Supporting Information for –

Computational Study of the Mechanism of Cyclometallation by Palladium Acetate

David L. Davies,[b] Steven M. A. Donald[a] and Stuart A. Macgregor.[a]

[a]School of Engineering and Physical Sciences, William Perkin Building, Heriot-Watt University, Edinburgh, EH14 4AS, UK.

[b]Department of Chemistry, University of Leicester, Leicester,LE1 7RH, UK

Contents:

Computational Details

Calculations were performed with the Gaussian 98 program[1] and used the BP86 functional. Pd and P centres were described using the Stuttgart RECPs and the associated basis sets.[2a] For P and Cl an extra set of polarisation functions was added (ζ = 0.387 and 0.640 respectively).[2b] 6-31G** basis sets were used for C, N, O and H atoms.[3c] The nature of all stationary points was confirmed via frequency analyses and, for transition states, via subsequent IRC calculations which showed they linked to the expected minima. All quoted energies include a correction for zero-point energies.

A value for the H/D kinetic isotope effect was computed for the activation barrier corresponding to species **1a** to **$TS_{1a\text{-}2a}$**. Free energies and frequency calculations were computed for these species and the corresponding deuterated systems based on $Pd(OAc)_2(Me_2NCD_2C_6D_5)$. All results are corrected to 298.15 K. The kinetic isotope effect was then computed according to the Eyring approach:

$$\frac{k_H}{k_D} = \exp\left[\Delta G_D^{act} - \Delta G_H^{act} / RT\right]$$

Using the values of ΔG_D^{act} = +14.33 and ΔG_H^{act} = +14.24 kcal/mol leads to a value of $\frac{k_H}{k_D} = 1.17$.

Free energies of activation were computed for **1a** to **$TS_{1a\text{-}2a}$** as well as their Me- and Cl-*para*-substituted analogues - **1a(Me)**, **$TS_{1a\text{-}2a}$(Me)** and **1a(Cl)**, **$TS_{1a\text{-}2a}$(Cl)** . Rate constants were then calculated according to the Eyring model:

$$k_X = A\exp\left[-\Delta G_X^{act} / RT\right] \; where \; A = \frac{RT}{Nh}$$

References:

(1) Gaussian 98, Revision A.11.4, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, V. G. Zakrzewski, J. A. Montgomery, Jr., R. E. Stratmann, J. C. Burant, S. Dapprich, J. M. Millam, A. D. Daniels, K. N. Kudin, M. C. Strain, O. Farkas, J. Tomasi, V. Barone, M. Cossi, R. Cammi, B. Mennucci, C. Pomelli, C. Adamo, S. Clifford, J. Ochterski, G. A. Petersson, P. Y. Ayala, Q. Cui, K. Morokuma, N. Rega, P. Salvador, J. J. Dannenberg, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. Cioslowski, J. V. Ortiz, A. G. Baboul, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. Gomperts, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, J. L. Andres, C. Gonzalez, M. Head-Gordon, E. S. Replogle, and J. A. Pople, Gaussian, Inc., Pittsburgh PA, 2002.

2 (a) Andrae, D.; Häusserman, U.; Dolg, M.; Stoll, H.; Preuss, H̃. *Theor. Chim. Acta* **1990**, *77*, 123. (b) Hehre, W. J.; Ditchfield, R.; Pople, J. A. *J. Chem. Phys*. **1972**, *56*, 2257 (c) Hariharan, P. C.; Pople, J. A. *Theor. Chim. Acta* **1973**, *28*, 213.

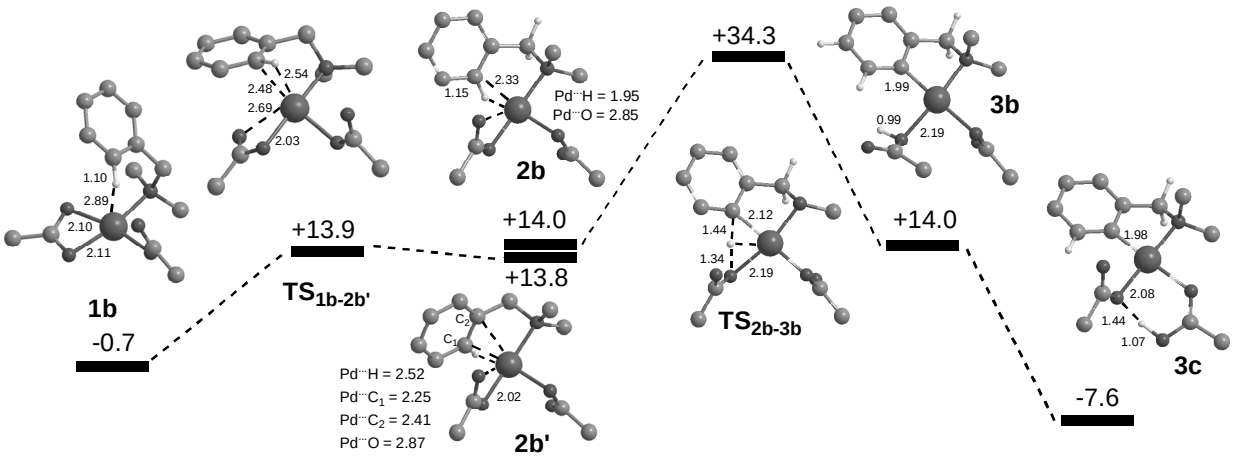

Figure S1. Computed reaction profile (kcal/mol) and key distances (Å) for the cyclometallation of $Pd(OAc)_2$(DMBA-H) via a 4-membered transition state. Methyl and non-participating phenyl hydrogens are omitted for clarity.
As shown, acetate displacement in 1b did not lead directly to 2b, but to a new intermediate, 2b' (E = +13.8) which features an η^2-arene moiety. Interconversion of 2b' to 2b is presumably facile, although we have not studied this process.

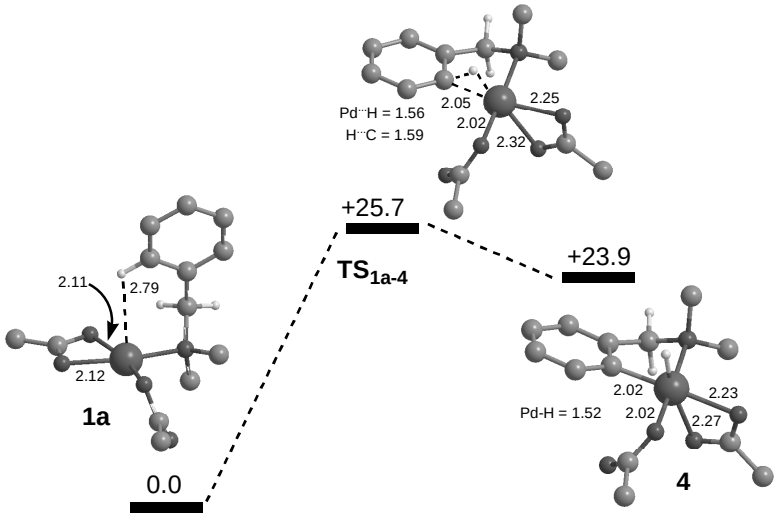

Figure S2. Computed reaction profile (kcal/mol) and key distances (Å) for the cyclometallation of $Pd(OAc)_2$(DMBA-H) via oxidative addition. Methyl and non-participating phenyl hydrogens are omitted for clarity.

Tables of computed Cartesian coordinates (Å) and energies (hartrees) with corrections for zero-point energies, temperatures effects to 298.15 K and free energies at 298.,15 K. Natural charges are also reported for selected stationary points. For transition states the value of the unique imaginary frequency is also given. Species are numbered according to the the main text or in Figures S1 and S2.

$Pd(OAc)_2$(DMBA-H), 1a, **(equivalent data for 1a-d_7 in parenthesis)** Energy = -990.563748 (-990.563748) Enthalpy (0K) = -990.264403 (-990.287034) Enthalpy (298.15 K) = -990.241346 (-990.262992) Free Energy = -990.318466 (-990.341830)	**Natural charges for 1a**
Pd 0.897708 0.282686 -0.003169	Pd1 0.74563
C -2.383467 0.944294 -0.541972	C2 -0.22304
C -2.556156 0.027881 0.516488	C3 -0.07304
C -3.704206 -0.790013 0.525743	C4 -0.22169
C -4.652122 -0.708861 -0.506514	C5 -0.24073
C -4.462236 0.196251 -1.562677	C6 -0.24061
C -3.327219 1.023893 -1.576813	C7 -0.24022
C -1.542762 -0.062061 1.638906	C8 -0.30252
N -0.289205 -0.849310 1.309740	N9 -0.42558
C 1.543467 2.669111 -0.050813	C10 0.77967
C 1.977933 4.108453 -0.035208	C11 -0.81954
O 0.725192 2.209706 0.844895	O12 -0.64791
O 1.987767 1.844019 -0.931234	O13 -0.60988
O 1.356366 -1.243677 -1.237000	O14 -0.65787
C 2.226274 -2.136044 -0.794210	C15 0.77064
C 2.767948 -3.021294 -1.917131	C16 -0.81067
O 2.594237 -2.269410 0.386731	O17 -0.65150
H 2.857146 4.215062 0.623682	H18 0.28054
H 2.263904 4.429667 -1.047467	H19 0.27528
H 1.173733 4.746359 0.361010	H20 0.27260
H 3.586258 -2.486494 -2.429181	H21 0.26860
H 3.168062 -3.953715 -1.493494	H22 0.25899
H 1.992312 -3.238225 -2.667551	H23 0.25869
C -0.636567 -2.216433 0.827250	C24 -0.52262
C 0.545534 -0.968880 2.547591	C25 -0.53699
H -3.859070 -1.493442 1.352670	H26 0.24092
H -5.538967 -1.350674 -0.483634	H27 0.24891
H -5.200074 0.261442 -2.369144	H28 0.25032
H -3.178181 1.737947 -2.393336	H29 0.25318
H -1.500907 1.593089 -0.548162	H30 0.25607
H -2.005295 -0.551620 2.520359	H31 0.24234
H -1.201681 0.940654 1.945715	H32 0.28035
H -0.009152 -1.540285 3.319206	H33 0.22693
H 1.476371 -1.485948 2.271736	H34 0.29021
H 0.769912 0.038016 2.931081	H35 0.25743
H -1.293184 -2.710204 1.570322	H36 0.22518
H -1.154665 -2.148819 -0.137742	H37 0.27092
H 0.296324 -2.784078 0.720583	H38 0.27098

$Pd(OAc)_2$(DMBA-H), $TS_{1a\text{-}2a}$. **(equivalent data for $TS_{1a\text{-}2a}$-d_7 in parenthesis)** Energy = -990.541727 (-990.541727) Enthalpy (0K) = -990.243711 (-990.266248) Enthalpy (298.15 K) = -990.221172 (-990.242727) Free Energy = -990.295781 (-990.318999) Nimag = 1, -79.9 cm^{-1} (-81.6 cm^{-1})	**Natural charges for $TS_{1a\text{-}2a}$**
Pd 0.387414 0.062963 -0.021635	Pd1 0.75233
C -2.058405 0.747365 0.332450	C2 -0.30662
C -2.551330 -0.568728 0.503301	C3 -0.05998
C -3.722218 -0.960332 -0.164411	C4 -0.23978
C -4.399259 -0.049769 -0.996147	C5 -0.22244
C -3.895878 1.248749 -1.180825	C6 -0.23551
C -2.724471 1.648687 -0.517995	C7 -0.20225
C -1.716276 -1.519606 1.325072	C8 -0.30427
N -0.403127 -1.793111 0.631157	N9 -0.45322
C 1.094911 2.618851 0.427621	C10 0.77310
C 1.816478 3.947614 0.303548	C11 -0.81364
O 0.452441 2.294290 1.458005	O12 -0.65258
O 1.213347 1.816478 -0.605627	O13 -0.61917
O 1.799151 -0.926092 -1.128023	O14 -0.64985
C 2.987308 -0.958594 -0.535308	C15 0.76878
C 4.085386 -1.438986 -1.490129	C16 -0.80444
O 3.221777 -0.635844 0.635627	O17 -0.62133
H 2.849974 3.823571 0.670359	H18 0.27450
H 1.865442 4.277495 -0.745322	H19 0.26169
H 1.317696 4.705791 0.925120	H20 0.26258
H 4.442112 -0.573664 -2.074267	H21 0.26962
H 4.927120 -1.843282 -0.909610	H22 0.25905
H 3.710166 -2.190255 -2.201629	H23 0.25349
C -0.609609 -2.683676 -0.547114	C24 -0.52352
C 0.546940 -2.428008 1.589971	C25 -0.52047
H -4.106420 -1.979152 -0.038280	H26 0.24981
H -5.316777 -0.359597 -1.506878	H27 0.25330
H -4.421946 1.951210 -1.835250	H28 0.25516
H -2.330634 2.661583 -0.644157	H29 0.26414
H -1.235038 1.134698 0.977364	H30 0.27703
H -2.232959 -2.481578 1.512561	H31 0.24852
H -1.465240 -1.067233 2.300435	H32 0.27602
H 0.125260 -3.381551 1.966202	H33 0.22574
H 1.502594 -2.610273 1.082482	H34 0.27486
H 0.729011 -1.739842 2.427908	H35 0.26765
H -0.956146 -3.681093 -0.210311	H36 0.22384
H -1.361847 -2.235739 -1.211913	H37 0.26115
H 0.343303 -2.767658 -1.087751	H38 0.27671

$Pd(OAc)_2$(DMBA-H), agostic, 2a. Energy = -990.544416 Enthalpy (0K) = -990.246945 Enthalpy (298.15 K) = -990.223795 Free Energy = -990.299792	**Natural charges for 2a**
Pd 0.334688 -0.040474 -0.120828	Pd1 0.72702
C -1.818711 0.577969 0.310250	C2 -0.33931
C -2.473871 -0.665830 0.512961	C3 -0.04095
C -3.782719 -0.841318 0.042578	C4 -0.23839
C -4.444956 0.213889 -0.612694	C5 -0.21477
C -3.794751 1.441814 -0.819098	C6 -0.24051
C -2.482660 1.626358 -0.357060	C7 -0.18389
C -1.659637 -1.774094 1.132336	C8 -0.29930
N -0.407321 -1.981949 0.322058	N9 -0.45080
C 0.922543 2.693422 0.349743	C10 0.77776
C 1.727297 3.965230 0.089088	C11 -0.80447
O 0.187963 2.577469 1.350491	O12 -0.65044
O 1.118769 1.770025 -0.572644	O13 -0.63215
O 1.997600 -0.874094 -0.951384	O14 -0.66175
C 3.071984 -0.757081 -0.175054	C15 0.76890
C 4.357926 -1.134747 -0.915098	C16 -0.80676
O 3.069856 -0.379012 1.002288	O17 -0.62015
H 2.727012 3.842446 0.539658	H18 0.27106
H 1.861059 4.145139 -0.987997	H19 0.25806
H 1.232249 4.822305 0.568210	H20 0.25770
H 4.705008 -0.256327 -1.485520	H21 0.26922
H 5.134771 -1.411781 -0.187936	H22 0.25862
H 4.191525 -1.952827 -1.632754	H23 0.25243
C -0.709639 -2.668682 -0.966260	C24 -0.52398
C 0.582409 -2.778212 1.100228	C25 -0.51627
H -4.287446 -1.804488 0.179289	H26 0.25092
H -5.470226 0.070563 -0.969206	H27 0.25470
H -4.314277 2.257119 -1.332431	H28 0.25800
H -1.969181 2.583536 -0.478910	H29 0.27561
H -0.920221 0.917349 0.954231	H30 0.28964
H -2.221869 -2.726203 1.203143	H31 0.24742
H -1.331401 -1.492186 2.148698	H32 0.27846
H 0.140128 -3.751024 1.393269	H33 0.22505
H 1.465493 -2.944566 0.470144	H34 0.26917
H 0.887450 -2.210506 1.990294	H35 0.27169
H -1.052581 -3.705567 -0.775381	H36 0.22587
H -1.493631 -2.113769 -1.501113	H37 0.26101
H 0.206942 -2.681157 -1.573527	H38 0.27559

Pd(OAc)(OAc)$_2$(DMBA-H), TS$_{2a-3a}$. Energy = -990.540707 Enthalpy (0K) = -990.246758 Enthalpy (298.15 K) = -990.224310 Free Energy = -990.298371 Nimag =1, -706.95 cm^{-1}	**Natural charges for TS$_{2a-3a}$**
Pd 0.355368 -0.046929 -0.269347	Pd1 0.71211
C -1.695193 0.452638 0.064154	C2 -0.36449
C -2.347677 -0.701657 0.590243	C3 -0.05291
C -3.726454 -0.887639 0.415624	C4 -0.23595
C -4.483676 0.071355 -0.280911	C5 -0.22633
C -3.853175 1.198748 -0.832046	C6 -0.24914
C -2.472264 1.384880 -0.664014	C7 -0.19054
C -1.449290 -1.744992 1.201635	C8 -0.29786
N -0.287203 -1.983108 0.266580	N9 -0.43836
C 0.659309 2.675055 0.341590	C10 0.79760
C 1.350147 4.025059 0.381526	C11 -0.79902
O -0.212043 2.393009 1.227199	O12 -0.62605
O 1.029546 1.872013 -0.603662	O13 -0.61899
O 2.162849 -0.769018 -0.933721	O14 -0.68819
C 3.131551 -0.575914 -0.050713	C15 0.76839
C 4.521095 -0.862674 -0.624863	C16 -0.80942
O 2.968719 -0.189478 1.117928	O17 -0.63882
H 2.243771 3.932836 1.022285	H18 0.28055
H 1.678427 4.325403 -0.623573	H19 0.26629
H 0.685607 4.782178 0.821322	H20 0.26477
H 4.868770 0.029320 -1.173964	H21 0.26596
H 5.228045 -1.068412 0.191967	H22 0.25696
H 4.500253 -1.702007 -1.337332	H23 0.25252
C -0.723898 -2.724125 -0.951640	C24 -0.52219
C 0.784775 -2.748821 0.962571	C25 -0.52547
H -4.211871 -1.788329 0.809503	H26 0.24913
H -5.561887 -0.072154 -0.406212	H27 0.25296
H -4.439646 1.936755 -1.389388	H28 0.25499
H -1.988594 2.277873 -1.072695	H29 0.26119
H -0.793635 1.161730 0.736667	H30 0.34092
H -1.972244 -2.702689 1.396633	H31 0.24586
H -1.012274 -1.388695 2.151784	H32 0.28000
H 0.377072 -3.708002 1.338109	H33 0.22707
H 1.594173 -2.940047 0.245738	H34 0.26876
H 1.185085 -2.144082 1.788091	H35 0.27690
H -1.045761 -3.749205 -0.677665	H36 0.22708
H -1.558618 -2.190652 -1.427103	H37 0.26331
H 0.122761 -2.775018 -1.651160	H38 0.27042

Pd(OAc)(HOAc)(DMBA), 3a Energy = -990.582894 Enthalpy (0K) = -990.285391 Enthalpy (298.15 K) = -990.262769 Free Energy = -990.337613	**Natural charges for 3a**
Pd 0.161345 -0.094090 -0.294586	Pd1 0.56968
C -1.754481 0.331010 -0.055967	C2 -0.12060
C -2.524524 -0.716255 0.513912	C3 -0.12145
C -3.915162 -0.583667 0.667499	C4 -0.24403
C -4.551723 0.601643 0.263027	C5 -0.25358
C -3.795953 1.640422 -0.305231	C6 -0.23761
C -2.404326 1.507106 -0.471124	C7 -0.27278
C -1.745943 -1.926441 0.957162	C8 -0.28542
N -0.525256 -2.068812 0.076534	N9 -0.44641
C 1.199072 2.607400 0.167993	C10 0.81264
C 1.085508 4.112247 -0.026105	C11 -0.80653
O 1.875678 2.176841 1.154697	O12 -0.68324
O 0.559262 1.888693 -0.691784	O13 -0.64102
O 2.195938 -0.811046 -0.679633	O14 -0.67638
C 3.225401 -0.617532 0.027361	C15 0.82328
C 4.487022 -1.409682 -0.260477	C16 -0.81039
O 3.326847 0.228403 1.009489	O17 -0.67950
H 1.989605 4.615886 0.344996	H18 0.26284
H 0.908047 4.357703 -1.083202	H19 0.26281
H 0.223961 4.478542 0.559270	H20 0.27065
H 5.235999 -0.739931 -0.716206	H21 0.27494
H 4.919661 -1.786996 0.679446	H22 0.26898
H 4.279669 -2.238699 -0.950482	H23 0.25984
C -0.910670 -2.671575 -1.234286	C24 -0.52209
C 0.483888 -2.936209 0.738328	C25 -0.51317
H -4.501145 -1.401958 1.104329	H26 0.24251
H -5.634863 0.708942 0.382978	H27 0.24565
H -4.293034 2.561997 -0.629590	H28 0.24462
H -1.819438 2.313520 -0.924544	H29 0.26181
H 2.524787 1.000351 1.057725	H30 0.50467
H -2.334114 -2.867180 0.933571	H31 0.23971
H -1.369947 -1.791674 1.987920	H32 0.26686
H 0.062055 -3.944680 0.921466	H33 0.22767
H 1.365966 -3.014844 0.087970	H34 0.26208
H 0.780610 -2.482301 1.695464	H35 0.25722
H -1.270620 -3.710374 -1.084361	H36 0.22352
H -1.707500 -2.065231 -1.686377	H37 0.26957
H -0.035239 -2.677199 -1.899849	H38 0.26261

$Pd(OAc)_2$(DMBA-H), 1b Energy = -990.564780 Enthalpy (0K) = -990.265572 Enthalpy (298.15 K) = -990.243329 Free Energy = -990.318154	**Natural charge for 1b**
Pd -0.974416 0.354769 0.362816	Pd1 0.71626
N 0.207349 -0.913189 1.553190	N2 -0.41255
C 0.989801 -0.058656 2.490537	C3 -0.52644
C -0.680575 -1.819458 2.341068	C4 -0.52417
C 1.127567 -1.765337 0.691349	C5 -0.30952
H 0.468290 -2.309014 -0.003191	H6 0.28740
H 1.612627 -2.496346 1.370928	H7 0.23757
C 2.181453 -0.992416 -0.072364	C8 -0.07378
C 3.489102 -0.868126 0.440155	C9 -0.24206
H 3.744043 -1.339440 1.397410	H10 0.24201
C 4.470433 -0.157301 -0.268146	C11 -0.25072
H 5.482933 -0.070227 0.139969	H12 0.25033
C 4.152067 0.431780 -1.502608	C13 -0.25151
H 4.916860 0.983879 -2.059385	H14 0.25148
C 2.856076 0.296387 -2.028238	C15 -0.24811
H 2.609723 0.736825 -3.000205	H16 0.25597
C 1.872807 -0.414649 -1.322405	C17 -0.22740
H 0.865611 -0.554728 -1.735544	H18 0.28734
O -2.201196 -1.192842 -0.092760	O19 -0.66093
C -2.038491 -1.742116 -1.288955	C20 0.76638
O -1.085751 -1.537934 -2.056641	O21 -0.63849
C -3.193627 -2.672209 -1.662332	C22 -0.81125
H -2.844527 -3.424519 -2.384529	H23 0.25971
H -3.629712 -3.158880 -0.776713	H24 0.25462
H -3.987159 -2.072895 -2.141071	H25 0.26921
O -1.885773 1.975017 -0.629482	O26 -0.59026
C -1.017232 2.771955 -0.109746	C27 0.77357
O -0.124787 2.254533 0.672283	O28 -0.62120
C -1.056434 4.250993 -0.374791	C29 -0.81801
H -1.745268 4.731729 0.341351	H30 0.27848
H -1.431913 4.442665 -1.391043	H31 0.27666
H -0.055942 4.688494 -0.243323	H32 0.27245
H 1.623873 -0.693646 3.140159	H33 0.22735
H 1.622956 0.634493 1.921821	H34 0.27679
H 0.289670 0.517868 3.112182	H35 0.26183
H -1.303138 -2.399921 1.647820	H36 0.27541
H -0.067386 -2.489374 2.974926	H37 0.22556
H -1.337487 -1.209299 2.978214	H38 0.26003

$Pd(OAc)_2$(DMBA-H), $TS_{1b-2b'}$ Energy = -990.540195 Enthalpy (0K) = -990.242273 Enthalpy (298.15 K) = -990.219595 Free Energy = -990.294455 Nimag =1, -28.60 cm^{-1}	**Natural charges for $TS_{1b-2b'}$**
Pd -0.340788 0.113333 0.083954	Pd1 0.78754
N -0.576422 -1.933655 0.566740	N2 -0.43809
C -0.234381 -2.025474 2.014259	C3 -0.53281
C -1.922384 -2.515318 0.314673	C4 -0.52313
C 0.472366 -2.601907 -0.279595	C5 -0.29924
H -0.004258 -2.863249 -1.238939	H6 0.27481
H 0.812207 -3.537439 0.206302	H7 0.24758
C 1.607226 -1.620481 -0.509524	C8 -0.08084
C 2.819282 -1.691048 0.206346	C9 -0.23720
H 2.971162 -2.495784 0.934646	H10 0.25188
C 3.829365 -0.746587 -0.018400	C11 -0.21548
H 4.767782 -0.810731 0.541329	H12 0.25709
C 3.637660 0.288058 -0.953828	C13 -0.23266
H 4.429592 1.025121 -1.119981	H14 0.25756
C 2.445531 0.366867 -1.679978	C15 -0.20600
H 2.295858 1.158533 -2.419819	H16 0.26600
C 1.417517 -0.581720 -1.466287	C17 -0.31980
H 0.554586 -0.607412 -2.145078	H18 0.29285
O -2.312337 0.558693 0.491650	O19 -0.64232
C -3.069453 0.432363 -0.585667	C20 0.75729
O -2.720336 -0.064357 -1.669683	O21 -0.63839
C -4.476580 0.999439 -0.374382	C22 -0.80792
H -5.183283 0.500030 -1.053190	H23 0.25764
H -4.805828 0.898533 0.670829	H24 0.25505
H -4.458335 2.075257 -0.619176	H25 0.26944
O -0.035299 2.092722 -0.235274	O26 -0.62519
C 0.860211 2.454055 0.662005	C27 0.75547
O 1.414143 1.642507 1.436227	O28 -0.64401
C 1.144212 3.948284 0.700450	C29 -0.81528
H 0.358346 4.449811 1.291071	H30 0.26918
H 1.127129 4.381443 -0.311923	H31 0.25985
H 2.116173 4.132591 1.180950	H32 0.25944
H -0.245750 -3.084729 2.342896	H33 0.22810
H 0.761177 -1.590408 2.185736	H34 0.26921
H -0.974307 -1.450303 2.589317	H35 0.27269
H -2.207111 -2.314855 -0.727449	H36 0.27762
H -1.911138 -3.602865 0.524859	H37 0.22553
H -2.645618 -2.016997 0.974770	H38 0.26653

$Pd(OAc)_2$(DMBA-H), η^2-arene, 2b' Energy = -990.540941212 Enthalpy (0K) = -990.243120 Enthalpy (298.15 K) = -990.219485 Free Energy = -990.297151	**Natural charges for 2b'**
Pd -0.246798 -0.028936 -0.076700	Pd1 0.76193
N -0.730970 -2.032830 0.414666	N2 -0.44209
C -0.770982 -2.081746 1.902740	C3 -0.52926
C -1.985985 -2.579883 -0.162183	C4 -0.51286
C 0.498303 -2.701634 -0.131275	C5 -0.29320
H 0.242523 -3.134437 -1.112536	H6 0.26853
H 0.826278 -3.523292 0.532947	H7 0.25253
C 1.557945 -1.617807 -0.293650	C8 -0.09876
C 2.636581 -1.480286 0.618033	C9 -0.21900
H 2.691670 -2.140432 1.490498	H10 0.25080
C 3.625559 -0.522164 0.398981	C11 -0.20449
H 4.452042 -0.422388 1.109171	H12 0.25808
C 3.563918 0.324051 -0.731487	C13 -0.23400
H 4.346125 1.072520 -0.891668	H14 0.25862
C 2.519797 0.201208 -1.645693	C15 -0.19781
H 2.473563 0.844338 -2.528815	H16 0.26700
C 1.501368 -0.769200 -1.444578	C17 -0.32398
H 0.800053 -0.985650 -2.259828	H18 0.28740
O -2.064147 0.662679 0.585666	O19 -0.64161
C -2.946530 0.709001 -0.402389	C20 0.75540
O -2.782350 0.247592 -1.542394	O21 -0.63328
C -4.231405 1.437323 0.001681	C22 -0.81037
H -5.066888 1.093573 -0.625449	H23 0.25868
H -4.463810 1.296020 1.068219	H24 0.25625
H -4.088048 2.517998 -0.169427	H25 0.27008
O 0.246411 1.900845 -0.450443	O26 -0.62676
C 0.851448 2.422718 0.605812	C27 0.75630
O 1.174230 1.790196 1.625120	O28 -0.63800
C 1.095634 3.924622 0.460996	C29 -0.81307
H 0.184771 4.466215 0.768984	H30 0.26752
H 1.312121 4.200652 -0.582659	H31 0.25619
H 1.922269 4.230389 1.119071	H32 0.25832
H -0.934671 -3.122893 2.247184	H33 0.22794
H 0.175825 -1.696024 2.308232	H34 0.26537
H -1.588276 -1.433409 2.250612	H35 0.27772
H -1.994991 -2.406763 -1.246478	H36 0.27166
H -2.070981 -3.661129 0.065583	H37 0.22489
H -2.837125 -2.042150 0.276364	H38 0.26736

$Pd(OAc)_2$(DMBA-H), agostic, 2b Energy = -990.539706391 Enthalpy (0K) = -990.242107 Enthalpy (298.15 K) = -990.218713 Free Energy = -990.295958	**Natural charges for 2b**
Pd -0.376288 0.018232 -0.148868	Pd1 0.72372
N 0.120325 -1.987119 0.347845	N2 -0.44509
C 0.395740 -1.982372 1.814683	C3 -0.53720
C -0.960330 -2.964264 0.037843	C4 -0.52376
C 1.363955 -2.327274 -0.428297	C5 -0.30450
H 1.039193 -2.551439 -1.460211	H6 0.27793
H 1.827484 -3.241381 -0.007323	H7 0.24999
C 2.310583 -1.149110 -0.414588	C8 -0.04134
C 3.590304 -1.196427 0.155034	C9 -0.23787
H 3.971735 -2.138863 0.563762	H10 0.25311
C 4.379915 -0.032423 0.210782	C11 -0.20528
H 5.381425 -0.079984 0.650666	H12 0.25660
C 3.886251 1.190535 -0.273762	C13 -0.23734
H 4.501022 2.093417 -0.208640	H14 0.26005
C 2.602543 1.254511 -0.834612	C15 -0.17392
H 2.201161 2.197935 -1.213767	H16 0.27156
C 1.821179 0.085463 -0.916409	C17 -0.33392
H 0.922949 0.082460 -1.603726	H18 0.27368
O -2.256309 -0.193649 0.643731	O19 -0.64713
C -3.143591 -0.486284 -0.299220	C20 0.75447
O -2.882103 -0.788986 -1.472297	O21 -0.62642
C -4.583223 -0.393671 0.214923	C22 -0.80826
H -5.232181 -1.050813 -0.382233	H23 0.25928
H -4.654651 -0.645788 1.283821	H24 0.25577
H -4.931231 0.646017 0.090400	H25 0.27062
O -0.813265 1.944062 -0.576360	O26 -0.63397
C -0.409878 2.722638 0.418877	C27 0.75921
O 0.245478 2.328863 1.398183	O28 -0.63103
C -0.858725 4.172775 0.255553	C29 -0.81289
H -1.882187 4.275911 0.655250	H30 0.26797
H -0.882294 4.472082 -0.803739	H31 0.25727
H -0.192679 4.834171 0.828832	H32 0.25880
H 0.664174 -3.002990 2.155198	H33 0.22945
H 1.219032 -1.287452 2.032640	H34 0.27095
H -0.508555 -1.639330 2.337460	H35 0.27783
H -1.258774 -2.854152 -1.013407	H36 0.27677
H -0.610823 -3.994834 0.246305	H37 0.22617
H -1.826577 -2.730713 0.670832	H38 0.26874

$Pd(OAc)_2$(DMBA-H) TS_{2b-3b} Energy = -990.502455 Enthalpy (0K) = -990.209708 Enthalpy (298.15 K) = -990.186708 Free Energy = -990.262627 Nimag =1, -1223.20 cm^{-1}	**Natural charges for TS_{2b-3b}**
Pd -0.391031 -0.026875 0.152839	Pd1 0.66868
N 0.181186 -2.037389 0.350959	N2 -0.41137
C 0.771261 -2.304204 1.695098	C3 -0.52556
C -0.918274 -3.006747 0.085967	C4 -0.52567
C 1.227762 -2.128442 -0.739766	C5 -0.29960
H 0.675872 -2.070748 -1.694512	H6 0.28780
H 1.728845 -3.116703 -0.684890	H7 0.24654
C 2.203553 -0.985607 -0.589920	C8 -0.06517
C 3.590333 -1.180172 -0.669597	C9 -0.23676
H 3.987408 -2.169471 -0.925995	H10 0.25087
C 4.473933 -0.118426 -0.403707	C11 -0.22399
H 5.554405 -0.274386 -0.486932	H12 0.25384
C 3.968030 1.122001 0.007299	C13 -0.23641
H 4.651446 1.941402 0.253813	H14 0.25628
C 2.579743 1.317989 0.122845	C15 -0.22416
H 2.192452 2.278109 0.476489	H16 0.27050
C 1.672648 0.287627 -0.218765	C17 -0.32745
H 0.609542 1.160233 -0.657373	H18 0.39322
O -2.360889 -0.317622 0.641881	O19 -0.68262
C -3.124052 -0.642549 -0.388979	C20 0.76033
O -2.705780 -0.967981 -1.514971	O21 -0.64837
C -4.618242 -0.563516 -0.073430	C22 -0.81234
H -5.183977 -1.182719 -0.784708	H23 0.25806
H -4.827704 -0.874605 0.961791	H24 0.25659
H -4.951938 0.483270 -0.178985	H25 0.26569
O -0.453548 1.973679 -0.732460	O26 -0.70423
C -0.478785 2.972911 0.192162	C27 0.79104
O -0.087543 2.861507 1.349743	O28 -0.57727
C -1.071223 4.245341 -0.394232	C29 -0.81491
H -2.124692 4.063942 -0.664882	H30 0.27667
H -0.543515 4.524748 -1.320277	H31 0.26915
H -1.011161 5.058175 0.342055	H32 0.26630
H 1.113239 -3.357164 1.751858	H33 0.23123
H 1.619232 -1.629119 1.870599	H34 0.26853
H 0.000757 -2.126702 2.458976	H35 0.26804
H -1.418333 -2.733054 -0.854026	H36 0.28367
H -0.502350 -4.032497 0.041886	H37 0.22776
H -1.648429 -2.938659 0.904435	H38 0.26509

Pd(OAc)(HOAc)(DMBA), 3b Energy = -990.541058208 Enthalpy (0K) = -990.242082 Enthalpy (298.15 K) = -990.219028 Free Energy = -990.295031	**Natural charges for 3b**
Pd -0.247417 -0.045694 0.069112	Pd1 0.60557
N 0.481094 -1.937222 0.588983	N2 -0.41052
C 0.882180 -1.943257 2.028096	C3 -0.51949
C -0.514843 -3.017893 0.343242	C4 -0.52252
C 1.694848 -2.134641 -0.294509	C5 -0.29097
H 1.304341 -2.386366 -1.296738	H6 0.27902
H 2.280253 -3.002619 0.073137	H7 0.24382
C 2.477851 -0.847313 -0.322913	C8 -0.11296
C 3.868460 -0.777620 -0.499460	C9 -0.23637
H 4.456587 -1.695966 -0.618682	H10 0.24632
C 4.507051 0.475147 -0.524172	C11 -0.25623
H 5.590934 0.534048 -0.666859	H12 0.24991
C 3.754333 1.644975 -0.342803	C13 -0.23927
H 4.252110 2.621182 -0.335838	H14 0.25045
C 2.359434 1.575253 -0.148483	C15 -0.31240
H 1.814446 2.509257 0.046779	H16 0.24306
C 1.697599 0.330048 -0.159058	C17 -0.17702
H 0.078190 2.281658 -1.036534	H18 0.53742
O -2.307561 -0.457433 0.396363	O19 -0.75221
C -2.898491 -0.981356 -0.659217	C20 0.76526
O -2.307371 -1.367879 -1.687442	O21 -0.65670
C -4.422725 -1.075379 -0.539448	C22 -0.81428
H -4.821848 -1.765401 -1.296793	H23 0.25749
H -4.722930 -1.400004 0.469832	H24 0.25271
H -4.866141 -0.078076 -0.707813	H25 0.25605
O -0.770614 1.952864 -0.655349	O26 -0.70956
C -1.203707 2.967078 0.241252	C27 0.79034
O -0.506885 3.946473 0.410622	O28 -0.52429
C -2.559553 2.665898 0.807783	C29 -0.83719
H -2.701259 1.579768 0.950237	H30 0.30242
H -3.315014 3.004666 0.075921	H31 0.28479
H -2.695982 3.234530 1.737692	H32 0.27616
H 1.249215 -2.951409 2.308134	H33 0.22819
H 1.676301 -1.201314 2.187769	H34 0.26783
H 0.008376 -1.685626 2.643361	H35 0.26268
H -0.901489 -2.920304 -0.681268	H36 0.28309
H -0.036749 -4.003850 0.505615	H37 0.22678
H -1.350974 -2.889539 1.044578	H38 0.26263

Pd(OAc)(HOAc)(DMBA), 3c Energy = -990.574762570 Enthalpy (0K) = -990.276533 Enthalpy (298.15 K) = -990.253666 Free Energy = -990.329242	**Natural charges for 3c**
Pd -0.178114 -0.227442 -0.030758	Pd1 0.55039
N 0.834926 -2.041982 0.345378	N2 -0.43367
C 1.114443 -2.093062 1.812605	C3 -0.52715
C 0.059073 -3.245565 -0.052548	C4 -0.51897
C 2.132227 -1.974605 -0.424931	C5 -0.28850
H 2.845478 -2.724339 -0.024023	H6 0.24186
H 1.891144 -2.263997 -1.464321	H7 0.26614
C 2.650032 -0.561703 -0.373218	C8 -0.12233
C 4.011965 -0.232593 -0.487402	C9 -0.23946
H 4.762737 -1.026923 -0.583286	H10 0.24148
C 4.406489 1.114797 -0.483477	C11 -0.25139
H 5.466192 1.375490 -0.573631	H12 0.24583
C 3.437726 2.123101 -0.351581	C13 -0.24247
H 3.743284 3.175523 -0.337638	H14 0.24676
C 2.074340 1.798384 -0.223880	C15 -0.26633
H 1.337728 2.594229 -0.093975	H16 0.26136
C 1.665962 0.452877 -0.238979	C17 -0.10707
O -2.188867 -1.179335 0.133076	O18 -0.65354
C -3.239357 -0.725973 -0.389738	C19 0.81539
O -3.334104 0.444996 -0.980218	O20 -0.67946
C -4.521233 -1.528386 -0.376982	C21 -0.81279
H -5.294820 -0.978558 0.184171	H22 0.27662
H -4.893412 -1.650110 -1.407296	H23 0.27534
H -4.355740 -2.510839 0.083738	H24 0.26623
O -1.161904 1.558560 -0.439876	O25 -0.73759
C -1.261918 2.462237 0.558769	C26 0.77046
C -2.153857 3.644264 0.184381	C27 -0.81787
H -1.752337 4.155157 -0.706445	H28 0.26576
H -2.209627 4.349233 1.024963	H29 0.26413
H -3.168451 3.294627 -0.072416	H30 0.25976
O -0.688995 2.365421 1.641802	O31 -0.58156
H -2.419876 0.976139 -0.844070	H32 0.51409
H -0.140233 -3.205280 -1.133513	H33 0.25625
H 0.629596 -4.165359 0.186119	H34 0.22928
H -0.899629 -3.248440 0.484194	H35 0.26905
H 1.640695 -3.036500 2.065451	H36 0.22548
H 1.737632 -1.231863 2.089404	H37 0.27491
H 0.164011 -2.041763 2.363405	H38 0.26360

$Pd(OAc)_2(DMBA)(H)$, TS_{1-4} Energy = -990.517746803 Enthalpy (0K) = -990.223412 Enthalpy (298.15 K) = -990.200741 Free Energy = -990.274784 Nimag =1, -582.89 cm^{-1}	**Natural charges for TS_{1a-4}**
Pd 0.371742 -0.102568 -0.395911	Pd1 0.80186
O 0.133292 2.471607 1.255502	O2 -0.59223
O 0.911666 1.799982 -0.796717	O3 -0.61308
O 2.479460 -0.705398 -0.882399	O4 -0.68142
O 2.014786 -0.194741 1.237406	O5 -0.67905
C 0.730622 2.674404 0.197774	C6 0.77126
C 2.861447 -0.492560 0.327227	C7 0.76640
C 1.401176 4.013643 -0.130978	C8 -0.80047
C 4.340685 -0.569251 0.662732	C9 -0.80707
N -0.255999 -2.131653 -0.056166	N10 -0.43876
C -2.294808 -0.813808 0.436108	C11 -0.09530
C -3.658582 -0.707513 0.754641	C12 -0.23633
C -4.364404 0.467407 0.446758	C13 -0.23790
C -3.707308 1.539017 -0.179790	C14 -0.23063
C -2.345487 1.443067 -0.509151	C15 -0.22162
C -1.633549 0.271205 -0.194610	C16 -0.19106
C -1.449493 -1.992240 0.854267	C17 -0.29281
H 0.896387 4.815799 0.426772	H18 0.25928
H 2.454146 3.970342 0.195583	H19 0.26424
H 1.390142 4.225828 -1.210563	H20 0.25459
H 4.787893 0.427568 0.507227	H21 0.27401
H 4.486398 -0.846804 1.716977	H22 0.26115
H 4.856430 -1.278897 -0.001035	H23 0.25968
C -0.654468 -2.759960 -1.350360	C24 -0.52121
C 0.791211 -2.967569 0.592371	C25 -0.52130
H -4.167455 -1.538559 1.257445	H26 0.25000
H -5.427976 0.543651 0.694153	H27 0.25340
H -4.256571 2.455731 -0.418418	H28 0.25468
H -1.833432 2.271236 -1.005425	H29 0.27111
H -0.745305 -0.010070 -1.482981	H30 0.15394
H -2.015795 -2.945319 0.876492	H31 0.24639
H -1.042665 -1.814758 1.866390	H32 0.28282
H 0.377841 -3.966490 0.830743	H33 0.23005
H 1.637299 -3.068516 -0.101593	H34 0.26823
H 1.136092 -2.463119 1.505064	H35 0.27446
H -0.954523 -3.812271 -1.179401	H36 0.23224
H -1.501581 -2.207467 -1.781590	H37 0.25938
H 0.198656 -2.724851 -2.043038	H38 0.27112

$Pd(OAc)_2(DMBA)(H)$, 4 Energy = -990.522637995 Enthalpy (0K) = -990.226265 Enthalpy (298.15 K) = -990.203629 Free Energy = -990.277357	**Natural charges for 4**
Pd 0.370437 -0.129755 -0.503795	Pd1 0.82882
O 0.367359 2.456061 1.203321	O2 -0.60146
O 1.026090 1.746836 -0.879903	O3 -0.62099
O 2.489559 -0.770647 -0.747437	O4 -0.66889
O 1.717402 -0.359675 1.302817	O5 -0.67868
C 0.932297 2.625947 0.123576	C6 0.76885
C 2.694317 -0.631866 0.515130	C7 0.76801
C 1.662484 3.925414 -0.240242	C8 -0.80454
C 4.098679 -0.761008 1.068097	C9 -0.81025
N -0.400922 -2.122987 -0.177771	N10 -0.43325
C -2.221740 -0.664029 0.586469	C11 -0.11500
C -3.568690 -0.486075 0.950894	C12 -0.23026
C -4.228359 0.709614 0.626192	C13 -0.24204
C -3.548233 1.718585 -0.075547	C14 -0.23298
C -2.203273 1.547598 -0.451398	C15 -0.25625
C -1.540545 0.365613 -0.098937	C16 -0.08606
C -1.421148 -1.898450 0.913951	C17 -0.29455
H 1.332717 4.725064 0.437945	H18 0.26081
H 2.748571 3.776361 -0.118128	H19 0.26422
H 1.482069 4.209176 -1.288419	H20 0.25857
H 4.570560 0.236598 1.068850	H21 0.27660
H 4.074181 -1.123906 2.106356	H22 0.26349
H 4.706774 -1.425816 0.436926	H23 0.26288
C -1.061635 -2.647073 -1.410327	C24 -0.51626
C 0.630797 -3.096284 0.272398	C25 -0.51485
H -4.098486 -1.281602 1.488615	H26 0.24589
H -5.276264 0.848636 0.910621	H27 0.25026
H -4.065179 2.648125 -0.337280	H28 0.25273
H -1.677145 2.333188 -0.999362	H29 0.26854
H -0.274248 -0.060935 -1.883093	H30 0.07561
H -2.047461 -2.805552 1.028766	H31 0.24636
H -0.844548 -1.754152 1.845248	H32 0.28436
H 0.153801 -4.072964 0.481611	H33 0.23174
H 1.386041 -3.210459 -0.517583	H34 0.26898
H 1.109737 -2.707982 1.181148	H35 0.26731
H -1.470153 -3.657031 -1.212152	H36 0.23104
H -1.877829 -1.972659 -1.703079	H37 0.26737
H -0.319782 -2.702966 -2.219943	H38 0.26387

$Pd(OAc)_2(NMe_2C_6H_4$-*p*-Me), 1a(Me)			**$Pd(OAc)_2(NMe_2C_6H_4$-*p*-Me), $TS_{1a\text{-}2a}$(Me)**		
Energy = -1029.881317			Energy = -1029.859527		
Enthalpy (0K) = -1029.555517			Enthalpy (0K) = -1029.535044		
Enthalpy (298.15 K) = -1029.531363			Enthalpy (298.15 K) = -1029.510534		
Free Energy = -1029.611229			Free Energy = -1029.590170		
Pd	1.133489	0.290256 -0.039665	Pd	-0.581539	0.073165 -0.035188
C	-2.214461	0.926556 -0.063823	C	1.894004	0.257539 -0.643836
C	-2.191785	-0.029187 0.971600	C	2.116359	-1.138265 -0.734423
C	-3.295539	-0.896724 1.103433	C	3.239584	-1.689263 -0.101498
C	-4.376754	-0.827311 0.215314	C	4.128826	-0.863346 0.609456
C	-4.393926	0.114699 -0.834822	C	3.907973	0.523906 0.724166
C	-3.296708	0.990631 -0.953645	C	2.774575	1.071720 0.086835
C	-1.028945	-0.110120 1.936539	C	1.056611	-1.967743 -1.414382
N	0.178412	-0.873094 1.425103	N	-0.223392	-1.936670 -0.610496
C	1.731305	2.686295 -0.161757	C	-0.843049	2.680102 -0.640401
C	2.144024	4.131816 -0.198055	C	-1.273187	4.133439 -0.567427
O	1.069056	2.207718 0.845857	O	-0.398650	2.161605 -1.695860
O	2.043587	1.875491 -1.109547	O	-0.994372	1.992098 0.467943
O	1.402541	-1.219175 -1.347277	O	-2.008627	-0.543752 1.299296
C	2.353945	-2.092848 -1.062323	C	-3.247317	-0.442804 0.833152
C	2.714057	-2.967707 -2.263781	C	-4.288536	-0.628892 1.942304
O	2.921721	-2.216500 0.037505	O	-3.565466	-0.215539 -0.341109
H	3.112597	4.245445 0.319091	H	-2.344930	4.198653 -0.822778
H	2.266732	4.465954 -1.238721	H	-1.140497	4.537134 0.447815
H	1.402151	4.754590 0.323888	H	-0.707370	4.729778 -1.298390
H	3.422946	-2.416974 -2.905616	H	-4.436993	0.340716 2.447369
H	3.198316	-3.892102 -1.917361	H	-5.244183	-0.946121 1.500583
H	1.826526	-3.199952 -2.872207	H	-3.953795	-1.352648 2.700929
C	-0.208621	-2.243235 0.983630	C	-0.091670	-2.786659 0.607470
C	1.183623	-0.982747 2.529521	C	-1.358386	-2.416882 -1.450813
H	-3.309618	-1.633549 1.915573	H	3.423466	-2.768667 -0.155504
H	-5.222937	-1.513366 0.338874	H	5.005866	-1.307751 1.093721
C	-5.562655	0.181644 -1.794377	C	4.868969	1.410789 1.486220
H	-3.291729	1.738915 -1.754533	H	2.579370	2.147684 0.149693
H	-1.374720	1.622035 -0.168962	H	1.109932	0.748110 -1.265699
H	-1.352467	-0.615172 2.869986	H	1.369117	-3.021325 -1.554656
H	-0.662131	0.895524 2.200824	H	0.813058	-1.546461 -2.405451
H	0.756374	-1.568751 3.368222	H	-1.178642	-3.463482 -1.768502
H	2.075699	-1.479720 2.120857	H	-2.290416	-2.343460 -0.876102
H	1.441798	0.026198 2.885456	H	-1.452578	-1.767742 -2.333425
H	-0.761730	-2.748123 1.799810	H	0.017502	-3.849986 0.314964
H	-0.841350	-2.178269 0.089630	H	0.792856	-2.467351 1.177159
H	0.710929	-2.798256 0.759365	H	-0.987786	-2.644820 1.226629
H	-5.417881	0.966669 -2.553801	H	4.331201	2.089618 2.169807
H	-5.701591	-0.777376 -2.324516	H	5.580429	0.817839 2.083000
H	-6.507864	0.395319 -1.264026	H	5.457333	2.044221 0.797851

$Pd(OAc)_2(NMe_2C_6H_4$-*p*-Cl), 1a(Cl)	**$Pd(OAc)_2(NMe_2C_6H_4$-*p*-Cl), $TS_{1a\text{-}2a}$(Cl)**
Energy = -1004.990793	Energy = -1004.967481
Enthalpy (0K) = -1004.701010	Enthalpy (0K) = -1004.679220
Enthalpy (298.15 K) = -1004.676668	Enthalpy (298.15 K) = -1004.655401
Free Energy = -1004.757303	Free Energy = -1004.733501
Pd 1.369656 0.289191 -0.071415	Pd -0.787062 0.052892 -0.038913
C -1.953315 0.867294 0.119972	C 1.625491 0.007198 -0.770897
C -1.869562 -0.040285 1.196839	C 1.757126 -1.401257 -0.831503
C -2.976254 -0.869968 1.465042	C 2.897483 -2.007719 -0.282989
C -4.135474 -0.817201 0.676491	C 3.903223 -1.230607 0.317880
C -4.180006 0.084360 -0.395576	C 3.741913 0.161693 0.383678
C -3.100364 0.932091 -0.683289	C 2.613269 0.795664 -0.154419
C -0.632331 -0.107252 2.067498	C 0.595154 -2.182244 -1.392583
N 0.529876 -0.870988 1.467955	N -0.619817 -2.008380 -0.512576
C 1.977622 2.680846 -0.225508	C -0.859247 2.657721 -0.750226
C 2.401628 4.121786 -0.283477	C -1.183809 4.139190 -0.708775
O 1.389709 2.200424 0.827152	O -0.484854 2.078934 -1.800596
O 2.206329 1.873403 -1.199840	O -1.025107 2.017375 0.385691
O 1.515677 -1.212255 -1.405057	O -2.225645 -0.377635 1.349391
C 2.474721 -2.100379 -1.198406	C -3.454408 -0.123456 0.910682
C 2.733129 -2.969337 -2.429004	C -4.483439 -0.169287 2.044410
O 3.120014 -2.237977 -0.143731	O -3.764863 0.136753 -0.257831
H 3.408267 4.221471 0.158414	H -2.256256 4.271836 -0.932945
H 2.447537 4.462803 -1.328078	H -0.989788 4.561778 0.288642
H 1.708981 4.747992 0.298562	H -0.601935 4.671997 -1.475232
H 3.396849 -2.420428 -3.118882	H -4.503054 0.818339 2.535807
H 3.232841 -3.900916 -2.126725	H -5.480027 -0.375306 1.628158
H 1.799724 -3.188158 -2.969903	H -4.220265 -0.917317 2.807498
C 0.113729 -2.247403 1.072971	C -0.470748 -2.793455 0.746765
C 1.622704 -0.967550 2.487729	C -1.839907 -2.449281 -1.248825
H -2.938841 -1.569525 2.308036	H 3.009901 -3.097155 -0.317012
H -4.991340 -1.462460 0.889198	H 4.796398 -1.698198 0.739574
Cl -5.635280 0.162338 -1.399936	Cl 4.999604 1.137865 1.151446
H -3.160493 1.633398 -1.519153	H 2.507786 1.881766 -0.108057
H -1.105760 1.527676 -0.093437	H 0.830860 0.538448 -1.353319
H -0.880919 -0.600366 3.029455	H 0.821749 -3.261980 -1.490967
H -0.251609 0.903365 2.290329	H 0.318648 -1.797376 -2.389879
H 1.267290 -1.546137 3.364218	H -1.747481 -3.516799 -1.531878
H 2.478376 -1.467968 2.011426	H -2.718638 -2.302234 -0.608491
H 1.907422 0.045300 2.810313	H -1.962758 -1.829477 -2.148611
H -0.358303 -2.750127 1.939779	H -0.456659 -3.877385 0.517095
H -0.598386 -2.195390 0.239732	H 0.467471 -2.508203 1.243942
H 1.013635 -2.796917 0.769154	H -1.314502 -2.549177 1.406712