	3.082376000
H	0.258955000	-0.046091000	1.870499000

Figure 3, Pt, 6-endo TS, Black

HF: -1500.68505506

C	-2.772318000	-1.220238000	0.610800000
C	-1.860632000	-1.107374000	-0.461573000
C	-1.358892000	1.308456000	-0.517938000
C	-0.925027000	0.884456000	0.713212000
C	-1.836388000	0.664026000	1.879433000
C	-2.224629000	-0.843988000	1.959101000
H	-0.823026000	-1.424222000	-0.354625000
H	-2.187797000	-0.954458000	-1.491127000
H	-3.743223000	-0.744275000	0.424613000
H	-1.321892000	0.932742000	2.811738000
H	-2.749979000	1.265255000	1.831826000
H	-1.318245000	-1.414516000	2.209930000
H	-2.949305000	-1.010692000	2.764044000
C	-0.425885000	1.474328000	-1.683335000
H	0.067640000	2.456249000	-1.639826000
H	0.363563000	0.715994000	-1.728151000
H	-0.981561000	1.438181000	-2.628677000
C	0.511824000	0.566453000	0.996738000
H	0.606162000	-0.254399000	1.721478000
H	1.100062000	0.309565000	0.110214000
H	0.991844000	1.441243000	1.460076000
C	-2.735394000	1.839974000	-0.789309000
H	-3.199473000	1.320763000	-1.640815000
H	-3.424303000	1.790775000	0.057671000
H	-2.653271000	2.894783000	-1.089760000
Pt	-3.084303000	-3.362265000	0.148504000
P	-1.210097000	-4.020738000	1.426888000
H	-0.018088000	-3.310778000	1.214814000
H	-1.373858000	-3.911355000	2.815386000
H	-0.772025000	-5.347089000	1.297153000
P	-4.963456000	-2.662148000	-1.076066000
H	-6.093166000	-2.386437000	-0.293767000
H	-4.796671000	-1.458076000	-1.778620000
H	-5.482768000	-3.511544000	-2.062374000

P	-3.543401000	-5.638473000	-0.283936000
H	-2.507146000	-6.343174000	-0.913761000
H	-3.782346000	-6.431571000	0.847345000
H	-4.642004000	-5.958997000	-1.093397000

Figure 3, Pt, Reactant, Black

HF: -1500.69226886

C	-2.797740000	-1.134914000	0.502330000
C	-2.258641000	-1.418028000	-0.738156000
C	-1.178285000	1.783749000	-0.314136000
C	-0.782179000	1.076082000	0.761992000
C	-1.713322000	0.616591000	1.849585000
C	-2.006545000	-0.904324000	1.740427000
H	-1.181258000	-1.530724000	-0.862193000
H	-2.814451000	-1.218554000	-1.654463000
H	-3.834104000	-0.786855000	0.550612000
H	-1.253198000	0.776498000	2.835517000
H	-2.663794000	1.162857000	1.860212000
H	-1.045661000	-1.437381000	1.714845000
H	-2.561032000	-1.241784000	2.625159000
C	-0.237403000	2.160356000	-1.421209000
H	-0.176133000	3.254170000	-1.526243000
H	0.778129000	1.775731000	-1.289462000
H	-0.615246000	1.783775000	-2.384305000
C	0.644441000	0.605797000	0.933929000
H	0.805765000	0.187319000	1.935911000
H	0.925223000	-0.177119000	0.211723000
H	1.369715000	1.419780000	0.809986000
C	-2.573940000	2.278132000	-0.561016000
H	-2.982421000	1.831402000	-1.481028000
H	-3.282829000	2.076875000	0.247955000
H	-2.566928000	3.365162000	-0.730707000
Pt	-3.097002000	-3.430014000	-0.052549000
P	-0.970374000	-4.063184000	0.780105000
H	0.108926000	-3.264621000	0.374052000
H	-0.848436000	-4.060984000	2.176250000
H	-0.529657000	-5.350425000	0.442898000
P	-5.213775000	-2.882770000	-0.958182000
H	-6.300027000	-3.013622000	-0.083646000
H	-5.352509000	-1.573176000	-1.439907000
H	-5.604119000	-3.661560000	-2.054655000
P	-3.791474000	-5.671685000	0.176266000
H	-5.130651000	-5.969438000	-0.105478000
H	-3.095364000	-6.570031000	-0.641541000
H	-3.614409000	-6.208857000	1.457204000

Figure 3, Pt, 5-exo, Black

HF: -1500.67741546

C	-1.618501000	0.352098000	0.388653000
C	-3.669053000	0.509068000	-0.471326000
C	-3.686493000	0.854225000	0.864337000
C	-3.377964000	-0.188404000	1.918657000
C	-1.974060000	-0.636368000	1.480306000

H	-1.452029000	1.377164000	0.733939000
H	-3.373757000	0.272843000	2.911635000
H	-4.103632000	-1.009024000	1.948953000
H	-1.226293000	-0.605271000	2.284677000
H	-1.979569000	-1.657637000	1.076639000
C	-3.671303000	1.549136000	-1.551381000
H	-3.275498000	1.129351000	-2.484473000
H	-4.698287000	1.881196000	-1.759289000
H	-3.078129000	2.435752000	-1.296361000
C	-0.871980000	-0.028926000	-0.789706000
H	-1.144747000	-1.008649000	-1.194934000
H	-0.865184000	0.719954000	-1.589639000
P	1.303927000	2.208813000	-0.386780000
H	1.638246000	2.991191000	0.728132000
H	2.263564000	2.630273000	-1.318905000
H	0.147065000	2.854075000	-0.855686000
P	3.436963000	-0.175618000	0.654075000
H	4.211201000	-1.255375000	0.202305000
H	4.259826000	0.905349000	0.300806000
H	3.659463000	-0.240450000	2.037784000
P	0.967930000	-2.434012000	0.214126000
H	2.103126000	-3.209232000	-0.065826000
H	0.640862000	-2.877355000	1.504995000
H	-0.007736000	-3.079666000	-0.560856000
Pt	1.164615000	-0.109043000	-0.049534000
C	-3.936685000	-0.879148000	-0.960482000
H	-3.199644000	-1.193810000	-1.711038000
H	-3.997222000	-1.637060000	-0.175414000
H	-4.906857000	-0.861970000	-1.477821000
C	-3.843639000	2.247340000	1.357248000
H	-3.970586000	2.996090000	0.572019000
H	-4.738746000	2.271010000	1.997017000
H	-3.006795000	2.539476000	2.009053000

Figure 3, Pt, 5-exo Int, Black

HF: -1500.69847172

C	-1.772611000	0.379297000	0.191347000
C	-3.221764000	0.659433000	-0.314933000
C	-4.015049000	0.702343000	0.912552000
C	-3.296019000	0.084953000	2.026457000
C	-1.991671000	-0.462525000	1.451942000
H	-1.398534000	1.367990000	0.516665000
H	-3.105575000	0.947773000	2.700963000
H	-3.923137000	-0.588003000	2.627274000
H	-1.156766000	-0.386635000	2.157199000
H	-2.111755000	-1.525333000	1.194762000
C	-3.354950000	1.840737000	-1.260175000
H	-2.760073000	1.652255000	-2.162525000
H	-4.390814000	2.006491000	-1.580061000
H	-2.983218000	2.760405000	-0.790069000
C	-0.825206000	-0.220948000	-0.831265000
H	-1.156488000	-1.235215000	-1.096085000
H	-0.837677000	0.358877000	-1.767172000

P	1.221356000	2.056527000	-0.548443000
H	1.221885000	2.865118000	0.599769000
H	2.308261000	2.602175000	-1.249730000
H	0.136215000	2.601317000	-1.257717000
P	3.514423000	-0.271633000	0.493015000
H	4.265106000	-1.426543000	0.211113000
H	4.375730000	0.705564000	-0.035537000
H	3.798262000	-0.127407000	1.861803000
P	0.983666000	-2.554818000	0.123247000
H	2.136229000	-3.355488000	0.070588000
H	0.450599000	-2.952651000	1.360338000
H	0.135364000	-3.238302000	-0.762253000
Pt	1.199054000	-0.253833000	-0.187057000
C	-3.856577000	-0.618220000	-0.973245000
H	-3.262541000	-0.817213000	-1.874181000
H	-3.828686000	-1.512301000	-0.340495000
H	-4.891512000	-0.429072000	-1.276024000
C	-5.325799000	1.318649000	1.039021000
H	-5.900829000	1.291273000	0.106470000
H	-5.904362000	0.938900000	1.885575000
H	-5.123487000	2.390853000	1.227991000

Figure 3, Pt, 6-endo Int, Blue

HF: -1461.41874572

C	-3.221514000	-1.016757000	0.852192000
C	-2.114098000	-0.901250000	-0.158443000
C	-1.528790000	0.612568000	-0.239361000
C	-1.143450000	0.815087000	1.142845000
C	-2.209074000	0.929297000	2.122085000
C	-2.756282000	-0.569358000	2.214631000
H	-1.266974000	-1.571045000	0.053853000
H	-2.436106000	-1.104959000	-1.189046000
H	-4.031017000	-0.329496000	0.555700000
H	-1.857023000	1.240803000	3.110386000
H	-3.039703000	1.558349000	1.784948000
H	-1.940898000	-1.187582000	2.618437000
H	-3.557363000	-0.551071000	2.963293000
H	-2.406156000	1.226690000	-0.482872000
Pt	-4.051998000	-3.002509000	0.804978000
C	0.243411000	0.656080000	1.581003000
H	0.767747000	1.594506000	1.322243000
H	0.338252000	0.505277000	2.660225000
H	0.772937000	-0.128908000	1.024953000
C	-0.461841000	0.704690000	-1.311263000
H	-0.919554000	0.543215000	-2.293242000
H	0.011360000	1.693527000	-1.319138000
H	0.322579000	-0.051680000	-1.183883000
P	-2.353554000	-3.831102000	2.202068000
H	-1.039747000	-3.399566000	1.952776000
H	-2.474848000	-3.543132000	3.570600000
H	-2.166505000	-5.222250000	2.238732000
P	-5.053294000	-5.177542000	0.723870000
H	-5.515108000	-5.701604000	1.942424000

H	-6.184781000	-5.374656000	-0.084443000
H	-4.240896000	-6.237129000	0.285857000
P	-5.657286000	-2.063627000	-0.604388000
H	-5.153537000	-1.204657000	-1.594207000
H	-6.495136000	-2.900492000	-1.356512000
H	-6.589152000	-1.227099000	0.028334000

Figure 3, Pt, 6-endo TS, Blue

HF: -1461.40212987

C	-2.771996000	-1.199398000	0.576314000
C	-1.871331000	-1.082521000	-0.507236000
C	-1.278882000	1.218606000	-0.485507000
C	-0.849217000	0.881234000	0.765337000
C	-1.839738000	0.676031000	1.861243000
C	-2.227111000	-0.833402000	1.927945000
H	-0.834326000	-1.409288000	-0.423358000
H	-2.221194000	-0.932198000	-1.529400000
H	-3.738724000	-0.712524000	0.395767000
H	-1.417172000	0.967086000	2.831993000
H	-2.748631000	1.268809000	1.694829000
H	-1.323325000	-1.404868000	2.185589000
H	-2.958852000	-1.001419000	2.726266000
C	-0.430493000	1.430939000	-1.694724000
H	-0.128870000	2.484941000	-1.772557000
H	0.485674000	0.828515000	-1.687376000
H	-0.987206000	1.193019000	-2.609008000
C	0.574729000	0.580062000	1.095789000
H	0.654469000	-0.259609000	1.800877000
H	1.189337000	0.357211000	0.217207000
H	1.025456000	1.447460000	1.599806000
Pt	-3.091129000	-3.343659000	0.128417000
P	-1.199515000	-3.995977000	1.385441000
H	-0.010845000	-3.281136000	1.170744000
H	-1.355813000	-3.893451000	2.775306000
H	-0.756615000	-5.319945000	1.247654000
P	-5.001628000	-2.661696000	-1.054413000
H	-6.093512000	-2.336832000	-0.237830000
H	-4.852978000	-1.494047000	-1.817245000
H	-5.573385000	-3.547290000	-1.977935000
P	-3.546438000	-5.622428000	-0.294425000
H	-2.518204000	-6.323371000	-0.941163000
H	-3.764917000	-6.417136000	0.839896000
H	-4.657212000	-5.944442000	-1.086496000
H	-2.328037000	1.510398000	-0.583103000

Figure 3, Pt, Reactant, Blue

HF: -1461.41069934

C	-2.504935000	-1.249631000	0.320290000
C	-1.923460000	-1.752669000	-0.824554000
C	-1.266368000	1.941195000	-0.171953000
C	-0.717102000	1.107514000	0.723688000
C	-1.574176000	0.496587000	1.801127000
C	-1.803266000	-1.019027000	1.615557000

H	-0.869174000	-2.031392000	-0.836352000
H	-2.374331000	-1.600690000	-1.805031000
H	-3.477764000	-0.755178000	0.236949000
H	-1.105226000	0.631033000	2.787960000
H	-2.551937000	0.998042000	1.842175000
H	-0.837562000	-1.543799000	1.640641000
H	-2.411219000	-1.393142000	2.451080000
C	-0.604024000	2.654421000	-1.302527000
H	-0.685910000	3.743504000	-1.177159000
H	0.458748000	2.411149000	-1.406675000
H	-1.095394000	2.418169000	-2.256769000
C	0.729514000	0.714395000	0.757226000
H	1.175015000	0.965197000	1.731421000
H	0.863304000	-0.371368000	0.631323000
H	1.325437000	1.204056000	-0.019251000
Pt	-3.092945000	-3.532136000	0.003749000
P	-1.126373000	-4.333655000	1.079220000
H	0.085685000	-3.829045000	0.586962000
H	-1.050398000	-4.052413000	2.449909000
H	-0.904254000	-5.717106000	1.046898000
P	-5.061031000	-2.803495000	-1.083201000
H	-6.211321000	-2.788543000	-0.284232000
H	-5.025585000	-1.504567000	-1.610322000
H	-5.458237000	-3.574770000	-2.182432000
P	-4.034758000	-5.684300000	0.223527000
H	-5.380002000	-5.847794000	-0.128644000
H	-3.382775000	-6.641508000	-0.562975000
H	-3.980100000	-6.240221000	1.507567000
H	-2.335805000	2.150000000	-0.062433000

Figure 3, Pt, 5-exo TS, Blue

HF: -1461.39433979

C	-1.499733000	0.452692000	0.368366000
C	-3.582488000	0.514485000	-0.367452000
C	-3.743855000	0.947997000	0.921213000
C	-3.192053000	0.081375000	2.026066000
C	-1.913987000	-0.524483000	1.439359000
H	-1.373426000	1.481307000	0.722305000
H	-2.955731000	0.715931000	2.890585000
H	-3.914102000	-0.667920000	2.374892000
H	-1.115672000	-0.637812000	2.186673000
H	-2.091131000	-1.514036000	0.995745000
C	-3.855006000	1.309761000	-1.597865000
H	-3.200156000	0.984352000	-2.416134000
H	-4.887490000	1.155735000	-1.940862000
H	-3.704831000	2.384524000	-1.446682000
C	-0.781403000	0.097537000	-0.822465000
H	-1.095474000	-0.847382000	-1.277680000
H	-0.726265000	0.888823000	-1.577290000
P	1.516190000	2.210788000	-0.244127000
H	1.958299000	2.892603000	0.899110000
H	2.462196000	2.616757000	-1.196117000
H	0.390443000	2.962055000	-0.616320000

P	3.488510000	-0.358292000	0.681543000
H	4.300283000	-1.167530000	-0.127320000
H	4.282199000	0.792847000	0.802576000
H	3.671547000	-0.951956000	1.939317000
P	0.929290000	-2.444060000	0.062379000
H	2.042508000	-3.250511000	-0.217626000
H	0.522270000	-2.952179000	1.305322000
H	-0.035865000	-2.986012000	-0.799327000
Pt	1.239782000	-0.110248000	-0.042787000
C	-4.249099000	2.290300000	1.295118000
H	-4.705656000	2.838901000	0.466986000
H	-4.997222000	2.174930000	2.093006000
H	-3.443060000	2.900594000	1.731633000
H	-3.437476000	-0.556336000	-0.522669000

Figure 3, Pt, 5-exo Int, Blue

HF: -1461.41305484

C	-3.197461000	-1.152667000	0.706948000
C	-2.053103000	-0.150843000	0.434735000
C	-1.563451000	0.233755000	1.756809000
C	-2.515206000	-0.168953000	2.784828000
C	-3.759291000	-0.638679000	2.034949000
H	-2.709957000	-2.127194000	0.904468000
H	-1.994746000	-1.029928000	3.261566000
H	-2.632815000	0.564024000	3.593136000
H	-4.327739000	-1.390683000	2.591352000
H	-4.408988000	0.232587000	1.858667000
H	-2.569487000	0.814949000	0.173324000
C	-0.289990000	0.882155000	2.013740000
H	-0.196183000	1.277549000	3.027658000
H	0.490014000	0.113922000	1.855588000
H	-0.075726000	1.652057000	1.259773000
C	-1.023256000	-0.491291000	-0.625758000
H	-1.516544000	-0.755720000	-1.567257000
H	-0.339767000	0.340119000	-0.831269000
H	-0.431791000	-1.361672000	-0.314911000
C	-4.175064000	-1.359960000	-0.442420000
H	-3.626295000	-1.739010000	-1.316410000
H	-4.862325000	-2.173674000	-0.169545000
P	-6.914742000	-0.313268000	0.604965000
H	-7.171995000	0.592758000	1.647375000
H	-8.216056000	-0.534870000	0.126254000
H	-6.678119000	-1.497732000	1.320741000
P	-6.750398000	2.185022000	-1.680170000
H	-6.919838000	2.422121000	-3.055698000
H	-8.094600000	2.201638000	-1.268197000
H	-6.354597000	3.465856000	-1.259358000
P	-3.851193000	0.726575000	-2.768481000
H	-4.351282000	1.370600000	-3.911570000
H	-2.726575000	1.526826000	-2.500883000
H	-3.243412000	-0.400274000	-3.346152000
Pt	-5.360178000	0.317514000	-1.024254000

Figure 3, Pt, 6-endo Int, Red

HF: -1461.41639450

C	-3.256583000	-1.064114000	0.908123000
C	-2.185179000	-0.947146000	-0.143574000
C	-1.607682000	0.572952000	-0.249363000
C	-1.157324000	0.723463000	1.118964000
C	-2.140929000	0.846248000	2.177360000
C	-2.728014000	-0.643271000	2.256256000
H	-1.340096000	-1.623760000	0.047594000
H	-2.537596000	-1.152097000	-1.164246000
H	-4.080768000	-0.376862000	0.663810000
H	-1.700368000	1.098703000	3.147022000
H	-2.970421000	1.519162000	1.940996000
H	-1.910418000	-1.284354000	2.617772000
H	-3.498921000	-0.618850000	3.035767000
Pt	-4.106038000	-3.041938000	0.840435000
P	-2.408227000	-3.904661000	2.215355000
H	-1.089162000	-3.511036000	1.933787000
H	-2.494778000	-3.600389000	3.582964000
H	-2.259646000	-5.300267000	2.262043000
P	-5.108863000	-5.211724000	0.713827000
H	-5.379493000	-5.863729000	1.928217000
H	-6.346223000	-5.353221000	0.064878000
H	-4.361178000	-6.204436000	0.058371000
P	-5.710711000	-2.068581000	-0.548652000
H	-5.209249000	-1.156921000	-1.492542000
H	-6.526213000	-2.884742000	-1.346549000
H	-6.664101000	-1.277545000	0.110113000
H	-0.753766000	0.515962000	-0.936151000
C	-2.666856000	1.522345000	-0.787368000
H	-2.263775000	2.538053000	-0.865115000
H	-2.960703000	1.198065000	-1.792581000
H	-3.571287000	1.563655000	-0.172249000
C	0.241599000	0.461703000	1.462806000
H	0.725764000	1.454016000	1.523324000
H	0.358512000	0.005978000	2.453411000
H	0.775537000	-0.101888000	0.689873000

Figure 3, Pt, 6-endo TS, Red

HF: -1461.40135362

C	-2.742862000	-1.242866000	0.647307000
C	-1.842645000	-1.099822000	-0.437440000
C	-1.408466000	1.233578000	-0.462134000
C	-0.935379000	0.885176000	0.771781000
C	-1.821906000	0.641649000	1.946031000
C	-2.184495000	-0.876481000	1.994592000
H	-0.805261000	-1.422632000	-0.349829000
H	-2.191864000	-0.968293000	-1.461845000
H	-3.714742000	-0.761874000	0.478189000
H	-1.304518000	0.901071000	2.878663000
H	-2.745214000	1.230469000	1.904952000
H	-1.264613000	-1.433434000	2.226402000
H	-2.896360000	-1.067948000	2.805467000

C	0.518537000	0.610747000	0.976905000
H	0.687803000	-0.332360000	1.517242000
H	1.075584000	0.582044000	0.033571000
H	0.955062000	1.400577000	1.604764000
Pt	-3.083329000	-3.376288000	0.185832000
P	-1.214830000	-4.063547000	1.456685000
H	-0.002563000	-3.395846000	1.223901000
H	-1.360883000	-3.928474000	2.844871000
H	-0.817683000	-5.404365000	1.344192000
P	-4.960318000	-2.652218000	-1.026926000
H	-6.091674000	-2.397049000	-0.239894000
H	-4.798177000	-1.431351000	-1.701570000
H	-5.477333000	-3.480272000	-2.032498000
P	-3.564094000	-5.645054000	-0.262527000
H	-2.539066000	-6.350550000	-0.909842000
H	-3.797329000	-6.449406000	0.862109000
H	-4.672389000	-5.950909000	-1.064572000
H	-0.666169000	1.309329000	-1.261793000
C	-2.763975000	1.753256000	-0.808304000
H	-2.701258000	2.836144000	-0.983742000
H	-3.136860000	1.311295000	-1.741883000
H	-3.513357000	1.590390000	-0.027166000

Figure 3, Pt, Reactant, Red

HF: -1461.41081370

C	-2.655256000	-1.232686000	0.458932000
C	-2.105030000	-1.609717000	-0.749321000
C	-1.193891000	1.827195000	-0.145225000
C	-0.745770000	1.044087000	0.846848000
C	-1.623281000	0.467596000	1.924551000
C	-1.894596000	-1.042752000	1.725200000
H	-1.036280000	-1.809086000	-0.833774000
H	-2.617897000	-1.413276000	-1.690777000
H	-3.661134000	-0.801597000	0.461732000
H	-1.132877000	0.574549000	2.903512000
H	-2.584467000	0.992160000	1.999184000
H	-0.935518000	-1.578431000	1.697978000
H	-2.469816000	-1.423910000	2.579536000
C	0.703764000	0.663897000	0.935680000
H	1.134872000	0.970755000	1.900356000
H	0.853345000	-0.425630000	0.865989000
H	1.293734000	1.126758000	0.136063000
Pt	-3.107369000	-3.519950000	-0.000555000
P	-1.037433000	-4.288974000	0.863824000
H	0.106275000	-3.614128000	0.413708000
H	-0.909341000	-4.224885000	2.257763000
H	-0.718323000	-5.627620000	0.596746000
P	-5.172083000	-2.854217000	-0.944842000
H	-6.273453000	-2.877062000	-0.079749000
H	-5.214647000	-1.555757000	-1.472264000
H	-5.608801000	-3.638663000	-2.019993000
P	-3.943559000	-5.715653000	0.229055000
H	-5.320818000	-5.903782000	0.060398000

H	-3.386751000	-6.616446000	-0.686651000
H	-3.692882000	-6.324316000	1.464779000
C	-2.584889000	2.306551000	-0.397320000
H	-2.976212000	1.898659000	-1.341452000
H	-3.292524000	2.039185000	0.395843000
H	-2.606884000	3.399793000	-0.504085000
H	-0.452772000	2.174981000	-0.870949000

Figure 3, Pt, 5-exo TS, Red

HF: -1461.39080750

C	-1.625206000	0.370718000	0.372989000
C	-3.678258000	0.482189000	-0.415506000
C	-3.725209000	0.831228000	0.910576000
C	-3.365428000	-0.189997000	1.961179000
C	-1.951271000	-0.590833000	1.500353000
H	-1.478677000	1.408528000	0.684359000
H	-3.370650000	0.261616000	2.958085000
H	-4.055437000	-1.041183000	1.983013000
H	-1.191572000	-0.510396000	2.289922000
H	-1.929623000	-1.624454000	1.131806000
C	-0.884602000	-0.035281000	-0.797876000
H	-1.158730000	-1.022606000	-1.181910000
H	-0.878895000	0.699022000	-1.610616000
P	1.313598000	2.200190000	-0.385816000
H	1.610258000	2.976542000	0.743889000
H	2.313248000	2.614869000	-1.277836000
H	0.183865000	2.855677000	-0.900134000
P	3.426557000	-0.197674000	0.650200000
H	4.199118000	-1.268119000	0.174288000
H	4.250660000	0.890179000	0.322368000
H	3.645342000	-0.294890000	2.032468000
P	0.957179000	-2.443107000	0.213366000
H	2.079960000	-3.219246000	-0.110474000
H	0.678892000	-2.887946000	1.515008000
H	-0.048612000	-3.085822000	-0.524612000
Pt	1.153929000	-0.116994000	-0.051801000
C	-3.898132000	-0.871433000	-0.997658000
H	-3.248495000	-1.046266000	-1.863756000
H	-3.769439000	-1.689702000	-0.281947000
H	-4.930589000	-0.918648000	-1.370155000
C	-3.884984000	2.240907000	1.343106000
H	-3.908925000	2.942210000	0.502433000
H	-4.834251000	2.328305000	1.892984000
H	-3.099154000	2.536925000	2.053072000
H	-3.721511000	1.308711000	-1.130021000

Figure 3, Pt, 5-exo Int, Red

HF: -1461.41279070

C	-1.983075000	0.543663000	0.230487000
C	-3.418854000	0.930611000	-0.214582000
C	-4.221466000	0.845165000	1.002605000
C	-3.492330000	0.135381000	2.050207000
C	-2.241282000	-0.432973000	1.384367000
H	-1.558106000	1.463743000	0.669515000

H	-3.215956000	0.970243000	2.733912000
H	-4.117736000	-0.524879000	2.665406000
H	-1.392602000	-0.507918000	2.072762000
H	-2.448239000	-1.443159000	1.000345000
C	-1.072526000	0.029038000	-0.869874000
H	-1.483659000	-0.907020000	-1.277117000
H	-1.041851000	0.738820000	-1.711199000
P	3.224021000	-0.548687000	0.474032000
H	4.190140000	0.358134000	0.002869000
H	3.487644000	-0.485413000	1.853075000
H	3.863097000	-1.762024000	0.164076000
Pt	0.939566000	-0.247987000	-0.234566000
P	1.132337000	2.084484000	-0.198945000
H	2.325324000	2.653322000	-0.672231000
H	0.174983000	2.805173000	-0.932633000
H	1.026159000	2.704239000	1.056899000
P	0.522065000	-2.532262000	-0.403303000
H	1.556903000	-3.456486000	-0.187221000
H	-0.470421000	-3.036243000	0.453247000
H	0.034285000	-2.956102000	-1.649138000
H	-3.506207000	1.908095000	-0.708542000
C	-4.094734000	-0.116564000	-1.156647000
H	-5.113244000	0.187908000	-1.416587000
H	-3.499976000	-0.153178000	-2.075248000
H	-4.124116000	-1.121568000	-0.720082000
C	-5.578671000	1.344616000	1.147211000
H	-6.242862000	0.475007000	0.983944000
H	-5.785162000	1.667118000	2.174877000
H	-5.839933000	2.114009000	0.415280000

Figure 3, Pd, 6-endo Int, Black

HF: -1533.25889349

C	-0.685090000	0.991146000	-1.197959000
C	-1.115493000	0.206768000	-0.003652000
C	-0.662248000	0.833933000	1.277174000
C	0.940655000	1.034485000	1.230693000
C	1.105725000	1.854690000	0.049920000
C	0.949753000	1.247495000	-1.261920000
H	-0.854751000	0.215039000	2.161886000
H	-0.771940000	-0.834188000	-0.066909000
H	-1.163602000	1.978203000	-1.236585000
H	-0.876222000	0.478128000	-2.152072000
H	1.394052000	0.042240000	1.170652000
H	1.243156000	1.541544000	2.151518000
H	-1.118137000	1.818177000	1.440201000
Pd	-3.197426000	0.041675000	-0.031224000
Cl	-3.420799000	2.369976000	0.166980000
Cl	-5.642125000	-0.284405000	-0.100200000
N	-2.978134000	-1.973353000	-0.174470000
C	-2.911573000	-3.125554000	-0.240041000
C	-2.836443000	-4.567504000	-0.320049000
H	-2.983685000	-5.004196000	0.673202000
H	-1.856742000	-4.873043000	-0.701060000

H	-3.613640000	-4.944827000	-0.992462000
C	1.098885000	3.319214000	0.205181000
H	0.228824000	3.761089000	-0.306821000
H	1.091878000	3.632253000	1.252523000
H	1.978698000	3.747907000	-0.298462000
C	1.214627000	2.159948000	-2.450754000
H	0.941842000	1.637427000	-3.375530000
H	0.637576000	3.091077000	-2.416327000
H	2.280526000	2.416568000	-2.515637000
C	1.645853000	-0.096809000	-1.473296000
H	2.733653000	0.042352000	-1.510145000
H	1.421326000	-0.840868000	-0.704300000
H	1.327989000	-0.511325000	-2.437959000

Figure 3, Pd, 6-endo TS, Black

HF: -1533.25228340

C	0.354341000	0.913500000	1.239993000
C	-0.712687000	0.144094000	0.516552000
C	-1.270290000	0.837879000	-0.607231000
C	0.286609000	1.192796000	-2.039384000
C	0.783185000	1.928357000	-0.975401000
C	1.454606000	1.289973000	0.190853000
H	-1.800557000	0.278145000	-1.381942000
H	-0.412968000	-0.885420000	0.286774000
H	-0.049803000	1.836736000	1.673337000
H	0.807597000	0.334738000	2.053279000
H	2.150359000	1.999066000	0.657266000
H	-1.639640000	1.855052000	-0.466050000
Pd	-2.581938000	-0.088381000	1.499082000
Cl	-2.643602000	2.163480000	2.110444000
Cl	-4.641075000	-0.534250000	2.700067000
N	-2.561288000	-2.037947000	0.928047000
C	-2.620734000	-3.156171000	0.643055000
C	-2.705029000	-4.556497000	0.294517000
H	-2.053794000	-4.773545000	-0.557942000
H	-2.395048000	-5.170083000	1.146641000
H	-3.736754000	-4.810921000	0.030781000
H	2.024264000	0.395818000	-0.081215000
C	0.548459000	3.393131000	-0.821173000
H	1.510001000	3.913854000	-0.939033000
H	-0.150210000	3.820756000	-1.544376000
H	0.193554000	3.627953000	0.193334000
C	-0.436410000	1.844354000	-3.188416000
H	0.284669000	2.283228000	-3.892222000
H	-1.013883000	1.094908000	-3.743777000
H	-1.127964000	2.636295000	-2.881762000
C	0.751147000	-0.200379000	-2.366755000
H	-0.095628000	-0.833291000	-2.663983000
H	1.423591000	-0.149319000	-3.235090000
H	1.286316000	-0.706241000	-1.560022000

Figure 3, Pd, Reactant, Black

HF: -1533.27116579

C	-0.919955000	0.534847000	-1.403483000
C	-0.944744000	0.213318000	-0.060138000
C	-0.818855000	1.196053000	1.054363000
C	0.680055000	1.384223000	1.392164000
C	1.406748000	2.088005000	0.278055000
C	2.243177000	1.473270000	-0.580552000
H	-1.353125000	0.832062000	1.942146000
H	-0.767605000	-0.831358000	0.212840000
H	-0.897313000	1.575415000	-1.726204000
H	-0.679438000	-0.217531000	-2.154836000
H	1.119989000	0.410144000	1.639318000
H	0.730315000	1.988535000	2.310520000
H	-1.257882000	2.161051000	0.772628000
Pd	-3.035251000	0.061618000	-0.959494000
Cl	-3.466565000	2.324984000	-0.805708000
Cl	-5.338046000	-0.376780000	-1.188892000
N	-2.693906000	-1.940086000	-1.141697000
C	-2.556704000	-3.082352000	-1.241346000
C	-2.390462000	-4.511938000	-1.361626000
H	-1.508864000	-4.736808000	-1.970189000
H	-3.275247000	-4.948521000	-1.835949000
H	-2.262312000	-4.954579000	-0.368408000
C	1.028667000	3.543485000	0.139246000
H	1.879226000	4.179423000	-0.132109000
H	0.252692000	3.704025000	-0.627024000
H	0.621671000	3.933023000	1.081927000
C	2.864118000	2.170166000	-1.756888000
H	3.960600000	2.076257000	-1.736517000
H	2.535727000	1.690728000	-2.692820000
H	2.615436000	3.232868000	-1.829667000
C	2.632687000	0.023999000	-0.519967000
H	2.256400000	-0.515328000	0.354211000
H	2.272849000	-0.506841000	-1.415747000
H	3.728500000	-0.077854000	-0.526663000

Figure 3, Pd, 5-exo TS, Black

HF: -1533.24140514

C	-1.884486000	-0.133741000	0.355287000
C	-4.019502000	0.191621000	0.015339000
C	-4.056877000	-1.050897000	0.863964000
C	-2.550156000	-1.335316000	1.015458000
H	-1.948380000	0.795814000	0.931752000
H	-4.545176000	-0.842495000	1.821852000
H	-4.607271000	-1.874070000	0.392185000
H	-2.228771000	-1.424129000	2.061024000
H	-2.248330000	-2.261052000	0.509314000
C	-0.614282000	-0.266873000	-0.335970000
H	-0.519801000	-1.154981000	-0.969191000
H	-0.247408000	0.641979000	-0.821912000
Pd	0.657050000	-0.539959000	1.308553000
Cl	2.233064000	-0.893364000	3.136574000
Cl	0.540416000	1.763831000	1.682956000
N	0.713611000	-2.532786000	0.920839000

C	0.794328000	-3.671861000	0.742391000
C	0.900443000	-5.097167000	0.524099000
H	0.857937000	-5.316838000	-0.547488000
H	1.849884000	-5.465266000	0.926332000
H	0.077141000	-5.614440000	1.027364000
C	-3.216318000	0.172897000	-1.119957000
C	-4.592324000	1.421500000	0.604288000
H	-4.513536000	2.307365000	-0.030020000
H	-5.656114000	1.226267000	0.807734000
H	-4.142511000	1.630104000	1.587825000
C	-3.114166000	-1.054574000	-1.988063000
H	-3.836173000	-0.939783000	-2.808522000
H	-2.121018000	-1.135685000	-2.445540000
H	-3.343742000	-1.993106000	-1.475183000
C	-2.883572000	1.450859000	-1.840061000
H	-2.047869000	1.288443000	-2.530977000
H	-3.739181000	1.791959000	-2.439056000
H	-2.601198000	2.259408000	-1.154638000

Figure 3, Pd, 5-exo Int, Black

HF: -1533.25212134

C	-1.701082000	-0.102261000	0.183905000
C	-4.039172000	0.214716000	0.454394000
C	-3.598250000	-0.660717000	1.539650000
C	-2.212593000	-1.170744000	1.153173000
H	-1.383546000	0.776495000	0.771222000
H	-3.530636000	0.049234000	2.393682000
H	-4.360023000	-1.387048000	1.854588000
H	-1.554668000	-1.296539000	2.019520000
H	-2.286168000	-2.148695000	0.654792000
C	-0.556839000	-0.522854000	-0.703473000
H	-0.742945000	-1.495734000	-1.181176000
H	-0.334319000	0.229038000	-1.472457000
Pd	1.159532000	-0.697353000	0.405523000
Cl	3.264516000	-0.964601000	1.743552000
Cl	1.269425000	1.655218000	0.375115000
N	0.943904000	-2.720389000	0.369518000
C	0.855629000	-3.873487000	0.356258000
C	0.756027000	-5.316762000	0.341224000
H	-0.096809000	-5.629238000	-0.269820000
H	1.671064000	-5.748680000	-0.077197000
H	0.621151000	-5.694021000	1.360109000
C	-2.995910000	0.363969000	-0.556533000
C	-5.324950000	0.896192000	0.435519000
H	-5.705072000	1.045914000	-0.581933000
H	-6.073870000	0.430068000	1.081304000
H	-5.125207000	1.912714000	0.824097000
C	-2.886383000	1.713480000	-1.243170000
H	-2.107264000	1.663094000	-2.013413000
H	-3.820548000	2.012358000	-1.734605000
H	-2.601110000	2.492412000	-0.524484000
C	-3.479556000	-0.719182000	-1.584890000
H	-4.403269000	-0.405476000	-2.082954000

H	-2.682264000	-0.790434000	-2.335828000
H	-3.627854000	-1.714536000	-1.151152000

Figure 3, Pd, 6-endo Int, Blue

HF: -1493.97729621

C	-0.705172000	1.003320000	-1.177449000
C	-1.118338000	0.208512000	0.020428000
C	-0.648443000	0.830175000	1.299450000
C	0.952019000	1.067249000	1.249952000
C	1.094689000	1.850399000	0.044250000
C	0.923612000	1.203882000	-1.236308000
H	-0.819210000	0.199190000	2.180019000
H	-0.770589000	-0.830092000	-0.055299000
H	-1.168523000	1.997729000	-1.188868000
H	-0.929698000	0.509466000	-2.133074000
H	1.432649000	0.085759000	1.210048000
H	1.239144000	1.608496000	2.156983000
H	-1.118915000	1.804521000	1.478327000
Pd	-3.197688000	0.034030000	0.019418000
Cl	-3.425421000	2.360013000	0.241440000
Cl	-5.643830000	-0.299078000	-0.022334000
N	-2.973870000	-1.978041000	-0.157678000
C	-2.904168000	-3.128638000	-0.244826000
C	-2.824983000	-4.568753000	-0.350589000
H	-2.970587000	-5.023042000	0.635022000
H	-1.844541000	-4.864659000	-0.737234000
H	-3.601391000	-4.936577000	-1.029159000
C	1.088076000	3.316927000	0.130394000
H	0.654038000	3.789815000	-0.758086000
H	0.608720000	3.681413000	1.047031000
H	2.143243000	3.637615000	0.178675000
C	1.624871000	-0.117123000	-1.502595000
H	2.710486000	0.026702000	-1.548072000
H	1.414519000	-0.879993000	-0.746506000
H	1.295435000	-0.510128000	-2.471412000
H	1.092246000	1.910185000	-2.059378000

Figure 3, Pd, 6-endo TS, Blue

HF: -1493.96929388

C	-0.633359000	1.195433000	1.370942000
C	-1.169427000	0.261684000	0.327241000
C	-0.991450000	0.701430000	-1.024331000
C	1.105868000	0.872214000	-1.346761000
C	1.035700000	1.804111000	-0.334438000
C	0.898249000	1.409733000	1.088089000
H	-1.062290000	-0.018998000	-1.841830000
H	-0.871693000	-0.780042000	0.493275000
H	-1.137894000	2.168723000	1.330401000
H	-0.756374000	0.797555000	2.385040000
H	1.262401000	2.204285000	1.751257000
H	-1.293418000	1.714232000	-1.292068000
Pd	-3.285736000	0.140404000	0.104402000
Cl	-3.521513000	2.456373000	0.233080000

Cl	-5.681296000	-0.164686000	-0.056547000
N	-3.078131000	-1.876654000	-0.012008000
C	-3.023769000	-3.029640000	-0.064158000
C	-2.962863000	-4.472398000	-0.127389000
H	-2.518854000	-4.867805000	0.791921000
H	-3.971742000	-4.882065000	-0.240645000
H	-2.353325000	-4.783916000	-0.981657000
H	1.443934000	0.489806000	1.325412000
C	0.841547000	3.246463000	-0.647991000
H	1.715052000	3.815857000	-0.299470000
H	0.720697000	3.429166000	-1.721596000
H	-0.027981000	3.659184000	-0.113950000
C	1.588485000	-0.540370000	-1.232013000
H	1.040719000	-1.202681000	-1.913656000
H	2.645820000	-0.585723000	-1.525593000
H	1.507170000	-0.950351000	-0.220851000
H	1.109065000	1.273171000	-2.364717000

Figure 3, Pd, Reactant, Blue

HF: -1493.99023491

C	-1.254741000	0.623595000	-1.389281000
C	-1.032896000	0.275730000	-0.071528000
C	-0.823543000	1.241257000	1.045837000
C	0.689419000	1.415881000	1.301921000
C	1.408866000	2.041011000	0.137930000
C	2.200147000	1.367371000	-0.709113000
H	-1.299417000	0.864406000	1.961942000
H	-0.737432000	-0.756829000	0.139393000
H	-1.360431000	1.669716000	-1.676744000
H	-1.084383000	-0.093366000	-2.192284000
H	1.122127000	0.443742000	1.573362000
H	0.794602000	2.061270000	2.187538000
H	-1.287871000	2.206047000	0.809619000
Pd	-3.225437000	-0.020654000	-0.618336000
Cl	-3.793199000	2.195280000	-0.302515000
Cl	-5.488795000	-0.636321000	-0.450158000
N	-2.774162000	-1.979839000	-0.956710000
C	-2.567232000	-3.096290000	-1.167046000
C	-2.311565000	-4.493099000	-1.430819000
H	-1.263507000	-4.726982000	-1.218018000
H	-2.522918000	-4.715883000	-2.481793000
H	-2.953915000	-5.113312000	-0.797339000
C	1.157471000	3.509054000	-0.046834000
H	1.720633000	3.915431000	-0.895479000
H	0.091515000	3.721633000	-0.224497000
H	1.437090000	4.076744000	0.853623000
C	2.545642000	-0.085449000	-0.698572000
H	2.153844000	-0.619395000	0.174981000
H	2.152181000	-0.588926000	-1.594618000
H	3.634774000	-0.231851000	-0.716832000
H	2.656300000	1.940637000	-1.522061000

Figure 3, Pd, 5-exo TS, Blue

HF: -1493.95583409

C	-1.895296000	-0.133617000	0.363676000
C	-4.049532000	0.159740000	0.031284000
C	-4.079522000	-1.083278000	0.873431000
C	-2.563624000	-1.323756000	1.048159000
H	-1.956068000	0.808327000	0.917011000
H	-4.596084000	-0.902388000	1.821441000
H	-4.583852000	-1.920454000	0.376060000
H	-2.253342000	-1.373789000	2.099542000
H	-2.242231000	-2.260278000	0.575217000
C	-0.644769000	-0.288644000	-0.349844000
H	-0.565414000	-1.191839000	-0.962686000
H	-0.284930000	0.607954000	-0.862651000
Pd	0.647471000	-0.542867000	1.286384000
Cl	2.258130000	-0.874373000	3.083736000
Cl	0.547715000	1.762405000	1.639918000
N	0.702788000	-2.539765000	0.920489000
C	0.791078000	-3.679876000	0.752932000
C	0.906823000	-5.106367000	0.548262000
H	0.868009000	-5.336240000	-0.521325000
H	1.857832000	-5.464457000	0.955787000
H	0.085827000	-5.624209000	1.054676000
C	-3.262611000	0.146911000	-1.103667000
C	-4.559350000	1.417070000	0.619154000
H	-4.305703000	2.299856000	0.023587000
H	-5.655192000	1.344525000	0.693030000
H	-4.198814000	1.546384000	1.650673000
C	-3.090435000	-1.015648000	-2.032165000
H	-3.884576000	-0.974474000	-2.789148000
H	-2.134441000	-0.957127000	-2.564072000
H	-3.156108000	-1.988882000	-1.534592000
H	-3.065860000	1.124147000	-1.553228000

Figure 3, Pd, 5-exo Int, Blue

HF: -1493.96642380

C	-1.649889000	0.046158000	0.282220000
C	-4.003836000	0.254017000	0.569788000
C	-3.513548000	-0.563925000	1.678601000
C	-2.108866000	-1.019551000	1.288090000
H	-1.359386000	0.948259000	0.845369000
H	-3.472559000	0.167268000	2.515730000
H	-4.237226000	-1.317319000	2.018992000
H	-1.436927000	-1.092621000	2.149735000
H	-2.141797000	-2.012648000	0.816552000
C	-0.498998000	-0.352345000	-0.607844000
H	-0.704190000	-1.285721000	-1.151199000
H	-0.245122000	0.442670000	-1.321538000
Pd	1.172145000	-0.684879000	0.536064000
Cl	3.163022000	-1.162428000	1.988200000
Cl	1.442523000	1.648138000	0.637489000
N	0.861041000	-2.690098000	0.361882000
C	0.742897000	-3.837665000	0.279888000
C	0.609035000	-5.275090000	0.184500000

H	-0.412778000	-5.576233000	0.436855000
H	0.835507000	-5.605572000	-0.834404000
H	1.304459000	-5.759539000	0.877583000
C	-2.972970000	0.409787000	-0.446676000
C	-5.318033000	0.874030000	0.519662000
H	-5.189741000	1.853463000	1.018620000
H	-5.639879000	1.098754000	-0.502686000
H	-6.079766000	0.325930000	1.082351000
C	-3.397331000	-0.649958000	-1.514099000
H	-4.362394000	-0.400660000	-1.966108000
H	-2.628584000	-0.628926000	-2.294296000
H	-3.446259000	-1.665828000	-1.106246000
H	-2.992999000	1.392578000	-0.936858000

Figure 3, Pd, 6-endo Int, Red

HF: -1493.97996560

C	-0.724405000	1.036214000	-1.210181000
C	-1.133503000	0.227068000	-0.023345000
C	-0.672421000	0.833331000	1.264870000
C	0.930827000	1.029310000	1.209171000
C	1.080948000	1.893784000	0.061944000
C	0.891444000	1.299620000	-1.243185000
H	-0.855142000	0.197493000	2.139651000
H	-0.757038000	-0.802227000	-0.114652000
H	-1.208351000	2.021638000	-1.233805000
H	-0.918926000	0.534631000	-2.167642000
H	1.372750000	0.036739000	1.074532000
H	1.252951000	1.485252000	2.150161000
H	-1.130573000	1.812654000	1.450487000
Pd	-3.208865000	0.033435000	-0.014924000
Cl	-3.453472000	2.358852000	0.201121000
Cl	-5.652768000	-0.319210000	-0.046590000
N	-2.968476000	-1.978061000	-0.170980000
C	-2.893438000	-3.129568000	-0.239336000
C	-2.807797000	-4.570786000	-0.321882000
H	-2.962179000	-5.010528000	0.668953000
H	-1.822231000	-4.868876000	-0.693498000
H	-3.575557000	-4.951943000	-1.002922000
C	1.106253000	3.352464000	0.234328000
H	0.307070000	3.832448000	-0.351782000
H	1.031787000	3.657596000	1.281755000
H	2.046985000	3.743879000	-0.185807000
H	1.331485000	0.294326000	-1.280075000
C	1.241966000	2.119427000	-2.468348000
H	2.311192000	2.361985000	-2.495314000
H	1.002005000	1.549108000	-3.372574000
H	0.675460000	3.058122000	-2.509531000

Figure 3, Pd, 6-endo TS, Red

HF: -1493.97081732

C	-0.252608000	1.090662000	1.368187000
C	-1.020308000	0.229716000	0.412571000
C	-1.206235000	0.779983000	-0.891985000

C	0.735417000	1.131787000	-1.693767000
C	0.942393000	1.958696000	-0.613272000
C	1.152902000	1.353549000	0.725615000
H	-1.451407000	0.123037000	-1.729263000
H	-0.665802000	-0.807858000	0.400321000
H	-0.755687000	2.050940000	1.537372000
H	-0.116528000	0.607948000	2.343177000
H	1.051305000	0.092351000	-1.571907000
H	1.716303000	2.028173000	1.382873000
H	-1.582544000	1.799014000	-0.993397000
Pd	-3.115354000	0.055315000	0.755544000
Cl	-3.356323000	2.356059000	1.052206000
Cl	-5.434840000	-0.320217000	1.325753000
N	-2.923654000	-1.943542000	0.437303000
C	-2.882500000	-3.084732000	0.260864000
C	-2.840270000	-4.512687000	0.040595000
H	-1.802037000	-4.857556000	0.007517000
H	-3.362820000	-5.028972000	0.852438000
H	-3.328647000	-4.756431000	-0.908476000
H	1.695645000	0.402158000	0.653714000
C	0.745178000	3.431941000	-0.655142000
H	1.712669000	3.930675000	-0.497307000
H	0.332103000	3.795484000	-1.600791000
H	0.092757000	3.761520000	0.167613000
C	0.494852000	1.573983000	-3.103837000
H	1.442768000	1.814327000	-3.603843000
H	0.017580000	0.774234000	-3.681857000
H	-0.147197000	2.460845000	-3.166081000

Figure 3, Pd, Reactant, Red

HF: -1493.98982233

C	-1.507729000	0.814177000	-1.482332000
C	-1.146214000	0.441848000	-0.203679000
C	-0.953582000	1.365493000	0.952729000
C	0.548528000	1.488507000	1.272367000
C	1.356042000	2.082791000	0.148449000
C	2.225486000	1.319765000	-0.529160000
H	-1.470189000	0.964953000	1.837030000
H	-0.740834000	-0.565524000	-0.063717000
H	-1.731251000	1.854997000	-1.716385000
H	-1.339368000	0.146030000	-2.326560000
H	0.940241000	0.493968000	1.534004000
H	0.639935000	2.113661000	2.174636000
H	-1.395768000	2.346794000	0.739960000
Pd	-3.342394000	-0.044866000	-0.587500000
Cl	-4.081773000	2.093791000	-0.132839000
Cl	-5.510209000	-0.888032000	-0.231033000
N	-2.742482000	-1.935220000	-1.054943000
C	-2.449631000	-3.015943000	-1.337299000
C	-2.089921000	-4.369293000	-1.691188000
H	-1.020199000	-4.425054000	-1.915980000
H	-2.658955000	-4.683657000	-2.572104000
H	-2.318369000	-5.042642000	-0.858877000

H	2.313547000	0.274176000	-0.215675000
C	1.094725000	3.533864000	-0.122789000
H	1.763707000	3.959198000	-0.877762000
H	0.063688000	3.702000000	-0.469353000
H	1.206755000	4.124716000	0.798635000
C	3.108100000	1.707115000	-1.668795000
H	4.162470000	1.499068000	-1.436913000
H	2.869398000	1.120538000	-2.567693000
H	3.029933000	2.766458000	-1.937085000

Figure 3, Pd, 5-exo TS, Red

HF: -1493.96025986

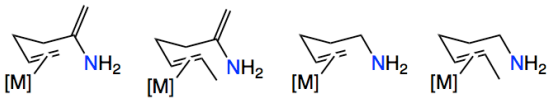
C	-1.721074000	-0.053065000	0.368860000
C	-4.007774000	0.310158000	0.359250000
C	-3.775714000	-0.741406000	1.407687000
C	-2.335606000	-1.201115000	1.148960000
H	-1.703553000	0.902027000	0.905768000
H	-3.877135000	-0.284102000	2.401060000
H	-4.516035000	-1.550935000	1.357183000
H	-1.776574000	-1.394392000	2.073704000
H	-2.292400000	-2.120253000	0.548543000
C	-0.630722000	-0.222106000	-0.557273000
H	-0.691722000	-1.109146000	-1.197583000
H	-0.329633000	0.678280000	-1.099231000
Pd	0.902570000	-0.538152000	0.840453000
Cl	2.791617000	-0.947129000	2.319867000
Cl	0.966211000	1.764188000	1.207916000
N	0.794544000	-2.533921000	0.468437000
C	0.779040000	-3.673791000	0.278340000
C	0.766942000	-5.100397000	0.044058000
H	-0.264170000	-5.466047000	0.007420000
H	1.259030000	-5.325547000	-0.907674000
H	1.299479000	-5.614271000	0.850857000
C	-3.349962000	0.128691000	-0.838117000
H	-3.181201000	-0.902737000	-1.155459000
C	-4.662790000	1.574308000	0.758967000
H	-4.939823000	2.212377000	-0.085074000
H	-5.559398000	1.347126000	1.351960000
H	-3.999596000	2.144534000	1.430686000
C	-3.248827000	1.165652000	-1.909757000
H	-2.432009000	0.925465000	-2.599705000
H	-4.172426000	1.213271000	-2.502539000
H	-3.061112000	2.163819000	-1.495008000

Figure 3, Pd, 5-exo Int, Red

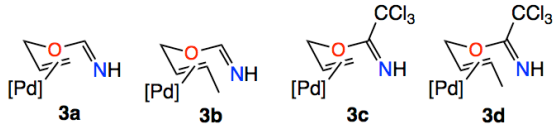
HF: -1493.97031420

C	-1.688792000	0.138156000	0.277465000
C	-4.062432000	0.301935000	0.439904000
C	-3.602357000	-0.465437000	1.592896000
C	-2.186927000	-0.927816000	1.257100000
H	-1.426406000	1.052772000	0.836654000
H	-3.577744000	0.311894000	2.389686000
H	-4.333932000	-1.200431000	1.954477000

H	-1.549875000	-1.023461000	2.142355000
H	-2.216854000	-1.908766000	0.757549000
C	-0.525518000	-0.267688000	-0.590270000
H	-0.778309000	-1.156961000	-1.189788000
H	-0.209424000	0.546045000	-1.255409000
Pd	1.111276000	-0.721503000	0.555474000
Cl	3.107480000	-1.342100000	1.945284000
Cl	1.395198000	1.593572000	0.863637000
N	0.761137000	-2.700933000	0.235356000
C	0.609160000	-3.838782000	0.094707000
C	0.428306000	-5.264275000	-0.073085000
H	-0.637709000	-5.513211000	-0.062809000
H	0.859189000	-5.587742000	-1.026219000
H	0.926887000	-5.800578000	0.740902000
C	-2.984149000	0.457971000	-0.526756000
H	-3.181393000	-0.476279000	-1.120531000
C	-5.389522000	0.881713000	0.308919000
H	-5.771087000	0.762816000	-0.714725000
H	-6.105557000	0.509118000	1.045227000
H	-5.270246000	1.973082000	0.437307000
C	-2.988226000	1.656673000	-1.450853000
H	-2.209792000	1.542719000	-2.212062000
H	-3.945877000	1.783777000	-1.968382000
H	-2.774204000	2.570764000	-0.881911000



	1a	1b	2a	2b
5-*exo*	**4.2 (-13.7)**	**6.7 (-7.8)**	**2.7 (-24.2)**	**-3.2 (-20.7)**
6-*endo*	***5.8 (-11.5)***	***3.4 (-10.5)***	***2.4 (-22.9)***	***-1.8 (-24.0)***
5-*exo*	4.6 (-12.9)	6.3 (-6.9)	2.4 (-24.1)	-3.0 (-18.8)
6-*endo*	*5.8 (-9.8)*	*3.7 (-10.3)*	*1.5 (-21.7)*	*-1.1 (-22.4)*



	3a	3b	3c	3d
5-*exo*	1.8 (-15.6)	4.0 (-12.0)	9.4 (-3.9)	12.4 (0.3)
6-*endo*	*5.1 (-19.1)*	*2.6 (-19.1)*	*10.8 (-8.2)*	*8.7 (-7.9)*

Figure 4. Free energy barriers and exergonicities (kcal/mol; in DCE; exergonities in parentheses) for systems with nitrogen nucleophiles. For **1a/b** and **2a/b**, bold values are for [M]=[Pt(PH$_3$)$_3$]$^{2+}$ and plain text values are for [M]=[Pd(PH$_3$)$_3$]$^{2+}$. For **3a-d**, [M]=[PdCl$_2$(NCMe)]. Note that barriers for **2b** are negative because they are based on an extended rather than productive conformation of the reactant.

Figure-4-structures

1a
M=Pt(CH3)3
reactant

Zero-point correction= 0.248510 (Hartree/Particle)
Thermal correction to Energy= 0.266223
Thermal correction to Enthalpy= 0.267167
Thermal correction to Gibbs Free Energy= 0.202063
Sum of electronic and zero-point Energies= -1437.926519
Sum of electronic and thermal Energies= -1437.908806
Sum of electronic and thermal Enthalpies= -1437.907862
Sum of electronic and thermal Free Energies= -1437.972967

C	-0.68050000	1.60609800	0.85246600
C	-3.58724800	0.89887200	0.04452400
C	-3.09821800	1.25525800	1.41627200
C	-1.64127700	0.80646300	1.67536100
H	-0.21073900	2.44604400	1.37152200
H	-3.19584400	2.33680400	1.57334900
H	-3.72336900	0.76494800	2.17793000
H	-1.40222900	0.93525300	2.73635200
H	-1.56544100	-0.26638700	1.46132900
C	-0.54821300	1.56695700	-0.52253900
H	-1.22146400	0.96760500	-1.13370100
H	-0.02066500	2.36487000	-1.04591100
P	2.49945800	1.95940800	1.05275300
H	2.35700200	2.22796700	2.42044900
H	3.88667200	1.82245300	0.91404900
H	2.26157900	3.21217300	0.46991600
P	2.93468500	-1.30550300	0.43249000
H	2.82171000	-2.11515700	1.56906600
H	3.09021500	-2.23978800	-0.59897800
H	4.22165800	-0.76609100	0.55213000
P	-0.12981200	-1.50221800	-0.83441900
H	0.15122000	-2.83146200	-0.48893500
H	-1.53000800	-1.37628200	-0.65510500
H	0.02927400	-1.51206500	-2.22687500
Pt	1.16198900	0.20507000	0.19148800
C	-3.92557000	1.82935200	-0.85865600
H	-4.28354300	1.56353000	-1.85252700
H	-3.85338400	2.88652900	-0.61661500
N	-3.54857800	-0.47527800	-0.24335200
H	-4.06421300	-0.72258300	-1.08391400
H	-3.85826600	-1.06182100	0.52855100

1a
M=Pt(CH3)3
5-exo-TS

Zero-point correction= 0.247908 (Hartree/Particle)
Thermal correction to Energy= 0.266000
Thermal correction to Enthalpy= 0.266944
Thermal correction to Gibbs Free Energy= 0.200680
Sum of electronic and zero-point Energies= -1437.919101
Sum of electronic and thermal Energies= -1437.901009
Sum of electronic and thermal Enthalpies= -1437.900065
Sum of electronic and thermal Free Energies= -1437.966329

C	-1.49465900	0.07849300	0.29299400
C	-3.98204300	0.96396300	1.07585200
C	-3.39581300	-0.09126300	1.96688100
C	-2.15074900	-0.75880800	1.33585500
H	-1.46223300	1.15313500	0.49175700
H	-3.15615100	0.35093000	2.94023700
H	-4.13653400	-0.88074900	2.15878700
H	-1.41956300	-0.94931900	2.13682300
H	-2.39719500	-1.73723500	0.89993300
C	-0.85598300	-0.41325800	-0.84359600
H	-1.11978300	-1.42030000	-1.17499000
H	-0.62738000	0.27739100	-1.65761600
P	1.30321400	1.88731700	0.14977200
H	1.12522400	2.59895100	1.34428900
H	2.55285000	2.34598700	-0.28705200
H	0.42279400	2.54167000	-0.72453300
P	3.16792600	-0.62091500	1.33272700
H	4.12712200	-1.34952000	0.61692300
H	3.85853100	0.56092700	1.63340900
H	3.15243200	-1.28242100	2.56788100
P	0.88185300	-2.80994900	0.24728500
H	1.88877400	-3.58113300	0.84490500
H	-0.27717000	-3.34633900	0.82565500
H	0.83646700	-3.33481600	-1.05120500
Pt	1.07115800	-0.45480400	0.29269700
C	-4.39198300	2.15772300	1.51701600
H	-4.82186100	2.89983800	0.84625500
H	-4.30969100	2.41737700	2.56911000
N	-3.89761700	0.62116500	-0.28071500
H	-4.30067100	1.30518900	-0.91555400
H	-4.23538700	-0.31230700	-0.50708900

Figure-4-structures

1a
M=Pt(CH3)3
6-endo-TS

Zero-point correction=	0.248226 (Hartree/Particle)
Thermal correction to Energy=	0.266073
Thermal correction to Enthalpy=	0.267017
Thermal correction to Gibbs Free Energy=	0.201475
Sum of electronic and zero-point Energies=	-1437.916919
Sum of electronic and thermal Energies=	-1437.899072
Sum of electronic and thermal Enthalpies=	-1437.898128
Sum of electronic and thermal Free Energies=	-1437.963670

C	-2.84526600	-1.30670100	0.52853500
C	-2.11390700	-1.31420400	-0.65928700
C	-0.87264500	0.94269100	0.73438600
C	-1.84276000	0.57805900	1.82344800
C	-2.15966800	-0.93223300	1.81649100
H	-1.04344800	-1.51296200	-0.66063600
H	-2.58399900	-1.23197300	-1.63715600
H	-3.86139900	-0.90192300	0.45811400
H	-1.41333800	0.83936100	2.79773400
H	-2.77834100	1.15006300	1.71933200
H	-1.20183400	-1.46073500	1.93504700
H	-2.78802600	-1.18901400	2.67831400
C	0.44058100	1.08347300	0.94596800
H	0.85133900	0.98575400	1.94768900
H	1.13626100	1.29522800	0.13543600
Pt	-3.09863800	-3.49996400	0.11910500
P	-1.04546600	-4.04781400	1.15807800
H	0.06746500	-3.27493000	0.79359100
H	-1.04864700	-3.92508400	2.55468900
H	-0.55720600	-5.35074300	0.98329600
P	-5.16166600	-2.93838100	-0.87790600
H	-6.19738200	-2.72356600	0.04152700
H	-5.17538800	-1.74983800	-1.62367100
H	-5.73636500	-3.85486800	-1.76836700
P	-3.56815100	-5.81807100	-0.06548100
H	-3.71537800	-6.48940000	1.15583400
H	-4.72497200	-6.20261200	-0.75675100
H	-2.57815300	-6.57888000	-0.70271400
N	-1.43748700	0.94569500	-0.55854600
H	-0.80521600	1.27407400	-1.28538900
H	-2.32720600	1.43690800	-0.62255400

1a
M=Pt(CH3)3
5-exo-int

Zero-point correction=	0.251772 (Hartree/Particle)
Thermal correction to Energy=	0.269514
Thermal correction to Enthalpy=	0.270459
Thermal correction to Gibbs Free Energy=	0.203882
Sum of electronic and zero-point Energies=	-1437.946832
Sum of electronic and thermal Energies=	-1437.929090
Sum of electronic and thermal Enthalpies=	-1437.928146
Sum of electronic and thermal Free Energies=	-1437.994722

C	-1.74361300	0.50707500	0.23934000
C	-4.06310100	0.66186100	0.99877700
C	-3.16520500	0.42150600	2.17562500
C	-1.91257700	-0.20559900	1.57143400
H	-1.45996000	1.55437300	0.41871100
H	-2.91730200	1.37870200	2.65774900
H	-3.65235600	-0.20632400	2.92827100
H	-1.02006100	-0.08329300	2.19428600
H	-2.06174500	-1.28239900	1.39816100
C	-0.88244100	-0.15398800	-0.80446000
H	-1.28503300	-1.15787900	-1.01445600
H	-0.91211100	0.40366700	-1.75143100
P	1.28491400	2.06301700	-0.54151300
H	1.12838700	2.88536300	0.58573100
H	2.47944300	2.56853800	-1.07722000
H	0.33364100	2.61382400	-1.41584100
P	3.44835000	-0.37424300	0.48739500
H	4.15980300	-1.54046500	0.15930600
H	4.34134500	0.60285300	0.01638300
H	3.70311700	-0.30499000	1.86671700
P	0.84008700	-2.55518000	-0.00869500
H	1.91737700	-3.38578400	0.33671000
H	-0.13443100	-2.97184600	0.91139200
H	0.37905100	-3.17045400	-1.18225200
Pt	1.15556000	-0.24930800	-0.19245700
C	-5.36515300	0.86944200	0.90714800
H	-5.86873300	1.02982800	-0.04315100
H	-5.97275900	0.88347000	1.80803300
N	-3.21126800	0.61032700	-0.22887300
H	-3.35833100	1.41986100	-0.84176800
H	-3.44332800	-0.22009100	-0.79005700

Figure-4-structures

1a
M=Pt(CH3)3
6-endo-in

Zero-point correction=	0.253330 (Hartree/Particle)
Thermal correction to Energy=	0.270621
Thermal correction to Enthalpy=	0.271565
Thermal correction to Gibbs Free Energy=	0.207275
Sum of electronic and zero-point Energies=	-1437.945289
Sum of electronic and thermal Energies=	-1437.927998
Sum of electronic and thermal Enthalpies=	-1437.927053
Sum of electronic and thermal Free Energies=	-1437.991343

C	-2.68016500	-1.45282800	0.48635200
C	-1.78269500	-1.00530000	-0.64282400
C	-0.97806500	0.89323000	0.77370300
C	-1.84988800	0.45639400	1.90153800
C	-2.09205800	-1.06003500	1.83707200
H	-0.78159800	-1.45221500	-0.60472600
H	-2.20765100	-1.17254800	-1.63820900
H	-3.63348200	-0.90298100	0.38830100
H	-1.37479600	0.74238900	2.84688500
H	-2.81698800	0.98366600	1.85357800
H	-1.12264400	-1.55509900	2.00861000
H	-2.75883300	-1.36463500	2.65368900
C	0.20093400	1.49635300	0.81894400
H	0.63294200	1.76419700	1.77936800
H	0.76932700	1.75254300	-0.07286200
Pt	-3.12163100	-3.53602400	0.20672500
P	-1.08652100	-4.13109600	1.21962000
H	0.06151700	-3.41200000	0.85039200
H	-1.04922100	-3.99756400	2.61655600
H	-0.63118100	-5.45019100	1.06368900
P	-5.10934400	-2.77922400	-0.75984200
H	-6.00887100	-2.17783600	0.13340300
H	-4.95560700	-1.76073300	-1.71462700
H	-5.94595600	-3.67643600	-1.44103900
P	-3.64984200	-5.84613100	-0.16031600
H	-4.01810600	-6.60216200	0.96520800
H	-4.70314800	-6.16757900	-1.03280300
H	-2.63257000	-6.66206500	-0.68361000
N	-1.53161600	0.50601600	-0.54296800
H	-0.90370100	0.80544100	-1.29831200
H	-2.42484600	0.99186100	-0.70334000

1b
M=Pt(CH3)3
reactant

Zero-point correction=	0.277987 (Hartree/Particle)
Thermal correction to Energy=	0.297495
Thermal correction to Enthalpy=	0.298439
Thermal correction to Gibbs Free Energy=	0.230353
Sum of electronic and zero-point Energies=	-1477.184617
Sum of electronic and thermal Energies=	-1477.165110
Sum of electronic and thermal Enthalpies=	-1477.164165
Sum of electronic and thermal Free Energies=	-1477.232251

C	-0.60597100	1.60612800	0.69657800
C	-3.54242400	1.05505700	0.19023600
C	-2.95578600	1.36771300	1.53520600
C	-1.49904900	0.87943700	1.66327100
H	-0.19179500	2.55399000	1.05748500
H	-3.00886000	2.44903100	1.71553100
H	-3.54064300	0.87974300	2.32987800
H	-1.13932000	1.04897200	2.68549400
H	-1.47207600	-0.20504800	1.49739300
C	-0.63973300	1.45213900	-0.67869400
H	-1.32750600	0.70679300	-1.08433000
P	2.35112100	1.83343100	1.44881200
H	1.79096300	2.14786900	2.69477200
H	3.68979800	1.58311000	1.77867200
H	2.42977600	3.08737700	0.82779600
P	2.99917700	-1.28453700	0.38476300
H	2.73964200	-2.44465000	1.12495500
H	3.44379800	-1.79370800	-0.84208100
H	4.18102800	-0.80010500	0.95812900
P	0.01465600	-1.49318500	-0.97230400
H	0.47722500	-2.81344100	-0.87771200
H	-1.35447800	-1.59222800	-0.65727500
H	0.00252500	-1.27431400	-2.35701600
Pt	1.18503600	0.17873200	0.23682900
C	-3.89848100	2.01737700	-0.67356100
H	-4.31533500	1.78651200	-1.65332300
H	-3.78849700	3.06595500	-0.40858400
N	-3.54988000	-0.30914400	-0.13221900
H	-4.12739300	-0.53246400	-0.93785500
H	-3.79685300	-0.91409700	0.64710200
C	-0.06883000	2.41738300	-1.65772400
H	0.59036900	3.15327300	-1.18338200
H	0.48047900	1.90544900	-2.45772300
H	-0.89990900	2.95624600	-2.13527900

Figure-4-structures

1b
M=Pt(CH3)3
5-exo-TS

Zero-point correction=	0.276892 (Hartree/Particle)
Thermal correction to Energy=	0.296236
Thermal correction to Enthalpy=	0.297181
Thermal correction to Gibbs Free Energy=	0.228415
Sum of electronic and zero-point Energies=	-1477.173158
Sum of electronic and thermal Energies=	-1477.153814
Sum of electronic and thermal Enthalpies=	-1477.152869
Sum of electronic and thermal Free Energies=	-1477.221635

C	-1.40527300	0.56400700	0.51876300
C	-4.05989600	0.88516900	1.13598900
C	-3.47171900	-0.40335900	1.59775100
C	-1.94118700	-0.20869500	1.69136600
H	-1.21792700	1.62959000	0.66249900
H	-3.87695800	-0.72510300	2.56240100
H	-3.68370300	-1.19961900	0.86626200
H	-1.70170400	0.32858100	2.61781300
H	-1.45547200	-1.19173900	1.74011200
C	-0.84940400	-0.04585900	-0.63075400
H	-1.29218900	-1.03319600	-0.82493200
P	1.47592600	1.79267100	1.11156900
H	0.80382000	2.13167900	2.29593100
H	2.79232800	2.15961500	1.42941300
H	1.10007400	2.84143100	0.25883900
P	3.32220100	-0.94072700	1.05576800
H	3.73677800	-2.27669500	0.96105800
H	4.36178900	-0.26635300	0.39876800
H	3.59782800	-0.64640600	2.39925800
P	0.84046600	-2.55595500	-0.58594700
H	1.88566400	-3.48532600	-0.48786600
H	-0.24176600	-3.27662900	-0.05904600
H	0.55705400	-2.56683100	-1.95952300
C	-4.87854000	1.67470600	1.82983500
H	-5.22516800	2.62984200	1.43969400
H	-5.22481700	1.37892600	2.81675500
N	-3.45367700	1.25140000	-0.09184000
H	-3.64903600	2.20491500	-0.39345900
H	-3.66481500	0.60512600	-0.85305900
C	-0.64607000	0.77356800	-1.88039000
H	0.04903900	0.28875200	-2.57622900
H	-1.60313100	0.90138100	-2.40806500
H	-0.25706000	1.77558600	-1.65901900
Pt	1.15280700	-0.41164100	0.30421500

1b
M=Pt(CH3)3
6-endo-TS

Zero-point correction=	0.276722 (Hartree/Particle)
Thermal correction to Energy=	0.295785
Thermal correction to Enthalpy=	0.296730
Thermal correction to Gibbs Free Energy=	0.228976
Sum of electronic and zero-point Energies=	-1477.179084
Sum of electronic and thermal Energies=	-1477.160021
Sum of electronic and thermal Enthalpies=	-1477.159077
Sum of electronic and thermal Free Energies=	-1477.226831

C	-2.90771700	-1.25555800	0.18870600
C	-1.85356000	-1.27583500	-0.74111300
C	-1.01818800	0.93884200	0.97560500
C	-2.27904000	0.64242300	1.73253300
C	-2.65776400	-0.84687500	1.62296900
H	-3.82365200	-0.81673700	-0.22997100
H	-2.14291300	0.89334100	2.79108900
H	-3.10918100	1.26113300	1.35640600
H	-1.84635300	-1.44049000	2.06897200
H	-3.55800000	-1.04180300	2.22129800
C	0.18983200	0.99235700	1.54726800
H	0.29422000	0.88177700	2.62370200
H	1.09767100	1.15210100	0.96750800
Pt	-3.13874200	-3.48850500	0.11639400
P	-0.86764000	-3.98301800	0.54303800
H	-0.16866600	-3.11444200	1.39665300
H	-0.59487000	-5.23057500	1.12237100
H	-0.03594800	-4.00431600	-0.58713500
P	-5.40038100	-2.96450700	-0.27237300
H	-5.94729500	-2.07358400	0.66253100
H	-5.66730800	-2.32020600	-1.48870700
H	-6.34293700	-4.00299800	-0.27776600
P	-3.70343300	-5.75756900	0.31450100
H	-2.67481100	-6.69883700	0.46393000
H	-4.52198400	-6.04495000	1.41569200
H	-4.44469900	-6.29805000	-0.74549000
N	-1.19875200	0.95715800	-0.42337800
H	-0.37076500	1.24025100	-0.94435200
H	-2.00563300	1.49774700	-0.73126800
H	-0.84063200	-1.44055400	-0.36477500
C	-2.03474900	-1.31487700	-2.21311000
H	-1.34125100	-0.61792700	-2.69639600
H	-1.79009100	-2.31550700	-2.59689700
H	-3.06225000	-1.06870200	-2.50404000

Figure-4-structures

1b
M=Pt(CH3)3
5-exo-int

Zero-point correction=	0.279115 (Hartree/Particle)
Thermal correction to Energy=	0.297709
Thermal correction to Enthalpy=	0.298653
Thermal correction to Gibbs Free Energy=	0.231196
Sum of electronic and zero-point Energies=	-1477.196747
Sum of electronic and thermal Energies=	-1477.178154
Sum of electronic and thermal Enthalpies=	-1477.177210
Sum of electronic and thermal Free Energies=	-1477.244666

C	-1.78129400	0.53930800	0.13947200
C	-4.04935300	0.76894300	1.00073200
C	-3.08764000	0.75592100	2.15317100
C	-1.82357700	0.10546300	1.59636900
H	-1.59566400	1.62241100	0.06468600
H	-2.87881000	1.78754200	2.47128400
H	-3.50418400	0.22841300	3.01731900
H	-0.91509100	0.40597000	2.12873000
H	-1.88406800	-0.99297400	1.64430800
C	-0.91311000	-0.26026000	-0.79896400
H	-1.28474700	-1.29880800	-0.73466400
P	1.16279700	2.08196000	0.01219900
H	0.61712600	2.65151900	1.17517300
H	2.41392900	2.71770900	-0.02475400
H	0.47643700	2.80411400	-0.97866700
P	3.44625600	-0.36899300	0.51525000
H	4.18204000	-1.52063700	0.18900100
H	4.31462100	0.62545000	0.03309300
H	3.71262100	-0.28554900	1.89211500
P	0.97570600	-2.57146400	-0.44892300
H	2.12297000	-3.37642800	-0.37839800
H	0.11296700	-3.22970500	0.44210100
H	0.43460400	-2.95765500	-1.68566300
Pt	1.13964800	-0.26463600	-0.15095200
C	-5.34499700	1.02008000	0.93041100
H	-5.89693500	0.99945200	-0.00624700
H	-5.89792700	1.26000400	1.83468600
N	-3.27682000	0.42621200	-0.23084900
H	-3.53191400	1.02608700	-1.02277600
H	-3.47891200	-0.54212900	-0.51826400
C	-0.99499100	0.19021600	-2.25121100
H	-2.00492900	0.06365100	-2.67448100
H	-0.71896400	1.24645700	-2.37596900
H	-0.31900500	-0.39797900	-2.88448400

1b
M=Pt(CH3)3
6-endo-int

Zero-point correction=	0.281612 (Hartree/Particle)
Thermal correction to Energy=	0.300040
Thermal correction to Enthalpy=	0.300984
Thermal correction to Gibbs Free Energy=	0.235213
Sum of electronic and zero-point Energies=	-1477.202607
Sum of electronic and thermal Energies=	-1477.184179
Sum of electronic and thermal Enthalpies=	-1477.183235
Sum of electronic and thermal Free Energies=	-1477.249006

C	-2.68501900	-1.43789100	0.28558600
C	-1.63136800	-0.98944900	-0.70961500
C	-1.06303000	0.90234000	0.86276100
C	-2.10094000	0.46918000	1.83809500
C	-2.33896300	-1.04315800	1.71836500
H	-0.63887300	-1.39213700	-0.46557300
H	-3.60356700	-0.88439600	0.01176600
H	-1.77933700	0.74201400	2.84953600
H	-3.04529800	1.00380000	1.64238200
H	-1.43090000	-1.56232300	2.06447900
H	-3.14947200	-1.34206000	2.39629000
C	0.10918200	1.47657500	1.09228700
H	0.39651400	1.72661800	2.10996300
H	0.81192100	1.72386600	0.29936300
Pt	-3.12084600	-3.53832100	0.15059800
P	-0.91956800	-4.10040900	0.76294900
H	0.14203900	-3.24964900	0.41226200
H	-0.71232200	-4.21492600	2.14677200
H	-0.41728900	-5.33283400	0.31645900
P	-5.28260600	-2.83262100	-0.35940200
H	-5.84352400	-1.96336700	0.58959700
H	-5.40565300	-2.06970700	-1.53107500
H	-6.31102500	-3.77233800	-0.52872800
P	-3.71100000	-5.86012300	0.00897000
H	-3.99642900	-6.53312800	1.20838100
H	-4.84866200	-6.19662400	-0.74336100
H	-2.77157200	-6.74104200	-0.55355500
N	-1.42223800	0.53630100	-0.52264000
H	-0.70177700	0.86470500	-1.17759500
H	-2.29278200	1.01471500	-0.79801600
C	-1.97006300	-1.22685100	-2.16368100
H	-1.99615400	-2.30519600	-2.36077400
H	-2.95759000	-0.81343300	-2.41177700
H	-1.22671300	-0.78352000	-2.83737400

Figure-4-structures

2a
M=Pt(CH3)3
reactant

Zero-point correction=	0.243347 (Hartree/Particle)
Thermal correction to Energy=	0.261712
Thermal correction to Enthalpy=	0.262656
Thermal correction to Gibbs Free Energy=	0.194886
Sum of electronic and zero-point Energies=	-1399.862792
Sum of electronic and thermal Energies=	-1399.844427
Sum of electronic and thermal Enthalpies=	-1399.843483
Sum of electronic and thermal Free Energies=	-1399.911253

C	-0.86523100	1.16298600	0.31516400
C	-3.14181900	1.00281000	1.30813500
C	-1.87640400	0.23856100	0.90334700
H	-0.61850200	2.02867500	0.93869600
H	-2.89031100	1.74848500	2.07921300
H	-3.84440100	0.29690600	1.77010100
H	-1.45395400	-0.24360600	1.79743500
H	-2.13761600	-0.55159900	0.18246700
C	-0.40301500	1.13053000	-0.98504700
H	-0.83375200	0.43050800	-1.70165600
H	0.11397800	1.98602500	-1.41989100
P	2.23693300	2.09591600	0.81105700
H	2.31291000	2.30404600	2.19422800
H	3.55779100	2.30183600	0.39453300
H	1.58533400	3.25065800	0.35570800
P	3.16538800	-1.09640700	0.91085400
H	2.90328400	-2.27320600	1.62289700
H	4.00408900	-1.53250100	-0.12201700
H	4.04007100	-0.40566000	1.75831700
P	0.37598500	-2.04415100	-0.54990100
H	1.32002400	-3.00941600	-0.92714700
H	-0.37336000	-2.72620000	0.41836700
H	-0.48427100	-2.02323900	-1.65601900
Pt	1.25862200	0.04836600	0.14905900
N	-5.09075800	2.25510000	0.56179500
H	-5.56822600	2.67146400	-0.23456800
H	-4.91494900	3.02153900	1.21009200
C	-3.82238500	1.68542700	0.13467500
H	-4.02226800	0.93793300	-0.64932700
H	-3.12718900	2.42436900	-0.31464700

1b
M=Pt(CH3)3
5-exo-TS

Zero-point correction=	0.243322 (Hartree/Particle)
Thermal correction to Energy=	0.259953
Thermal correction to Enthalpy=	0.260897
Thermal correction to Gibbs Free Energy=	0.198288
Sum of electronic and zero-point Energies=	-1399.861956
Sum of electronic and thermal Energies=	-1399.845325
Sum of electronic and thermal Enthalpies=	-1399.844380
Sum of electronic and thermal Free Energies=	-1399.906989

C	-1.38903700	0.12085400	0.29633100
C	-3.29013600	-0.00966800	1.96003500
C	-2.10422400	-0.72441000	1.29178800
H	-1.35537300	1.19141500	0.51972300
H	-2.93985800	0.59108100	2.81007800
H	-3.93619700	-0.79048800	2.38330700
H	-1.40301700	-1.02214000	2.08782600
H	-2.43169600	-1.64828300	0.79504300
C	-0.84512600	-0.31962500	-0.89749600
H	-1.10830600	-1.31502300	-1.25964900
H	-0.57895200	0.39578600	-1.67667700
P	1.37943600	1.92542800	0.17520800
H	1.33384800	2.63455900	1.38305200
H	2.61284900	2.32032200	-0.35846700
H	0.46475400	2.62426900	-0.62613000
P	3.15230600	-0.62610200	1.35471200
H	4.08840500	-1.37749700	0.63299200
H	3.86671000	0.54117800	1.65381000
H	3.11291700	-1.28823100	2.58821000
P	0.81637100	-2.76195300	0.26219900
H	1.79757700	-3.55146800	0.87759900
H	-0.36486500	-3.27993300	0.81048700
H	0.79426200	-3.27368600	-1.04211800
Pt	1.05572000	-0.40568300	0.32019000
N	-4.13912900	0.30710000	-0.32178000
H	-4.62247800	0.93763300	-0.95753800
H	-4.68034400	-0.55697700	-0.31188900
C	-4.09059500	0.88384000	1.01653900
H	-3.60367000	1.86598200	0.93026700
H	-5.08118100	1.07387100	1.46391000

Figure-4-structures

2a
M=Pt(CH3)3
5-endo-TS

Zero-point correction=	0.243481 (Hartree/Particle)
Thermal correction to Energy=	0.260764
Thermal correction to Enthalpy=	0.261708
Thermal correction to Gibbs Free Energy=	0.197658
Sum of electronic and zero-point Energies=	-1399.861625
Sum of electronic and thermal Energies=	-1399.844342
Sum of electronic and thermal Enthalpies=	-1399.843398
Sum of electronic and thermal Free Energies=	-1399.907448

C	-2.79178400	-1.34268700	0.45928600
C	-1.99901000	-1.49331400	-0.66538900
C	-1.95426400	0.54344200	1.83946500
C	-2.19123700	-0.97224700	1.78519100
H	-0.93261300	-1.69228500	-0.58199300
H	-2.38826600	-1.39351300	-1.67651300
H	-3.79511300	-0.93106300	0.30909500
H	-1.69609400	0.81178000	2.87232300
H	-2.89140800	1.07598300	1.60957900
H	-1.21996400	-1.46988500	1.93580400
H	-2.85133100	-1.28158000	2.60598200
Pt	-3.07940600	-3.55569900	0.05907100
P	-1.14606600	-4.15649800	1.28786000
H	0.04268700	-3.48532300	0.96668900
H	-1.24457300	-3.94986100	2.67109200
H	-0.74368100	-5.49810700	1.22364600
P	-5.02628900	-2.99848300	-1.14870000
H	-6.20139200	-2.99048500	-0.38575700
H	-5.04305400	-1.72857100	-1.74464300
H	-5.36731200	-3.83671000	-2.21819300
P	-3.70203000	-5.84604300	0.03007000
H	-2.75704700	-6.71114900	-0.53776200
H	-3.89802600	-6.41039800	1.29757300
H	-4.87783300	-6.20444000	-0.64280800
N	-1.18715100	0.89138600	-0.49492600
H	-0.40693300	1.18639900	-1.07881600
H	-1.96870600	1.50464700	-0.72476700
C	-0.84092700	1.03506000	0.92211900
H	-0.59064600	2.07542800	1.19023300
H	0.06650800	0.43934900	1.10608800

1b
M=Pt(CH3)3
5-exo-int

Zero-point correction=	0.248391 (Hartree/Particle)
Thermal correction to Energy=	0.265175
Thermal correction to Enthalpy=	0.266119
Thermal correction to Gibbs Free Energy=	0.202081
Sum of electronic and zero-point Energies=	-1399.903566
Sum of electronic and thermal Energies=	-1399.886782
Sum of electronic and thermal Enthalpies=	-1399.885838
Sum of electronic and thermal Free Energies=	-1399.949876

C	-1.73358500	0.53179400	0.25435000
C	-3.14557300	0.46275100	2.18447400
C	-1.90014900	-0.17586600	1.58692300
H	-1.43239600	1.57393400	0.43370100
H	-2.91417200	1.46593700	2.56513400
H	-3.57917200	-0.11536300	3.00558100
H	-1.00508000	-0.05568300	2.20749100
H	-2.05726400	-1.25323300	1.41901300
C	-0.88463100	-0.13485800	-0.79732200
H	-1.29879000	-1.13354800	-1.00926300
H	-0.91339900	0.42742200	-1.74172500
P	1.30639100	2.05934100	-0.54668100
H	1.18321000	2.88560700	0.58175800
H	2.49793600	2.54772900	-1.10472100
H	0.34747800	2.62271200	-1.40455600
P	3.44765900	-0.39576300	0.48602800
H	4.14361200	-1.57745200	0.18065700
H	4.35342700	0.55991200	-0.00451900
H	3.70568700	-0.30270400	1.86338400
P	0.81395300	-2.55282500	-0.00734200
H	1.88455700	-3.39575200	0.32927200
H	-0.15688400	-2.95869100	0.92144000
H	0.33568000	-3.16345100	-1.17644300
Pt	1.15438800	-0.25106400	-0.19284800
N	-3.20473600	0.65519300	-0.21421100
H	-3.35144100	1.53110600	-0.72403200
H	-3.41008200	-0.09522200	-0.88222300
C	-4.10683900	0.54820200	1.00613800
H	-4.69826300	-0.36279500	0.88725000
H	-4.77770300	1.40869500	1.02318000

Figure-4-structures

2a
M=Pt(CH3)3
5-endo-int

Zero-point correction= 0.249720 (Hartree/Particle)
Thermal correction to Energy= 0.266036
Thermal correction to Enthalpy= 0.266980
Thermal correction to Gibbs Free Energy= 0.204795
Sum of electronic and zero-point Energies= -1399.902825
Sum of electronic and thermal Energies= -1399.886509
Sum of electronic and thermal Enthalpies= -1399.885565
Sum of electronic and thermal Free Energies= -1399.947750

C	-2.68069700	-1.45718600	0.48959600
C	-1.78773300	-0.99495900	-0.64101700
C	-1.86578000	0.44697900	1.90934400
C	-2.09262600	-1.06330900	1.84193100
H	-0.78850000	-1.44845700	-0.61258500
H	-2.21605700	-1.16703300	-1.63426100
H	-3.63591300	-0.90939500	0.39649200
H	-1.40192700	0.73326700	2.86115600
H	-2.82754000	0.97991600	1.85510600
H	-1.11976900	-1.55587100	2.00892100
H	-2.75416300	-1.38408000	2.65687100
Pt	-3.12036000	-3.53916100	0.20648400
P	-1.08749600	-4.13113300	1.22423400
H	0.06192600	-3.41353200	0.85600000
H	-1.05226400	-3.99378600	2.62096700
H	-0.63128900	-5.45062200	1.07345800
P	-5.10445700	-2.77885100	-0.76325300
H	-6.00683000	-2.17971200	0.12874000
H	-4.94885100	-1.75725400	-1.71450800
H	-5.94014200	-3.67298000	-1.44983900
P	-3.65082100	-5.85127300	-0.16155300
H	-4.03652300	-6.60413500	0.96047100
H	-4.69424500	-6.17208200	-1.04634200
H	-2.63111200	-6.67390700	-0.66975900
N	-1.54453900	0.50382800	-0.53818700
H	-0.93000900	0.81030000	-1.30063300
H	-2.43590500	0.99483200	-0.67975500
C	-0.95987700	0.91084300	0.78815400
H	-0.82765900	1.99601300	0.76384100
H	0.02819500	0.43787700	0.84082400

Figure-4-structures

2b
M=Pt(CH3)3
reactant

Zero-point correction=	0.272467 (Hartree/Particle)
Thermal correction to Energy=	0.291795
Thermal correction to Enthalpy=	0.292740
Thermal correction to Gibbs Free Energy=	0.224579
Sum of electronic and zero-point Energies=	-1439.118651
Sum of electronic and thermal Energies=	-1439.099322
Sum of electronic and thermal Enthalpies=	-1439.098378
Sum of electronic and thermal Free Energies=	-1439.166539

C	-0.80813400	1.16588300	0.41946800
C	-3.11183900	0.99100100	1.33944600
C	-1.82350400	0.23229300	1.00345100
H	-0.58777400	2.04076400	1.03987800
H	-2.90015200	1.75661800	2.10315300
H	-3.82553800	0.28782200	1.78933700
H	-1.43142300	-0.23321200	1.91850900
H	-2.06126400	-0.57245500	0.29029200
C	-0.44795000	1.21950000	-0.91545900
H	-0.86639100	0.46193100	-1.58342000
P	2.32815300	2.05247800	0.93988900
H	1.52083600	3.06192200	1.48160200
H	3.31216200	1.90123900	1.92537500
H	3.01920100	2.72600000	-0.07640700
P	3.23087300	-1.13212400	0.66342300
H	3.05027700	-2.38425700	1.26469500
H	3.96603900	-1.44105300	-0.48737000
H	4.18053600	-0.52791500	1.49640300
P	0.29807900	-1.99318200	-0.48753400
H	1.18806300	-2.94669600	-1.00208400
H	-0.34289800	-2.70474600	0.53577400
H	-0.68093500	-1.93710700	-1.48849700
Pt	1.25282400	0.06632400	0.21860900
N	-5.05994900	2.18091200	0.48759700
H	-5.50389100	2.58395900	-0.33481500
H	-4.93334500	2.95483500	1.13859600
C	-3.75798300	1.63938000	0.12692400
H	-3.90455100	0.87567500	-0.65396800
H	-3.06627900	2.39234200	-0.30426300
C	0.12638100	2.41386700	-1.60048300
H	0.97236900	2.15436100	-2.24815500
H	-0.65144400	2.84006200	-2.25035900
H	0.42842900	3.20001200	-0.89814400

1b
M=Pt(CH3)3
5-TS-exo

Zero-point correction=	0.272264 (Hartree/Particle)
Thermal correction to Energy=	0.290997
Thermal correction to Enthalpy=	0.291941
Thermal correction to Gibbs Free Energy=	0.224324
Sum of electronic and zero-point Energies=	-1439.123710
Sum of electronic and thermal Energies=	-1439.104977
Sum of electronic and thermal Enthalpies=	-1439.104033
Sum of electronic and thermal Free Energies=	-1439.171651

C	-1.26677800	0.57889800	0.38100500
C	-3.37228000	-0.06607900	1.59987500
C	-1.85587800	0.17502200	1.69525900
H	-1.11518800	1.64207900	0.19327800
H	-3.74974000	-0.32651100	2.59670800
H	-3.55860900	-0.93607200	0.95022500
H	-1.65530000	0.95367800	2.44412500
H	-1.38408200	-0.75015800	2.05372400
C	-0.92371700	-0.30187200	-0.64307100
H	-1.36776300	-1.30062100	-0.54782600
P	1.47498300	1.92781700	0.67937400
H	2.80231700	2.34091800	0.85886700
H	1.06084900	2.75427300	-0.37522300
H	0.83880900	2.51641600	1.78201600
P	3.24714900	-0.84413000	1.23722600
H	4.09107500	-1.54194200	0.36245500
H	4.05499300	0.23049700	1.63330600
H	3.25220200	-1.66527000	2.37297400
P	0.79156800	-2.69816000	0.02110700
H	1.83746800	-3.57666900	0.33992900
H	-0.29005400	-3.26771800	0.70771400
H	0.51582400	-3.03330200	-1.31159300
Pt	1.11208600	-0.38795200	0.39045200
N	-3.57565900	1.42072300	-0.28969400
H	-3.86271400	2.33986000	-0.61889600
H	-3.93808000	0.74113000	-0.95756000
C	-4.09386000	1.14333400	1.04652500
H	-3.88921800	2.01899200	1.67871700
H	-5.18339900	0.97698700	1.06746200
C	-0.72019400	0.16881200	-2.05320700
H	-0.08728500	-0.51632700	-2.62928700
H	-1.69630500	0.22333600	-2.55733200
H	-0.26980500	1.16814900	-2.09266100

Figure-4-structures

2b
M=Pt(CH3)3
6-TS-endo

Zero-point correction=	0.272280 (Hartree/Particle)
Thermal correction to Energy=	0.290638
Thermal correction to Enthalpy=	0.291582
Thermal correction to Gibbs Free Energy=	0.226144
Sum of electronic and zero-point Energies=	-1439.123323
Sum of electronic and thermal Energies=	-1439.104965
Sum of electronic and thermal Enthalpies=	-1439.104021
Sum of electronic and thermal Free Energies=	-1439.169459

C	-2.83215500	-1.30830200	0.09274400
C	-1.68502100	-1.54750800	-0.65549200
C	-2.47858600	0.66954200	1.59936800
C	-2.75551200	-0.83531900	1.52214500
H	-0.74802800	-1.69620900	-0.11360700
H	-3.65069000	-0.85878800	-0.48431900
H	-2.60182100	0.98831400	2.64294200
H	-3.24079700	1.21647900	1.02016800
H	-1.96595900	-1.37789400	2.06643800
H	-3.70033100	-1.05957800	2.03694700
Pt	-3.14565700	-3.56523100	0.06755400
P	-0.96708500	-4.25303100	0.71486000
H	-0.36654400	-3.52857500	1.75486300
H	-0.82986300	-5.57131800	1.17445900
H	0.01236500	-4.19936600	-0.28758700
P	-5.30371600	-2.88857900	-0.56309700
H	-5.89272500	-1.95135100	0.29777500
H	-5.38559700	-2.24546400	-1.80607800
H	-6.30161300	-3.86672100	-0.67159900
P	-3.84401800	-5.79496900	0.29250600
H	-5.17012800	-6.09690200	-0.04477500
H	-3.12431000	-6.73202600	-0.46213100
H	-3.73582100	-6.31447200	1.58994100
N	-0.92080900	0.85232700	-0.30751700
H	0.02174500	1.10835600	-0.59647500
H	-1.55556000	1.45777600	-0.82834200
C	-1.08997900	1.07767400	1.13038400
H	-0.90412500	2.12606700	1.41845800
H	-0.33672400	0.47030200	1.65586100
C	-1.62328800	-1.63348700	-2.13358000
H	-0.93451800	-0.86066400	-2.49752000
H	-1.21620100	-2.59947300	-2.46073500
H	-2.60423200	-1.48305000	-2.59753700

1b
M=Pt(CH3)3
5-int-exo

Zero-point correction=	0.276388 (Hartree/Particle)
Thermal correction to Energy=	0.294584
Thermal correction to Enthalpy=	0.295528
Thermal correction to Gibbs Free Energy=	0.229253
Sum of electronic and zero-point Energies=	-1439.152347
Sum of electronic and thermal Energies=	-1439.134151
Sum of electronic and thermal Enthalpies=	-1439.133207
Sum of electronic and thermal Free Energies=	-1439.199483

C	-1.77590600	0.60870700	0.16957300
C	-3.12706400	0.67747100	2.14917000
C	-1.83461500	0.09388600	1.59764000
H	-1.54386800	1.68297600	0.17066100
H	-3.00786300	1.74942100	2.35373000
H	-3.46423000	0.19361400	3.07045800
H	-0.94281400	0.39491100	2.15878700
H	-1.87717700	-1.00679200	1.59579800
C	-0.91786200	-0.15229500	-0.81249500
H	-1.31150300	-1.18457700	-0.82404900
P	1.34456900	2.11104600	-0.18120100
H	1.80627700	2.71548900	0.99896100
H	2.29415700	2.58201400	-1.10183900
H	0.25132900	2.93661200	-0.49131500
P	3.41938200	-0.41901100	0.55689100
H	4.12160300	-1.57930400	0.19036900
H	4.33281200	0.56241600	0.13321900
H	3.66577500	-0.40415400	1.93974700
P	0.83242700	-2.54337300	-0.23691200
H	1.92148300	-3.39852000	-0.00766200
H	-0.12869900	-3.08015700	0.63387400
H	0.36426700	-3.01052700	-1.47550600
Pt	1.12092900	-0.23397700	-0.14087500
N	-3.27619900	0.56919000	-0.24349300
H	-3.52476900	1.40379200	-0.78236200
H	-3.45165600	-0.22959800	-0.86213200
C	-4.11706200	0.45568100	1.01889200
H	-4.53297100	-0.55501800	1.03292100
H	-4.93351900	1.17770100	0.96397900
C	-0.97031600	0.38843200	-2.23584300
H	-1.97205600	0.29626200	-2.68688100
H	-0.69086300	1.45019100	-2.29137500
H	-0.28447900	-0.16587700	-2.88857300

Figure-4-structures

2b
M=Pt(CH3)3
6-endo-int

Zero-point correction=	0.277991 (Hartree/Particle)
Thermal correction to Energy=	0.295405
Thermal correction to Enthalpy=	0.296349
Thermal correction to Gibbs Free Energy=	0.233037
Sum of electronic and zero-point Energies=	-1439.159850
Sum of electronic and thermal Energies=	-1439.142437
Sum of electronic and thermal Enthalpies=	-1439.141492
Sum of electronic and thermal Free Energies=	-1439.204805

C	-2.69869700	-1.44096300	0.29470800
C	-1.60142000	-0.98423200	-0.65062800
C	-2.20169700	0.46026600	1.87111900
C	-2.41878700	-1.04590000	1.74319600
H	-0.62438200	-1.39934800	-0.36651800
H	-3.60310700	-0.88568300	-0.02029400
H	-1.94116000	0.73564800	2.90031700
H	-3.12885900	1.00064500	1.62453400
H	-1.52242800	-1.56407000	2.12381600
H	-3.25352100	-1.35992200	2.38432800
Pt	-3.12770100	-3.54038700	0.14268300
P	-0.94607500	-4.11458500	0.81443800
H	0.13654800	-3.28059400	0.48893900
H	-0.78005300	-4.22425800	2.20440600
H	-0.44697300	-5.35781800	0.39361200
P	-5.27088300	-2.82404000	-0.42045900
H	-5.84207700	-1.93757100	0.50637800
H	-5.36163400	-2.07428000	-1.60378600
H	-6.30462500	-3.75666400	-0.59707300
P	-3.70714600	-5.86514900	-0.02395100
H	-3.17306600	-6.75890400	0.92015900
H	-5.06559300	-6.21765900	0.04185900
H	-3.33688700	-6.51526200	-1.21307600
N	-1.40259400	0.52583700	-0.45778900
H	-0.65608000	0.85209800	-1.08269300
H	-2.25583100	1.01276300	-0.76400100
C	-1.08763700	0.92132900	0.95898700
H	-0.94561300	2.00568000	0.96734700
H	-0.13296100	0.44021500	1.20279000
C	-1.87914300	-1.22914100	-2.11737400
H	-1.91023000	-2.30811100	-2.31078300
H	-2.85117000	-0.80732800	-2.40931000
H	-1.10378600	-0.79616100	-2.76133900

1a
M=Pd(PH3)3
reactant

Zero-point correction=	0.248452 (Hartree/Particle)
Thermal correction to Energy=	0.266857
Thermal correction to Enthalpy=	0.267801
Thermal correction to Gibbs Free Energy=	0.201548
Sum of electronic and zero-point Energies=	-1446.446559
Sum of electronic and thermal Energies=	-1446.428154
Sum of electronic and thermal Enthalpies=	-1446.427210
Sum of electronic and thermal Free Energies=	-1446.493463

C	-0.67617400	1.68376000	0.82950500
C	-3.57687400	0.85566800	0.04063400
C	-3.10027900	1.31372100	1.38593000
C	-1.63672600	0.91345400	1.68275600
H	-0.18392900	2.52735600	1.32045300
H	-3.21779800	2.40147400	1.46838000
H	-3.72152100	0.86601000	2.17658600
H	-1.41438000	1.10536800	2.73781600
H	-1.53304800	-0.16877800	1.53123500
C	-0.55234700	1.59600000	-0.53661400
H	-1.22769700	0.97863700	-1.12695400
H	0.02092800	2.34216600	-1.08775100
P	2.50384200	1.91637100	1.17491500
H	2.26402400	2.15992100	2.53451200
H	3.89628500	1.76025900	1.14210600
H	2.33729700	3.18868000	0.60699900
P	2.91788700	-1.30546100	0.29601200
H	2.71303400	-2.34671800	1.21074400
H	3.17152500	-1.98972700	-0.89964600
H	4.18686800	-0.82705100	0.64636100
P	-0.14288500	-1.48138200	-0.79551400
H	0.16735500	-2.81342000	-0.48227400
H	-1.53630800	-1.36742300	-0.54194500
H	-0.05676600	-1.47567200	-2.19497700
C	-3.91999400	1.71475900	-0.92913100
H	-4.26937900	1.37387700	-1.90300400
H	-3.86118500	2.78724200	-0.76287100
N	-3.52313000	-0.53511000	-0.14853600
H	-4.03863500	-0.84905600	-0.96666000
H	-3.81951700	-1.07028900	0.66472800
Pd	1.15640800	0.22638400	0.20467500

Figure-4-structures

1a
M=Pd(PH3)3
5-exo-TS

Zero-point correction=	0.247413 (Hartree/Particle)
Thermal correction to Energy=	0.264682
Thermal correction to Enthalpy=	0.265626
Thermal correction to Gibbs Free Energy=	0.201545
Sum of electronic and zero-point Energies=	-1446.440328
Sum of electronic and thermal Energies=	-1446.423059
Sum of electronic and thermal Enthalpies=	-1446.422115
Sum of electronic and thermal Free Energies=	-1446.486196

C	-1.39466500	0.54283300	0.49891900
C	-4.17778800	0.69681800	1.02098500
C	-3.43055400	-0.47776300	1.55860700
C	-1.97022100	-0.02020300	1.76093300
H	-1.15238700	1.60518000	0.49400500
H	-3.85166500	-0.83095500	2.50567300
H	-3.45561200	-1.32247800	0.85130400
H	-1.93769400	0.73635600	2.55297700
H	-1.36651000	-0.87329600	2.09650900
C	-0.93295100	-0.24734700	-0.56900700
H	-1.38416100	-1.23688800	-0.68810600
H	-0.73350200	0.25240200	-1.52002800
P	1.64326300	1.77368200	-0.21597500
H	1.73793500	2.64260800	0.88083100
H	2.87722500	1.97924300	-0.84969600
H	0.76958800	2.47398400	-1.06311400
P	3.28201200	-0.85469500	1.06888500
H	4.01344700	-1.82936900	0.37437400
H	4.19637400	0.20884100	1.10731700
H	3.34885400	-1.33493900	2.38498100
P	0.57874700	-2.75896900	0.50542300
H	1.48741400	-3.61636600	1.14457900
H	-0.61279500	-3.06036000	1.18452500
H	0.38163100	-3.41461400	-0.71828600
C	-5.16507900	1.33500800	1.65158300
H	-5.63544300	2.22239800	1.23184500
H	-5.52835700	0.98119700	2.61307200
N	-3.55566000	1.17274300	-0.15561900
H	-3.87819600	2.09010600	-0.45867800
H	-3.60446800	0.52178800	-0.93899300
Pd	1.09416500	-0.46935500	0.26015800

1a
M=Pd(PH3)3
6-endo-TS

Zero-point correction=	0.247707 (Hartree/Particle)
Thermal correction to Energy=	0.265695
Thermal correction to Enthalpy=	0.266640
Thermal correction to Gibbs Free Energy=	0.200973
Sum of electronic and zero-point Energies=	-1446.437437
Sum of electronic and thermal Energies=	-1446.419449
Sum of electronic and thermal Enthalpies=	-1446.418505
Sum of electronic and thermal Free Energies=	-1446.484172

C	-2.87215800	-1.24707600	0.40060200
C	-1.98829500	-1.30795000	-0.67494900
C	-0.86264300	0.90003200	0.78032600
C	-1.98534700	0.65438300	1.74697400
C	-2.39073600	-0.83737900	1.76537100
H	-0.92999000	-1.51575400	-0.53333200
H	-2.34072500	-1.30225000	-1.70533400
H	-3.86530500	-0.84943700	0.16390400
H	-1.67309900	0.94261300	2.75748100
H	-2.86167300	1.26978700	1.49040900
H	-1.51123600	-1.41404300	2.08426300
H	-3.17638000	-0.99891500	2.51315200
C	0.42413100	0.93970300	1.14450600
H	0.70319900	0.86024300	2.19214800
H	1.22494000	1.06100900	0.41689300
P	-0.95155200	-3.99821700	1.08368500
H	0.01885000	-2.98875700	1.21163400
H	-1.03518700	-4.48028700	2.39867800
H	-0.21881200	-5.01665800	0.45630700
P	-5.15960700	-2.98459800	-0.82370100
H	-6.08464700	-2.43556700	0.07542400
H	-5.14479500	-2.02936300	-1.85162600
H	-5.90304900	-4.02105400	-1.40840000
P	-3.54790100	-5.78538700	0.00441500
H	-2.63993900	-6.71285000	0.53766400
H	-4.74381300	-6.16927700	0.62807000
H	-3.73054300	-6.27858800	-1.29577200
N	-1.26275000	0.88602200	-0.57219300
H	-0.52356800	1.12504200	-1.23014500
H	-2.10202000	1.42755600	-0.77046100
Pd	-3.05165100	-3.46557400	0.12216200

Figure-4-structures

1a
M=Pd(PH3)3
5-exo-int

Zero-point correction=	0.250391 (Hartree/Particle)
Thermal correction to Energy=	0.268607
Thermal correction to Enthalpy=	0.269551
Thermal correction to Gibbs Free Energy=	0.201961
Sum of electronic and zero-point Energies=	-1446.465618
Sum of electronic and thermal Energies=	-1446.447403
Sum of electronic and thermal Enthalpies=	-1446.446459
Sum of electronic and thermal Free Energies=	-1446.514048

C	-1.73710100	0.50172500	0.21947900
C	-4.04961300	0.65847200	1.00176000
C	-3.13632000	0.44330400	2.17132000
C	-1.89085200	-0.19348500	1.56300500
H	-1.45836400	1.55253400	0.38244400
H	-2.88351300	1.41029700	2.63088300
H	-3.61208700	-0.17025800	2.94270200
H	-0.99214900	-0.06265800	2.17530600
H	-2.04297900	-1.27214700	1.40629700
C	-0.88630100	-0.16733400	-0.82289500
H	-1.27655500	-1.17560400	-1.02734900
H	-0.88118100	0.38680700	-1.77053900
P	1.26234400	2.07410200	-0.53276700
H	1.25721100	2.88965600	0.61100700
H	2.40708700	2.55890800	-1.18593300
H	0.24964200	2.68606000	-1.29221600
P	3.42636300	-0.36707700	0.52981500
H	4.13856300	-1.55046800	0.26815700
H	4.34760500	0.57800700	0.04517000
H	3.65637300	-0.24563700	1.91048200
P	0.81687900	-2.56330100	-0.04346800
H	1.88458400	-3.40316100	0.31399000
H	-0.17400500	-3.00442600	0.84842000
H	0.38297400	-3.17292300	-1.23121400
C	-5.35402700	0.85508500	0.92128200
H	-5.86893000	0.99705000	-0.02583800
H	-5.95165100	0.87900300	1.82861500
N	-3.21143200	0.59271200	-0.23551400
H	-3.36733700	1.39386100	-0.85726600
H	-3.44839900	-0.24531700	-0.78319900
Pd	1.13473800	-0.25192500	-0.19294100

1a
M=Pd(PH3)3
6-endo-min

Zero-point correction=	0.252283 (Hartree/Particle)
Thermal correction to Energy=	0.269080
Thermal correction to Enthalpy=	0.270024
Thermal correction to Gibbs Free Energy=	0.207467
Sum of electronic and zero-point Energies=	-1446.464185
Sum of electronic and thermal Energies=	-1446.447387
Sum of electronic and thermal Enthalpies=	-1446.446443
Sum of electronic and thermal Free Energies=	-1446.509001

C	-2.67493600	-1.45098300	0.48560500
C	-1.78682500	-1.01089600	-0.64874900
C	-0.98988800	0.89464100	0.76829200
C	-1.85351400	0.44879600	1.89919800
C	-2.08127400	-1.07159600	1.83308500
H	-0.78471200	-1.45495200	-0.61316600
H	-2.21530400	-1.17866300	-1.64239600
H	-3.63926900	-0.92239200	0.39599900
H	-1.37552200	0.73433700	2.84324500
H	-2.82550200	0.96710900	1.85871300
H	-1.10462000	-1.55529600	1.99211800
H	-2.73809600	-1.38492400	2.65426300
C	0.18208300	1.51147800	0.81211800
H	0.61183800	1.78423700	1.77216100
H	0.74618300	1.77498400	-0.08020200
P	-1.09695700	-4.13428900	1.26488000
H	0.08049700	-3.44213600	0.93250200
H	-1.08942400	-3.99569200	2.66285800
H	-0.64905000	-5.46056700	1.13774100
P	-5.07503200	-2.75478600	-0.81511300
H	-6.01640500	-2.20847500	0.07209800
H	-4.92807300	-1.69036800	-1.72118900
H	-5.88409500	-3.62714500	-1.56079400
P	-3.65432100	-5.84861800	-0.14570400
H	-3.80805700	-6.64229400	1.00434700
H	-4.82234400	-6.20133400	-0.84404800
H	-2.71080600	-6.62197800	-0.84473800
N	-1.54146500	0.50325200	-0.54851400
H	-0.91464600	0.80485700	-1.30411900
H	-2.43683300	0.98495600	-0.70986800
Pd	-3.10993500	-3.52385400	0.19753000

Figure-4-structures

1b
M=Pd(PH3)3
reactant

Zero-point correction=	0.277071 (Hartree/Particle)
Thermal correction to Energy=	0.296829
Thermal correction to Enthalpy=	0.297773
Thermal correction to Gibbs Free Energy=	0.229569
Sum of electronic and zero-point Energies=	-1485.706274
Sum of electronic and thermal Energies=	-1485.686517
Sum of electronic and thermal Enthalpies=	-1485.685572
Sum of electronic and thermal Free Energies=	-1485.753776

C	-0.60314400	1.64637300	0.68324200
C	-3.52973300	1.01927900	0.19371900
C	-2.94326900	1.35280800	1.53368400
C	-1.47285900	0.90094600	1.65511000
H	-0.17827700	2.58853400	1.04595100
H	-3.02030700	2.43353100	1.70826500
H	-3.51129100	0.85540500	2.33456100
H	-1.11515200	1.08040100	2.67621000
H	-1.42337900	-0.18345700	1.49111900
C	-0.65028200	1.49534000	-0.68799400
H	-1.33537400	0.74828000	-1.09326100
P	2.35895700	1.82623000	1.46918900
H	1.80463300	2.13926600	2.71883000
H	3.69716200	1.56978600	1.79886200
H	2.44700400	3.08560200	0.85888400
P	2.95633300	-1.29562800	0.38922000
H	2.67576600	-2.43587500	1.15344000
H	3.38284600	-1.84201000	-0.82859700
H	4.15714200	-0.83593600	0.94522100
P	-0.01136600	-1.46109000	-0.98071000
H	0.43128500	-2.78960200	-0.89254300
H	-1.38435700	-1.54085500	-0.66594700
H	-0.01790200	-1.24112000	-2.36583600
C	-3.89808200	1.96808000	-0.68012500
H	-4.31073300	1.72116100	-1.65774500
H	-3.80366900	3.02071000	-0.42568900
N	-3.51876700	-0.34770300	-0.11639400
H	-4.09476100	-0.58685600	-0.91866500
H	-3.75454100	-0.94949000	0.66888900
C	-0.06013000	2.44517000	-1.66881200
H	0.59287200	3.18579500	-1.19314900
H	0.50124900	1.92123200	-2.45316200
H	-0.88024400	2.97856500	-2.17075300
Pd	1.16514200	0.20192400	0.23882200

1a
M=Pd(PH3)3
5-exo-TS

Zero-point correction=	0.275661 (Hartree/Particle)
Thermal correction to Energy=	0.295313
Thermal correction to Enthalpy=	0.296257
Thermal correction to Gibbs Free Energy=	0.226989
Sum of electronic and zero-point Energies=	-1485.695136
Sum of electronic and thermal Energies=	-1485.675483
Sum of electronic and thermal Enthalpies=	-1485.674539
Sum of electronic and thermal Free Energies=	-1485.743807

C	-1.40048200	0.58705400	0.50374200
C	-4.04160600	0.87178300	1.13141100
C	-3.43578400	-0.39689700	1.62341700
C	-1.90850400	-0.17208700	1.69913800
H	-1.20993500	1.65441000	0.62801300
H	-3.83161000	-0.69828500	2.59835200
H	-3.64070000	-1.21482900	0.91435100
H	-1.67083200	0.38911000	2.61170800
H	-1.40338100	-1.14452800	1.76463600
C	-0.85171300	-0.04404100	-0.63678800
H	-1.29194800	-1.03462100	-0.81560700
P	1.45648600	1.78013600	1.16813700
H	0.76833400	2.08481000	2.35368600
H	2.76575200	2.14348400	1.52263100
H	1.09685500	2.86533100	0.35297400
P	3.32243900	-0.94083400	1.04303400
H	3.77072800	-2.26631000	0.93959400
H	4.35157000	-0.24469400	0.39064700
H	3.60730100	-0.65424400	2.38727200
P	0.82058300	-2.55969300	-0.59445200
H	1.86081600	-3.49783400	-0.51787400
H	-0.25193700	-3.28124300	-0.04737400
H	0.50937600	-2.58250000	-1.96275500
C	-4.87513800	1.66678400	1.80045000
H	-5.23094700	2.60819200	1.38623100
H	-5.22659100	1.38783500	2.79042100
N	-3.43202000	1.21871600	-0.10150800
H	-3.62327000	2.16814000	-0.41930600
H	-3.63878900	0.56032400	-0.85396900
C	-0.61264300	0.75263500	-1.89136700
H	0.07808000	0.24381400	-2.57452200
H	-1.56079100	0.89349500	-2.43273600
H	-0.20488100	1.74869500	-1.67770900
Pd	1.13725200	-0.41059900	0.29712200

Figure-4-structures

1b
M=Pd(PH3)3
6-TS-endo

Zero-point correction=	0.275941 (Hartree/Particle)
Thermal correction to Energy=	0.295227
Thermal correction to Enthalpy=	0.296171
Thermal correction to Gibbs Free Energy=	0.228463
Sum of electronic and zero-point Energies=	-1485.700323
Sum of electronic and thermal Energies=	-1485.681038
Sum of electronic and thermal Enthalpies=	-1485.680093
Sum of electronic and thermal Free Energies=	-1485.747801

C	-2.88693700	-1.25956700	0.19581000
C	-1.82439100	-1.29227900	-0.72109300
C	-1.04787300	0.96880200	0.96726800
C	-2.29540400	0.64404600	1.73336600
C	-2.64320300	-0.85551500	1.62836500
H	-3.80007500	-0.82523200	-0.23233500
H	-2.15692000	0.89926700	2.79046500
H	-3.14294800	1.24250200	1.36341200
H	-1.81530900	-1.43131100	2.06771900
H	-3.53485100	-1.06545100	2.23444300
C	0.15708000	1.09213000	1.53470000
H	0.26750000	1.01780700	2.61347200
H	1.05602700	1.27542000	0.94826100
P	-0.85430500	-4.02685000	0.53525200
H	-0.13170600	-3.19796000	1.40968700
H	-0.59285500	-5.29276400	1.08077200
H	-0.01801600	-4.03632300	-0.59280300
P	-5.39041300	-2.92519100	-0.22128300
H	-5.91727400	-2.03748000	0.72894800
H	-5.66703100	-2.26016000	-1.42490700
H	-6.35844800	-3.94153300	-0.23018400
P	-3.72770500	-5.76019400	0.26541000
H	-2.72451400	-6.73060800	0.41016600
H	-4.57613500	-6.07071500	1.33853900
H	-4.45542400	-6.26355000	-0.82302300
N	-1.22617600	0.94105500	-0.43211700
H	-0.40611100	1.23318400	-0.96093000
H	-2.04926400	1.44566900	-0.75854100
H	-0.81558300	-1.45004400	-0.33092900
C	-1.99374700	-1.35821300	-2.19316700
H	-1.28092000	-0.68986100	-2.68837900
H	-1.77049100	-2.37269300	-2.55401400
H	-3.01337700	-1.09614700	-2.49837200
Pd	-3.13068700	-3.47953400	0.13041400

1a
M=Pd(PH3)3
5-exo-int

Zero-point correction=	0.278558 (Hartree/Particle)
Thermal correction to Energy=	0.298085
Thermal correction to Enthalpy=	0.299029
Thermal correction to Gibbs Free Energy=	0.229768
Sum of electronic and zero-point Energies=	-1485.716025
Sum of electronic and thermal Energies=	-1485.696498
Sum of electronic and thermal Enthalpies=	-1485.695554
Sum of electronic and thermal Free Energies=	-1485.764815

C	-1.76709300	0.58152000	0.13208800
C	-4.05476500	0.71155000	0.99884900
C	-3.08400100	0.74761200	2.13978800
C	-1.81713100	0.11088800	1.57816800
H	-1.56270000	1.66204800	0.08698400
H	-2.88820200	1.79013600	2.43120600
H	-3.48140700	0.23159500	3.01937700
H	-0.91204000	0.40050300	2.12266700
H	-1.88291300	-0.98762500	1.60308600
C	-0.91327000	-0.20819600	-0.82398900
H	-1.28614300	-1.24579500	-0.78858600
P	1.19823500	2.11052200	-0.02988900
H	0.73037900	2.68005300	1.16816900
H	2.45565800	2.73073300	-0.12185600
H	0.47978500	2.87796000	-0.96403600
P	3.45163700	-0.40476900	0.45364200
H	4.16163900	-1.57052300	0.11694400
H	4.34029700	0.56709400	-0.03983800
H	3.75328000	-0.33012700	1.82461500
P	0.86858200	-2.57015600	-0.31236500
H	1.96441000	-3.43114400	-0.13596800
H	-0.05810600	-3.13143900	0.58209400
H	0.35817700	-3.03246300	-1.53746900
C	-5.37171800	0.81082700	0.95289100
H	-5.93315200	0.76467600	0.02288200
H	-5.93239200	0.94594500	1.87392300
N	-3.26519700	0.49897100	-0.25478800
H	-3.51110300	1.17978600	-0.98226000
H	-3.46585300	-0.43213000	-0.64558500
C	-0.93718800	0.27317400	-2.26316400
H	-1.92812700	0.13504200	-2.72715200
H	-0.68046300	1.33676200	-2.35774800
H	-0.22723000	-0.29282900	-2.87955700
Pd	1.12690600	-0.25053400	-0.16828800

Figure-4-structures

1b
M=Pd(PH3)3
6-TS-int

Zero-point correction=	0.279945 (Hartree/Particle)
Thermal correction to Energy=	0.298940
Thermal correction to Enthalpy=	0.299884
Thermal correction to Gibbs Free Energy=	0.232388
Sum of electronic and zero-point Energies=	-1485.722595
Sum of electronic and thermal Energies=	-1485.703601
Sum of electronic and thermal Enthalpies=	-1485.702657
Sum of electronic and thermal Free Energies=	-1485.7701531

C	-2.70143800	-1.41420200	0.27590200
C	-1.63153500	-1.00356000	-0.71295700
C	-1.05818100	0.89348700	0.84705000
C	-2.12639000	0.49823800	1.80607000
C	-2.38904700	-1.01439900	1.70965600
H	-0.64634600	-1.41720000	-0.45791900
H	-3.61787700	-0.87671000	-0.02882600
H	-1.82295000	0.78181100	2.82011100
H	-3.05586600	1.04600700	1.57899500
H	-1.50201000	-1.54238300	2.09127600
H	-3.22664800	-1.28329800	2.36694000
C	0.12492700	1.43711700	1.09454200
H	0.39892300	1.68941400	2.11531400
H	0.84994500	1.65632300	0.31354100
P	-0.89501800	-4.07510400	0.73004800
H	0.09910200	-3.09739300	0.91600300
H	-0.76888000	-4.78409200	1.93637600
H	-0.22975900	-4.95166600	-0.14353700
P	-5.29368300	-2.81046500	-0.32200000
H	-5.85059000	-1.92576300	0.61660100
H	-5.43781900	-2.06245200	-1.50233000
H	-6.33255200	-3.74415800	-0.46928600
P	-3.68199200	-5.85071000	0.06413900
H	-3.98334400	-6.49695400	1.27516600
H	-4.80332600	-6.22476200	-0.69640400
H	-2.73156000	-6.74736200	-0.45564500
N	-1.39991500	0.52243000	-0.54160200
H	-0.66255300	0.82990100	-1.18802300
H	-2.25682500	1.01371600	-0.83628400
C	-1.97231000	-1.25708300	-2.16339800
H	-2.02519400	-2.33765100	-2.34064200
H	-2.95011300	-0.82569400	-2.41908100
H	-1.21737700	-0.84455300	-2.84331500
Pd	-3.11672100	-3.50621700	0.16721400

2a
M=Pd(PH3)3
reactant

Zero-point correction=	0.242887 (Hartree/Particle)
Thermal correction to Energy=	0.261337
Thermal correction to Enthalpy=	0.262281
Thermal correction to Gibbs Free Energy=	0.194788
Sum of electronic and zero-point Energies=	-1408.383165
Sum of electronic and thermal Energies=	-1408.364716
Sum of electronic and thermal Enthalpies=	-1408.363771
Sum of electronic and thermal Free Energies=	-1408.431265

C	-0.87452800	1.19043800	0.33482600
C	-3.15854300	1.01920800	1.30849100
C	-1.87991900	0.26409400	0.92723700
H	-0.60922400	2.04905800	0.96105600
H	-2.92454000	1.77996700	2.07014200
H	-3.85778200	0.31198100	1.77347900
H	-1.46122600	-0.20207600	1.83178500
H	-2.12590500	-0.53838100	0.21456300
C	-0.41711500	1.14913900	-0.95905200
H	-0.83780100	0.43877600	-1.67129400
H	0.13780900	1.98143900	-1.39186100
P	2.26313300	2.07799900	0.84561400
H	2.28370300	2.28832500	2.23089100
H	3.60488500	2.26587900	0.48918000
H	1.65651300	3.24697800	0.36328200
P	3.18469300	-1.09550500	0.83997900
H	2.96472400	-2.30692100	1.50807200
H	3.99560000	-1.47175500	-0.23804300
H	4.08008100	-0.43643300	1.69215500
P	0.36875700	-2.04638100	-0.51227400
H	1.29119700	-3.03124300	-0.89486600
H	-0.36920500	-2.70806300	0.47950500
H	-0.51247200	-2.03816400	-1.60273000
N	-5.11512000	2.23266300	0.51585100
H	-5.58813400	2.62655300	-0.29453300
H	-4.95989800	3.01354700	1.15201600
C	-3.83318500	1.67431400	0.11583400
H	-4.01210800	0.91236600	-0.65945300
H	-3.14209600	2.41575200	-0.33549300
Pd	1.25370300	0.05259900	0.16155900

Figure-4-structures

2a
M=Pd(PH3)3
5-TS-exo

Zero-point correction=	0.243110 (Hartree/Particle)
Thermal correction to Energy=	0.260536
Thermal correction to Enthalpy=	0.261480
Thermal correction to Gibbs Free Energy=	0.197763
Sum of electronic and zero-point Energies=	-1408.382090
Sum of electronic and thermal Energies=	-1408.364665
Sum of electronic and thermal Enthalpies=	-1408.363721
Sum of electronic and thermal Free Energies=	-1408.427438

C	-1.39817500	0.11093200	0.25209800
C	-3.27217700	-0.00716700	1.95156200
C	-2.10386000	-0.72677900	1.26134100
H	-1.37312400	1.18596200	0.45567100
H	-2.90274700	0.59533800	2.79227400
H	-3.91403200	-0.78264800	2.39060700
H	-1.38780500	-1.03220100	2.04163700
H	-2.44303200	-1.65023300	0.77132800
C	-0.84017400	-0.34329900	-0.92217200
H	-1.08443400	-1.34450100	-1.28042200
H	-0.50496800	0.35926500	-1.68610200
P	1.29195900	1.92142100	0.44829200
H	0.78262000	2.51967400	1.60900500
H	2.59040400	2.44757800	0.38869800
H	0.64077500	2.63069800	-0.57228900
P	3.20163300	-0.62895800	1.23843100
H	3.66413500	-1.90605900	1.58175900
H	4.20938000	-0.15561900	0.38755400
H	3.43131900	0.09914100	2.41363100
P	0.83688800	-2.77564700	0.16048700
H	1.76783500	-3.58826000	0.82186400
H	-0.38127300	-3.29830300	0.61837900
H	0.89643700	-3.25969900	-1.15358400
N	-4.15056600	0.30986200	-0.31830700
H	-4.64401300	0.93814100	-0.94843600
H	-4.68707000	-0.55703900	-0.30123000
C	-4.08545600	0.88675700	1.01904200
H	-3.60026200	1.86918400	0.92655100
H	-5.07059200	1.07655200	1.47837200
Pd	1.04134500	-0.43194300	0.33551900

2a
M=Pd(PH3)3
6-TS-endo

Zero-point correction=	0.242407 (Hartree/Particle)
Thermal correction to Energy=	0.260003
Thermal correction to Enthalpy=	0.260948
Thermal correction to Gibbs Free Energy=	0.196381
Sum of electronic and zero-point Energies=	-1408.382780
Sum of electronic and thermal Energies=	-1408.365183
Sum of electronic and thermal Enthalpies=	-1408.364239
Sum of electronic and thermal Free Energies=	-1408.428805

C	-2.76955100	-1.32034700	0.47333000
C	-2.00835400	-1.49377500	-0.66275600
C	-1.91014800	0.55398800	1.84462600
C	-2.14398500	-0.96388400	1.78760500
H	-0.94149800	-1.70057400	-0.60259700
H	-2.42266200	-1.41044100	-1.66575000
H	-3.78841900	-0.94074500	0.34942000
H	-1.63071900	0.81642100	2.87335700
H	-2.85330700	1.08492800	1.63758900
H	-1.16842500	-1.45908200	1.91421400
H	-2.78687800	-1.27541300	2.62103800
P	-1.19836300	-4.17744700	1.34774300
H	0.01537600	-3.53278100	1.06456700
H	-1.33430400	-3.95663800	2.72637900
H	-0.80880400	-5.52512100	1.31582000
P	-5.02275000	-3.00231400	-1.17818200
H	-6.22999300	-3.16869200	-0.48542200
H	-5.12912400	-1.68438100	-1.65030300
H	-5.25027900	-3.74968000	-2.34179300
P	-3.72713500	-5.83226400	0.00848100
H	-2.81175600	-6.67168900	-0.64178700
H	-3.85295700	-6.44909600	1.26113200
H	-4.93550000	-6.18563200	-0.60966800
N	-1.19015200	0.90185000	-0.50307800
H	-0.42219900	1.19087900	-1.10573000
H	-1.97931400	1.50887200	-0.72271600
C	-0.81761200	1.04979500	0.90563400
H	-0.56917700	2.09247400	1.16695700
H	0.09699700	0.46051500	1.07277700
Pd	-3.09196800	-3.54459400	0.07001500

Figure-4-structures

2a
M=Pd(PH3)3
5-int-exo

Zero-point correction=	0.247000 (Hartree/Particle)
Thermal correction to Energy=	0.264284
Thermal correction to Enthalpy=	0.265228
Thermal correction to Gibbs Free Energy=	0.199693
Sum of electronic and zero-point Energies=	-1408.422431
Sum of electronic and thermal Energies=	-1408.405148
Sum of electronic and thermal Enthalpies=	-1408.404203
Sum of electronic and thermal Free Energies=	-1408.469738

C	-1.72792700	0.52520700	0.23779900
C	-3.11979800	0.48550800	2.18247300
C	-1.87867800	-0.16054600	1.58395400
H	-1.43481900	1.57248400	0.39654200
H	-2.88668100	1.49525900	2.54403900
H	-3.54338400	-0.07995000	3.01743300
H	-0.97848600	-0.02620900	2.19433200
H	-2.03397900	-1.24082200	1.43641500
C	-0.88769000	-0.15213300	-0.80909700
H	-1.28865800	-1.15663800	-1.01123700
H	-0.88229600	0.40200000	-1.75687200
P	1.27816700	2.07145400	-0.53212700
H	1.26785400	2.88810300	0.61092600
H	2.42920100	2.55246900	-1.17716200
H	0.27300700	2.68667200	-1.29902200
P	3.43202700	-0.39200000	0.51502000
H	4.13256600	-1.58011900	0.24318600
H	4.35839700	0.54709400	0.02822100
H	3.67461900	-0.27912300	1.89440300
P	0.79601000	-2.56152000	-0.03956600
H	1.85751100	-3.41187800	0.31198900
H	-0.19386200	-2.99366700	0.85783200
H	0.34961500	-3.16733800	-1.22469600
N	-3.20514400	0.63011200	-0.21990000
H	-3.36049500	1.49273900	-0.74962600
H	-3.41489800	-0.13749400	-0.86672100
C	-4.09358700	0.54948900	1.01277900
H	-4.68903100	-0.36166300	0.91860200
H	-4.76158000	1.41233400	1.02035300
Pd	1.13584000	-0.25376000	-0.19038300

2a
M=Pd(PH3)3
6-int-endo

Zero-point correction=	0.249056 (Hartree/Particle)
Thermal correction to Energy=	0.265544
Thermal correction to Enthalpy=	0.266488
Thermal correction to Gibbs Free Energy=	0.204615
Sum of electronic and zero-point Energies=	-1408.421439
Sum of electronic and thermal Energies=	-1408.404952
Sum of electronic and thermal Enthalpies=	-1408.404007
Sum of electronic and thermal Free Energies=	-1408.465880

C	-2.67596900	-1.45498300	0.48816000
C	-1.79412800	-0.99561600	-0.64728200
C	-1.86994900	0.43437900	1.91231400
C	-2.08348800	-1.07933000	1.83907500
H	-0.79319500	-1.44480000	-0.62492900
H	-2.22780200	-1.16557400	-1.63844200
H	-3.64253300	-0.92914900	0.40504000
H	-1.40276000	0.71722600	2.86352900
H	-2.83625300	0.95936200	1.86701000
H	-1.10462000	-1.56228400	1.99464900
H	-2.73700300	-1.41033300	2.65615700
P	-1.07310900	-4.12674500	1.22513800
H	0.09121500	-3.41512500	0.88756000
H	-1.04720000	-4.00630200	2.62475400
H	-0.60907300	-5.44492900	1.07478200
P	-5.08210000	-2.75252900	-0.79619300
H	-6.00762100	-2.18441400	0.09411700
H	-4.93466600	-1.70104000	-1.71731000
H	-5.91005600	-3.62432300	-1.52192600
P	-3.66356400	-5.85383800	-0.14158600
H	-3.98827100	-6.59509500	1.00796000
H	-4.75065300	-6.20001500	-0.96348000
H	-2.67453000	-6.69010000	-0.68927900
N	-1.55781600	0.50531300	-0.53865200
H	-0.94551600	0.81733700	-1.30089000
H	-2.45164200	0.99276900	-0.67760600
C	-0.97270100	0.91008200	0.78884500
H	-0.85017800	1.99646100	0.76944800
H	0.01960000	0.44567000	0.83584800
Pd	-3.10738100	-3.52694000	0.19408700

Figure-4-structures

2b
M=Pd(PH3)3
reactant

Zero-point correction=	0.271041 (Hartree/Particle)
Thermal correction to Energy=	0.290955
Thermal correction to Enthalpy=	0.291900
Thermal correction to Gibbs Free Energy=	0.221593
Sum of electronic and zero-point Energies=	-1447.640091
Sum of electronic and thermal Energies=	-1447.620176
Sum of electronic and thermal Enthalpies=	-1447.619232
Sum of electronic and thermal Free Energies=	-1447.689539

C	-0.82623900	1.21208300	0.36074000
C	-3.09872600	1.01159200	1.35831200
C	-1.81069800	0.27173100	0.98228400
H	-0.59498800	2.09930800	0.95903500
H	-2.87037200	1.79241700	2.10168200
H	-3.78186600	0.30381900	1.84648300
H	-1.38402500	-0.18061100	1.88932600
H	-2.05425700	-0.54453000	0.28367000
C	-0.46352000	1.22614300	-0.96786700
H	-0.87613000	0.44990000	-1.61744500
P	2.30772200	2.04273900	1.00852600
H	1.50410700	3.05697300	1.54866800
H	3.27786500	1.88307800	2.00702900
H	3.01967200	2.72443100	0.01072900
P	3.19406800	-1.12591700	0.68822600
H	3.00217800	-2.38070200	1.28200500
H	3.93556200	-1.43617600	-0.45883200
H	4.14666000	-0.53883200	1.53108500
P	0.33433900	-1.98635900	-0.53948400
H	1.23772600	-2.91975400	-1.06878500
H	-0.28268000	-2.72287100	0.48202500
H	-0.65606200	-1.95067700	-1.53094400
N	-5.08997300	2.17110600	0.56834600
H	-5.57385900	2.55221500	-0.24183400
H	-4.94157200	2.95993500	1.19648100
C	-3.80075100	1.63140100	0.16259100
H	-3.97407900	0.85205200	-0.59692100
H	-3.13231300	2.37968200	-0.31118800
C	0.17399800	2.37438000	-1.67145300
H	1.03135100	2.06193400	-2.28062800
H	-0.56228600	2.80575300	-2.36463900
H	0.48516800	3.16975400	-0.98366800
Pd	1.23295800	0.08043500	0.21790800

2b
M=Pd(PH3)3
5-exo-TS

Zero-point correction=	0.271316 (Hartree/Particle)
Thermal correction to Energy=	0.290252
Thermal correction to Enthalpy=	0.291197
Thermal correction to Gibbs Free Energy=	0.222592
Sum of electronic and zero-point Energies=	-1447.645593
Sum of electronic and thermal Energies=	-1447.626657
Sum of electronic and thermal Enthalpies=	-1447.625712
Sum of electronic and thermal Free Energies=	-1447.694317

C	-1.28329700	0.61434200	0.38132900
C	-3.36730500	-0.11271900	1.58901700
C	-1.86369300	0.19335300	1.69522400
H	-1.11394600	1.67710100	0.21020500
H	-3.74504600	-0.39731800	2.57895000
H	-3.51441700	-0.98198100	0.92846700
H	-1.70100600	0.98296800	2.44132900
H	-1.35474100	-0.70894800	2.06204100
C	-0.93569300	-0.26367700	-0.64214300
H	-1.37898500	-1.26310900	-0.55880200
P	1.50096900	1.94768500	0.65727100
H	2.83845200	2.34566100	0.79953800
H	1.06848500	2.79732500	-0.37222400
H	0.91174300	2.54197500	1.78367000
P	3.24609100	-0.85989100	1.18885200
H	4.05411000	-1.57225600	0.29119800
H	4.09180200	0.19150000	1.57127100
H	3.27251200	-1.68730400	2.32103900
P	0.73286700	-2.68442900	0.08706600
H	1.74955800	-3.58341500	0.44555700
H	-0.37124200	-3.21434800	0.77118800
H	0.46884100	-3.06179700	-1.23776900
N	-3.56637600	1.40850700	-0.26965100
H	-3.83700300	2.34124000	-0.57328600
H	-3.89943300	0.75409900	-0.97649200
C	-4.12109600	1.07882300	1.03923800
H	-3.97551100	1.94571400	1.69844200
H	-5.20258200	0.86877800	1.01295600
C	-0.67933100	0.20461600	-2.04266500
H	0.00123900	-0.46314900	-2.58462800
H	-1.62899300	0.22134900	-2.59795900
H	-0.26178400	1.21837700	-2.07019700
Pd	1.08822600	-0.37093400	0.38793900

Figure-4-structures

2b
M=Pd(PH3)3
6-TS-endo

Zero-point correction=	0.271329 (Hartree/Particle)
Thermal correction to Energy=	0.289949
Thermal correction to Enthalpy=	0.290893
Thermal correction to Gibbs Free Energy=	0.225216
Sum of electronic and zero-point Energies=	-1447.645157
Sum of electronic and thermal Energies=	-1447.626537
Sum of electronic and thermal Enthalpies=	-1447.625593
Sum of electronic and thermal Free Energies=	-1447.691270

C	-2.83664000	-1.29026100	0.08835100
C	-1.68969200	-1.54650100	-0.65132400
C	-2.46993400	0.66409700	1.61221300
C	-2.76749700	-0.83792700	1.52141600
H	-0.75428900	-1.69232100	-0.10637500
H	-3.65589300	-0.84725400	-0.49140700
H	-2.57545200	0.97145900	2.66099500
H	-3.23184900	1.22713800	1.04883700
H	-1.98868600	-1.39374900	2.06718800
H	-3.71921100	-1.05097300	2.02808900
P	-0.96733500	-4.22581900	0.72742000
H	-0.33706400	-3.46436600	1.72377700
H	-0.83477000	-5.52223600	1.24897100
H	0.00452000	-4.23811000	-0.28483900
P	-5.31235000	-2.87779300	-0.56474800
H	-5.91045800	-1.94432600	0.29531100
H	-5.40783000	-2.23312700	-1.80672600
H	-6.31074000	-3.85656200	-0.67298100
P	-3.82819400	-5.78666700	0.27109900
H	-5.14366500	-6.12291600	-0.07918900
H	-3.08422800	-6.71367800	-0.47368800
H	-3.72571000	-6.31198800	1.56754700
N	-0.93604400	0.84770200	-0.31314100
H	0.00564300	1.09044600	-0.61587200
H	-1.57305800	1.46102500	-0.82151500
C	-1.08190900	1.05738100	1.12878800
H	-0.87744500	2.09979800	1.42561500
H	-0.32911400	0.43422300	1.63622600
C	-1.62686000	-1.65037000	-2.12820800
H	-0.92245600	-0.89685900	-2.50233800
H	-1.23874300	-2.62833100	-2.44364600
H	-2.60422200	-1.48716700	-2.59571400
Pd	-3.14612600	-3.53541100	0.06689200

2b
M=Pd(PH3)3
5-exo-int

Zero-point correction=	0.274862 (Hartree/Particle)
Thermal correction to Energy=	0.292690
Thermal correction to Enthalpy=	0.293634
Thermal correction to Gibbs Free Energy=	0.228751
Sum of electronic and zero-point Energies=	-1447.673326
Sum of electronic and thermal Energies=	-1447.655498
Sum of electronic and thermal Enthalpies=	-1447.654553
Sum of electronic and thermal Free Energies=	-1447.719437

C	-1.75749600	0.67422700	0.12657500
C	-3.07372400	0.82532100	2.13641900
C	-1.75035800	0.29889500	1.60170200
H	-1.54441200	1.74573000	0.00281600
H	-3.04461500	1.91836200	2.23671700
H	-3.34699400	0.40363300	3.10799300
H	-0.87762300	0.72385200	2.10990500
H	-1.69743200	-0.79623700	1.70530900
C	-0.93195000	-0.17625900	-0.80411700
H	-1.32777200	-1.20265200	-0.72000300
P	1.23060900	2.11803800	-0.09718700
H	0.78252100	2.73725700	1.08361500
H	2.50238800	2.70343400	-0.21257800
H	0.52634600	2.87319600	-1.05199600
P	3.42529200	-0.48512000	0.47801000
H	4.20878900	-1.33712300	-0.32033700
H	4.27629900	0.63305800	0.53991200
H	3.67474900	-1.04936300	1.74132700
P	0.81741700	-2.56203800	-0.26166600
H	1.90109100	-3.43579400	-0.07023900
H	-0.11653500	-3.09763200	0.64103200
H	0.30296800	-3.03679800	-1.48027300
N	-3.27739400	0.57617600	-0.23050000
H	-3.57794200	1.41273200	-0.74002200
H	-3.45036000	-0.21525900	-0.85897300
C	-4.05904200	0.41295500	1.06096200
H	-4.32304200	-0.64530300	1.13830600
H	-4.97193500	1.00815200	1.00200500
C	-0.95400300	0.24674300	-2.26124800
H	-1.95690300	0.14350000	-2.70842100
H	-0.64679300	1.29144900	-2.40279300
H	-0.28233100	-0.37878600	-2.86298800
Pd	1.10970600	-0.24171400	-0.15710700

Figure-4-structures

2b
M=Pd(PH3)3
6-TS-int

Zero-point correction=	0.276168 (Hartree/Particle)
Thermal correction to Energy=	0.293405
Thermal correction to Enthalpy=	0.294349
Thermal correction to Gibbs Free Energy=	0.231531
Sum of electronic and zero-point Energies=	-1447.680575
Sum of electronic and thermal Energies=	-1447.663338
Sum of electronic and thermal Enthalpies=	-1447.662394
Sum of electronic and thermal Free Energies=	-1447.725212

C	-2.70438800	-1.43091500	0.27292200
C	-1.53218700	-1.04330500	-0.60673400
C	-2.30637200	0.52868100	1.78643100
C	-2.54469900	-0.98063700	1.71786200
H	-0.58126300	-1.44975100	-0.23027500
H	-3.57985800	-0.90578600	-0.15108300
H	-2.11961100	0.84813400	2.81884200
H	-3.20068500	1.07186300	1.44451400
H	-1.69928500	-1.49430600	2.20204200
H	-3.44049100	-1.24221100	2.29727300
P	-0.89890000	-4.05777600	0.73919900
H	-0.16180000	-3.20056900	1.57595200
H	-0.67122500	-5.28559700	1.38244700
H	-0.00439400	-4.17514700	-0.33967200
P	-5.29599200	-2.81783700	-0.33934700
H	-5.84177900	-1.88795900	0.56153000
H	-5.42872300	-2.11855700	-1.55041900
H	-6.34899600	-3.74170800	-0.44710200
P	-3.76874600	-5.84713100	0.06931800
H	-2.85800900	-6.87024800	0.38845900
H	-4.85626200	-6.23469500	0.87192900
H	-4.22051900	-6.30679100	-1.17978600
N	-1.32560400	0.47270500	-0.47495600
H	-0.52624100	0.75813200	-1.05307500
H	-2.14372400	0.95469200	-0.87209500
C	-1.11542500	0.92746600	0.94416600
H	-0.95319700	2.00853500	0.91546700
H	-0.19222500	0.44231200	1.28390800
C	-1.71095900	-1.36208800	-2.07451000
H	-1.75357600	-2.44863800	-2.21353100
H	-2.65148500	-0.94011400	-2.45567000
H	-0.88189700	-0.98031300	-2.68264400
Pd	-3.12675000	-3.52398600	0.18318000

Figure-4-structures

3a
M=PdCl2MeCN
reactant

Zero-point correction=	0.159815 (Hartree/Particle)
Thermal correction to Energy=	0.176112
Thermal correction to Enthalpy=	0.177056
Thermal correction to Gibbs Free Energy=	0.113102
Sum of electronic and zero-point Energies=	-1467.221268
Sum of electronic and thermal Energies=	-1467.204972
Sum of electronic and thermal Enthalpies=	-1467.204027
Sum of electronic and thermal Free Energies=	-1467.267982

C	-0.33449400	1.11839400	-0.64203100
C	-1.41080600	0.37140600	0.09547000
C	-2.43941100	0.96613100	0.80309000
C	1.14417900	1.65853500	1.10850900
H	-2.99986800	0.40073600	1.54610600
H	-1.18181400	-0.67959700	0.28518300
H	-0.55580000	2.19219400	-0.71124800
H	-0.20487500	0.72866700	-1.65682800
H	-2.56433000	2.04930400	0.80533200
Pd	-3.27860900	0.24809700	-1.08225200
Cl	-3.03498400	2.38429100	-2.00669900
Cl	-3.61239000	-1.87642200	-0.16656200
N	-4.60649100	-0.21771800	-2.60540000
C	-5.35311500	-0.47920300	-3.44601600
C	-6.28650800	-0.80687500	-4.49792700
H	-6.40628500	-1.89279500	-4.56442700
H	-5.91572200	-0.42563300	-5.45477600
H	-7.25869200	-0.35097200	-4.28447500
N	2.17228600	1.44150400	1.80713800
O	0.90168600	0.88812900	0.02723400
H	2.21709600	2.12265400	2.56398600
H	0.38868000	2.44515000	1.26773100

3a
M=PdCl2MeCN
6-endo-TS

Zero-point correction=	0.159944 (Hartree/Particle)
Thermal correction to Energy=	0.175337
Thermal correction to Enthalpy=	0.176281
Thermal correction to Gibbs Free Energy=	0.114975
Sum of electronic and zero-point Energies=	-1467.214838
Sum of electronic and thermal Energies=	-1467.199446
Sum of electronic and thermal Enthalpies=	-1467.198501
Sum of electronic and thermal Free Energies=	-1467.259808

C	0.22008900	0.88441900	-0.84137900
C	-1.02922200	0.35362000	-0.19206100
C	-1.74435400	1.29886700	0.56355400
C	1.10392700	1.43646900	1.30815100
H	-2.36619100	0.99907300	1.40535900
H	-0.88767300	-0.62573900	0.27451400
H	0.08981200	1.91572500	-1.18919300
H	0.58171800	0.26512900	-1.66540600
H	-1.84935200	2.31990400	0.20709100
Pd	-2.78627900	0.15716000	-1.32064600
Cl	-2.13871500	1.87955800	-2.78386000
Cl	-3.46179400	-1.53914100	0.15824400
N	-4.48791100	-0.20235500	-2.52048200
C	-5.41208200	-0.41068200	-3.18166500
C	-6.57013300	-0.66986100	-4.00700400
H	-6.28421600	-0.66245100	-5.06361600
H	-7.32739300	0.10253500	-3.83823400
H	-6.99543800	-1.64715400	-3.75790900
N	0.02778000	2.01461100	1.67272700
O	1.28911900	0.85443000	0.13148800
H	0.08108000	2.37123400	2.62488500
H	2.00614800	1.34735300	1.92196800

Figure-4-structures

3a
M=PdCl2MeCN
5-TS-exo

Zero-point correction=	0.159815 (Hartree/Particle)
Thermal correction to Energy=	0.176112
Thermal correction to Enthalpy=	0.177056
Thermal correction to Gibbs Free Energy=	0.113102
Sum of electronic and zero-point Energies=	-1467.221268
Sum of electronic and thermal Energies=	-1467.204972
Sum of electronic and thermal Enthalpies=	-1467.204027
Sum of electronic and thermal Free Energies=	-1467.267982

C	-1.47111300	0.18862200	0.46455800
C	-4.07017100	0.41667000	0.17258400
C	-2.38427900	-0.79862800	1.13342800
H	-1.46134700	1.19877500	0.87558800
H	-2.06526200	-0.99600400	2.16111900
H	-2.40456500	-1.74391300	0.57538200
C	-0.38844800	-0.20147700	-0.35038800
H	-0.47237200	-1.15533900	-0.87404000
H	0.12104400	0.59196000	-0.89838000
Pd	0.79221500	-0.48705300	1.36070700
Cl	0.37665300	-2.80098500	1.22485800
Cl	1.21069700	1.82880100	1.44672700
N	2.11098300	-0.80272200	2.97453300
C	2.85697700	-0.98055200	3.83882800
C	3.79048100	-1.20234000	4.92045700
H	3.99114900	-0.25991100	5.43987000
H	3.37382300	-1.92191300	5.63251100
H	4.73110900	-1.59830100	4.52411000
O	-3.72438000	-0.28976100	1.24058700
N	-3.18846400	0.68288200	-0.69752700
H	-3.46785100	1.27010100	-1.47910800
H	-5.12158300	0.71178000	0.17886000

3a
M=PdCl2MeCN
6-endo-int

Zero-point correction=	0.163806 (Hartree/Particle)
Thermal correction to Energy=	0.179055
Thermal correction to Enthalpy=	0.180000
Thermal correction to Gibbs Free Energy=	0.118591
Sum of electronic and zero-point Energies=	-1467.253182
Sum of electronic and thermal Energies=	-1467.237932
Sum of electronic and thermal Enthalpies=	-1467.236988
Sum of electronic and thermal Free Energies=	-1467.298397

C	0.07897100	0.61238700	-0.85544300
C	-1.15930500	0.43007000	-0.03598400
C	-1.34883500	1.61573200	0.88022100
C	1.08019600	1.45009900	1.13871700
H	-2.10475800	1.42657600	1.64882100
H	-1.06920000	-0.48583500	0.56348800
H	0.04355200	1.49315400	-1.50645400
H	0.36020400	-0.27137500	-1.43188800
H	-1.61865700	2.52835000	0.33429800
Pd	-2.76000700	0.13394400	-1.26888500
Cl	-2.48106700	2.30479100	-2.19673900
Cl	-3.01111000	-2.02831800	-0.33618800
N	-4.44803400	-0.20966600	-2.54626900
C	-5.36798000	-0.39928100	-3.22057200
C	-6.51922100	-0.63731300	-4.06376000
H	-6.21962200	-0.63119500	-5.11667300
H	-7.26856000	0.14464900	-3.90414000
H	-6.96325400	-1.60923700	-3.82620500
N	-0.06866900	1.86688500	1.58326400
O	1.26459100	0.83903100	0.02615900
H	-0.07274400	2.35486200	2.47427400
H	1.97697700	1.62123900	1.73206600

Figure-4-structures

3a
M=PdCl2MeCN
5-int-exo

Zero-point correction=	0.162512 (Hartree/Particle)
Thermal correction to Energy=	0.178048
Thermal correction to Enthalpy=	0.178992
Thermal correction to Gibbs Free Energy=	0.115812
Sum of electronic and zero-point Energies=	-1467.246077
Sum of electronic and thermal Energies=	-1467.230540
Sum of electronic and thermal Enthalpies=	-1467.229596
Sum of electronic and thermal Free Energies=	-1467.292776

C	-1.80441000	0.42615400	0.11063500
C	-4.09104300	0.23859800	0.32518500
C	-2.20470200	-0.68408500	1.09502100
H	-1.35963600	1.29060500	0.61995800
H	-1.79860800	-0.56134600	2.10036000
H	-1.98108200	-1.68575100	0.71108300
C	-0.92427900	-0.03964600	-1.01730600
H	-1.40122800	-0.85816300	-1.57191700
H	-0.67358000	0.79000700	-1.68958700
Pd	0.82231900	-0.71360200	-0.22604800
Cl	0.09830500	-2.94941600	-0.57125200
Cl	1.43594900	1.55215000	0.12834500
N	2.69718200	-1.40623500	0.60977300
C	3.70160500	-1.76510100	1.05743700
C	4.95844000	-2.21401800	1.61693200
H	5.46435800	-1.38241100	2.11782700
H	4.78171900	-3.01216400	2.34500300
H	5.60674100	-2.59645700	0.82204100
O	-3.67269200	-0.60107400	1.21069800
N	-3.16773600	0.84291100	-0.34653000
H	-3.34676200	1.53806700	-1.06454100
H	-5.16012400	0.38446100	0.19958300

3b
M=PdCl2MeCN
reactant

Zero-point correction=	0.187701 (Hartree/Particle)
Thermal correction to Energy=	0.205637
Thermal correction to Enthalpy=	0.206582
Thermal correction to Gibbs Free Energy=	0.139082
Sum of electronic and zero-point Energies=	-1506.479430
Sum of electronic and thermal Energies=	-1506.461494
Sum of electronic and thermal Enthalpies=	-1506.460550
Sum of electronic and thermal Free Energies=	-1506.528049

C	-0.37571600	0.99190600	-0.65700900
C	-1.44333200	0.26398500	0.11353000
C	-2.42657900	0.88878100	0.86773400
C	1.11006200	1.64538300	1.05119400
H	-1.20982500	-0.78098900	0.33313600
H	-0.61252200	2.05833700	-0.77615600
H	-0.23678400	0.55861700	-1.65293800
H	-2.52025100	1.97432500	0.77688100
Pd	-3.26426300	0.18222100	-1.10315400
Cl	-3.17541900	2.42108500	-1.80023300
Cl	-3.42669700	-2.08261100	-0.52419400
N	-4.61880500	-0.18219500	-2.62819900
C	-5.35745800	-0.41675300	-3.48367400
C	-6.28159100	-0.71344900	-4.55314900
H	-6.41645700	-1.79642000	-4.63764500
H	-5.89191600	-0.32448800	-5.49933500
H	-7.24987800	-0.24626900	-4.34684900
N	2.14599200	1.47940200	1.75330600
O	0.86944900	0.81621200	0.01619900
H	2.18681500	2.20191600	2.47097200
H	0.34729800	2.43157500	1.17495600
C	-3.17137000	0.26124400	1.99314600
H	-4.24486500	0.47942700	1.93380900
H	-3.02611000	-0.82210500	2.03677900
H	-2.80886100	0.70680200	2.93139100

Figure-4-structures

3b
M=PdCl2MeCN
6-TS-endo

Zero-point correction=	0.187945 (Hartree/Particle)
Thermal correction to Energy=	0.204883
Thermal correction to Enthalpy=	0.205827
Thermal correction to Gibbs Free Energy=	0.141309
Sum of electronic and zero-point Energies=	-1506.477240
Sum of electronic and thermal Energies=	-1506.460302
Sum of electronic and thermal Enthalpies=	-1506.459358
Sum of electronic and thermal Free Energies=	-1506.523876

C	0.11273400	0.81766100	-0.81129100
C	-1.10777500	0.32285300	-0.08077100
C	-1.76802800	1.28943300	0.71671800
C	1.17130900	1.39064200	1.23499600
H	-0.94146500	-0.64189300	0.41037400
H	-0.01636700	1.84860400	-1.16193500
H	0.39197800	0.18133500	-1.65447400
H	-1.86201200	2.29275800	0.30117500
Pd	-2.80883300	0.06684400	-1.27812500
Cl	-2.41371600	2.07421000	-2.45403100
Cl	-3.22699400	-1.95130300	-0.13771200
N	-4.46071500	-0.30408700	-2.53679100
C	-5.35526600	-0.49572200	-3.24242100
C	-6.47526600	-0.72997500	-4.12610600
H	-7.23958700	0.03803300	-3.96940900
H	-6.91147300	-1.71390900	-3.92697900
H	-6.14162800	-0.69125300	-5.16803100
N	0.13517300	2.01401200	1.63833800
O	1.25797300	0.76856400	0.06933900
H	0.25382400	2.40055500	2.57332600
C	-2.57964300	0.97769800	1.91650100
H	-2.34515000	-0.01020700	2.32558000
H	-2.43038600	1.74794800	2.68134700
H	-3.64538200	1.00180700	1.64934000
H	2.10681100	1.29073500	1.79500300

3b
M=PdCl2MeCN
5-TS-exo

Zero-point correction=	0.186947 (Hartree/Particle)
Thermal correction to Energy=	0.204244
Thermal correction to Enthalpy=	0.205189
Thermal correction to Gibbs Free Energy=	0.139428
Sum of electronic and zero-point Energies=	-1506.474077
Sum of electronic and thermal Energies=	-1506.456779
Sum of electronic and thermal Enthalpies=	-1506.455835
Sum of electronic and thermal Free Energies=	-1506.521596

C	-1.48926000	0.19794100	0.49930700
C	-4.03648500	-0.04694200	-0.00253600
C	-2.21352000	-1.02595700	0.98699400
H	-1.67952900	1.12857800	1.03676100
H	-1.95204500	-1.26079700	2.02315700
H	-1.98158900	-1.89019700	0.35081000
C	-0.32701800	0.12727400	-0.30466200
H	-0.24885100	-0.78953300	-0.89696300
Pd	0.79433100	-0.30365500	1.43899300
Cl	0.95369100	-2.53414500	0.67788000
Cl	0.62548500	1.90127500	2.28568800
N	2.11399700	-0.76603700	3.03499000
C	2.85842400	-1.01055100	3.88446000
C	3.78859500	-1.31525700	4.94893000
H	3.52889000	-0.74419400	5.84603900
H	3.75321200	-2.38402800	5.18257600
H	4.80566200	-1.05129400	4.64151600
O	-3.64026100	-0.82630900	0.99160500
N	-3.16353200	0.53185400	-0.71707100
H	-3.49511900	1.16581900	-1.43930600
H	-5.12307200	0.02210500	-0.08544400
C	0.15350400	1.36099700	-1.01411400
H	-0.43245600	1.49209600	-1.93806300
H	0.03719500	2.26007100	-0.39952700
H	1.20780900	1.27367800	-1.30275800

Figure-4-structures

3b
M=PdCl2MeCN
6-int-endo

Zero-point correction=	0.191427 (Hartree/Particle)
Thermal correction to Energy=	0.208096
Thermal correction to Enthalpy=	0.209041
Thermal correction to Gibbs Free Energy=	0.144938
Sum of electronic and zero-point Energies=	-1506.511947
Sum of electronic and thermal Energies=	-1506.495278
Sum of electronic and thermal Enthalpies=	-1506.494334
Sum of electronic and thermal Free Energies=	-1506.558437

C	0.06446200	0.63303400	-0.86925500
C	-1.16233400	0.44372700	-0.03590700
C	-1.34900100	1.61126900	0.91104800
C	1.10046200	1.40560600	1.13007300
H	-1.06557300	-0.47888200	0.55574800
H	0.02574200	1.52541900	-1.50410800
H	0.32812800	-0.24247600	-1.46650300
H	-1.55186000	2.53552400	0.35164500
Pd	-2.76504200	0.14474400	-1.26854200
Cl	-2.52443500	2.33857200	-2.15072300
Cl	-2.99036500	-2.03348900	-0.36158400
N	-4.44856700	-0.20337100	-2.55097400
C	-5.36768800	-0.39628700	-3.22551200
C	-6.51822900	-0.63858700	-4.06849200
H	-6.21857500	-0.63391000	-5.12139000
H	-7.26936300	0.14199000	-3.91048100
H	-6.96006400	-1.61104600	-3.82900500
N	-0.03984700	1.81660700	1.60043200
O	1.26729800	0.83213400	-0.00472100
H	-0.02871200	2.27102100	2.51038100
H	2.00559000	1.54704700	1.71867200
C	-2.41391400	1.37927000	1.96016800
H	-2.22641900	0.44366100	2.50412300
H	-2.46274000	2.20602600	2.68002000
H	-3.38947900	1.29878500	1.46621100

3b
M=PdCl2MeCN
5-int-exo

Zero-point correction=	0.190351 (Hartree/Particle)
Thermal correction to Energy=	0.207463
Thermal correction to Enthalpy=	0.208407
Thermal correction to Gibbs Free Energy=	0.141949
Sum of electronic and zero-point Energies=	-1506.498807
Sum of electronic and thermal Energies=	-1506.481695
Sum of electronic and thermal Enthalpies=	-1506.480750
Sum of electronic and thermal Free Energies=	-1506.547209

C	-1.82322700	0.52028100	0.07917100
C	-4.08239000	0.18952900	0.37895500
C	-2.11484800	-0.52009900	1.16757700
H	-1.44082100	1.46025500	0.49728400
H	-1.68625100	-0.28370600	2.14280100
H	-1.84043600	-1.53657100	0.86471800
C	-0.92214300	0.00880000	-1.01890500
H	-1.38719100	-0.88517300	-1.46056700
Pd	0.81851500	-0.67727500	-0.18179200
Cl	0.45146000	-2.76471700	-1.26797700
Cl	1.14339000	1.40316500	0.94750900
N	2.69845600	-1.41196800	0.64121000
C	3.69561000	-1.79356000	1.08672500
C	4.94242200	-2.27114700	1.64555600
H	5.46023300	-1.45478200	2.15921700
H	4.74823900	-3.07476800	2.36315800
H	5.58767700	-2.65560300	0.84924500
O	-3.58057500	-0.52421600	1.32922600
N	-3.22378800	0.78137200	-0.38433800
H	-3.47999100	1.39998600	-1.14719700
H	-5.16211800	0.25166500	0.27836400
C	-0.60984400	1.03779700	-2.08296400
H	-1.51294100	1.33805900	-2.64315000
H	-0.16405300	1.94321600	-1.65074900
H	0.09428200	0.63296900	-2.82131900

Figure-4-structures

3c
M=PdCl2MeCN
reactant

Zero-point correction=	0.159365 (Hartree/Particle)
Thermal correction to Energy=	0.180296
Thermal correction to Enthalpy=	0.181240
Thermal correction to Gibbs Free Energy=	0.104670
Sum of electronic and zero-point Energies=	-2885.186557
Sum of electronic and thermal Energies=	-2885.165625
Sum of electronic and thermal Enthalpies=	-2885.164681
Sum of electronic and thermal Free Energies=	-2885.241252

C	-0.74435600	1.91236500	-0.80117300
C	-1.51375400	0.83367400	-0.09127300
C	-2.61069900	1.05970700	0.71645400
C	0.73941800	2.49641800	0.93577800
H	-2.94755300	0.30127000	1.42143600
H	-0.98856800	-0.12204400	-0.01758800
H	-1.21314000	2.89547000	-0.69321000
H	-0.61280400	1.68159200	-1.86241200
H	-3.01850100	2.06352700	0.82823900
Pd	-3.35108700	0.27534100	-1.18619800
Cl	-3.76770300	2.45621800	-1.92384200
Cl	-3.02444500	-1.91969500	-0.44898200
N	-4.63131400	-0.43594600	-2.65385600
C	-5.35608700	-0.84980100	-3.45128700
C	-6.26439400	-1.36904300	-4.44684100
H	-6.13230500	-2.45134800	-4.54267300
H	-6.06811000	-0.89484200	-5.41371300
H	-7.29692400	-1.15891000	-4.14947100
N	-0.19322200	3.06379900	1.56522600
O	0.58682000	1.93530400	-0.26793600
C	2.20039600	2.30177300	1.37929500
H	0.11128500	3.43725700	2.46298200
Cl	2.53546700	0.54671800	1.47244000
Cl	2.48678000	3.03275700	2.97557400
Cl	3.29094500	3.06164400	0.18664500

3c
M=PdCl2MeCN
6-TS-endo

Zero-point correction=	0.159181 (Hartree/Particle)
Thermal correction to Energy=	0.179371
Thermal correction to Enthalpy=	0.180315
Thermal correction to Gibbs Free Energy=	0.105804
Sum of electronic and zero-point Energies=	-2885.170714
Sum of electronic and thermal Energies=	-2885.150523
Sum of electronic and thermal Enthalpies=	-2885.149579
Sum of electronic and thermal Free Energies=	-2885.224090

C	0.16622900	1.17690800	-0.87640700
C	-0.97620500	0.40639300	-0.28003300
C	-1.72173500	1.14050300	0.66673600
C	1.06858700	1.46411600	1.32470500
H	-2.26193400	0.63843200	1.46824900
H	-0.69389000	-0.60649100	0.02390900
H	-0.08940300	2.22598200	-1.06188600
H	0.57898200	0.73148800	-1.78346800
H	-1.98094300	2.17841900	0.47186900
Pd	-2.74096700	0.16618200	-1.37523100
Cl	-2.34756400	2.13858500	-2.58940000
Cl	-3.15497800	-1.78714100	-0.13813700
N	-4.46071900	-0.19900700	-2.53622300
C	-5.39500000	-0.41565200	-3.18012400
C	-6.56627900	-0.68655600	-3.98277600
H	-7.40593400	-0.96089000	-3.33619300
H	-6.36239900	-1.51295000	-4.67112800
H	-6.83619300	0.20202500	-4.56221700
N	-0.05223400	1.82598100	1.80469800
O	1.27665000	1.14354800	0.06553700
H	-0.06006800	2.01278600	2.80586300
C	2.37563200	1.28573800	2.12381500
Cl	2.18180700	1.82910700	3.80509500
Cl	3.67671900	2.22351500	1.35151800
Cl	2.78256600	-0.45353600	2.10870900

Figure-4-structures

3c
M=PdCl2MeCN
5-TS-exo

Zero-point correction=	0.158684 (Hartree/Particle)
Thermal correction to Energy=	0.178938
Thermal correction to Enthalpy=	0.179882
Thermal correction to Gibbs Free Energy=	0.105704
Sum of electronic and zero-point Energies=	-2885.173328
Sum of electronic and thermal Energies=	-2885.153075
Sum of electronic and thermal Enthalpies=	-2885.152131
Sum of electronic and thermal Free Energies=	-2885.226309

C	-1.55460300	0.42222700	0.62627600
C	-4.08200600	0.20406400	0.15401000
C	-2.22884500	-0.89635400	0.89514300
H	-1.75046800	1.22005200	1.34520900
H	-1.92147100	-1.31704900	1.85596800
H	-2.01873900	-1.61684300	0.09495800
C	-0.37016800	0.51446100	-0.14467700
H	-0.24861800	-0.21100700	-0.95120400
H	-0.02473900	1.52390700	-0.37237700
Pd	0.80993100	-0.09829800	1.47081000
Cl	0.87966100	-2.26779500	0.55570100
Cl	0.72777600	2.08728000	2.34305500
N	2.12220200	-0.69138000	3.01246500
C	2.85739300	-1.01782500	3.84204700
C	3.77473100	-1.42658700	4.88217000
H	4.75878300	-0.97953100	4.70806700
H	3.40247400	-1.09658300	5.85734400
H	3.87356600	-2.51660600	4.88686900
O	-3.65887100	-0.72645400	0.98902200
N	-3.22287200	0.91101900	-0.44874000
H	-3.51828000	1.66442800	-1.06513700
C	-5.60496900	0.28267500	0.08303300
Cl	-6.11367000	1.51801000	-1.08590600
Cl	-6.20676700	0.70799600	1.70619400
Cl	-6.23244200	-1.30748700	-0.41199000

3c
M=PdCl2MeCN
6-int-endo

Zero-point correction=	0.162485 (Hartree/Particle)
Thermal correction to Energy=	0.182600
Thermal correction to Enthalpy=	0.183544
Thermal correction to Gibbs Free Energy=	0.109287
Sum of electronic and zero-point Energies=	-2885.201086
Sum of electronic and thermal Energies=	-2885.180971
Sum of electronic and thermal Enthalpies=	-2885.180027
Sum of electronic and thermal Free Energies=	-2885.254284

C	0.02928700	0.64368500	-0.81054300
C	-1.19151600	0.40949500	0.01269100
C	-1.39440800	1.56008200	0.96512700
C	1.03682000	1.44467300	1.21517300
H	-2.14307600	1.34155600	1.73222800
H	-1.08394700	-0.52532700	0.57831800
H	-0.02371000	1.54265100	-1.43442800
H	0.34193200	-0.21829800	-1.40281200
H	-1.66810600	2.49077200	0.45251200
Pd	-2.77924600	0.12858800	-1.24490800
Cl	-2.58545200	2.35907000	-2.03643700
Cl	-2.91940600	-2.10527700	-0.48128700
N	-4.44133800	-0.20104700	-2.54497800
C	-5.34411600	-0.38682000	-3.24286400
C	-6.47306200	-0.61921700	-4.11694900
H	-6.14872900	-0.58871900	-5.16211000
H	-7.23372100	0.15212500	-3.95929100
H	-6.91225700	-1.60025700	-3.90968700
N	-0.11658800	1.81175500	1.68450000
O	1.22111900	0.88351100	0.07969400
H	-0.14316300	2.26518600	2.59618000
C	2.33983200	1.69840400	1.98515800
Cl	3.25166100	0.17952000	2.06495300
Cl	2.03290400	2.29478000	3.63063100
Cl	3.24382400	2.92373600	1.06187800

Figure-4-structures

3c
M=PdCl2MeCN
5-int-exo

Zero-point correction=	0.161272 (Hartree/Particle)
Thermal correction to Energy=	0.181645
Thermal correction to Enthalpy=	0.182589
Thermal correction to Gibbs Free Energy=	0.106597
Sum of electronic and zero-point Energies=	-2885.192751
Sum of electronic and thermal Energies=	-2885.172378
Sum of electronic and thermal Enthalpies=	-2885.171434
Sum of electronic and thermal Free Energies=	-2885.247426

C	-1.75285100	0.42799800	0.38517500
C	-3.94939000	0.13778200	-0.24672400
C	-2.51062700	-0.50003500	1.34518700
H	-1.55032000	1.41150900	0.82859500
H	-2.50810400	-0.17256800	2.38575400
H	-2.18537300	-1.54344700	1.26728900
C	-0.50171400	-0.17335100	-0.18778000
H	-0.71721100	-1.12302000	-0.69392300
H	-0.00199700	0.52716600	-0.86726700
Pd	0.77926500	-0.52118200	1.35326900
Cl	0.22644200	-2.82908500	1.27064300
Cl	1.19961500	1.81294900	1.41177500
N	2.17459800	-0.86854900	2.96487100
C	2.93619100	-1.05005800	3.81625900
C	3.88997800	-1.27703000	4.88064400
H	4.10143400	-0.33751500	5.40116400
H	3.48669900	-1.99876300	5.59826000
H	4.82386600	-1.67205400	4.46773700
O	-3.91627100	-0.46771600	0.89182900
N	-2.82961300	0.64373600	-0.64242000
H	-2.69883800	1.15877500	-1.50995700
C	-5.27710300	0.17660700	-0.97717900
Cl	-5.74830500	-1.50434800	-1.30452500
Cl	-5.12900800	1.08234600	-2.49258700
Cl	-6.45031300	0.96170300	0.10018300

3d
M=PdCl2MeCN
reactant

Zero-point correction=	0.187123 (Hartree/Particle)
Thermal correction to Energy=	0.209693
Thermal correction to Enthalpy=	0.210637
Thermal correction to Gibbs Free Energy=	0.130596
Sum of electronic and zero-point Energies=	-2924.445143
Sum of electronic and thermal Energies=	-2924.422573
Sum of electronic and thermal Enthalpies=	-2924.421629
Sum of electronic and thermal Free Energies=	-2924.501670

C	-0.74862400	1.85598700	-0.84140300
C	-1.50270200	0.77132300	-0.12354800
C	-2.56820600	1.01517700	0.72983700
C	0.68535800	2.47096400	0.93008700
H	-0.94994500	-0.16581500	-0.01233700
H	-1.24613400	2.82814000	-0.76047000
H	-0.58356800	1.61307300	-1.89514800
H	-2.97156000	2.02983100	0.74226600
Pd	-3.27823200	0.22298400	-1.26582300
Cl	-3.89832800	2.42832100	-1.77284700
Cl	-2.70466400	-2.01873600	-0.88490000
N	-4.62525300	-0.43919100	-2.70171600
C	-5.36759000	-0.84124100	-3.48904600
C	-6.29795200	-1.34752700	-4.47129600
H	-6.19388200	-2.43379400	-4.55656900
H	-6.09755700	-0.88938100	-5.44505600
H	-7.32251700	-1.10812700	-4.16877900
N	-0.27403500	3.00254200	1.55227700
O	0.57390800	1.93111100	-0.28555000
C	2.13883800	2.29445100	1.40634100
H	0.00507500	3.36380700	2.46334400
Cl	2.48208100	0.54057200	1.51381000
Cl	2.38518200	3.03285100	3.00580200
Cl	3.25154600	3.05569000	0.23652400
C	-3.01607100	0.11645700	1.82521600
H	-2.70008300	0.57323200	2.77568300
H	-4.10946100	0.03709200	1.86074300
H	-2.58135000	-0.88486100	1.75144800

Figure-4-structures

3d
M=PdCl2MeCN
6-TS-endo

Zero-point correction=	0.187343 (Hartree/Particle)
Thermal correction to Energy=	0.208962
Thermal correction to Enthalpy=	0.209906
Thermal correction to Gibbs Free Energy=	0.132633
Sum of electronic and zero-point Energies=	-2924.433062
Sum of electronic and thermal Energies=	-2924.411443
Sum of electronic and thermal Enthalpies=	-2924.410499
Sum of electronic and thermal Free Energies=	-2924.487772

C	0.09995400	0.80255200	-0.82770400
C	-1.12305800	0.34050700	-0.08695700
C	-1.72329800	1.33807700	0.73151800
C	1.14931500	1.34532500	1.23732200
H	-0.96440100	-0.62021200	0.41648000
H	-0.00191900	1.82903700	-1.19768400
H	0.38657100	0.14215800	-1.64848300
H	-1.82283100	2.33439600	0.29881300
Pd	-2.80932200	0.08557900	-1.29433700
Cl	-2.40305100	2.09970300	-2.45451700
Cl	-3.23574700	-1.93024000	-0.15449000
N	-4.45833000	-0.28042000	-2.54989100
C	-5.35266300	-0.49178000	-3.25001500
C	-6.47293500	-0.75600900	-4.12479600
H	-7.38940700	-0.34271200	-3.69137400
H	-6.59694100	-1.83554800	-4.25666600
H	-6.30152400	-0.29342100	-5.10197000
N	0.11967900	1.97842000	1.63449000
O	1.24866400	0.75830000	0.06653900
H	0.17804100	2.35354300	2.58035900
C	2.42065100	1.08044900	2.06597700
Cl	2.45111000	2.08136800	3.53323800
Cl	3.86925400	1.42075500	1.09248800
Cl	2.38110000	-0.64825800	2.52386200
C	-2.54015600	1.04060000	1.93240700
H	-2.28085400	0.07298700	2.37460000
H	-2.43869100	1.83693800	2.67750900
H	-3.59934100	1.01621700	1.63991700

3d
M=PdCl2MeCN
5-TS-exo

Zero-point correction=	0.186545 (Hartree/Particle)
Thermal correction to Energy=	0.208483
Thermal correction to Enthalpy=	0.209427
Thermal correction to Gibbs Free Energy=	0.131895
Sum of electronic and zero-point Energies=	-2924.427247
Sum of electronic and thermal Energies=	-2924.405310
Sum of electronic and thermal Enthalpies=	-2924.404365
Sum of electronic and thermal Free Energies=	-2924.481897

C	-1.53646800	0.51675700	0.66674100
C	-4.06060300	0.32148800	0.24044100
C	-2.24336200	-0.72009800	1.15728600
H	-1.66350300	1.42145900	1.26501300
H	-1.96819300	-0.96623800	2.18651400
H	-2.03493000	-1.57703700	0.50469300
C	-0.38541800	0.43756200	-0.16333700
H	-0.36781600	-0.44842400	-0.80610900
Pd	0.78612100	-0.12320300	1.50190600
Cl	0.85269400	-2.31271100	0.61832700
Cl	0.70828200	2.03560600	2.46824100
N	2.11120800	-0.72285900	3.04721700
C	2.84673300	-1.05152400	3.87583600
C	3.76633700	-1.46476200	4.91255500
H	3.41696400	-2.39493800	5.37191100
H	4.75961800	-1.63120900	4.48329900
H	3.83642800	-0.68973400	5.68229800
O	-3.67437900	-0.51347900	1.18376800
N	-3.17794600	0.93490200	-0.42885900
H	-3.44887100	1.61738100	-1.13280400
C	-5.58048400	0.41440200	0.12246500
Cl	-6.04081400	1.59557400	-1.12040200
Cl	-6.23725300	0.91441100	1.69981100
Cl	-6.19607200	-1.19678000	-0.32305000
C	0.11112300	1.68835100	-0.83388800
H	-0.50798600	1.89557200	-1.72175900
H	0.06473600	2.55730000	-0.16831200
H	1.14617800	1.57240300	-1.17686300

Figure-4-structures

3d
M=PdCl2MeCN
6-int-endo

Zero-point correction=	0.190229 (Hartree/Particle)
Thermal correction to Energy=	0.211778
Thermal correction to Enthalpy=	0.212722
Thermal correction to Gibbs Free Energy=	0.135757
Sum of electronic and zero-point Energies=	-2924.459843
Sum of electronic and thermal Energies=	-2924.438294
Sum of electronic and thermal Enthalpies=	-2924.437350
Sum of electronic and thermal Free Energies=	-2924.514315

C	0.02573800	0.67523200	-0.81939200
C	-1.18567700	0.42285700	0.01129800
C	-1.40340000	1.55394900	0.99028800
C	1.05103700	1.43079700	1.21163300
H	-1.06528600	-0.51720800	0.56935300
H	-0.03637800	1.58208700	-1.43066500
H	0.33313200	-0.17726400	-1.42802500
H	-1.61589500	2.49368700	0.46049000
Pd	-2.77983300	0.13066200	-1.23857700
Cl	-2.59178300	2.35860600	-2.03838300
Cl	-2.95355600	-2.08041800	-0.41248500
N	-4.44226000	-0.20730800	-2.53708300
C	-5.34280900	-0.39057800	-3.23854800
C	-6.46871700	-0.61897100	-4.11763200
H	-6.14131200	-0.57954400	-5.16154700
H	-7.23148700	0.14954700	-3.95634500
H	-6.90646400	-1.60251000	-3.91937700
N	-0.09997700	1.77731300	1.70090000
O	1.22812400	0.90501000	0.05853900
H	-0.11989300	2.19792100	2.62955500
C	2.36051700	1.67090500	1.97598500
Cl	3.28749000	0.15970900	2.00008600
Cl	2.06659300	2.21461000	3.64208900
Cl	3.24292300	2.93298300	1.08123600
C	-2.46481100	1.27118000	2.03012500
H	-2.26155600	0.32437800	2.54783900
H	-2.53611500	2.07644200	2.77175000
H	-3.43542400	1.18505800	1.52779900

3d
M=PdCl2MeCN
5-TS-int

Zero-point correction=	0.189210 (Hartree/Particle)
Thermal correction to Energy=	0.211149
Thermal correction to Enthalpy=	0.212093
Thermal correction to Gibbs Free Energy=	0.133725
Sum of electronic and zero-point Energies=	-2924.445630
Sum of electronic and thermal Energies=	-2924.423691
Sum of electronic and thermal Enthalpies=	-2924.422747
Sum of electronic and thermal Free Energies=	-2924.501114

C	-1.73559800	0.59985600	0.28781800
C	-3.94071200	0.15667500	-0.20075300
C	-2.42673700	-0.17880100	1.41109400
H	-1.55712200	1.64760500	0.55989900
H	-2.37526600	0.30249500	2.38826300
H	-2.09396700	-1.22125400	1.47146100
C	-0.48008100	-0.05702200	-0.22749600
H	-0.74508200	-1.04757300	-0.62590500
Pd	0.76180200	-0.45691200	1.35538500
Cl	0.92261200	-2.69728100	0.57354800
Cl	0.55371700	1.78798200	2.14361700
N	2.13232800	-0.90214900	2.98152800
C	2.86261300	-1.14350600	3.84562000
C	3.77567200	-1.44700000	4.92663600
H	4.00282400	-0.53833500	5.49328500
H	3.32664300	-2.18319900	5.60109600
H	4.70793200	-1.85720700	4.52510000
O	-3.85238400	-0.23167200	1.02671800
N	-2.84827300	0.60388300	-0.72458100
H	-2.76729800	0.96124300	-1.67345300
C	-5.29049200	0.02116100	-0.87529300
Cl	-5.67799900	-1.71300500	-0.90870000
Cl	-5.23606900	0.67198300	-2.52209600
Cl	-6.47449400	0.91220800	0.10144000
C	0.26047500	0.76810100	-1.25596700
H	-0.34548800	0.94458500	-2.16234900
H	0.55044600	1.74659100	-0.85098100
H	1.17140900	0.25115900	-1.58316900

FigS1-structures

B-Pd-Cl2MeCN-reactant

Zero-point correction=	0.278635 (Hartree/Particle)
Thermal correction to Energy=	0.298940
Thermal correction to Enthalpy=	0.299884
Thermal correction to Gibbs Free Energy=	0.228903
Sum of electronic and zero-point Energies=	-1532.997887
Sum of electronic and thermal Energies=	-1532.977582
Sum of electronic and thermal Enthalpies=	-1532.976637
Sum of electronic and thermal Free Energies=	-1533.047619

C	-1.33083800	0.78577900	-1.53900900
C	-1.11080700	0.30466400	-0.25907200
C	-0.97842800	1.14494200	0.97029900
C	0.51593700	1.40613500	1.24583800
C	1.17795400	2.23381100	0.17554600
C	2.02637800	1.66023900	-0.69022000
H	-1.41828000	0.62309500	1.83186800
H	-0.68719500	-0.70312300	-0.17731200
H	-1.57614400	1.84487000	-1.64948700
H	1.03371700	0.44090100	1.35379200
H	0.59066700	1.91744100	2.21848000
H	-1.52177900	2.09046500	0.85349100
Pd	-3.26462800	-0.08496000	-0.75175000
Cl	-3.96134100	2.09811100	-0.41381400
Cl	-5.50442400	-0.81708200	-0.62997200
N	-2.73413500	-2.03303000	-1.05137900
C	-2.51375500	-3.15745300	-1.19597100
C	-2.23988800	-4.56451600	-1.37403500
H	-1.16082100	-4.74345700	-1.33261200
H	-2.62257300	-4.89837100	-2.34390700
H	-2.72983200	-5.13803000	-0.58053600
H	2.21167900	0.58786000	-0.56342500
C	-0.95429300	0.06295100	-2.78774600
H	-1.73937800	0.13000000	-3.55115700
H	-0.05710500	0.54088300	-3.20875800
H	-0.72315900	-0.99201800	-2.60289000
C	2.77783400	2.29656700	-1.81210900
H	3.86250200	2.18208800	-1.67165600
H	2.54160300	1.81355900	-2.77117000
H	2.56933300	3.36652100	-1.92122800
C	0.79316500	3.68284700	0.16625700
H	1.32681400	4.26773400	-0.58966400
H	-0.28401200	3.81185500	-0.02215300
H	0.98837000	4.14147400	1.14718000

B-Pd-Cl2MeCN 5-exo-TS

Zero-point correction=	0.277913 (Hartree/Particle)
Thermal correction to Energy=	0.298392
Thermal correction to Enthalpy=	0.299336
Thermal correction to Gibbs Free Energy=	0.226938
Sum of electronic and zero-point Energies=	-1532.961136
Sum of electronic and thermal Energies=	-1532.940657
Sum of electronic and thermal Enthalpies=	-1532.939713
Sum of electronic and thermal Free Energies=	-1533.012111

C	-1.85445200	-0.00686600	0.16704100
C	-4.11581000	0.28755600	0.64745400
C	-3.53992000	-0.40235000	1.84458900
C	-2.16986900	-0.89293800	1.36314100
H	-1.79281500	1.06132000	0.40709200
H	-3.44080600	0.32443800	2.66252300
H	-4.19298800	-1.20397400	2.21574200
H	-1.39801800	-0.80337900	2.13823100
H	-2.19016600	-1.94608100	1.04909500
C	-0.94347900	-0.41699800	-0.88225300
H	-1.09960800	-1.45861400	-1.19263100
Pd	0.80626700	-0.53731500	0.32767300
Cl	2.92503800	-0.82455100	1.51616800
Cl	0.81888800	1.77979800	0.70103000
N	0.76135800	-2.55456000	0.03482100
C	0.78417900	-3.70059400	-0.11432700
C	0.81821400	-5.13410300	-0.30030900
H	0.33211100	-5.40078800	-1.24419700
H	1.85597300	-5.48180100	-0.32257600
H	0.29472600	-5.63080700	0.52305300
C	-3.70627000	-0.19335400	-0.58331700
H	-3.53264000	-1.26979200	-0.65408000
C	-0.67483800	0.50493800	-2.04522400
H	-1.43727700	0.38887800	-2.82923200
H	-0.65749800	1.55523900	-1.73094900
H	0.29396800	0.27739700	-2.50831100
C	-4.02669800	0.50859200	-1.86789200
H	-3.55293500	0.01006500	-2.71890600
H	-5.10975700	0.50937700	-2.05415700
H	-3.69216600	1.55445700	-1.85201700
C	-4.80350500	1.58254500	0.83080900
H	-5.40583500	1.88538800	-0.03104300
H	-5.43296900	1.55115200	1.72943000
H	-4.05212100	2.36942700	1.01775600

FigS1-structures

B-Pd-Cl2MeCN
6-endo-TS

Zero-point correction=	0.278637 (Hartree/Particle)
Thermal correction to Energy=	0.298906
Thermal correction to Enthalpy=	0.299850
Thermal correction to Gibbs Free Energy=	0.228192
Sum of electronic and zero-point Energies=	-1532.976856
Sum of electronic and thermal Energies=	-1532.956588
Sum of electronic and thermal Enthalpies=	-1532.955644
Sum of electronic and thermal Free Energies=	-1533.027301

C	-0.22707300	0.91744100	1.21091200
C	-1.05195300	0.12287500	0.24279300
C	-1.25083800	0.70645400	-1.06596800
C	0.67094000	1.06551400	-1.83011700
C	0.96538200	1.82640600	-0.71682000
C	1.18477100	1.15450400	0.58021800
H	-0.71338800	-0.92077000	0.17362300
H	-0.68896700	1.88932600	1.42730300
H	-0.10426800	0.39074500	2.16519800
H	0.95800300	0.01119400	-1.78230100
H	1.77689800	1.77952800	1.26051900
Pd	-3.06581000	-0.02447100	0.90299700
Cl	-3.28936000	2.30431000	0.99199400
Cl	-5.31725600	-0.34676400	1.75648500
N	-2.87254100	-2.04491100	0.78813300
C	-2.81399100	-3.19771000	0.73160800
C	-2.74649000	-4.64037100	0.66508100
H	-2.13055000	-4.94800300	-0.18596600
H	-2.30614900	-5.03575700	1.58623300
H	-3.75268000	-5.05499900	0.54587900
H	1.68840200	0.18774500	0.45495800
C	-1.78413000	-0.14194200	-2.18260000
H	-1.34768700	-1.14884800	-2.16605200
H	-2.87159800	-0.23990300	-2.05707600
H	-1.62531700	0.30752500	-3.16713500
H	-1.58743700	1.74809600	-1.08094600
C	0.84630800	3.30579500	-0.70449600
H	0.39896100	3.71621700	-1.61483700
H	0.26356800	3.64160600	0.16630900
H	1.84778200	3.74721800	-0.59011200
C	0.51853800	1.65306800	-3.20521900
H	1.42101300	2.20996400	-3.49040500
H	0.36945200	0.86959200	-3.95470000
H	-0.32791000	2.35052300	-3.27333600

B-Pd-Cl2MeCN
6-endo-int

Zero-point correction=	0.280052 (Hartree/Particle)
Thermal correction to Energy=	0.300168
Thermal correction to Enthalpy=	0.301112
Thermal correction to Gibbs Free Energy=	0.230193
Sum of electronic and zero-point Energies=	-1532.982050
Sum of electronic and thermal Energies=	-1532.961934
Sum of electronic and thermal Enthalpies=	-1532.960989
Sum of electronic and thermal Free Energies=	-1533.031909

C	-0.74461500	0.95927800	-1.18109900
C	-1.16102900	0.12291600	-0.01257900
C	-0.66819400	0.64421900	1.30818300
C	0.96899900	0.85959300	1.23985700
C	1.10597200	1.69387500	0.06553400
C	0.86388700	1.08499000	-1.21784100
H	-0.81694300	-0.91557200	-0.14577900
H	-1.17111900	1.96991300	-1.14128100
H	-1.01270900	0.51479300	-2.14771400
H	1.35543500	-0.15002500	1.03946500
Pd	-3.24417000	-0.01057900	-0.05078100
Cl	-3.41331200	2.29830000	0.35080200
Cl	-5.69834300	-0.28819200	-0.13940700
N	-3.05244300	-2.00848500	-0.38231000
C	-2.99928300	-3.14796700	-0.57039000
C	-2.94040800	-4.57323100	-0.80806600
H	-3.26802000	-5.11497000	0.08513400
H	-1.91517000	-4.87145100	-1.04950500
H	-3.59492100	-4.83892600	-1.64448300
H	1.26722800	0.07193400	-1.31397700
H	1.14289500	1.71125500	-2.07039500
C	-0.96149500	-0.28538600	2.47450400
H	-2.04759300	-0.40610800	2.57509000
H	-0.52305000	-1.27913100	2.30170500
H	-0.58571500	0.10154700	3.42738300
H	-1.08468000	1.64331700	1.50865300
C	1.50660600	1.42363300	2.54509700
H	0.87639100	2.23400500	2.93428500
H	1.55212900	0.64016700	3.30717100
H	2.52372300	1.81409400	2.41896300
C	1.19478600	3.15495300	0.18181900
H	0.54881000	3.53791100	0.98479600
H	2.22376800	3.41203600	0.48561600
H	0.97942000	3.66733900	-0.76041400

FigS1-structures

B-Pd-Cl2MeCN
5-exo-int

Zero-point correction=	0.277225 (Hartree/Particle)
Thermal correction to Energy=	0.297870
Thermal correction to Enthalpy=	0.298814
Thermal correction to Gibbs Free Energy=	0.225698
Sum of electronic and zero-point Energies=	-1532.970271
Sum of electronic and thermal Energies=	-1532.949626
Sum of electronic and thermal Enthalpies=	-1532.948682
Sum of electronic and thermal Free Energies=	-1533.021798

C	-1.75349200	0.21801600	0.24034300
C	-4.14148700	0.31928200	0.43479800
C	-3.63550400	-0.26248500	1.66913400
C	-2.21203000	-0.71363000	1.36839000
H	-1.46759000	1.19646100	0.66150900
H	-3.62642800	0.62345800	2.34510600
H	-4.33030400	-0.96447500	2.14820300
H	-1.55805000	-0.66970700	2.24519400
H	-2.21949600	-1.75507600	1.01038000
C	-0.59193000	-0.34842300	-0.55428000
H	-0.89064500	-1.33753500	-0.94155500
Pd	0.97366600	-0.78526600	0.73469500
Cl	2.90525800	-1.43711200	2.23073500
Cl	1.11364800	1.50005300	1.34099800
N	0.78461800	-2.75546300	0.21917400
C	0.73045400	-3.88660500	-0.01715100
C	0.67416700	-5.30321200	-0.30640400
H	-0.36657500	-5.64129100	-0.33618500
H	1.14157700	-5.50613100	-1.27547400
H	1.20759100	-5.86268000	0.46892900
C	-3.07645900	0.44198200	-0.55937200
H	-3.26131900	-0.51321100	-1.12055200
C	-0.05834800	0.50293100	-1.68660600
H	-0.72434600	0.47545000	-2.56504100
H	0.07315500	1.54978900	-1.38325100
H	0.91661300	0.13260800	-2.03183000
C	-5.50753400	0.78356300	0.24931000
H	-6.20266200	0.39832900	0.99914800
H	-5.47386900	1.88545600	0.33357100
H	-5.86589100	0.58950700	-0.76998600
C	-3.18512100	1.61950900	-1.51573300
H	-2.98682300	2.55463800	-0.97615500
H	-2.45123800	1.53346600	-2.31989500
H	-4.17659500	1.68779900	-1.97772800

A-Pd-Cl2MeCN
reactant

Zero-point correction=	0.221969 (Hartree/Particle)
Thermal correction to Energy=	0.240436
Thermal correction to Enthalpy=	0.241380
Thermal correction to Gibbs Free Energy=	0.172664
Sum of electronic and zero-point Energies=	-1454.484985
Sum of electronic and thermal Energies=	-1454.466518
Sum of electronic and thermal Enthalpies=	-1454.465574
Sum of electronic and thermal Free Energies=	-1454.534290

C	-1.40209500	0.81000100	-1.51241200
C	-1.12586700	0.33278500	-0.24236000
C	-0.95451900	1.18342100	0.97660900
C	0.54626800	1.35837900	1.27126500
C	1.24943100	2.10199300	0.18093900
C	2.19221200	1.58165700	-0.60249700
H	-1.44073900	0.71072400	1.84168700
H	-0.69757600	-0.67355900	-0.16928800
H	-1.65224500	1.86967300	-1.60655800
H	1.01421700	0.37181000	1.41355800
H	0.64117000	1.89801300	2.22521600
H	-1.42967800	2.16225800	0.82807800
Pd	-3.29408500	-0.08115900	-0.65235800
Cl	-4.00358400	2.08425600	-0.24964500
Cl	-5.51563600	-0.84532700	-0.43183900
N	-2.75661000	-2.01724700	-1.01295800
C	-2.53848900	-3.13501600	-1.20465700
C	-2.26965400	-4.53306100	-1.44867300
H	-1.20380700	-4.67993100	-1.64986600
H	-2.84861400	-4.87426200	-2.31295100
H	-2.55420800	-5.12375300	-0.57198200
H	2.53216100	0.55271400	-0.47109400
H	2.66902400	2.15637900	-1.39446100
C	-1.07111500	0.09380100	-2.77791500
H	-1.89347100	0.14358900	-3.50245100
H	-0.20561700	0.58903800	-3.24263300
H	-0.81105600	-0.95616600	-2.60414400
H	0.92585600	3.13545900	0.02154300

FigS1-structures

A-Pd-Cl2MeCN
6-endo-TS

Zero-point correction=	0.222676 (Hartree/Particle)
Thermal correction to Energy=	0.239744
Thermal correction to Enthalpy=	0.240688
Thermal correction to Gibbs Free Energy=	0.176352
Sum of electronic and zero-point Energies=	-1454.457112
Sum of electronic and thermal Energies=	-1454.440043
Sum of electronic and thermal Enthalpies=	-1454.439099
Sum of electronic and thermal Free Energies=	-1454.503435

C	-0.21722100	0.96749800	1.34077300
C	-1.02685700	0.20524600	0.33998400
C	-1.23900600	0.86586300	-0.93155400
C	0.61594100	1.19827100	-1.62848000
C	1.03737400	1.87476600	-0.51048300
C	1.24183500	1.18218600	0.75861000
H	-0.66264200	-0.82402300	0.21067900
H	-0.66147400	1.94769000	1.55318100
H	-0.11650200	0.43001900	2.29142700
H	0.87370100	0.14355000	-1.74386000
H	1.81860800	1.77095200	1.47888500
Pd	-3.03614100	-0.04068600	0.99061600
Cl	-3.32358700	2.26048600	1.26188300
Cl	-5.27388000	-0.47854700	1.80540300
N	-2.80223600	-2.03958900	0.70098700
C	-2.72211200	-3.18107300	0.53949600
C	-2.62903400	-4.61006300	0.34132600
H	-3.61308100	-5.06923800	0.48084200
H	-2.27511000	-4.82500900	-0.67205700
H	-1.92803400	-5.04189800	1.06289900
H	1.70916900	0.19886100	0.62334600
H	0.42889400	1.74410700	-2.55246900
H	0.95916700	2.96408300	-0.49269900
C	-1.79207500	0.10284600	-2.10367500
H	-1.41185200	-0.92626900	-2.12578200
H	-2.88633100	0.06281800	-2.01547300
H	-1.56576900	0.59045500	-3.05755000
H	-1.58425200	1.90143200	-0.86501500

A-Pd-Cl2MeCN
5-exo-TS

Zero-point correction=	0.221322 (Hartree/Particle)
Thermal correction to Energy=	0.239025
Thermal correction to Enthalpy=	0.239969
Thermal correction to Gibbs Free Energy=	0.173527
Sum of electronic and zero-point Energies=	-1454.438978
Sum of electronic and thermal Energies=	-1454.421275
Sum of electronic and thermal Enthalpies=	-1454.420331
Sum of electronic and thermal Free Energies=	-1454.486773

C	-1.90968100	0.01286700	0.17222500
C	-4.12253400	0.32475100	0.32521900
C	-3.82245400	-0.42628500	1.57307100
C	-2.37656500	-0.89282600	1.31243500
H	-1.80756000	1.06102400	0.47259200
H	-3.89969800	0.23736700	2.44109500
H	-4.52618700	-1.25375500	1.74022900
H	-1.73025800	-0.79197000	2.19247700
H	-2.33469100	-1.94359600	0.99272700
C	-0.85228200	-0.41193300	-0.74931100
H	-1.01851500	-1.43903100	-1.10174700
Pd	0.75774500	-0.60413200	0.60786400
Cl	2.76287100	-0.95669200	1.97343500
Cl	0.71780000	1.68994900	1.10002300
N	0.75356400	-2.59996100	0.20059100
C	0.79908100	-3.73718000	-0.00151000
C	0.86354600	-5.15981600	-0.25196300
H	0.79320600	-5.35387000	-1.32709500
H	1.81149800	-5.56022500	0.12176400
H	0.03761700	-5.66763300	0.25652900
C	-3.47643300	-0.09912900	-0.82064700
H	-3.38252600	-1.17050000	-1.00876100
C	-0.46676300	0.51342500	-1.87523700
H	-1.21282800	0.48029600	-2.68583600
H	-0.37104200	1.55016300	-1.53134800
H	0.49274600	0.21241400	-2.31434800
H	-4.57839300	1.31511700	0.36778400
H	-3.50584100	0.52499600	-1.71234300

FigS1-structures

A-Pd-Cl2MeCN
6-endo-int

Zero-point correction=	0.223359 (Hartree/Particle)
Thermal correction to Energy=	0.240809
Thermal correction to Enthalpy=	0.241753
Thermal correction to Gibbs Free Energy=	0.176631
Sum of electronic and zero-point Energies=	-1454.459494
Sum of electronic and thermal Energies=	-1454.442044
Sum of electronic and thermal Enthalpies=	-1454.441099
Sum of electronic and thermal Free Energies=	-1454.506221

C	-0.79659100	1.03151900	-1.32370300
C	-1.17038200	0.21580700	-0.13768500
C	-0.71708900	0.81380800	1.15260900
C	0.93730100	1.00514100	1.05264000
C	1.09257100	1.76940000	-0.13919600
C	0.84929500	1.17117000	-1.40857400
H	-0.79052400	-0.81352100	-0.23298200
H	-1.22436300	2.03977700	-1.29665200
H	-1.04803500	0.56818000	-2.28550400
H	1.33100200	-0.01592600	0.98869600
H	1.24572800	1.51193100	1.97048200
Pd	-3.25696800	-0.00178100	-0.15477700
Cl	-3.53962000	2.30691300	0.11081700
Cl	-5.67756800	-0.38253100	-0.22703500
N	-2.98131500	-2.00807100	-0.32779900
C	-2.87176000	-3.15638800	-0.40184700
C	-2.74154700	-4.59355000	-0.49396600
H	-2.89635700	-5.04566600	0.49119100
H	-1.74201900	-4.85773000	-0.85374100
H	-3.48759000	-4.99187700	-1.18914700
H	1.22905500	0.15022900	-1.51325200
H	1.08104500	1.79271700	-2.27573800
H	1.10495900	2.85973200	-0.06758400
C	-0.95832000	-0.02844800	2.39211700
H	-2.03347200	-0.06839400	2.60779000
H	-0.59992900	-1.05639900	2.24025500
H	-0.45271800	0.39006400	3.27022800
H	-1.12980500	1.82278300	1.28280800

A-Pd-Cl2MeCN
5-exo-int

Zero-point correction=	0.220568 (Hartree/Particle)
Thermal correction to Energy=	0.238239
Thermal correction to Enthalpy=	0.239183
Thermal correction to Gibbs Free Energy=	0.173080
Sum of electronic and zero-point Energies=	-1454.442958
Sum of electronic and thermal Energies=	-1454.425287
Sum of electronic and thermal Enthalpies=	-1454.424343
Sum of electronic and thermal Free Energies=	-1454.490446

C	-1.72388000	0.22746700	0.31488700
C	-4.10433600	0.34096900	0.42903400
C	-3.65867900	-0.17489400	1.69586600
C	-2.22433300	-0.65464700	1.46554800
H	-1.42866500	1.21166300	0.71217100
H	-3.64827000	0.78996900	2.26976900
H	-4.37848200	-0.79808400	2.23906700
H	-1.60101600	-0.57842400	2.36157900
H	-2.23972500	-1.71090700	1.15354300
C	-0.58221800	-0.35610600	-0.49001800
H	-0.90250100	-1.33871600	-0.87772600
Pd	1.00655100	-0.81217900	0.75370700
Cl	2.93793100	-1.49150200	2.22907100
Cl	1.16986400	1.46125800	1.37883700
N	0.81004700	-2.77045500	0.20573400
C	0.75489700	-3.89499800	-0.05955200
C	0.69745500	-5.30332000	-0.38619200
H	-0.34327000	-5.64126700	-0.41753300
H	1.15793100	-5.47949500	-1.36380800
H	1.23702200	-5.88304600	0.36970600
C	-3.02148700	0.43893300	-0.50809000
H	-3.22052200	-0.49723600	-1.09974300
H	-3.09347300	1.25096700	-1.24081100
H	-5.13526000	0.63471500	0.21731000
C	-0.12406400	0.52105300	-1.63482600
H	-0.91419400	0.63127400	-2.39866800
H	0.15252600	1.52469900	-1.28718500
H	0.74801000	0.08849700	-2.14253100

FigS1-structures

B-Pt(PH3)3
reactant

Zero-point correction=	0.258841 (Hartree/Particle)
Thermal correction to Energy=	0.278023
Thermal correction to Enthalpy=	0.278968
Thermal correction to Gibbs Free Energy=	0.210453
Sum of electronic and zero-point Energies=	-1421.868029
Sum of electronic and thermal Energies=	-1421.848847
Sum of electronic and thermal Enthalpies=	-1421.847903
Sum of electronic and thermal Free Energies=	-1421.916417

C	-2.65612800	-1.25701700	0.35467100
C	-1.99926100	-1.64714200	-0.79852700
C	-1.19535000	1.91463900	-0.00908200
C	-0.84863300	1.04835200	0.94126400
C	-1.80013900	0.45347500	1.92953700
C	-2.00502600	-1.05382900	1.68840800
H	-3.61062000	-0.73486400	0.23338600
H	-1.42507200	0.58062300	2.95483500
H	-2.77242400	0.96630400	1.87646500
H	-1.02925500	-1.56189600	1.72787100
H	-2.63098700	-1.47219800	2.48853900
Pt	-3.16475900	-3.51153400	0.08300700
P	-1.07579300	-4.33918400	0.85331700
H	0.09195200	-3.75241400	0.34765100
H	-0.90700000	-4.21840200	2.23934900
H	-0.82756100	-5.70358100	0.64607000
P	-5.34346700	-2.83352500	-0.54617000
H	-6.31361600	-3.05828000	0.43971700
H	-5.55725900	-1.48986300	-0.88013300
H	-5.87829400	-3.50709800	-1.65262400
P	-3.98882200	-5.71172200	0.28452400
H	-5.35808600	-5.91484600	0.07004200
H	-3.39594400	-6.61149600	-0.60945600
H	-3.77568800	-6.31511300	1.52998400
H	-0.47217600	2.31407600	-0.71749900
H	-2.22219600	2.27306000	-0.10238500
H	0.18957500	0.70989300	1.01141600
C	-2.47508900	-1.40593400	-2.18884100
H	-1.84400100	-0.62158500	-2.63152700
H	-2.36453300	-2.29621600	-2.81923900
H	-3.51300400	-1.05782100	-2.22801100
H	-0.94729000	-1.93040200	-0.70906500

B-Pt(PH3)3
6-TS-endo

Zero-point correction=	0.258819 (Hartree/Particle)
Thermal correction to Energy=	0.276970
Thermal correction to Enthalpy=	0.277914
Thermal correction to Gibbs Free Energy=	0.212195
Sum of electronic and zero-point Energies=	-1421.854423
Sum of electronic and thermal Energies=	-1421.836272
Sum of electronic and thermal Enthalpies=	-1421.835328
Sum of electronic and thermal Free Energies=	-1421.901047

C	-2.73123600	-1.19568700	0.30378600
C	-1.49889300	-1.02063800	-0.42898500
C	-1.09141800	1.07624400	-0.25564600
C	-1.13606100	0.95765900	1.10185100
C	-2.39693000	0.75732000	1.82657400
C	-2.70952600	-0.77936300	1.75100900
H	-0.57604800	-1.35239200	0.05615600
H	-3.54704100	-0.68173400	-0.22712300
H	-2.32059300	1.04663000	2.88006300
H	-3.22316100	1.30758800	1.35911900
H	-1.94855300	-1.32080800	2.32904400
H	-3.67530600	-0.96209100	2.23827700
Pt	-3.12270700	-3.35884000	0.15230000
P	-1.04105700	-3.96814000	1.07524000
H	-0.46468800	-3.12865300	2.04137000
H	-0.96953300	-5.21387900	1.71525600
H	0.00352600	-4.07840000	0.14387200
P	-5.17371000	-2.69668400	-0.77546100
H	-5.87778400	-1.75944600	-0.00518700
H	-5.08161900	-2.04517900	-2.01377800
H	-6.15784300	-3.66465500	-1.02645700
P	-3.78609300	-5.61895100	0.03338500
H	-4.91164100	-5.93928700	0.80701700
H	-4.17934200	-6.08052500	-1.23145300
H	-2.88358600	-6.61664600	0.43180600
H	-0.13845600	1.17139800	-0.77350700
H	-1.97951100	1.38026000	-0.81214000
H	-0.20301500	0.78797200	1.64478700
C	-1.46967000	-1.08317800	-1.92365300
H	-0.56873800	-0.62341600	-2.34042400
H	-1.45617700	-2.14223600	-2.22177800
H	-2.35651700	-0.61565400	-2.36804800

FigS1-structures

B-Pt(PH3)3
5-exo-TS

Zero-point correction=	0.258742 (Hartree/Particle)
Thermal correction to Energy=	0.276817
Thermal correction to Enthalpy=	0.277761
Thermal correction to Gibbs Free Energy=	0.212639
Sum of electronic and zero-point Energies=	-1421.835356
Sum of electronic and thermal Energies=	-1421.817281
Sum of electronic and thermal Enthalpies=	-1421.816337
Sum of electronic and thermal Free Energies=	-1421.881460

C	-1.66995800	0.47277700	0.23757100
C	-3.59892900	0.19912000	-0.24351600
C	-3.85003200	0.90793100	0.90228300
C	-3.13404000	0.51599900	2.14847400
C	-1.85012000	-0.13439500	1.62065400
H	-1.58871900	1.56598500	0.23678400
H	-2.91721400	1.41524200	2.73791200
H	-3.73654800	-0.14030500	2.79122100
H	-0.97723600	0.06424700	2.25612400
H	-1.94262100	-1.22565500	1.53201400
C	-0.92468900	-0.18795600	-0.82042800
H	-1.21726400	-1.24599400	-0.87709100
P	1.13061700	2.19814600	0.30804700
H	0.57295500	2.63673300	1.51995300
H	2.38166800	2.83193400	0.34397200
H	0.44486100	3.00195300	-0.61614700
P	3.41173500	-0.26233700	0.61943200
H	4.28073900	-0.83922700	-0.31974800
H	4.10151700	0.91852600	0.93616100
H	3.67799200	-1.04933100	1.75043600
P	1.08406700	-2.44134600	-0.42996200
H	2.25411100	-3.19507500	-0.25275800
H	0.16050000	-3.16175000	0.34201800
H	0.70602900	-2.79875000	-1.73298200
Pt	1.13616700	-0.13082900	-0.04029500
H	-3.94418600	0.57943600	-1.20304500
C	-0.93321500	0.44200200	-2.19792500
H	-1.90514800	0.29037500	-2.69114300
H	-0.74508600	1.52301000	-2.16310500
H	-0.17015800	-0.00932900	-2.84377000
H	-3.42784300	-0.87655600	-0.19785700
H	-4.35951900	1.87128800	0.84747200

B-Pt(PH3)3
6-endo-int

Zero-point correction=	0.261053 (Hartree/Particle)
Thermal correction to Energy=	0.278805
Thermal correction to Enthalpy=	0.279749
Thermal correction to Gibbs Free Energy=	0.215837
Sum of electronic and zero-point Energies=	-1421.858474
Sum of electronic and thermal Energies=	-1421.840722
Sum of electronic and thermal Enthalpies=	-1421.839778
Sum of electronic and thermal Free Energies=	-1421.903690

C	-3.23475700	-1.07160700	0.71462200
C	-2.01057400	-0.99232400	-0.15644900
C	-1.45316800	0.56225000	-0.09878900
C	-1.31147000	0.79444200	1.30211200
C	-2.46221800	0.93824500	2.13206400
C	-2.96489200	-0.62185300	2.11896100
H	-1.19143800	-1.61085400	0.23610300
H	-3.98590100	-0.38829700	0.28254600
H	-2.26086400	1.21616600	3.16843900
H	-3.27575400	1.52250700	1.69166300
H	-2.20233600	-1.21956400	2.63464400
H	-3.85771200	-0.59825300	2.75631600
Pt	-4.10885600	-3.05609200	0.76110500
P	-2.20196800	-3.97937300	1.79563000
H	-0.93018200	-3.53186000	1.40474700
H	-2.13602300	-3.79935800	3.18614300
H	-2.03001700	-5.36945400	1.70205900
P	-5.14706000	-5.19992500	0.81620800
H	-5.30654600	-5.78667500	2.08207300
H	-6.44453200	-5.33523500	0.29716700
H	-4.48162800	-6.23231400	0.13509300
P	-5.97170200	-2.02240800	-0.19012300
H	-5.74697900	-1.41193700	-1.43358200
H	-7.13147200	-2.76860300	-0.44634100
H	-6.48083600	-0.94778300	0.55501900
H	-0.51691500	0.58462200	-0.66242100
H	-0.34810900	0.58655900	1.77627400
H	-2.23699200	1.16297900	-0.57452000
C	-2.23188200	-1.29906500	-1.62663000
H	-2.51141200	-2.35365300	-1.74651300
H	-3.04068000	-0.67888600	-2.03689700
H	-1.32638900	-1.11713500	-2.21607900

FigS1-structures

B-Pt(PH3)3
5-exo-int

Zero-point correction= 0.256758 (Hartree/Particle)
Thermal correction to Energy= 0.275411
Thermal correction to Enthalpy= 0.276355
Thermal correction to Gibbs Free Energy= 0.208569
Sum of electronic and zero-point Energies= -1421.850322
Sum of electronic and thermal Energies= -1421.831669
Sum of electronic and thermal Enthalpies= -1421.830725
Sum of electronic and thermal Free Energies= -1421.898511

C	-1.99212500	0.70816800	0.15701800
C	-3.48867100	0.74248900	-0.23691000
C	-4.22786600	0.73695700	0.99579700
C	-3.37924800	0.45302500	2.12155700
C	-2.03844900	0.01664800	1.52751700
H	-1.69377200	1.76314000	0.29182200
H	-3.30230900	1.48780500	2.54844200
H	-3.84246900	-0.12665800	2.92904600
H	-1.18830400	0.26729900	2.16960900
H	-2.04487900	-1.07612200	1.39345200
C	-1.10328600	0.02362500	-0.87143300
H	-1.53742000	-0.98519900	-1.00071700
P	3.19502200	-0.64359700	0.50918800
H	4.09517300	0.42635600	0.66149200
H	3.37271700	-1.28328600	1.74839500
H	3.96842300	-1.48905200	-0.30586900
Pt	0.91927400	-0.22677200	-0.19155700
P	1.09118600	2.07500000	0.23036200
H	2.37867500	2.63434300	0.26628000
H	0.45019800	2.96053500	-0.65187800
H	0.58489300	2.52832200	1.46104200
P	0.57185800	-2.46396200	-0.73708600
H	1.64038400	-3.37467600	-0.71033500
H	-0.38781400	-3.14322800	0.03051100
H	0.06635700	-2.66584700	-2.03201100
H	-3.84551300	1.44753800	-0.99736700
C	-1.12087600	0.70160200	-2.23316100
H	-2.13132500	0.69948000	-2.67298600
H	-0.79446800	1.74959000	-2.18421500
H	-0.46187900	0.18625500	-2.94403900
H	-3.79003100	-0.26656300	-0.63110400
H	-5.30048500	0.92964000	1.07061700

A-Pt(PH3)3
reactant

Zero-point correction= 0.315300 (Hartree/Particle)
Thermal correction to Energy= 0.337308
Thermal correction to Enthalpy= 0.338252
Thermal correction to Gibbs Free Energy= 0.263859
Sum of electronic and zero-point Energies= -1500.381569
Sum of electronic and thermal Energies= -1500.359561
Sum of electronic and thermal Enthalpies= -1500.358617
Sum of electronic and thermal Free Energies= -1500.433010

C	-2.62207100	-1.27534300	0.43310300
C	-2.02220900	-1.62447200	-0.76348200
C	-1.17231400	1.78198100	-0.00595200
C	-0.69288100	0.96392000	0.94316300
C	-1.62312400	0.38033300	1.97367100
C	-1.91152900	-1.11741400	1.74137000
H	-3.56831100	-0.72760100	0.37377500
H	-1.18984300	0.47888000	2.98067600
H	-2.57825400	0.92542000	1.98294600
H	-0.96324200	-1.67374700	1.75120400
H	-2.52903400	-1.50282200	2.56404500
Pt	-3.19985500	-3.49808800	0.10292800
P	-1.14377600	-4.34468900	0.93608200
H	0.03382000	-3.71692000	0.50561500
H	-1.02517200	-4.29981700	2.33184900
H	-0.87158400	-5.69207900	0.65951200
P	-5.29180100	-2.77505900	-0.74674000
H	-6.41631000	-3.49295000	-0.31868700
H	-5.67026200	-1.45176500	-0.48369600
H	-5.40180200	-2.85573600	-2.14166900
P	-4.04153100	-5.69469300	0.29248100
H	-5.41149500	-5.89191900	0.08155700
H	-3.45156800	-6.60126100	-0.59685900
H	-3.83077900	-6.29884300	1.53855400
H	-2.24371600	2.00750400	0.03068400
C	-2.54225100	-1.28055200	-2.11587000
H	-1.87516700	-0.52140900	-2.54901900
H	-2.52750600	-2.13980100	-2.79722700
H	-3.55037700	-0.85022600	-2.08538800
H	-0.98108400	-1.95668600	-0.73920000
C	0.74142900	0.54743200	1.07607500
H	0.86134500	-0.54243500	0.96831700
H	1.39938300	1.01819300	0.33928900
H	1.12401600	0.79832200	2.07646300
C	-0.42856500	2.46040000	-1.10694400
H	-0.86097200	2.21113700	-2.08635600
H	-0.50148500	3.55312600	-1.01037700
H	0.63475500	2.19944400	-1.13638100

FigS1-structures

A-Pt(PH3)3
6-endo-TS

Zero-point correction= 0.315241 (Hartree/Particle)
Thermal correction to Energy= 0.336108
Thermal correction to Enthalpy= 0.337052
Thermal correction to Gibbs Free Energy= 0.266201
Sum of electronic and zero-point Energies= -1500.374760
Sum of electronic and thermal Energies= -1500.353893
Sum of electronic and thermal Enthalpies= -1500.352948
Sum of electronic and thermal Free Energies= -1500.423800

C	-2.76803100	-1.20385900	0.26865700
C	-1.51951800	-1.07938300	-0.43295400
C	-0.99415600	1.12529700	-0.23943900
C	-1.05409400	0.88774900	1.10891500
C	-2.37152000	0.72900000	1.77438700
C	-2.77936700	-0.77171500	1.71230600
H	-0.60734300	-1.40053600	0.08116800
H	-3.55989200	-0.68579500	-0.29322700
H	-2.31961300	1.03781100	2.82647100
H	-3.14464100	1.32730900	1.27579200
H	-2.08331300	-1.35981500	2.32671600
H	-3.77452600	-0.89846600	2.15682300
Pt	-3.16047000	-3.37018300	0.12441300
P	-1.09454300	-3.98629000	1.09791000
H	-0.54921300	-3.14334600	2.08069900
H	-1.03741500	-5.23051100	1.74311200
H	-0.02242000	-4.09538100	0.19856500
P	-5.18820500	-2.69478000	-0.82603000
H	-5.90006300	-1.75506500	-0.06581100
H	-5.07177400	-2.03770300	-2.05987200
H	-6.17004800	-3.65814200	-1.09810600
P	-3.77250400	-5.64819900	0.03806300
H	-3.96276700	-6.26562500	1.28356400
H	-4.96332400	-5.97805200	-0.62605400
H	-2.86201900	-6.52743400	-0.56755800
H	-1.92561800	1.41987600	-0.73076500
C	-1.45685400	-1.13336700	-1.92183200
H	-0.52380800	-0.72036500	-2.31570100
H	-1.48361000	-2.18976800	-2.22969400
H	-2.31054700	-0.62393300	-2.38545600
C	0.15922700	0.64509200	1.93572200
H	1.03763100	0.36042200	1.34634500
H	0.41537700	1.56961700	2.47519800
H	-0.02183500	-0.11888600	2.70432300
C	0.27069000	1.36553000	-1.00255800
H	0.07888500	1.43620300	-2.07801400
H	0.72785100	2.31515900	-0.69149000
H	1.02353800	0.58156500	-0.84053700

A-Pt(PH3)3
5-exo-TS

Zero-point correction= 0.315040 (Hartree/Particle)
Thermal correction to Energy= 0.335977
Thermal correction to Enthalpy= 0.336921
Thermal correction to Gibbs Free Energy= 0.265642
Sum of electronic and zero-point Energies= -1500.357828
Sum of electronic and thermal Energies= -1500.336892
Sum of electronic and thermal Enthalpies= -1500.335947
Sum of electronic and thermal Free Energies= -1500.407226

C	-1.63352800	0.47078600	0.18788100
C	-3.70378500	0.21591900	-0.26959700
C	-3.86079800	0.96256800	0.87527500
C	-3.09962400	0.53069700	2.09343900
C	-1.84624000	-0.15358000	1.55036100
H	-1.58530300	1.56719900	0.18551900
H	-2.83383200	1.42450500	2.67562100
H	-3.70104400	-0.10417700	2.75766800
H	-0.96938100	-0.00415900	2.19543900
H	-1.97528200	-1.23925200	1.43919800
C	-0.90719000	-0.17911900	-0.87469000
H	-1.19418600	-1.23749100	-0.94906900
P	1.13556000	2.19876600	0.33242000
H	0.54691500	2.63075900	1.53200100
H	2.38708100	2.82838600	0.40559200
H	0.47685100	3.01022700	-0.60464100
P	3.40374600	-0.26454900	0.66280000
H	4.27613000	-0.84362700	-0.27168100
H	4.09078900	0.91774800	0.97961600
H	3.66260900	-1.04914200	1.79704000
P	1.08669400	-2.44419700	-0.40024200
H	2.24814500	-3.20037400	-0.18200800
H	0.13838200	-3.15524700	0.35020100
H	0.74605700	-2.80961500	-1.71114500
Pt	1.14066100	-0.13161700	-0.02175500
C	-0.84048500	0.47446100	-2.23903600
H	-1.77146400	0.31216200	-2.79925200
H	-0.68141400	1.55854800	-2.17112100
H	-0.02482100	0.05304100	-2.83942400
H	-3.48574300	-0.84704600	-0.15078900
C	-4.52133400	2.28687000	0.89978200
H	-5.25638200	2.42513000	0.10130700
H	-5.00351800	2.44440200	1.87351900
H	-3.76148300	3.08151300	0.80933400
C	-4.23562900	0.64096800	-1.60235300
H	-3.90845800	1.65510500	-1.86714300
H	-3.91482700	-0.04367100	-2.39364300
H	-5.33495000	0.64004600	-1.60234200

FigS1-structures

A-Pt(PH3)3
6-endo-int

Zero-point correction=	0.316862 (Hartree/Particle)
Thermal correction to Energy=	0.337639
Thermal correction to Enthalpy=	0.338583
Thermal correction to Gibbs Free Energy=	0.267585
Sum of electronic and zero-point Energies=	-1500.385099
Sum of electronic and thermal Energies=	-1500.364322
Sum of electronic and thermal Enthalpies=	-1500.363378
Sum of electronic and thermal Free Energies=	-1500.434376

C	-3.25420400	-1.08108100	0.66068800
C	-1.96258900	-1.06609000	-0.13034000
C	-1.32896000	0.44499500	-0.13456100
C	-1.26431000	0.74354400	1.28357400
C	-2.51185500	0.97363000	1.97784500
C	-3.10858300	-0.50761500	2.04672500
H	-1.18469000	-1.69013600	0.34329600
H	-3.95507100	-0.43400000	0.10421800
H	-2.38576600	1.35455000	2.99589800
H	-3.21926600	1.58527600	1.40826700
H	-2.45768400	-1.10990700	2.69624400
H	-4.07085900	-0.40461800	2.56485600
Pt	-4.15611400	-3.03525300	0.82359800
P	-2.13776900	-3.95996700	1.60180300
H	-1.31622100	-3.16637900	2.42154800
H	-2.19890700	-5.14125700	2.35799500
H	-1.22793500	-4.33448700	0.59913200
P	-5.23429400	-5.16955200	0.98616800
H	-5.16666900	-5.83058200	2.22419700
H	-6.61400200	-5.24257400	0.73306100
H	-4.76517600	-6.18217900	0.13343900
P	-6.05465000	-1.96336500	0.00140400
H	-5.91414500	-1.45734900	-1.30083500
H	-7.27605600	-2.64802600	-0.08799500
H	-6.42646300	-0.80631700	0.70444700
H	-2.10960800	1.05491500	-0.61211800
C	-2.14147900	-1.49408100	-1.57893600
H	-2.52933200	-2.51998900	-1.61782800
H	-2.86395200	-0.83962900	-2.08742200
H	-1.20134500	-1.47659300	-2.13810300
C	-0.02562300	0.57867300	2.04372600
H	0.64265600	-0.18111800	1.62065100
H	0.51935600	1.53751600	1.95575900
H	-0.20253900	0.40976000	3.11078400
C	-0.01932600	0.50123900	-0.90529200
H	0.63540400	-0.34832100	-0.67095500
H	-0.21450700	0.48595300	-1.98146600
H	0.52919300	1.42497100	-0.68697000

A-Pt(PH3)3
5-exo-int

Zero-point correction=	0.313934 (Hartree/Particle)
Thermal correction to Energy=	0.335260
Thermal correction to Enthalpy=	0.336204
Thermal correction to Gibbs Free Energy=	0.263339
Sum of electronic and zero-point Energies=	-1500.378001
Sum of electronic and thermal Energies=	-1500.356674
Sum of electronic and thermal Enthalpies=	-1500.355730
Sum of electronic and thermal Free Energies=	-1500.428595

C	-2.02130800	0.67948500	0.13146300
C	-3.52227100	0.78207900	-0.26727300
C	-4.26995800	0.70479200	0.99248200
C	-3.39248400	0.37082000	2.10379100
C	-2.06743400	-0.05185200	1.48014900
H	-1.68847100	1.72226700	0.28986900
H	-3.29071800	1.35761800	2.61218300
H	-3.85145400	-0.28056300	2.85815000
H	-1.20603400	0.17167500	2.11864200
H	-2.07837500	-1.13888000	1.30917300
C	-1.12701500	-0.03313000	-0.88026100
H	-1.55243800	-1.04983300	-0.96709900
P	3.19507900	-0.57643600	0.50234900
H	4.11876700	0.47171100	0.33820800
H	3.43647400	-0.89713100	1.84964200
H	3.90681200	-1.61747400	-0.12023400
Pt	0.89924800	-0.24296200	-0.18470300
P	1.02516800	2.07055500	0.18628000
H	2.29838600	2.66335800	0.18334500
H	0.34275900	2.91869400	-0.70198200
H	0.53124700	2.53680100	1.41716000
P	0.58053900	-2.49347200	-0.68657600
H	1.66465000	-3.38582500	-0.65844400
H	-0.35840000	-3.17837500	0.10151900
H	0.06337000	-2.72540900	-1.97207100
C	-1.10127600	0.56038100	-2.28149100
H	-2.06954200	0.43773000	-2.79189200
H	-0.86134400	1.63332500	-2.28344200
H	-0.35319500	0.05822200	-2.90954400
H	-3.81247700	-0.19267200	-0.73628300
C	-3.95349900	1.92282100	-1.18702400
H	-3.36638600	1.91301700	-2.10857100
H	-5.01083700	1.85201600	-1.46430400
H	-3.78645900	2.88694500	-0.69056100
C	-5.68569400	0.99948900	1.12747400
H	-6.12029100	0.61749800	2.05455800
H	-5.76406800	2.10343700	1.14394000
H	-6.26013600	0.68614800	0.24700100

FigS2-structures

M=Pt(PH3)3
6-Me:5-exo-int

Zero-point correction=	0.256139 (Hartree/Particle)
Thermal correction to Energy=	0.274085
Thermal correction to Enthalpy=	0.275029
Thermal correction to Gibbs Free Energy=	0.208898
Sum of electronic and zero-point Energies=	-1421.629765
Sum of electronic and thermal Energies=	-1421.611818
Sum of electronic and thermal Enthalpies=	-1421.610874
Sum of electronic and thermal Free Energies=	-1421.677006

C	-2.98006400	-1.10010100	0.70309200
C	-1.84529900	-0.10463500	0.33654100
C	-1.15306700	0.19317500	1.56312700
C	-1.86732900	-0.30560100	2.70970500
C	-3.23136400	-0.76528000	2.18216300
H	-2.52753500	-2.10628000	0.62587800
H	-1.21772400	-1.18609800	2.96544400
H	-1.80648700	0.31352600	3.61628800
H	-3.64650200	-1.59956000	2.75704200
H	-3.94601100	0.06915200	2.26146200
H	-2.29698900	0.90580300	0.12860800
C	-4.19940300	-0.98829700	-0.20750300
H	-4.53115400	0.06271100	-0.10493000
P	-4.49698500	-4.13532000	0.37058400
H	-3.69444000	-4.33356900	1.50953500
H	-5.11343700	-5.39501200	0.27854400
H	-3.53323100	-4.24659900	-0.64686000
P	-7.84391900	-3.56271800	0.85740100
H	-9.08954600	-3.08928000	0.40787800
H	-7.89912800	-4.88382600	0.37688900
H	-8.13690300	-3.77949500	2.21554800
P	-7.10768200	-0.25333500	0.15740300
H	-8.50952200	-0.27595400	0.24845300
H	-6.78822700	0.76001000	1.07730600
H	-6.91421500	0.41815400	-1.06203400
Pt	-5.87454100	-2.23245400	0.34185900
H	-0.19824100	0.72760700	1.62014800
H	-1.20682100	-0.28945600	-0.53825800
C	-3.86782000	-1.22792600	-1.67480400
H	-3.15926700	-0.47961900	-2.06447100
H	-3.41710700	-2.21513200	-1.84826100
H	-4.75858300	-1.16810700	-2.31274500

A-Pt(PH3)3
6-Me: 6-endo-int

Zero-point correction=	0.259433 (Hartree/Particle)
Thermal correction to Energy=	0.277675
Thermal correction to Enthalpy=	0.278619
Thermal correction to Gibbs Free Energy=	0.212628
Sum of electronic and zero-point Energies=	-1421.637537
Sum of electronic and thermal Energies=	-1421.619294
Sum of electronic and thermal Enthalpies=	-1421.618350
Sum of electronic and thermal Free Energies=	-1421.684341

C	-3.19558400	-1.04074200	0.58774500
C	-1.86881300	-0.98143000	-0.13064500
C	-1.38817300	0.60004300	-0.17802300
C	-1.41611900	0.96667900	1.20131900
C	-2.66009100	1.12724000	1.88793700
C	-3.12860100	-0.43863900	1.96416300
H	-1.08093500	-1.50811500	0.43361500
H	-3.90169400	-0.44430400	-0.01733900
H	-2.58527000	1.51356900	2.90772100
H	-3.42862100	1.65134500	1.30924600
H	-2.44015000	-0.96935700	2.63539900
H	-4.09857200	-0.38235600	2.47621100
H	-2.13878000	1.10988000	-0.79421300
Pt	-4.02990900	-3.04774000	0.72908900
P	-2.00130400	-3.92860700	1.55364900
H	-0.99946500	-4.11499700	0.58526300
H	-1.30510300	-3.19491300	2.52932500
H	-2.03073300	-5.19860900	2.15492300
P	-5.03932300	-5.22098600	0.89606900
H	-5.16847900	-5.74035900	2.19558600
H	-6.34459200	-5.39468900	0.40618700
H	-4.37271000	-6.27701600	0.25104800
P	-5.95771100	-2.07301300	-0.17391300
H	-5.78799500	-1.57964100	-1.47833100
H	-7.13840100	-2.82275200	-0.29793800
H	-6.41285000	-0.92827500	0.50194000
H	-0.49926000	0.86611600	1.79270100
H	-0.39790800	0.62536900	-0.64206000
C	-1.88326100	-1.45209900	-1.57554800
H	-2.66206200	-0.92977300	-2.14839400
H	-0.92294300	-1.28139800	-2.07421600
H	-2.09427100	-2.52871900	-1.62300900

FigS2-structures

M=Pt(PH3)3
1,5,6-Me:5-exo-int

Zero-point correction=	0.312804 (Hartree/Particle)
Thermal correction to Energy=	0.334586
Thermal correction to Enthalpy=	0.335530
Thermal correction to Gibbs Free Energy=	0.260632
Sum of electronic and zero-point Energies=	-1500.167799
Sum of electronic and thermal Energies=	-1500.146017
Sum of electronic and thermal Enthalpies=	-1500.145073
Sum of electronic and thermal Free Energies=	-1500.219971

C	-2.96362400	-1.08150600	0.64278900
C	-1.79933900	-0.10190300	0.29362900
C	-1.16596900	0.23914600	1.57516100
C	-1.92883100	-0.29970300	2.69513900
C	-3.26494600	-0.75288100	2.11268300
H	-2.52527900	-2.09617300	0.57196200
H	-1.31070900	-1.17804400	2.99692200
H	-1.93599800	0.33999700	3.58854400
H	-3.70635100	-1.58967000	2.66501300
H	-3.98375500	0.07954300	2.16590300
H	-2.26035400	0.88223100	0.02020400
C	-4.19974300	-0.96154000	-0.25099300
H	-4.53454700	0.08528100	-0.12372500
P	-4.46535400	-4.10849800	0.28911400
H	-3.65988100	-4.34953500	1.41762100
H	-5.07431800	-5.36735600	0.14590300
H	-3.50206200	-4.17261900	-0.73285900
P	-7.80313600	-3.56301300	0.91424000
H	-9.06153700	-3.10292100	0.48605700
H	-7.86154900	-4.88858800	0.44581800
H	-8.07156900	-3.77296800	2.27876100
P	-7.09589000	-0.23802000	0.24058600
H	-8.49187800	-0.26226900	0.39975300
H	-6.73539900	0.77300200	1.14782200
H	-6.96595500	0.44289600	-0.98230800
Pt	-5.85560000	-2.21762600	0.34716400
C	-3.95993000	-1.18614700	-1.73777700
H	-3.35743900	-0.37964900	-2.18243700
H	-3.44364500	-2.13424100	-1.94584000
H	-4.90029700	-1.20493700	-2.30398700
C	0.09233400	0.95387900	1.71073400
H	0.25841800	1.36821500	2.70966900
H	0.89404400	0.21180700	1.51888500
H	0.23156000	1.71433900	0.93003000
C	-0.80927800	-0.49583600	-0.80591700
H	-0.27514200	-1.41266700	-0.52459600
H	-1.32982700	-0.68767600	-1.74703700
H	-0.06892100	0.28850800	-0.99813600

A-Pt(PH3)3
1,5,6-Me: 6-endo-int

Zero-point correction=	0.315490 (Hartree/Particle)
Thermal correction to Energy=	0.336596
Thermal correction to Enthalpy=	0.337540
Thermal correction to Gibbs Free Energy=	0.265370
Sum of electronic and zero-point Energies=	-1500.171996
Sum of electronic and thermal Energies=	-1500.150890
Sum of electronic and thermal Enthalpies=	-1500.149946
Sum of electronic and thermal Free Energies=	-1500.222116

C	-3.19091100	-1.07031600	0.58598200
C	-1.84159100	-1.01223100	-0.10996800
C	-1.31217200	0.53586600	-0.15975900
C	-1.34253200	0.90178000	1.24635200
C	-2.64212300	1.06308900	1.87452100
C	-3.16250300	-0.44012200	1.96015400
H	-1.07109900	-1.55639000	0.46902700
H	-3.87400700	-0.47127900	-0.04394100
H	-2.59209100	1.48859900	2.88258000
H	-3.34947300	1.62576100	1.25404700
H	-2.51527300	-0.98965600	2.66062800
H	-4.15407200	-0.38325000	2.42888200
H	-2.11191400	1.06506400	-0.70061600
Pt	-4.05214000	-3.05664300	0.73029000
P	-2.03847200	-3.93499900	1.57847900
H	-1.03751700	-4.16052200	0.61702800
H	-1.32983300	-3.17940900	2.52930800
H	-2.07445500	-5.18534100	2.21997800
P	-5.09778200	-5.22183800	0.91967200
H	-5.23394600	-5.73530200	2.22133700
H	-6.40810300	-5.38405700	0.43783300
H	-4.45613000	-6.29868400	0.28276000
P	-5.94929400	-2.05445800	-0.19812100
H	-5.76171200	-1.57357000	-1.50488300
H	-7.14572700	-2.77846500	-0.32793000
H	-6.38861000	-0.89440900	0.46264500
C	-1.87565300	-1.53693700	-1.53767300
H	-2.56087900	-0.94002200	-2.15693100
H	-0.89181000	-1.53132800	-2.01549200
H	-2.23684800	-2.57413600	-1.54725000
C	-0.13319200	0.89720700	2.06668500
H	0.64545000	0.21699900	1.70007700
H	0.30520200	1.91151900	1.96777800
H	-0.33341900	0.75400100	3.13458000
C	0.02459400	0.66672300	-0.87363900
H	0.74370900	-0.10409000	-0.56642700
H	-0.11203600	0.58088500	-1.95532800
H	0.47942500	1.64748600	-0.69070900

FigS2-structures

M=H
6-Me:5-exo-int

Zero-point correction=	0.184660 (Hartree/Particle)
Thermal correction to Energy=	0.192279
Thermal correction to Enthalpy=	0.193223
Thermal correction to Gibbs Free Energy=	0.153328
Sum of electronic and zero-point Energies=	-273.931932
Sum of electronic and thermal Energies=	-273.924313
Sum of electronic and thermal Enthalpies=	-273.923369
Sum of electronic and thermal Free Energies=	-273.963263

C	-2.93282900	-1.05900800	0.85824000
C	-2.37436400	-0.57268900	-0.49114700
C	-1.36079800	0.40204800	-0.15979200
C	-1.40042300	0.75129100	1.23822000
C	-2.70839800	0.13899400	1.79913800
H	-2.12470600	-1.28427400	-1.28385000
H	-3.11157600	0.13253800	-0.96244900
H	-3.97811900	-1.36158500	0.78954600
H	-3.50265100	0.88163700	1.63991900
H	-2.35019300	-1.92433000	1.19555900
C	-2.64180000	-0.21479200	3.28221900
H	-3.59046000	-0.68619300	3.56093200
H	-1.86180400	-0.97311900	3.43248800
H	-0.54327300	0.10449000	1.57957600
H	-0.65863200	0.82298400	-0.88062200
H	-1.10256100	1.77217500	1.49397200
C	-2.38302800	0.99576700	4.17623000
H	-2.40396900	0.70668800	5.22887500
H	-1.40201100	1.44364300	3.98354500
H	-3.14484800	1.76737700	4.02754600

M=H
6-Me:6-endo-int

Zero-point correction=	0.187502 (Hartree/Particle)
Thermal correction to Energy=	0.194880
Thermal correction to Enthalpy=	0.195824
Thermal correction to Gibbs Free Energy=	0.156636
Sum of electronic and zero-point Energies=	-273.943733
Sum of electronic and thermal Energies=	-273.936355
Sum of electronic and thermal Enthalpies=	-273.935411
Sum of electronic and thermal Free Energies=	-273.974598

C	-2.97579600	-0.99119200	0.68796100
C	-1.87683200	-1.00191700	-0.36593900
C	-1.32536200	0.53922200	-0.56278300
C	-0.94311600	0.80008000	0.78537500
C	-1.92137000	1.06443900	1.80666600
C	-2.48260400	-0.43374700	2.01184800
H	-1.03515900	-1.61436000	-0.02317400
H	-3.83875500	-0.42016100	0.32376900
H	-1.50588400	1.41357900	2.75194100
H	-2.75556200	1.68038500	1.46465000
H	-1.69820000	-1.06177300	2.44447500
H	-3.27483400	-0.32624700	2.75694700
H	-2.18010600	1.11969900	-0.91571400
H	-3.31651100	-2.02239200	0.84085000
H	0.07244900	0.54438600	1.09541600
H	-0.50594700	0.50060300	-1.28020200
C	-2.32675300	-1.47331700	-1.74514800
H	-1.50886600	-1.44539600	-2.46833200
H	-2.67066400	-2.50916700	-1.66570100
H	-3.15338900	-0.86232200	-2.11832200

FigS2-structures

M=H
1,5,6-Me:5-exo-int

Zero-point correction=	0.241470 (Hartree/Particle)
Thermal correction to Energy=	0.252289
Thermal correction to Enthalpy=	0.253233
Thermal correction to Gibbs Free Energy=	0.205266
Sum of electronic and zero-point Energies=	-352.491412
Sum of electronic and thermal Energies=	-352.480592
Sum of electronic and thermal Enthalpies=	-352.479648
Sum of electronic and thermal Free Energies=	-352.527616

C	-2.84494600	-1.15706100	0.89895300
C	-3.23548700	-0.68604400	-0.50667900
C	-2.95388500	0.74831800	-0.53520500
C	-2.68936700	1.26056200	0.81529500
C	-3.03529400	0.09184900	1.77940900
H	-2.86867700	-1.23979200	-1.37686900
H	-4.34528800	-0.68331700	-0.60840900
H	-3.43881300	-2.00877500	1.23304500
H	-4.09836600	0.19664200	2.04294200
H	-1.79209800	-1.46163000	0.90144500
C	-2.20339400	0.01795000	3.06172300
H	-2.51994800	-0.88556800	3.59529100
H	-1.15196400	-0.14367000	2.78837600
H	-1.57234600	1.32162100	0.77213800
C	-2.31474100	1.21953000	3.99810400
H	-1.85951100	0.98719100	4.96339400
H	-1.79178300	2.09617300	3.60437500
H	-3.35948300	1.49162000	4.18208700
C	-3.00650800	1.57859700	-1.73856900
H	-3.97829700	2.10389200	-1.69917800
H	-2.25216400	2.37258500	-1.71482300
H	-2.95949100	1.00515300	-2.66448800
C	-3.25220800	2.65959000	1.09653900
H	-4.34538200	2.63449200	1.05670800
H	-2.96047400	2.98758400	2.09287900
H	-2.88961200	3.40000300	0.37917200

M=H
1,5,6-Me: 6-endo-int

Zero-point correction=	0.244404 (Hartree/Particle)
Thermal correction to Energy=	0.254466
Thermal correction to Enthalpy=	0.255410
Thermal correction to Gibbs Free Energy=	0.210279
Sum of electronic and zero-point Energies=	-352.500431
Sum of electronic and thermal Energies=	-352.490370
Sum of electronic and thermal Enthalpies=	-352.489426
Sum of electronic and thermal Free Energies=	-352.534557

C	-3.02333200	-0.97175000	0.67170700
C	-1.89806200	-1.03206000	-0.35869200
C	-1.24479600	0.44591700	-0.54610200
C	-0.84801600	0.71108100	0.82464600
C	-1.89116500	1.00551500	1.80089500
C	-2.54958100	-0.42182600	2.00830600
H	-1.10089100	-1.69490300	0.00582600
H	-3.84757800	-0.36238500	0.27936700
H	-1.49983600	1.37391300	2.75090900
H	-2.65925200	1.67372700	1.40368300
H	-1.81998200	-1.09377700	2.47335600
H	-3.36756400	-0.28021900	2.71873400
H	-2.09418400	1.07977900	-0.82493100
H	-3.41871600	-1.98322200	0.81657600
C	-2.37574600	-1.52435900	-1.72253000
H	-1.55270900	-1.66016100	-2.42579900
H	-2.86316000	-2.49513100	-1.59319200
H	-3.10359700	-0.83134600	-2.15617200
C	-0.14661300	0.46167700	-1.60563300
H	-0.59678700	0.42439100	-2.59864000
H	0.44590300	1.37873600	-1.54708000
H	0.52785300	-0.39529400	-1.51301100
C	0.53210500	0.49186300	1.27962900
H	1.03608600	1.46474200	1.12630800
H	0.59573000	0.26514900	2.34613200
H	1.07978800	-0.23362000	0.67416700

FigS3-structures

B-I-6

Zero-point correction= 0.377697 (Hartree/Particle)
Thermal correction to Energy= 0.402681
Thermal correction to Enthalpy= 0.403626
Thermal correction to Gibbs Free Energy= 0.321030
Sum of electronic and zero-point Energies= -1653.843552
Sum of electronic and thermal Energies= -1653.818567
Sum of electronic and thermal Enthalpies= -1653.817623
Sum of electronic and thermal Free Energies= -1653.900219

C	-2.97376300	-0.70399500	0.77289700
C	-1.93737500	-0.73630000	-0.32305800
C	-1.24431600	0.72627300	-0.65271100
C	-0.72494800	0.93222800	0.69338300
C	-1.65965900	1.21849200	1.78250200
C	-2.37427600	-0.17277600	2.05688800
H	-1.10825100	-1.43065400	-0.11116500
H	-2.34880600	-1.01330500	-1.30551700
H	-3.76449400	-0.00997100	0.44995300
H	-1.14384100	1.53356300	2.69692400
H	-2.42448700	1.95549800	1.51867500
H	-1.62414200	-0.86028100	2.47711400
H	-3.11616000	0.00175900	2.84713600
Pt	-3.95962900	-2.59785000	1.13226600
C	0.65659000	0.62160900	1.07563500
H	0.72236100	0.18487900	2.08155200
H	1.22347200	0.03818600	0.34539700
H	1.17024300	1.59980500	1.15947600
C	-0.21551900	0.49593500	-1.76240400
H	-0.76714900	0.15930800	-2.65396600
H	0.45144300	-0.34238100	-1.50302700
P	-1.90420100	-3.73478900	1.13076000
H	-0.79992500	-3.08309500	1.70992600
H	-1.83876400	-4.97868500	1.78120500
H	-1.38504200	-4.06744500	-0.13209400
P	-5.17278800	-4.64329000	1.55111300
H	-6.29878200	-4.55659100	2.38835800
H	-5.73266000	-5.28073300	0.43063100
H	-4.49695400	-5.71968200	2.15253200
P	-5.93304500	-1.33097700	1.13572900
H	-5.87913900	-0.16980400	1.92489500
H	-6.30783700	-0.80306100	-0.11017700
H	-7.13687700	-1.90910600	1.57138700
C	0.60981800	1.72770800	-2.11272200
H	-0.01887300	2.50902500	-2.56161000
H	1.06538600	2.17765500	-1.21567700
C	1.72976600	1.41602600	-3.08687100
H	1.30461100	0.99653100	-4.01789700
H	2.38945200	0.63639100	-2.65599700
O	2.40351000	2.61961500	-3.30015900
H	3.08759000	2.49893900	-3.97183800
C	-2.32390900	1.70539600	-1.12000700
H	-1.89696600	2.70515400	-1.26039100
H	-2.70830100	1.37370200	-2.09252700
H	-3.17432600	1.80428200	-0.44063300

B-I-5

Zero-point correction= 0.377282 (Hartree/Particle)
Thermal correction to Energy= 0.401999
Thermal correction to Enthalpy= 0.402943
Thermal correction to Gibbs Free Energy= 0.322465
Sum of electronic and zero-point Energies= -1653.853318
Sum of electronic and thermal Energies= -1653.828602
Sum of electronic and thermal Enthalpies= -1653.827657
Sum of electronic and thermal Free Energies= -1653.908135

C	-3.27279000	-0.89187900	0.77079100
C	-1.94684400	-0.06774700	0.87242600
C	-1.67323300	-0.01420400	2.30173100
C	-2.87354400	-0.36320000	3.07586800
C	-4.00796700	-0.52898800	2.06313800
H	-2.96293200	-1.94483700	0.88029900
H	-2.60462100	-1.34310900	3.52698100
H	-3.04929900	0.29293900	3.93975900
H	-4.72807300	-1.29502300	2.37293300
H	-4.55818300	0.41795000	1.95634500
C	-0.39514500	0.31968900	2.92087600
H	-0.50382000	0.79147100	3.90402300
H	0.11749000	-0.64653600	3.09674200
H	0.27171900	0.89966400	2.27336500
C	-0.82445300	-0.45508100	-0.09187700
H	0.08042200	0.13208000	0.12783400
H	-1.13623500	-0.12985100	-1.09754000
C	-4.04752200	-0.72662400	-0.53134500
H	-4.56062000	0.24808500	-0.53931900
H	-3.36061000	-0.69921700	-1.39083900
P	-3.62444400	-3.58740300	-1.72264100
H	-2.91782200	-4.34117100	-0.76900200
H	-3.89525400	-4.57496500	-2.68533500
H	-2.57522500	-2.88636200	-2.34358300
P	-7.04543000	-4.03760300	-1.43208600
H	-6.65219100	-5.14980000	-2.19828200
H	-7.63966900	-4.68940500	-0.33709000
H	-8.19615500	-3.65156800	-2.14303300
P	-7.08943000	-0.78907700	-0.27631600
H	-8.44086100	-1.17551800	-0.25872300
H	-6.95097900	-0.24087000	1.01041400
H	-7.14702700	0.37564700	-1.05889000
Pt	-5.43615400	-2.29802900	-0.94511100
C	-0.51030400	-1.94295400	-0.11807800
H	-0.06599900	-2.28794000	0.82880900
H	-1.44116400	-2.51537900	-0.23160700
C	0.36744000	-2.36378500	-1.28435800
H	1.42678700	-2.14327100	-1.07806600
H	0.08840700	-1.78283800	-2.18561000
O	0.13470000	-3.73822800	-1.46898400
H	0.84054400	-4.11766000	-2.01030400
C	-2.22970900	1.48449100	0.70897300
H	-2.69786400	1.58723900	-0.27892600
H	-2.91097100	1.92107300	1.44871000
H	-1.29252200	2.04973400	0.71344500

FigS3-structures

B-I-5-c

Zero-point correction= 0.382239 (Hartree/Particle)
Thermal correction to Energy= 0.405195
Thermal correction to Enthalpy= 0.406139
Thermal correction to Gibbs Free Energy= 0.329964
Sum of electronic and zero-point Energies= -1653.880793
Sum of electronic and thermal Energies= -1653.857838
Sum of electronic and thermal Enthalpies= -1653.856893
Sum of electronic and thermal Free Energies= -1653.933069

C	-3.15481900	0.28261300	0.14897900
C	-1.59073300	0.26794600	0.18347400
C	-1.29123200	0.82387100	1.58741800
C	-2.38776700	1.83171500	1.90211900
C	-3.53497300	1.55655700	0.91635900
H	-3.49093200	-0.57921000	0.75372100
H	-2.69671400	1.77453500	2.95546800
H	-1.97354700	2.84083300	1.78054800
H	-4.50785800	1.45885100	1.41393700
H	-3.62561300	2.40036200	0.21736400
C	0.10833500	1.25866100	1.92938900
H	0.20047800	1.50351300	2.99701600
H	0.87622800	0.52195500	1.66610300
H	0.34295400	2.17992900	1.38438600
C	-0.97321600	-1.11520100	-0.06516500
H	0.11874100	-1.00894400	-0.16288300
H	-1.31665500	-1.47818100	-1.04484500
C	-3.77774900	0.18404500	-1.23896300
H	-3.46047600	1.04843100	-1.84042500
H	-3.41559000	-0.70427700	-1.78085800
P	-5.64063600	-2.10957900	-0.38039300
H	-5.73477300	-2.26410200	1.01481700
H	-6.51824600	-3.12116400	-0.80726200
H	-4.39555400	-2.71904600	-0.62580200
P	-8.33110900	-0.12398700	-1.31724100
H	-9.03960400	0.28804500	-0.17448800
H	-9.01334700	0.61166000	-2.30362200
H	-8.91417500	-1.38835000	-1.52019400
P	-5.87704800	2.12909200	-2.30332800
H	-7.07983800	2.75171900	-2.67915800
H	-5.23908000	3.17084800	-1.60972000
H	-5.16795300	2.14260400	-3.51545400
Pt	-5.90939100	0.03987200	-1.25824000
C	-1.27656700	-2.16050200	1.00210900
H	-2.33873200	-2.44522800	1.00882800
H	-0.71187000	-3.08088900	0.80553800
C	-0.89377400	-1.66773500	2.36833400
H	0.17846700	-1.46429100	2.47552700
H	-1.23483800	-2.30866300	3.18625500
O	-1.62256000	-0.38122700	2.56943700
H	-1.50666400	-0.06279900	3.48844400
C	-1.00138400	1.24382100	-0.84069000
H	-1.21543700	0.89235000	-1.85669100
H	-1.40177700	2.26202000	-0.74678400
H	0.09009700	1.30234100	-0.75742900

B-I-5-t

Zero-point correction= 0.383505 (Hartree/Particle)
Thermal correction to Energy= 0.406021
Thermal correction to Enthalpy= 0.406965
Thermal correction to Gibbs Free Energy= 0.332270
Sum of electronic and zero-point Energies= -1653.868531
Sum of electronic and thermal Energies= -1653.846015
Sum of electronic and thermal Enthalpies= -1653.845071
Sum of electronic and thermal Free Energies= -1653.919766

C	-3.17676900	-0.72927100	0.51295200
C	-1.95688500	0.16747400	0.16320400
C	-1.49178200	0.46619700	1.59819900
C	-2.73228100	0.98119100	2.29883200
C	-3.81158600	0.02231200	1.71884100
H	-2.77269500	-1.69026300	0.87648800
H	-2.65457400	0.92309200	3.39119600
H	-2.93651300	2.02475700	2.03197600
H	-4.17410800	-0.68121100	2.47974500
H	-4.67840800	0.61353100	1.39285000
C	-0.85989200	-0.65371700	2.40545900
H	-0.41929100	-0.24703100	3.32712800
H	-1.63576900	-1.35326400	2.73423700
H	-0.09450100	-1.23467000	1.88338300
C	-0.80651500	-0.44711100	-0.63072600
H	-1.11962400	-0.66433300	-1.66112500
H	-0.49152800	-1.40718500	-0.19515400
C	-4.13115900	-1.02179500	-0.63744000
H	-3.56485700	-1.36101300	-1.52037000
P	-4.00436200	-4.00681500	-1.00990000
H	-4.06072100	-5.37487500	-0.69108700
H	-3.96523000	-4.06012000	-2.41314600
H	-2.65887600	-3.71292200	-0.72067500
P	-7.20618200	-4.25077400	0.33930900
H	-8.56501100	-4.00362600	0.07081900
H	-7.06134500	-5.49614800	-0.29914800
H	-7.29426700	-4.67718900	1.67651800
P	-7.07786400	-0.80846300	0.44179600
H	-8.44265000	-1.02018700	0.17894500
H	-7.12951900	-0.46382000	1.80431200
H	-6.88443000	0.45274200	-0.14723900
Pt	-5.59066600	-2.51196600	-0.17290000
C	0.36947500	0.54055700	-0.68388500
H	1.25946300	0.05793200	-1.10998200
H	0.13200400	1.37373100	-1.35605400
C	0.80104600	1.08833500	0.65864600
H	1.41145300	1.99124600	0.57560300
H	1.30551200	0.35313200	1.29395100
O	-0.41678200	1.55126500	1.43513900
H	-0.14749800	1.91857500	2.30337800
H	-4.65071600	-0.11000800	-0.96140600
C	-2.44972300	1.43577700	-0.55760900
H	-2.60449300	1.21040400	-1.62044100
H	-3.40440500	1.80900900	-0.17122100
H	-1.74364600	2.27028800	-0.50402700

FigS3-structures

B-I-6-t

Zero-point correction= 0.383409 (Hartree/Particle)
Thermal correction to Energy= 0.406088
Thermal correction to Enthalpy= 0.407032
Thermal correction to Gibbs Free Energy= 0.332056
Sum of electronic and zero-point Energies= -1653.875245
Sum of electronic and thermal Energies= -1653.852566
Sum of electronic and thermal Enthalpies= -1653.851622
Sum of electronic and thermal Free Energies= -1653.926597

C	-2.95288900	-0.81102000	0.71172200
C	-1.86017300	-0.92484000	-0.35696200
C	-1.15200400	0.42819300	-0.62831100
C	-0.57225800	0.88556200	0.72269800
C	-1.65601100	1.14084900	1.75015700
C	-2.43864100	-0.16908200	2.00323900
H	-1.08599000	-1.66065600	-0.08047500
H	-2.28852100	-1.27960700	-1.30725900
H	-3.70644800	-0.12752200	0.29044500
H	-1.21674700	1.48863900	2.69815300
H	-2.33609300	1.92652200	1.39625300
H	-1.79839100	-0.86578600	2.56620100
H	-3.27104700	0.06153600	2.68240600
Pt	-4.03685900	-2.62133200	1.14740500
C	0.55813700	0.06359300	1.31540800
H	0.99256600	0.58042600	2.18264600
H	0.17512100	-0.88906200	1.69321200
H	1.36375100	-0.17342200	0.61611800
C	-0.00865000	0.27502400	-1.64457400
H	-0.42517700	-0.06829300	-2.60134700
H	0.69496000	-0.50754200	-1.32700500
P	-2.04249600	-3.84947800	1.18563000
H	-0.92150600	-3.25555400	1.79320700
H	-2.04420900	-5.09804400	1.83262400
H	-1.50438000	-4.20580500	-0.06303500
P	-5.35228800	-4.60564600	1.64953200
H	-6.60850900	-4.43183500	2.25837500
H	-5.71724900	-5.42744200	0.56818100
H	-4.79993200	-5.56819200	2.51469500
P	-5.91970900	-1.23646100	1.08690700
H	-5.78314800	-0.01763800	1.77393300
H	-6.28936600	-0.78345700	-0.19029400
H	-7.15249100	-1.69493700	1.58190300
C	0.72319000	1.60070900	-1.87553200
H	1.62153700	1.44061800	-2.48618600
H	0.09184900	2.29135700	-2.44727000
C	1.18421100	2.27664700	-0.60575600
H	1.40845600	3.33815500	-0.74226900
H	2.02954400	1.78005600	-0.11839100
O	0.04979800	2.27472300	0.38716900
H	0.31081300	2.73872300	1.21018800
C	-2.16883200	1.43007600	-1.20101500
H	-2.45845100	1.10099400	-2.20774500
H	-3.08744300	1.51147100	-0.61399700
H	-1.76959900	2.44482100	-1.29242900

B-I-6-c

Zero-point correction= 0.383174 (Hartree/Particle)
Thermal correction to Energy= 0.405881
Thermal correction to Enthalpy= 0.406825
Thermal correction to Gibbs Free Energy= 0.330952
Sum of electronic and zero-point Energies= -1653.880442
Sum of electronic and thermal Energies= -1653.857735
Sum of electronic and thermal Enthalpies= -1653.856791
Sum of electronic and thermal Free Energies= -1653.932664

C	-2.92996300	-0.85963600	0.79324000
C	-1.82586300	-0.96151800	-0.25312100
C	-1.12755600	0.38820900	-0.56814200
C	-0.66936300	1.08333800	0.72991800
C	-1.66369800	1.00999500	1.87891000
C	-2.33167800	-0.34856100	2.09822400
H	-1.05960400	-1.67321300	0.09575700
H	-2.21091700	-1.35911900	-1.20502200
H	-3.64025800	-0.09732600	0.42797400
H	-1.18306200	1.37486600	2.80229200
H	-2.43492000	1.76290600	1.65571100
H	-1.59899200	-1.07113200	2.49358900
H	-3.09073200	-0.23632100	2.88510900
Pt	-4.09910700	-2.63666000	1.11700800
C	-0.11521400	2.48212500	0.57987500
H	0.36603000	2.81910500	1.50849600
H	0.59311300	2.59927200	-0.24622100
H	-0.94321200	3.17545500	0.39321900
C	0.06531600	0.13647500	-1.51481200
H	0.44236400	1.09647400	-1.89793800
H	-0.31240000	-0.40060400	-2.39585600
P	-2.17492100	-3.96834600	1.00745000
H	-1.04994200	-3.54643700	1.73854700
H	-2.26364200	-5.30407300	1.43857600
H	-1.60699100	-4.14778800	-0.26603700
P	-5.50360700	-4.58685400	1.51491600
H	-6.76875900	-4.39533600	2.09958500
H	-5.86632300	-5.36070500	0.39786900
H	-5.00265300	-5.59570300	2.35881100
P	-5.90645700	-1.15691400	1.20037900
H	-5.69641600	0.00616100	1.96157300
H	-6.28024800	-0.60270800	-0.03505600
H	-7.14975200	-1.58799900	1.69358600
C	1.21936300	-0.64609600	-0.89884300
H	0.94075400	-1.68624600	-0.68245500
H	2.06112800	-0.69725000	-1.60148900
C	1.71733200	0.01019700	0.35669700
H	2.15464200	1.00168100	0.19083300
H	2.40436300	-0.60835100	0.94122200
O	0.52987900	0.18845400	1.25194200
H	0.81348500	0.53975600	2.12138400
C	-2.10036100	1.32038900	-1.30288900
H	-2.51476700	0.79348600	-2.17213500
H	-2.94376000	1.65362900	-0.68641000
H	-1.59465500	2.21595100	-1.68251000

FigS3-structures

A-I-5

Zero-point correction= 0.348680 (Hartree/Particle)
Thermal correction to Energy= 0.371665
Thermal correction to Enthalpy= 0.372609
Thermal correction to Gibbs Free Energy= 0.295468
Sum of electronic and zero-point Energies= -1614.590374
Sum of electronic and thermal Energies= -1614.567389
Sum of electronic and thermal Enthalpies= -1614.566445
Sum of electronic and thermal Free Energies= -1614.643586

C	-3.04588700	-1.39764700	0.64509700
C	-1.94818100	-0.30740500	0.77462300
C	-1.55672000	-0.34131400	2.17940200
C	-2.56732500	-1.05303400	2.96351600
C	-3.73615300	-1.28804100	2.00466800
H	-2.50947000	-2.36725800	0.63697700
H	-2.06895900	-2.02072100	3.19975000
H	-2.77233100	-0.60545000	3.94565500
H	-4.33279600	-2.16732800	2.26946100
H	-4.39312800	-0.40378300	2.03671000
H	-2.54210700	0.65235500	0.83368400
C	-0.33115700	0.21872300	2.72820000
H	-0.38534900	0.42674300	3.80155000
H	0.45167300	-0.55394500	2.58890400
H	0.02397100	1.09120000	2.16496700
C	-0.88685200	-0.15107600	-0.31458000
H	-1.07124600	-0.93730900	-1.06380200
H	0.11958400	-0.35938600	0.07664500
C	-3.90294200	-1.39153000	-0.62063200
H	-3.27944900	-1.76347900	-1.44377000
H	-4.68280800	-2.15895900	-0.49960000
P	-6.48852100	0.10043100	0.38794600
H	-6.44627000	0.90475900	1.54144600
H	-7.81172200	0.33104000	-0.02705000
H	-6.61033900	-1.17915100	0.95584700
P	-6.01993500	2.36575500	-2.14547000
H	-7.39518200	2.51780000	-1.88883100
H	-5.54366900	3.60481900	-1.68263800
H	-6.01317900	2.60432300	-3.53221200
P	-3.55993300	0.32481600	-3.25437500
H	-4.31179200	0.36601800	-4.44142600
H	-2.60061000	1.34364600	-3.46757800
H	-2.79973700	-0.84096200	-3.45829400
Pt	-4.89512500	0.36912700	-1.31035400
C	-0.94049000	1.21900600	-0.98068400
H	-1.99488000	1.46222900	-1.19790400
H	-0.59812900	2.00966500	-0.29528400
C	-0.17905300	1.30591700	-2.29251000
H	-0.25984300	0.34350000	-2.83635800
H	0.89283100	1.48238500	-2.11884100
O	-0.76876300	2.35420200	-3.02897900
H	-0.16482100	2.64791000	-3.72628500

A-I-6

Zero-point correction= 0.350175 (Hartree/Particle)
Thermal correction to Energy= 0.373517
Thermal correction to Enthalpy= 0.374461
Thermal correction to Gibbs Free Energy= 0.296285
Sum of electronic and zero-point Energies= -1614.591262
Sum of electronic and thermal Energies= -1614.567920
Sum of electronic and thermal Enthalpies= -1614.566976
Sum of electronic and thermal Free Energies= -1614.645151

C	-2.87846300	-0.77070600	0.73143300
C	-1.75796800	-0.90100100	-0.27338600
C	-1.06931900	0.52971200	-0.59624900
C	-0.61083900	0.86287200	0.74249800
C	-1.62806700	1.20475000	1.73011400
C	-2.35981600	-0.17856200	2.02381300
H	-0.95155100	-1.57560400	0.05893800
H	-2.09391500	-1.25558500	-1.25791300
H	-3.59629700	-0.05426500	0.29603300
H	-1.20605200	1.59165000	2.66474200
H	-2.37667200	1.90201200	1.33514300
H	-1.64169100	-0.84501300	2.52615300
H	-3.14644400	0.04283800	2.75696700
H	-1.90631900	1.18349700	-0.88469000
Pt	-3.98816100	-2.58617300	1.11683000
C	0.76206000	0.63530500	1.18932700
H	0.81784300	0.34160200	2.24567500
H	1.34547200	-0.03256100	0.54697300
H	1.26254400	1.62339300	1.13615000
C	-0.05992400	0.41473600	-1.72808400
H	-0.60030500	0.04020900	-2.61102600
H	0.70028600	-0.35064200	-1.49968000
P	-2.00668900	-3.84280800	1.27026400
H	-0.92569800	-3.26471300	1.95873700
H	-2.07109300	-5.09927600	1.89607000
H	-1.39643300	-4.18215800	0.05059900
P	-5.32767100	-4.54862900	1.54641600
H	-6.59590600	-4.36034400	2.12272100
H	-5.66392100	-5.33492300	0.43110400
H	-4.80254100	-5.52786200	2.40824100
P	-5.87742100	-1.20808900	0.94307200
H	-5.81353700	-0.02980400	1.70580200
H	-6.11793300	-0.69372800	-0.34111400
H	-7.14441100	-1.70129400	1.29553800
C	0.59803800	1.74740200	-2.05785100
H	-0.16605500	2.51781100	-2.24245300
H	1.20634500	2.11080900	-1.21462000
C	1.50272800	1.67503000	-3.27245100
H	0.90723400	1.38414800	-4.15803800
H	2.26406400	0.88492500	-3.12311000
O	2.07263800	2.94307400	-3.40454900
H	2.63049900	2.97078500	-4.19304400

FigS3-structures

A-I-5-c

Zero-point correction= 0.354561 (Hartree/Particle)
Thermal correction to Energy= 0.375972
Thermal correction to Enthalpy= 0.376916
Thermal correction to Gibbs Free Energy= 0.303841
Sum of electronic and zero-point Energies= -1614.621691
Sum of electronic and thermal Energies= -1614.600280
Sum of electronic and thermal Enthalpies= -1614.599336
Sum of electronic and thermal Free Energies= -1614.672411

C	-3.19561400	-0.89100600	0.65158400
C	-2.11058500	0.16238200	0.36655600
C	-1.58630300	0.53304200	1.75520800
C	-2.74436000	0.30415000	2.72805500
C	-3.87685400	-0.31202800	1.89272500
H	-2.67848500	-1.81719700	0.96760100
H	-2.43904300	-0.36286500	3.54597200
H	-3.03162700	1.25099500	3.20114600
H	-4.44981100	-1.05620300	2.45962100
H	-4.57264100	0.48463400	1.58229000
H	-2.62715200	1.08083500	0.02553600
C	-0.85464300	1.83892600	1.89931800
H	-0.47145900	1.98304800	2.91893000
H	-0.02921400	1.96244600	1.18874300
H	-1.56688000	2.65313700	1.71512900
C	-1.02199700	-0.20125300	-0.64389400
H	-0.43742000	0.69490600	-0.90389500
H	-1.48349500	-0.53836400	-1.58217500
C	-4.09368000	-1.28751300	-0.51601200
H	-3.46790100	-1.58462500	-1.37156900
H	-4.63604600	-2.20527700	-0.24927300
P	-7.02411900	-0.75680100	0.46189800
H	-7.35860600	0.11024400	1.51736200
H	-8.30517700	-1.14126200	0.02980100
H	-6.62068900	-1.90378400	1.16610200
P	-7.34314500	1.54991900	-2.04550700
H	-6.97561400	2.85505500	-2.42098500
H	-8.00129700	1.13650500	-3.21765100
H	-8.45725600	1.84321200	-1.23722000
P	-4.11394100	0.69264900	-2.89916000
H	-4.57182200	1.50155900	-3.95426700
H	-2.96058500	1.40559400	-2.52321100
H	-3.53969400	-0.37529000	-3.60922200
Pt	-5.59535600	0.07922900	-1.20034300
C	-0.08399900	-1.29218400	-0.13958500
H	-0.60985400	-2.24851900	-0.01382100
H	0.72095000	-1.47267600	-0.86322700
C	0.55332000	-0.89630600	1.16172300
H	1.16853500	0.00895400	1.09345400
H	1.11760800	-1.70066100	1.64184700
O	-0.56404400	-0.61001800	2.11365700
H	-0.21967300	-0.45699900	3.01813400

A-I-5-t

Zero-point correction= 0.354583 (Hartree/Particle)
Thermal correction to Energy= 0.376100
Thermal correction to Enthalpy= 0.377044
Thermal correction to Gibbs Free Energy= 0.303507
Sum of electronic and zero-point Energies= -1614.613167
Sum of electronic and thermal Energies= -1614.591650
Sum of electronic and thermal Enthalpies= -1614.590706
Sum of electronic and thermal Free Energies= -1614.664243

C	-3.06716500	-0.84904200	0.58544400
C	-1.92377200	0.11324100	0.25623600
C	-1.37785600	0.38460400	1.65337900
C	-2.61376700	0.76536500	2.44366400
C	-3.68794900	-0.18742100	1.84527400
H	-2.60196300	-1.80457000	0.88999100
H	-2.48326200	0.64477200	3.52564800
H	-2.87272100	1.81415000	2.24685600
H	-4.02066600	-0.93183600	2.57906500
H	-4.56548800	0.40896400	1.55846200
H	-2.38596200	1.06948200	-0.06408500
C	-0.56011800	-0.69362500	2.32811900
H	-0.09001400	-0.30467700	3.24249500
H	-1.22285200	-1.50267800	2.65650800
H	0.21453100	-1.14330700	1.69906400
C	-0.83396500	-0.23702400	-0.73921500
H	-1.25093700	-0.43481900	-1.73650700
H	-0.30969200	-1.16001100	-0.45003200
C	-4.00834100	-1.21870900	-0.55987100
H	-3.40142300	-1.49569100	-1.43585900
H	-4.53520100	-2.14720800	-0.30028000
P	-6.92107400	-0.78140800	0.49966800
H	-7.31784700	0.04974000	1.56217500
H	-8.16868500	-1.25899900	0.06291700
H	-6.42705900	-1.89734300	1.19685400
P	-7.33943300	1.61232100	-1.91615400
H	-7.33951300	2.00998400	-3.26585400
H	-8.66647500	1.15726100	-1.80734100
H	-7.46434000	2.86787500	-1.29508000
P	-4.10693700	0.77252800	-2.88976100
H	-4.55658000	1.64932400	-3.89287300
H	-2.90059700	1.40109700	-2.52844000
H	-3.61990300	-0.29457400	-3.66360700
Pt	-5.54654200	0.14240400	-1.16894100
C	0.13249200	0.94943400	-0.82863600
H	0.99717900	0.71476400	-1.46350400
H	-0.37280200	1.80803700	-1.29515300
C	0.68803200	1.38502600	0.50528400
H	1.18746100	2.35650400	0.46366000
H	1.34548500	0.64488500	0.97345900
O	-0.46329900	1.61091000	1.45766900
H	-0.13143500	1.93963400	2.32026800

FigS3-structures

A-I-6-t

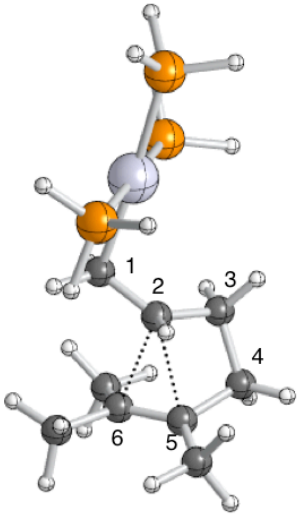
Zero-point correction= 0.355351 (Hartree/Particle)
Thermal correction to Energy= 0.376616
Thermal correction to Enthalpy= 0.377560
Thermal correction to Gibbs Free Energy= 0.305270
Sum of electronic and zero-point Energies= -1614.629339
Sum of electronic and thermal Energies= -1614.608073
Sum of electronic and thermal Enthalpies= -1614.607129
Sum of electronic and thermal Free Energies= -1614.679419

C	-2.87367400	-0.86512000	0.69740000
C	-1.72767300	-1.03808800	-0.30194400
C	-1.03800000	0.30906100	-0.56616700
C	-0.49689100	0.85047500	0.75305000
C	-1.61943200	1.08293000	1.74373300
C	-2.38424500	-0.23083400	1.99974100
H	-0.96732700	-1.75577500	0.05260700
H	-2.09859400	-1.43204500	-1.25934900
H	-3.55581500	-0.13650800	0.22106700
H	-1.22806200	1.47852300	2.69412200
H	-2.31036900	1.83185600	1.32845100
H	-1.74296100	-0.92786300	2.56239100
H	-3.22330400	-0.00567000	2.67241600
H	-1.82655000	1.01812300	-0.87832200
Pt	-4.05589300	-2.61293400	1.10888500
C	0.68558100	0.13062400	1.36130600
H	1.09532600	0.69467800	2.21043500
H	0.36282400	-0.83580800	1.76384800
H	1.49428100	-0.07395100	0.65288400
C	0.01243900	0.29401900	-1.67268100
H	-0.43849800	-0.10006000	-2.59246900
H	0.84375900	-0.38478400	-1.42746000
P	-2.12036400	-3.93279400	1.20409800
H	-1.01178200	-3.42162600	1.90309700
H	-2.21450600	-5.21090300	1.78300000
H	-1.52774500	-4.25048900	-0.03011000
P	-5.45957500	-4.53658200	1.60660700
H	-6.80750000	-4.32026900	1.94616600
H	-5.61574700	-5.50542500	0.59919400
H	-5.07071400	-5.35889900	2.68000800
P	-5.86875400	-1.14655200	0.95212100
H	-5.71230400	0.07446800	1.63102700
H	-6.15479000	-0.69549700	-0.34703900
H	-7.14262100	-1.54531600	1.39116700
C	0.51964600	1.71172200	-1.93190400
H	1.32374000	1.71820800	-2.67901200
H	-0.29132300	2.33153700	-2.33930000
C	1.06087000	2.36915000	-0.69079300
H	1.22905100	3.44358600	-0.80432200
H	1.95850400	1.88789800	-0.28585600
O	-0.00351000	2.27839900	0.36933800
H	0.26374400	2.76896100	1.17506400

A-I-6-c

Zero-point correction= 0.355106 (Hartree/Particle)
Thermal correction to Energy= 0.376318
Thermal correction to Enthalpy= 0.377262
Thermal correction to Gibbs Free Energy= 0.305376
Sum of electronic and zero-point Energies= -1614.626936
Sum of electronic and thermal Energies= -1614.605724
Sum of electronic and thermal Enthalpies= -1614.604780
Sum of electronic and thermal Free Energies= -1614.676666

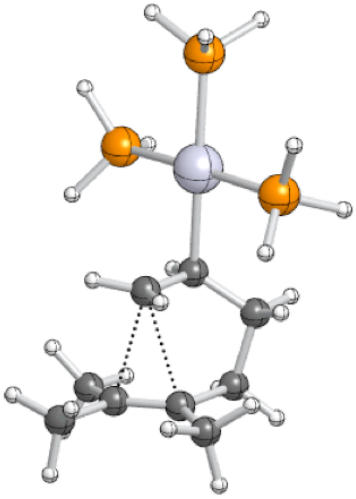
C	-2.88122800	-0.91621800	0.82624000
C	-1.77835400	-1.03696500	-0.21915500
C	-1.09650500	0.31491100	-0.50429800
C	-0.64740900	1.04370500	0.76289200
C	-1.61847300	0.94146200	1.92697300
C	-2.27514300	-0.42312800	2.13541400
H	-1.01450000	-1.75775200	0.11923200
H	-2.16751500	-1.42164400	-1.17349100
H	-3.55604800	-0.12031600	0.45736600
H	-1.13361500	1.30494200	2.84842900
H	-2.40172600	1.68610200	1.71239000
H	-1.53675900	-1.14753100	2.51660700
H	-3.02920900	-0.32313100	2.92876500
Pt	-4.11255800	-2.65218900	1.12708500
C	-0.20016700	2.47218200	0.55436000
H	0.19014700	2.91031400	1.48322800
H	0.54342300	2.60170300	-0.23705400
H	-1.07445100	3.06929600	0.26683500
C	0.04094800	0.17775900	-1.52572100
H	0.34026700	1.16512500	-1.90336800
H	-0.33375600	-0.37100900	-2.39889300
P	-2.22330800	-4.03643700	1.09938500
H	-1.09951100	-3.62492400	1.83742300
H	-2.35953200	-5.35478500	1.56956600
H	-1.63929800	-4.27183600	-0.15724100
P	-5.58954600	-4.55313400	1.49103200
H	-6.84883900	-4.31786400	2.07233100
H	-5.97736300	-5.29255400	0.35923800
H	-5.13606400	-5.59580500	2.32013900
P	-5.87596900	-1.11687700	1.13110200
H	-5.67115700	0.01939600	1.93336700
H	-6.15171700	-0.52013900	-0.11018100
H	-7.16151500	-1.51244700	1.53812300
C	1.25700000	-0.54857600	-0.95607900
H	1.03502100	-1.60451100	-0.75159100
H	2.08004300	-0.54672400	-1.68239000
C	1.76949700	0.10595300	0.29706000
H	2.16716700	1.11417300	0.13621500
H	2.49812400	-0.49827700	0.84471200
O	0.61222100	0.23019600	1.24661300
H	0.91544400	0.60254400	2.10073600
H	-1.86236800	0.98273300	-0.93612200



5-TS-exo

C2-C5: 2.18 (2.17) [2.23]
C2-C6: 2.23 (2.16) [2.26]

$\Delta G^{\ddagger}$ = 11.2 (12.1) [13.4]



6-TS-endo

C1-C5: 2.49 (2.42) [2.49]
C1-C6: 2.47 (2.38) [2.32]

$\Delta G^{\ddagger}$ = 6.8 (6.8) [7.6]

Method comparison for Pt(II)-catalyzed 5-TS-exo (left) and 6-TS-endo (right) at the M06/6-31G(d)-SDD level (M06/SDD-6-311++G(d,p) in parenthesis and MP2/6-31G(d)-SDD in brackets) in DCM with CPCM solvation model. Selected distances are in Ångstroms and free energies in kcal/mol.