SUPPORTING INFORMATION – PART II COMPUTATIONAL DETAILS

Palladium-Catalyzed Stereoselective Domino Arylation-Acylation: An Entry to Chiral Hydro-fluorenone Scaffolds

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Computational details

All geometry optimization and frequency analyses were conducted at the B3LYP[1,2]-D3[3]/def2-SVPD[4,5] level of theory using the Gaussian 16 package.[6] The inner 28 electrons of palladium were described using a Stuttgart-Dresden effective core potential.[7] Solvation effects from acetonitrile were accounted for implicitly using the Solvent Model Density (SMD) method.[8] Single point energies for all reported structures were obtained using the def2-TZVPD[4,5] basis set. Gibbs free energies were obtained by adding the thermal corrections from the frequency analyses to the single point energies. A correction term of 1.89 kcal/mol (1 atm → 1 M) was added to all Gibbs energies to account for a standard state of 298.15K and 1M. Calculation of the acetonitrile solvent is an exception, for which we added a correction term of 3.63 kcal/mol (1 atm → 19 M). As the reaction was conducted using a silver(I) additive in a polar solvent, a fast halide abstraction after oxidative addition was assumed. Therefore, all palladium complexes were modeled using acetonitrile and acetate ligands.

Extended reaction profiles for aldehyde insertion and β-hydride elimination pathways

TS1
28.6

IN1
0.0

IN2
1.2

TS2
8.3

+MeCN

IN7
-18.7

TS8
-8.8

-AcOH
-Pd(MeCN)₂

2
-26.4
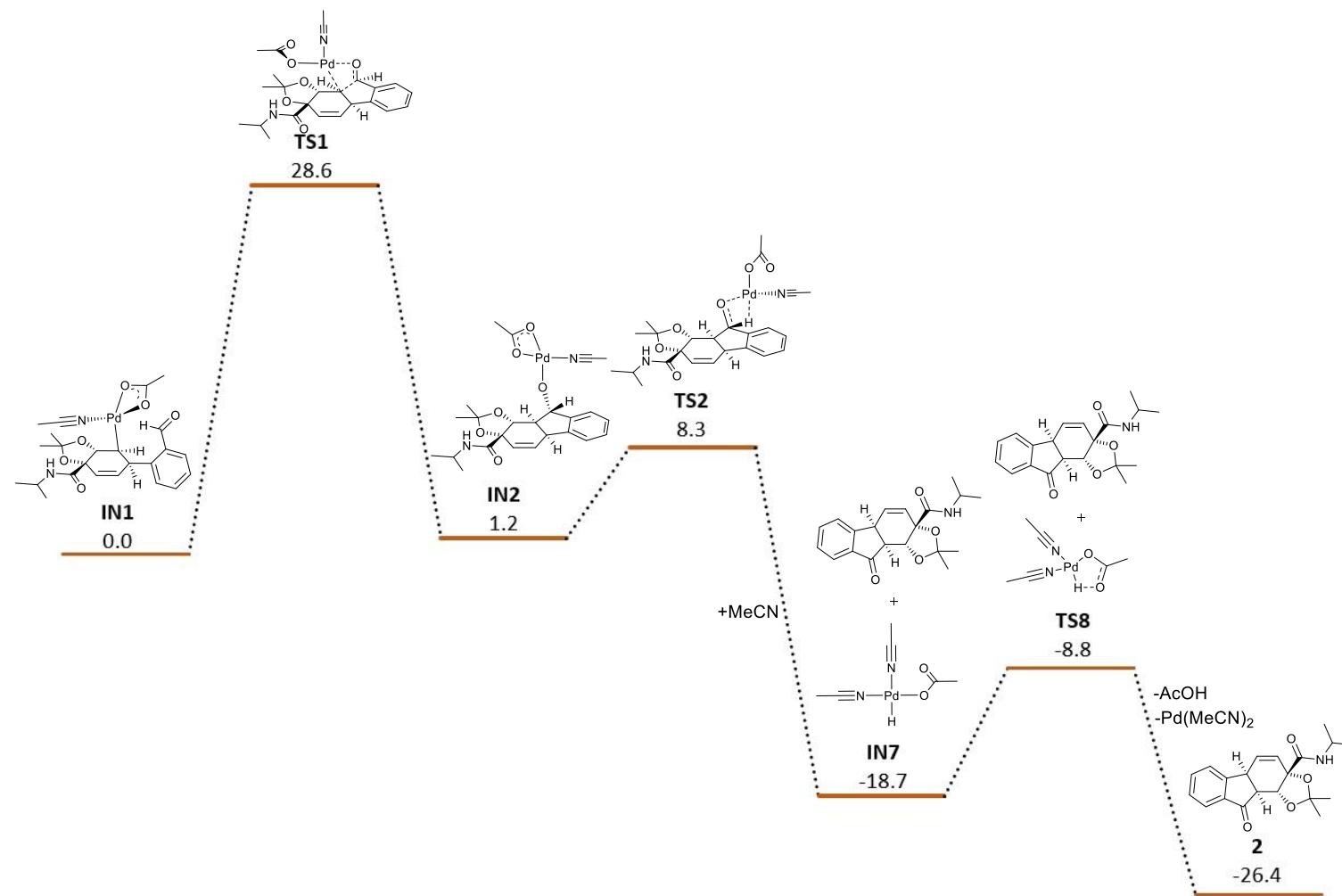
Figure 1 Extended reaction profile for the aldehyde insertion pathway.
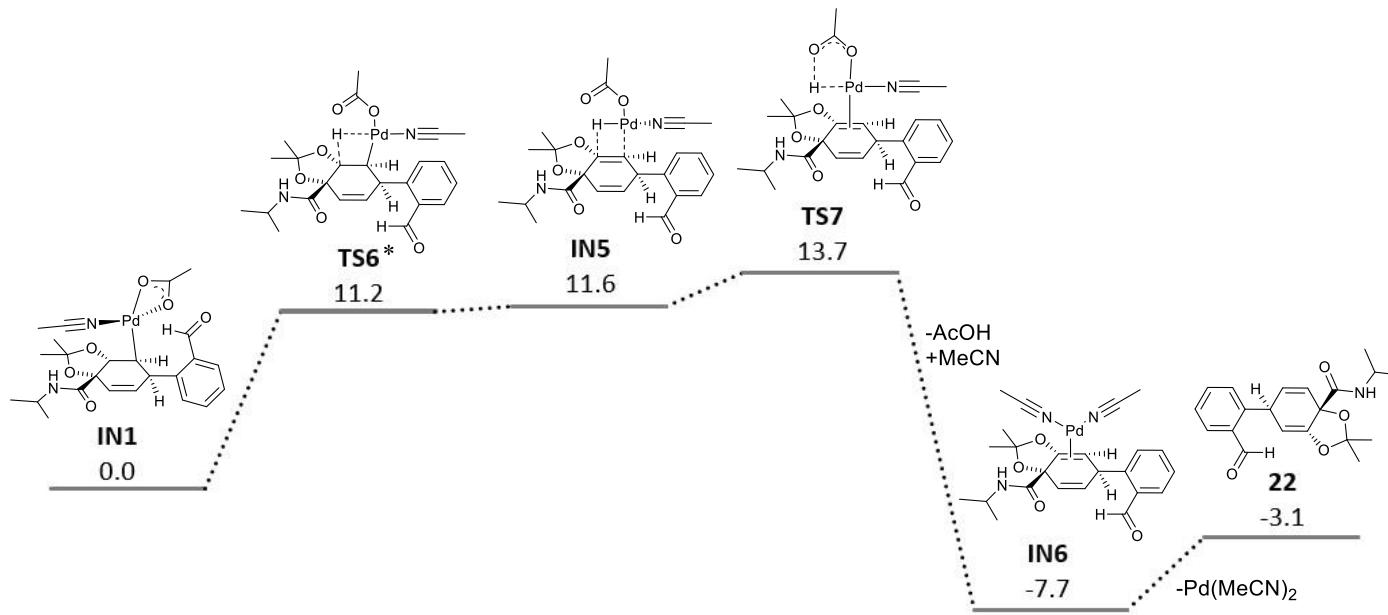
Figure 2 Extended reaction profile for the β-hydride elimination pathway.

The potential energy surface following **TS6 is shallow, and whereas the next stable intermediate in pathway C, **IN5**, has a slightly lower electronic energy, its computed Gibbs energy is 0.4 kcal/mol above **TS6**. Because our structure optimization proceeds on the electronic potential energy surface, and not the Gibbs energy surface, we cannot exclude the possibility that the true geometry of **TS6** is more similar to **IN5**. Our estimate to the activation barrier height of **TS6** is, therefore, likely to be a lower bound.*
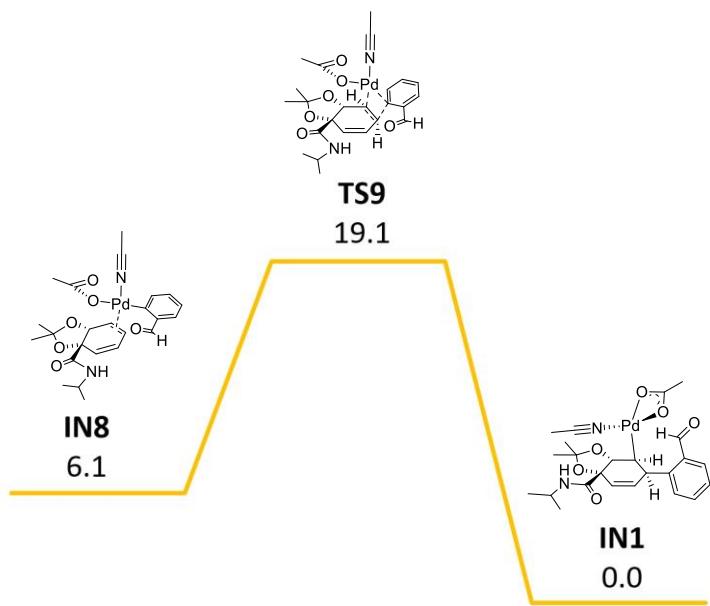
*Figure 3 Reaction profile for the formation of **IN1** through Heck-type migratory insertion.*

Geometries and energies

Optimized cartesian coordinates,energies and imaginary frequencies of all reported structures are reported here.

2
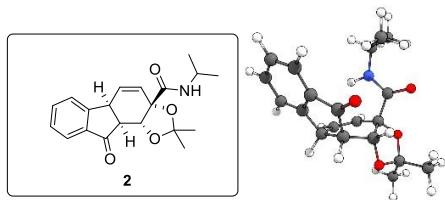
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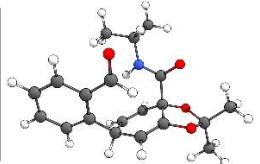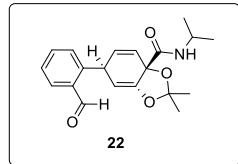
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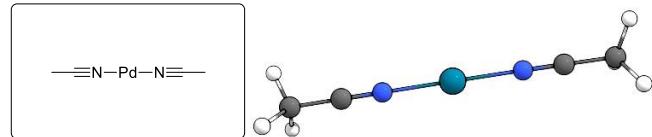
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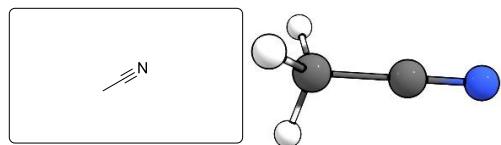
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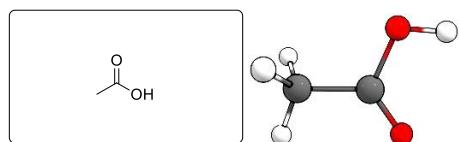
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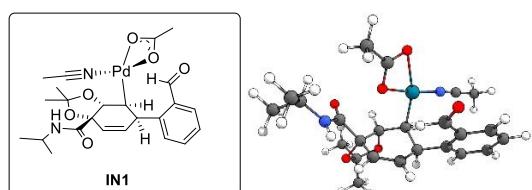
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IN2

IN2
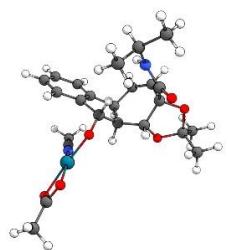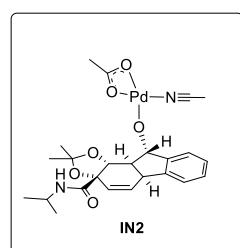
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H	4.606562000	0.571831000	-4.935631000
H	5.473010000	0.203699000	-3.422282000
C	2.010107000	0.445244000	-3.877159000
H	3.408725000	-1.173183000	-3.696586000
H	1.850812000	1.460140000	-3.490143000
H	1.157404000	-0.181215000	-3.582427000
H	2.039815000	0.491805000	-4.974365000

IN3

IN3
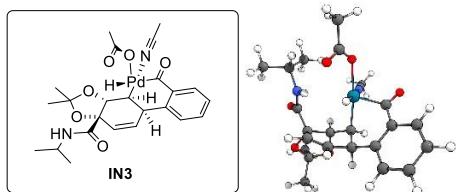
Charge: 0
Multiplicity: 1
EB3LYP-D3: -1622.148385 a.u.
ΔGcorr: 0.433315 a.u.
No imaginary frequencies

C	-0.556609000	1.607496000	-1.930166000
C	0.756656000	1.796747000	-1.756479000
C	1.412300000	1.873260000	-0.390227000
C	0.571440000	1.175351000	0.669814000
C	-1.551465000	1.530589000	-0.797087000
C	-0.878271000	1.620045000	0.607176000
H	-0.980452000	1.581551000	-2.935921000
H	1.400365000	1.925806000	-2.628018000
O	-2.352101000	2.713576000	-0.859530000
C	-2.511102000	0.307782000	-0.831587000
N	-2.065566000	-0.791942000	-1.469441000
O	-3.594652000	0.369724000	-0.254116000
O	-0.947838000	3.021630000	0.892418000
H	-1.484847000	1.069822000	1.340021000
C	-2.134226000	3.532733000	0.300201000
C	-1.877877000	4.961063000	-0.142888000
H	-1.014486000	4.988263000	-0.818652000
H	-2.759894000	5.352716000	-0.665530000
H	-1.678574000	5.596900000	0.729548000
C	-3.322004000	3.403629000	1.249271000
H	-3.471619000	2.355232000	1.529790000
H	-3.146815000	4.008721000	2.148869000
H	-4.233532000	3.762304000	0.753027000
C	-2.796707000	-2.069297000	-1.532299000
C	2.869571000	1.441930000	-0.433971000

C	4.744478000	-0.030530000	0.133584000
C	5.626070000	0.792501000	-0.555766000
C	5.139162000	1.949281000	-1.179378000
C	3.368000000	0.279199000	0.190024000
C	3.783984000	2.266936000	-1.106918000
H	5.102849000	-0.933269000	0.628038000
H	5.820999000	2.609310000	-1.718208000
H	3.417370000	3.179960000	-1.578600000
H	1.436571000	2.946855000	-0.124324000
H	6.686116000	0.540126000	-0.604685000
H	1.000597000	-5.380264000	-0.892762000
O	0.450170000	-2.981820000	0.006371000
C	0.220414000	-4.834970000	-1.441508000
H	-0.750613000	-5.149435000	-1.030692000
C	0.379978000	-3.338274000	-1.227864000
H	0.263344000	-5.088727000	-2.506453000
Pd	0.585631000	-0.890157000	0.475066000
O	0.408273000	-2.566361000	-2.202260000
H	0.956033000	1.405094000	1.672522000
H	-1.315675000	-0.640922000	5.411577000
C	-0.834425000	-1.354237000	3.507171000
C	-1.489377000	-1.528736000	4.787658000
N	-0.314693000	-1.214228000	2.486004000
H	-1.081758000	-2.416960000	5.290278000
H	-2.569022000	-1.660399000	4.629135000
C	2.519183000	-0.687726000	0.921859000
O	2.890605000	-1.451193000	1.766661000
H	1.026512000	-0.666191000	-0.945543000
H	-1.138718000	-0.787200000	-1.884398000
C	-4.104047000	-1.930665000	-2.317591000
H	-4.808924000	-1.274790000	-1.792325000
H	-4.569548000	-2.918893000	-2.438315000
H	-3.913551000	-1.515185000	-3.316879000
C	-3.003428000	-2.680315000	-0.142604000
H	-2.128650000	-2.728060000	-2.098142000
H	-3.692452000	-2.070585000	0.454349000
H	-2.046981000	-2.759638000	0.387928000
H	-3.427696000	-3.688918000	-0.243513000

IN4
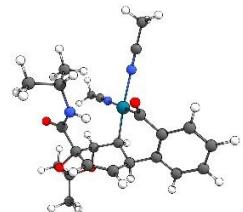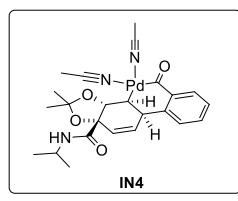
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Multiplicity: 1
E$_{B3LYP-D3}$: -1525.797505 a.u.
ΔG$_{corr}$: 0.416399 a.u.
No imaginary frequencies

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C	0.491713000	-2.361429000	-1.344168000
C	-0.046648000	-2.433368000	0.069444000
C	0.246300000	-1.143424000	0.857061000
C	2.126604000	-0.526145000	-0.826254000
C	1.679904000	-0.700238000	0.649457000

H	1.791768000	-1.513381000	-2.777085000
H	0.089756000	-3.082714000	-2.059756000
O	3.513004000	-0.869926000	-0.795966000
C	2.012463000	0.960812000	-1.258949000
N	0.900736000	1.270277000	-1.952067000
O	2.876719000	1.776815000	-0.943154000
O	2.596188000	-1.718219000	1.102204000
H	1.888580000	0.227090000	1.198313000
C	3.837739000	-1.511358000	0.451564000
C	4.472913000	-2.862673000	0.172958000
H	3.786805000	-3.474966000	-0.424688000
H	5.412648000	-2.728999000	-0.378432000
H	4.692742000	-3.378990000	1.116886000
C	4.741072000	-0.585207000	1.261843000
H	4.227468000	0.360430000	1.471121000
H	5.016831000	-1.066670000	2.209773000
H	5.657281000	-0.368133000	0.696650000
C	0.520930000	2.619933000	-2.394018000
C	-1.519947000	-2.797273000	0.043851000
C	-3.798139000	-2.200240000	-0.598660000
C	-4.251585000	-3.458116000	-0.187005000
C	-3.341839000	-4.386611000	0.328285000
C	-2.444486000	-1.864495000	-0.467396000
C	-1.983132000	-4.058422000	0.429546000
H	-4.495396000	-1.464879000	-1.004097000
H	-3.687594000	-5.370583000	0.650726000
H	-1.271938000	-4.793502000	0.811718000
H	0.484222000	-3.268706000	0.559510000
H	-5.309919000	-3.711570000	-0.270586000
Pd	-1.057340000	0.486889000	0.634183000
H	0.117221000	-1.354203000	1.930521000
H	2.443539000	2.847627000	3.777544000
C	0.602680000	2.210326000	3.023109000
C	1.372263000	2.961810000	3.995488000
N	0.001534000	1.608590000	2.241253000
H	1.162497000	2.582421000	5.005365000
H	1.098904000	4.024787000	3.940160000
C	-1.978009000	-0.483131000	-0.816964000
O	-2.261545000	0.032164000	-1.888761000
H	0.221429000	0.534842000	-2.103875000
C	1.471023000	3.134826000	-3.479556000
H	2.483096000	3.265766000	-3.074938000
H	1.118783000	4.105043000	-3.857529000
H	1.517304000	2.430628000	-4.321829000
C	0.386656000	3.601440000	-1.225291000
H	-0.473070000	2.486285000	-2.841350000
H	1.361379000	3.790855000	-0.759808000
H	-0.294107000	3.205414000	-0.462782000
H	-0.019420000	4.554837000	-1.591334000
N	-2.510207000	2.098285000	0.544036000
C	-3.298554000	2.939530000	0.472219000
H	-3.858748000	4.844037000	-0.185325000
C	-4.283562000	3.999394000	0.375309000
H	-5.175132000	3.625787000	-0.147573000
H	-4.564941000	4.335045000	1.383235000

IN5
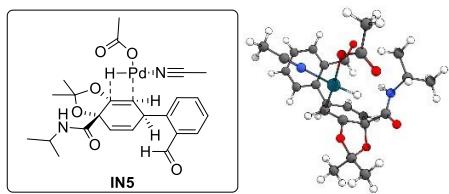
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Multiplicity: 1
$E_{B3LYP-D3}$: -1622.141366 a.u.
ΔG_{corr}: 0.431509 a.u.
No imaginary frequencies

C	-1.118148000	-1.722304000	2.047566000
C	0.209236000	-1.877407000	2.097885000
C	1.112022000	-1.966930000	0.896159000
C	0.401879000	-1.673297000	-0.420103000
C	-1.878283000	-1.446690000	0.777942000
C	-0.970925000	-1.450244000	-0.462132000
H	-1.711668000	-1.754745000	2.962309000
H	0.692484000	-2.041400000	3.062937000
O	-2.760069000	-2.525510000	0.464314000
C	-2.726060000	-0.135246000	0.876331000
N	-2.189823000	0.836227000	1.636018000
O	-3.776597000	-0.018652000	0.254890000
O	-1.749525000	-1.906915000	-1.497720000
H	-1.277631000	0.601529000	-0.847346000
C	-2.670711000	-2.868895000	-0.929735000
C	-2.076737000	-4.264590000	-1.046903000
H	-1.084536000	-4.291716000	-0.579046000
H	-2.729071000	-4.984288000	-0.535288000
H	-1.989184000	-4.553200000	-2.102166000
C	-4.011616000	-2.710700000	-1.611840000
H	-4.379135000	-1.692379000	-1.454897000
H	-3.907609000	-2.914817000	-2.685600000
H	-4.725269000	-3.429206000	-1.188166000
C	-2.663776000	2.222622000	1.623227000
C	2.504930000	-1.356673000	1.055189000
C	4.100469000	0.394642000	1.659353000
C	5.166456000	-0.401141000	1.254421000
C	4.907900000	-1.680541000	0.750008000
C	2.772608000	-0.059728000	1.556298000
C	3.595271000	-2.147607000	0.665177000
H	4.273956000	1.399344000	2.045145000
H	5.730212000	-2.318737000	0.422713000
H	3.409503000	-3.151723000	0.281348000
H	1.311502000	-3.050780000	0.811061000
H	6.189271000	-0.029097000	1.323783000
O	-2.005968000	2.674521000	-1.702012000
C	-0.569839000	4.569610000	-1.999971000
C	-0.845069000	3.092322000	-1.760936000
Pd	0.202253000	0.380106000	-1.061952000
O	0.224193000	2.381217000	-1.605551000
H	0.838617000	-2.156393000	-1.295042000
H	5.261128000	-0.590805000	-2.117686000
C	3.424530000	0.378208000	-1.897450000
C	4.825481000	0.406070000	-2.267737000
N	2.312739000	0.353408000	-1.589363000
H	5.354101000	1.131754000	-1.635038000

H	4.922731000	0.697689000	-3.322556000
C	1.691928000	0.880989000	1.927222000
O	1.877413000	1.953994000	2.478004000
H	0.668562000	0.574311000	1.647250000
H	-1.333213000	0.637255000	2.137361000
H	0.339805000	4.712862000	-2.596723000
H	-0.411410000	5.049870000	-1.021899000
H	-1.426689000	5.048018000	-2.488149000
C	-3.731468000	2.455190000	2.693739000
H	-4.579153000	1.771359000	2.552860000
H	-4.106162000	3.487642000	2.638839000
H	-3.314147000	2.292071000	3.698739000
C	-1.462063000	3.151235000	1.779418000
H	-3.103841000	2.377596000	0.629939000
H	-0.985115000	3.011708000	2.761081000
H	-1.782750000	4.198136000	1.699871000
H	-0.713015000	2.953203000	1.003384000

IN6
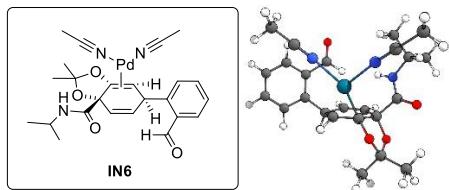
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Multiplicity: 1
$E_{B3LYP-D3}$: -1525.78831 a.u.
ΔG_{corr}: 0.418841 a.u.
No imaginary frequencies

C	-0.864765000	1.501682000	-2.033478000
C	0.453841000	1.729463000	-2.018553000
C	1.270626000	1.960583000	-0.773754000
C	0.512789000	1.644739000	0.516984000
C	-1.704547000	1.316987000	-0.794212000
C	-0.885724000	1.341248000	0.500455000
H	-1.393013000	1.428821000	-2.986226000
H	0.985302000	1.842133000	-2.966482000
O	-2.588491000	2.434291000	-0.631771000
C	-2.572412000	0.021988000	-0.859094000
N	-2.025536000	-0.994016000	-1.555902000
O	-3.655096000	-0.059274000	-0.283308000
O	-1.759135000	1.938465000	1.436491000
C	-2.525047000	2.912381000	0.724707000
C	-1.814965000	4.262935000	0.731929000
H	-0.801239000	4.155155000	0.326811000
H	-2.368391000	4.978802000	0.109578000
H	-1.755103000	4.656246000	1.755524000
C	-3.919781000	2.957488000	1.316931000
H	-4.373692000	1.964649000	1.229889000
H	-3.869679000	3.256297000	2.372590000
H	-4.533566000	3.690370000	0.776417000
C	-2.599832000	-2.335494000	-1.634158000
C	2.696898000	1.413953000	-0.796103000
C	4.405139000	-0.314014000	-1.097689000
C	5.403547000	0.559273000	-0.679266000
C	5.055295000	1.866481000	-0.319350000
C	3.057929000	0.090019000	-1.154472000

C	3.723273000	2.280059000	-0.385492000
H	4.647763000	-1.338863000	-1.378516000
H	5.823213000	2.568576000	0.010551000
H	3.468313000	3.304108000	-0.108094000
H	1.404316000	3.058505000	-0.763729000
H	6.441711000	0.228002000	-0.631239000
Pd	0.160145000	-0.310754000	1.146123000
H	0.850668000	2.249325000	1.364024000
C	2.053151000	-0.917463000	-1.566102000
O	2.330007000	-2.055580000	-1.915728000
H	0.999985000	-0.591547000	-1.541154000
H	-1.129939000	-0.842143000	-2.001693000
C	-3.581373000	-2.449230000	-2.803921000
H	-4.380687000	-1.701598000	-2.712664000
H	-4.040578000	-3.448391000	-2.821709000
H	-3.061223000	-2.290040000	-3.760263000
C	-1.468274000	-3.357215000	-1.722470000
H	-3.156532000	-2.486976000	-0.700165000
H	-0.890995000	-3.213442000	-2.648836000
H	-1.876052000	-4.376585000	-1.732328000
H	-0.783620000	-3.258129000	-0.870542000
H	-2.813429000	-4.552007000	1.062673000
C	-2.922475000	-3.853511000	1.904355000
C	-1.923809000	-2.807378000	1.788842000
N	-1.138139000	-1.968667000	1.657321000
H	-3.926378000	-3.407229000	1.876985000
H	-2.790553000	-4.398651000	2.848590000
C	3.035147000	-1.870297000	1.741770000
N	1.986525000	-1.395355000	1.627606000
C	4.361976000	-2.447564000	1.847202000
H	4.595294000	-2.990682000	0.920528000
H	4.403142000	-3.142717000	2.697163000
H	5.100440000	-1.646903000	1.991640000

IN7
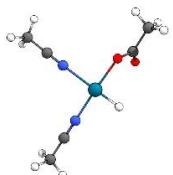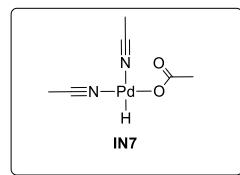
Charge: 0
Multiplicity: 1
$E_{B3LYP-D3}$: -622.8478021 a.u.
ΔG_{corr}: 0.103018 a.u.
No imaginary frequencies

H	4.976781000	-0.646198000	1.184643000
C	4.630440000	-1.197262000	0.298690000
H	5.167784000	-0.836201000	-0.589805000
C	3.208124000	-0.985709000	0.122976000
N	2.074833000	-0.816371000	-0.016706000
H	4.827394000	-2.270198000	0.434759000
H	1.015682000	4.666562000	-0.657728000
Pd	0.113654000	-0.514599000	-0.240677000
H	-0.055705000	-2.027659000	-0.358678000
N	0.309130000	1.658219000	-0.051206000
C	0.392149000	2.804302000	0.064133000
C	0.492149000	4.243162000	0.211070000

O	-1.880028000	-0.313037000	-0.592547000
H	-4.413662000	-1.108586000	-1.033928000
H	-0.516330000	4.675387000	0.276576000
H	1.051977000	4.480959000	1.126747000
C	-2.768485000	-0.666246000	0.279951000
C	-4.196312000	-0.434256000	-0.191703000
H	-4.312364000	0.595651000	-0.557792000
O	-2.532068000	-1.150662000	1.391584000
H	-4.909000000	-0.625451000	0.618760000

IN8
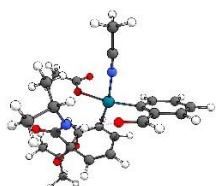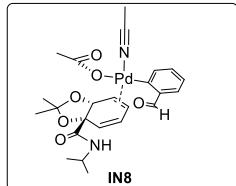
Charge: 0
Multiplicity: 1
$E_{B3LYP-D3}$: -1622.150488 a.u.
ΔG_{corr}: 0.431974 a.u.
No imaginary frequencies

C	1.480493000	-1.505160000	-1.762810000
C	0.390265000	-2.181423000	-1.367340000
C	-0.037239000	-2.188192000	0.034361000
C	0.691760000	-1.544266000	1.015236000
C	2.305873000	-0.657742000	-0.830130000
C	2.039420000	-0.950534000	0.677754000
H	1.813067000	-1.529568000	-2.801061000
H	-0.197280000	-2.760641000	-2.079352000
O	3.671588000	-1.033631000	-0.996119000
C	2.176171000	0.873907000	-1.127113000
N	1.015240000	1.247894000	-1.683844000
O	3.018309000	-1.952016000	0.970956000
H	2.232405000	-0.048849000	1.265674000
C	4.177218000	-1.640684000	0.204651000
C	4.883853000	-2.934194000	-0.151192000
H	4.191954000	-3.600117000	-0.680906000
H	5.746699000	-2.721520000	-0.795162000
H	5.242363000	-3.430525000	0.759927000
C	5.073844000	-0.649170000	0.940515000
H	4.518693000	0.262079000	1.188984000
H	5.459191000	-1.107513000	1.860973000
H	5.921454000	-0.373614000	0.299531000
C	-2.571139000	-1.235209000	0.106312000
C	-4.342490000	-1.957170000	-1.419617000
C	-4.973911000	-2.654730000	-0.395445000
C	-4.404617000	-2.644221000	0.883795000
C	-3.144907000	-1.241820000	-1.188496000
C	-3.215620000	-1.945630000	1.126959000
H	-4.772304000	-1.951756000	-2.423845000
H	-2.790455000	-1.963456000	2.132090000
H	-0.797012000	-2.909882000	0.321402000
H	-5.898350000	-3.200976000	-0.586983000
Pd	-1.001532000	-0.112361000	0.679201000
H	0.540276000	-1.803008000	2.063981000
H	-4.885876000	-3.184690000	1.701530000
O	0.399597000	1.286583000	1.432678000

O	-0.291441000	0.979586000	3.547177000
C	0.417150000	1.535244000	2.693880000
C	1.420869000	2.610549000	3.085490000
H	2.426838000	2.307159000	2.760623000
H	1.178803000	3.545637000	2.559966000
H	1.416508000	2.782007000	4.167607000
H	-3.144534000	4.403909000	-0.164887000
C	-3.741912000	3.630468000	0.337975000
H	-4.641821000	3.415363000	-0.254710000
C	-2.947100000	2.426977000	0.466084000
N	-2.299651000	1.477849000	0.561552000
H	-4.035057000	3.984068000	1.336333000
C	-2.585786000	-0.532443000	-2.350619000
O	-1.574144000	0.150601000	-2.378295000
H	-3.182654000	-0.656172000	-3.281786000
O	3.102758000	1.631144000	-0.850400000
C	0.642640000	2.623000000	-2.043526000
H	0.282992000	0.555170000	-1.808495000
C	1.537874000	3.163169000	-3.162889000
H	2.572579000	3.270269000	-2.812368000
H	1.177241000	4.148880000	-3.489263000
H	1.528796000	2.487241000	-4.029377000
C	0.590907000	3.560042000	-0.833672000
H	-0.376882000	2.522737000	-2.438492000
H	0.199333000	4.538590000	-1.145885000
H	1.592534000	3.700510000	-0.409344000
H	-0.053159000	3.144302000	-0.052824000

TS1
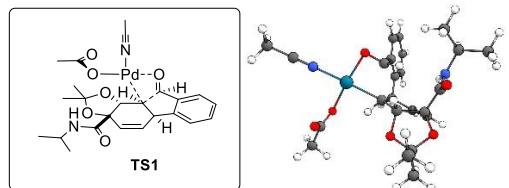
Charge: 0
Multiplicity: 1
$E_{B3LYP-D3}$: -1622.115675 a.u.
ΔG_{corr}: 0.433012 a.u.
One imaginary freq: -305.5699 cm^{-1}

C	2.473556000	1.315270000	1.603632000
C	1.738661000	0.532362000	2.398771000
C	0.516748000	-0.237118000	1.946618000
C	-0.133320000	0.364604000	0.683680000
C	2.141439000	1.589910000	0.160874000
C	0.617693000	1.425836000	-0.113729000
H	3.364604000	1.816689000	1.984368000
H	2.039561000	0.380597000	3.436814000
O	2.357424000	2.969328000	-0.111940000
C	2.984091000	0.769896000	-0.864533000
N	3.546831000	-0.350887000	-0.378234000
O	3.060757000	1.136134000	-2.034369000
O	0.133866000	2.713665000	0.274496000
H	0.459745000	1.296517000	-1.193695000
C	1.102452000	3.680585000	-0.106658000
C	1.135035000	4.771299000	0.948288000
H	1.359305000	4.331948000	1.927698000

H	1.906212000	5.510673000	0.697748000
H	0.163352000	5.280604000	0.992576000
C	0.831979000	4.211318000	-1.509484000
H	0.766550000	3.384414000	-2.226298000
H	-0.110020000	4.775247000	-1.520008000
H	1.647357000	4.879193000	-1.816972000
C	4.328459000	-1.324404000	-1.157587000
C	0.881716000	-1.702862000	1.763671000
C	0.966315000	-3.587874000	0.231266000
C	1.453901000	-4.399006000	1.258574000
C	1.651967000	-3.863000000	2.538260000
C	0.690973000	-2.238770000	0.490169000
C	1.364718000	-2.518900000	2.792550000
H	0.806301000	-3.991864000	-0.768810000
H	2.022804000	-4.499255000	3.343748000
H	1.501661000	-2.107718000	3.793778000
H	-0.222630000	-0.192750000	2.759892000
H	1.675484000	-5.449500000	1.063836000
H	-5.045094000	1.696222000	2.382153000
O	-3.130702000	0.584743000	1.088465000
C	-4.515276000	2.389388000	1.715344000
H	-3.790346000	2.949551000	2.325637000
C	-3.757631000	1.630404000	0.639521000
H	-5.220478000	3.095982000	1.262852000
Pd	-2.029311000	-0.552459000	-0.220758000
O	-3.745935000	2.014683000	-0.532268000
H	-1.027551000	0.892883000	1.027584000
H	-6.235302000	-3.119723000	-1.639477000
C	-4.701116000	-1.704105000	-1.547882000
C	-5.910757000	-2.209707000	-2.163498000
N	-3.738802000	-1.298087000	-1.058114000
H	-5.712887000	-2.444615000	-3.218828000
H	-6.699481000	-1.446846000	-2.098650000
C	0.222729000	-1.323913000	-0.592350000
O	-0.781161000	-1.659258000	-1.340331000
H	1.014552000	-0.758129000	-1.099191000
H	3.406009000	-0.553044000	0.603836000
C	5.619019000	-0.699586000	-1.694693000
H	5.394009000	0.076550000	-2.437203000
H	6.235771000	-1.472897000	-2.173493000
H	6.200333000	-0.248068000	-0.878791000
C	3.492087000	-1.980240000	-2.260194000
H	4.598470000	-2.099170000	-0.427416000
H	3.166399000	-1.236833000	-2.998107000
H	2.606798000	-2.471411000	-1.838178000
H	4.093993000	-2.741990000	-2.774152000

TS2
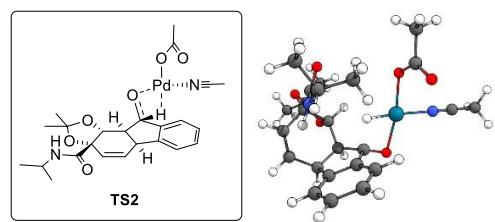
Charge: 0
Multiplicity: 1
$E_{B3LYP-D3}$: -1622.148074 a.u.
ΔG_{corr}: 0.433039 a.u.

One imaginary freq: -527.9217 cm⁻¹

C	3.715697000	-0.143145000	-0.106482000
C	3.639976000	0.496077000	-1.276910000
C	2.377080000	0.609950000	-2.086343000
C	1.263470000	-0.436992000	-1.758142000
C	2.561457000	-0.890142000	0.508882000
C	1.538273000	-1.359833000	-0.563253000
H	4.645939000	-0.166938000	0.462994000
H	4.516573000	1.013275000	-1.670944000
O	3.034460000	-2.125540000	1.028032000
C	1.855288000	-0.110553000	1.661790000
N	1.835185000	1.226181000	1.499996000
O	1.339889000	-0.706359000	2.601710000
O	2.160876000	-2.551476000	-1.029894000
H	0.589776000	-1.609593000	-0.064878000
C	2.772136000	-3.187207000	0.089803000
C	4.078092000	-3.811726000	-0.366108000
H	4.728886000	-3.039328000	-0.793212000
H	4.584467000	-4.281123000	0.486926000
H	3.882433000	-4.582104000	-1.123713000
C	1.821919000	-4.186132000	0.738660000
H	0.872953000	-3.700679000	0.996296000
H	1.627205000	-5.019231000	0.050518000
H	2.273529000	-4.584569000	1.656614000
C	1.174698000	2.194713000	2.389103000
C	1.699986000	1.961337000	-1.888130000
C	-0.489839000	2.941035000	-1.433806000
C	0.095216000	4.206971000	-1.444702000
C	1.474752000	4.347652000	-1.679894000
C	0.330195000	1.831661000	-1.655281000
C	2.285475000	3.230785000	-1.904452000
H	-1.553439000	2.808633000	-1.231855000
H	1.920136000	5.344007000	-1.678636000
H	3.354833000	3.348813000	-2.082566000
H	2.640224000	0.515411000	-3.150764000
H	-0.515186000	5.091725000	-1.259083000
H	-2.701533000	-0.637846000	3.959634000
O	-2.433731000	-0.613273000	1.474525000
C	-3.457090000	0.017046000	3.509324000
H	-3.517978000	0.963081000	4.061494000
C	-3.158614000	0.293975000	2.044684000
H	-4.435731000	-0.481801000	3.577611000
Pd	-1.942159000	-0.359930000	-0.486973000
O	-3.609854000	1.301254000	1.488981000
H	1.125028000	-1.110869000	-2.611106000
H	-5.984488000	-3.162156000	-2.080834000
C	-4.822987000	-1.579227000	-1.364599000
C	-6.110681000	-2.123132000	-1.745272000
N	-3.797380000	-1.145451000	-1.061566000
H	-6.534141000	-1.522993000	-2.562974000
H	-6.789101000	-2.096814000	-0.881008000
C	-0.048884000	0.390381000	-1.695897000
O	-1.105649000	-0.028219000	-2.314738000
H	-0.511068000	0.266675000	-0.156987000
H	2.326659000	1.609289000	0.703494000
C	1.802870000	2.195418000	3.785413000
H	1.619534000	1.239954000	4.293049000
H	1.364075000	3.001636000	4.389852000
H	2.887813000	2.359035000	3.724434000

C	-0.339351000	1.984714000	2.425215000
H	1.375775000	3.167371000	1.920398000
H	-0.584508000	1.006679000	2.853116000
H	-0.765226000	2.033908000	1.416626000
H	-0.811491000	2.765368000	3.036680000

TS3

TS3
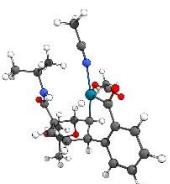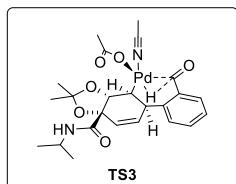
Charge: 0
Multiplicity: 1
$E_{B3LYP-D3}$: -1622.14127 a.u.
ΔG_{corr}: 0.433395 a.u.
One imaginary freq: -144.3141 cm^{-1}

C	-0.227891000	1.736429000	-2.057499000
C	1.090012000	1.551019000	-1.920082000
C	1.756519000	1.420436000	-0.565588000
C	0.807628000	0.848027000	0.476665000
C	-1.179957000	1.870590000	-0.890791000
C	-0.496397000	1.634841000	0.498384000
H	-0.667489000	1.867669000	-3.048275000
H	1.731952000	1.534217000	-2.802621000
O	-1.599302000	3.233026000	-0.832508000
C	-2.438317000	0.964527000	-0.997348000
N	-2.221773000	-0.238228000	-1.562979000
O	-3.517044000	1.322968000	-0.532647000
O	-0.206931000	2.968043000	0.931222000
H	-1.212716000	1.174141000	1.189815000
C	-1.216833000	3.825366000	0.417630000
C	-0.606471000	5.188059000	0.150589000
H	0.250106000	5.082511000	-0.526104000
H	-1.353525000	5.847178000	-0.309742000
H	-0.273339000	5.642936000	1.092469000
C	-2.418599000	3.881463000	1.356809000
H	-2.828685000	2.878073000	1.514435000
H	-2.117021000	4.314270000	2.320056000
H	-3.203871000	4.509552000	0.915931000
C	-3.185832000	-1.348349000	-1.604508000
C	3.111111000	0.744369000	-0.626301000
C	4.604584000	-1.193360000	-0.615701000
C	5.713275000	-0.369585000	-0.762431000
C	5.529170000	1.015295000	-0.854525000
C	3.301137000	-0.652631000	-0.550070000
C	4.245316000	1.555127000	-0.785093000
H	4.728663000	-2.273412000	-0.546916000
H	6.388586000	1.677496000	-0.972061000
H	4.111605000	2.635998000	-0.847058000
H	1.960249000	2.454583000	-0.236315000
H	6.713927000	-0.801367000	-0.805054000
H	-1.634447000	0.392020000	4.181382000
O	-0.701907000	-1.057424000	2.080403000
C	-1.123129000	-0.568060000	4.350651000
H	-1.891980000	-1.352645000	4.357504000
C	-0.139113000	-0.800988000	3.215417000

H	-0.607196000	-0.536365000	5.316665000
Pd	0.343679000	-1.136239000	0.263058000
O	1.081143000	-0.730253000	3.403181000
H	1.259753000	0.883674000	1.473910000
H	-1.445995000	-6.132696000	-0.593287000
C	-1.209223000	-4.080200000	-0.246573000
C	-2.058722000	-5.224946000	-0.507808000
N	-0.557250000	-3.149328000	-0.046202000
H	-2.605791000	-5.061135000	-1.446834000
H	-2.775388000	-5.341638000	0.316938000
C	2.206190000	-1.644109000	-0.420256000
O	2.357602000	-2.833203000	-0.496133000
H	0.818792000	-1.040487000	-1.219129000
H	-1.295514000	-0.422754000	-1.929058000
C	-4.311587000	-1.074296000	-2.605095000
H	-4.896377000	-0.198548000	-2.294538000
H	-4.985722000	-1.941155000	-2.658059000
H	-3.905373000	-0.888903000	-3.609013000
C	-3.716047000	-1.704405000	-0.211542000
H	-2.597641000	-2.199013000	-1.971541000
H	-4.433810000	-0.953542000	0.138764000
H	-2.896471000	-1.764387000	0.514272000
H	-4.220792000	-2.679321000	-0.250691000

TS4
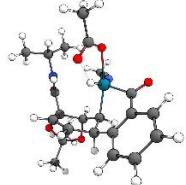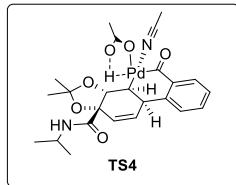
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Multiplicity: 1
$E_{B3LYP-D3}$: -1622.143178 a.u.
ΔG_{corr}: 0.432877 a.u.
One imaginary freq: -278.1558 cm^{-1}

C	-0.440285000	1.502380000	-1.930664000
C	0.854055000	1.721240000	-1.674926000
C	1.413485000	1.871141000	-0.273827000
C	0.507618000	1.221811000	0.765433000
C	-1.506885000	1.420502000	-0.865521000
C	-0.938235000	1.638531000	0.565333000
H	-0.794964000	1.440566000	-2.961629000
H	1.551940000	1.836024000	-2.506103000
O	-2.389490000	2.529679000	-1.043819000
C	-2.362288000	0.122530000	-0.903324000
N	-1.773246000	-0.944104000	-1.480595000
O	-3.476513000	0.098677000	-0.387357000
O	-1.058763000	3.060326000	0.716658000
H	-1.592501000	1.144061000	1.294353000
C	-2.235535000	3.469597000	0.034938000
C	-2.007209000	4.855631000	-0.539135000
H	-1.121689000	4.845396000	-1.186099000
H	-2.881497000	5.164245000	-1.126491000
H	-1.858301000	5.580769000	0.271634000
C	-3.457406000	3.392450000	0.945861000
H	-3.571036000	2.378823000	1.346696000
H	-3.351536000	4.105799000	1.774106000

H	-4.361388000	3.644194000	0.375562000
C	-2.386969000	-2.273426000	-1.634737000
C	2.879848000	1.472283000	-0.207357000
C	4.746701000	0.068527000	0.522670000
C	5.650784000	0.881420000	-0.149739000
C	5.177687000	2.002339000	-0.845808000
C	3.363335000	0.348757000	0.492787000
C	3.814501000	2.291168000	-0.861889000
H	5.093134000	-0.805997000	1.073437000
H	5.875517000	2.655665000	-1.372397000
H	3.456875000	3.176014000	-1.391165000
H	1.405625000	2.959101000	-0.069647000
H	6.716754000	0.650350000	-0.129432000
H	1.990995000	-4.918444000	-1.419610000
O	0.620773000	-2.988074000	0.163837000
C	1.000830000	-4.493697000	-1.643182000
H	0.242232000	-5.134649000	-1.178159000
C	0.942996000	-3.101029000	-1.059405000
H	0.869913000	-4.468520000	-2.730829000
Pd	0.575444000	-0.850452000	0.727401000
O	1.232637000	-2.118265000	-1.802602000
H	0.813740000	1.529707000	1.775100000
H	-3.651337000	-0.604263000	4.031043000
C	-2.037379000	-1.303333000	2.898710000
C	-3.354351000	-1.500702000	3.469297000
N	-0.997916000	-1.140984000	2.419710000
H	-3.341154000	-2.369601000	4.141679000
H	-4.071440000	-1.677301000	2.655445000
C	2.482702000	-0.607467000	1.207351000
O	2.850522000	-1.346412000	2.085812000
H	1.142714000	-0.930789000	-0.724247000
H	-0.867824000	-0.809414000	-1.915665000
C	-3.579473000	-2.221481000	-2.594837000
H	-4.388143000	-1.610420000	-2.174142000
H	-3.963235000	-3.236359000	-2.768846000
H	-3.281066000	-1.793586000	-3.561779000
C	-2.741419000	-2.912280000	-0.289902000
H	-1.601020000	-2.881602000	-2.100760000
H	-3.529836000	-2.345545000	0.218232000
H	-1.858791000	-2.960076000	0.356463000
H	-3.100950000	-3.936557000	-0.459957000

TS5
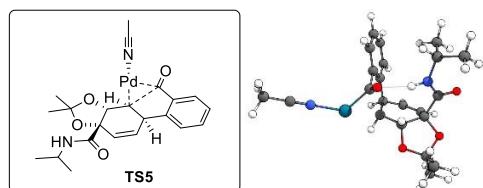
Charge: 0
Multiplicity: 1
$E_{B3LYP-D3}$: -1392.929152 a.u.
ΔG_{corr}: 0.379371 a.u.
One imaginary freq: -341.2578 cm^{-1}

C	-2.369325000	-0.383250000	1.883871000
C	-1.282252000	-0.019215000	2.569229000
C	0.099087000	0.040609000	1.959186000
C	0.270074000	-0.921210000	0.773606000

C	-2.338874000	-0.735997000	0.416521000
C	-0.973105000	-1.359119000	0.000602000
H	-3.355317000	-0.398557000	2.348225000
H	-1.374978000	0.264990000	3.619278000
O	-3.267194000	-1.796455000	0.145278000
C	-2.865667000	0.511794000	-0.346997000
N	-2.036676000	1.116112000	-1.212456000
O	-4.000072000	0.918567000	-0.087494000
O	-1.213691000	-2.749280000	0.263234000
H	-0.825614000	-1.240150000	-1.082517000
C	-2.562458000	-3.030310000	-0.073070000
C	-3.085683000	-4.090986000	0.878824000
H	-2.978081000	-3.743675000	1.913522000
H	-4.145150000	-4.289422000	0.671870000
H	-2.523187000	-5.024984000	0.748139000
C	-2.701919000	-3.427290000	-1.540546000
H	-2.284254000	-2.649364000	-2.191712000
H	-2.175002000	-4.372798000	-1.725747000
H	-3.762915000	-3.559838000	-1.790204000
C	-2.289095000	2.418216000	-1.849553000
C	0.481348000	1.462848000	1.552633000
C	1.357522000	2.898334000	-0.216266000
C	1.218469000	4.008595000	0.615723000
C	0.699126000	3.848649000	1.909553000
C	1.001811000	1.629549000	0.263894000
C	0.321359000	2.585294000	2.373026000
H	1.740919000	3.002072000	-1.232100000
H	0.579819000	4.719002000	2.557225000
H	-0.098789000	2.474296000	3.373440000
H	0.815244000	-0.261582000	2.739124000
H	1.500711000	4.999808000	0.257867000
Pd	2.367752000	-0.962760000	0.052105000
H	0.702587000	-1.861190000	1.155974000
C	1.093564000	0.405409000	-0.578946000
O	0.740949000	0.392910000	-1.757060000
H	-1.127664000	0.713965000	-1.411140000
C	-2.425696000	3.529836000	-0.804768000
H	-3.334484000	3.392331000	-0.205668000
H	-2.482445000	4.506223000	-1.305739000
H	-1.557607000	3.534361000	-0.132819000
C	-3.468594000	2.367600000	-2.823661000
H	-1.376309000	2.609906000	-2.429842000
H	-4.407610000	2.183640000	-2.287106000
H	-3.325082000	1.569201000	-3.565094000
H	-3.551154000	3.324676000	-3.357890000
N	4.334122000	-0.880566000	-0.543276000
C	5.442776000	-0.831240000	-0.869787000
H	6.911710000	-0.176774000	-2.206553000
C	6.830688000	-0.764448000	-1.281053000
H	7.426468000	-0.285565000	-0.491126000
H	7.210600000	-1.780374000	-1.459924000

TS6
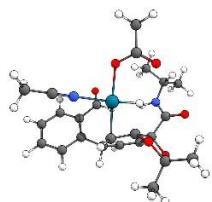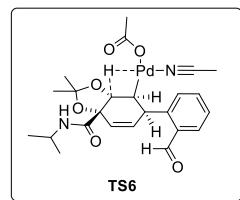

Charge: 0
Multiplicity: 1
$E_{B3LYP-D3}$: -1622.13955 a.u.
ΔG_{corr}: 0.429161 a.u.
One imaginary freq: -292.1967 cm^{-1}

C	-1.003021000	-1.786542000	2.003299000
C	0.325287000	-1.935331000	2.003406000
C	1.186539000	-1.979777000	0.769798000
C	0.448910000	-1.589333000	-0.509334000
C	-1.813311000	-1.499825000	0.766853000
C	-0.947125000	-1.369455000	-0.503441000
H	-1.564969000	-1.846516000	2.936198000
H	0.841445000	-2.122149000	2.947087000
O	-2.623648000	-2.620940000	0.427304000
C	-2.736937000	-0.252285000	0.967710000
N	-2.156838000	0.768462000	1.622880000
O	-3.876506000	-0.223981000	0.517777000
O	-1.737640000	-1.840437000	-1.534551000
H	-1.263997000	0.322908000	-0.815251000
C	-2.568522000	-2.887818000	-0.984433000
C	-1.895209000	-4.235550000	-1.195940000
H	-0.886825000	-4.224448000	-0.763622000
H	-2.483035000	-5.020639000	-0.702721000
H	-1.828882000	-4.462595000	-2.267634000
C	-3.944828000	-2.781262000	-1.604651000
H	-4.370043000	-1.799147000	-1.376161000
H	-3.874043000	-2.919466000	-2.691524000
H	-4.593750000	-3.565956000	-1.194687000
C	-2.732088000	2.113902000	1.699597000
C	2.591162000	-1.395390000	0.917639000
C	4.227815000	0.298730000	1.574118000
C	5.269881000	-0.481828000	1.086548000
C	4.978373000	-1.721832000	0.506892000
C	2.891597000	-0.134218000	1.487993000
C	3.657716000	-2.168519000	0.436046000
H	4.426681000	1.275640000	2.014817000
H	5.781561000	-2.346153000	0.112065000
H	3.446446000	-3.143424000	-0.005729000
H	1.365473000	-3.060600000	0.624604000
H	6.299269000	-0.126976000	1.147890000
O	-2.274621000	2.295527000	-1.704449000
C	-1.256545000	4.457599000	-1.898969000
C	-1.224236000	2.949706000	-1.696142000
Pd	0.251176000	0.443971000	-1.027230000
O	-0.042217000	2.470374000	-1.497980000
H	0.839019000	-2.064155000	-1.411668000
H	5.296191000	0.107452000	-2.232086000
C	3.414083000	0.890014000	-1.776027000
C	4.809781000	1.084995000	-2.112933000
N	2.306913000	0.730020000	-1.493296000

H	5.303599000	1.639216000	-1.303577000
H	4.887452000	1.653188000	-3.050055000
C	1.836203000	0.797870000	1.943601000
O	2.055571000	1.878419000	2.467369000
H	0.794439000	0.477126000	1.767338000
H	-1.208998000	0.644027000	1.954431000
H	-0.423662000	4.784334000	-2.535408000
H	-1.136321000	4.941401000	-0.917565000
H	-2.212497000	4.772359000	-2.332783000
C	-3.738999000	2.223677000	2.846008000
H	-4.538122000	1.479400000	2.733417000
H	-4.195299000	3.224113000	2.854544000
H	-3.241520000	2.061257000	3.813868000
C	-1.592989000	3.122867000	1.824105000
H	-3.250529000	2.275160000	0.744884000
H	-1.056339000	2.985707000	2.775378000
H	-1.991172000	4.145359000	1.802429000
H	-0.874934000	3.007475000	1.002792000

TS7
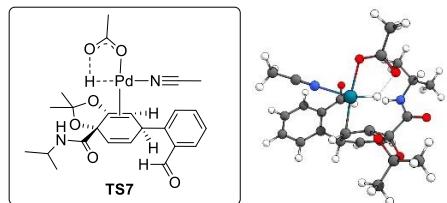


Charge: 0
Multiplicity: 1
$E_{B3LYP-D3}$: -1622.137719 a.u.
ΔG_{corr}: 0.431284 a.u.
One imaginary freq: -199.6920 cm^{-1}

C	0.840989000	1.711303000	2.022366000
C	-0.487236000	1.854875000	1.986828000
C	-1.306525000	1.931177000	0.726295000
C	-0.525980000	1.561079000	-0.532965000
C	1.691682000	1.479914000	0.799693000
C	0.868797000	1.350514000	-0.491531000
H	1.372890000	1.742204000	2.974261000
H	-1.033961000	2.008159000	2.919404000
O	2.465727000	2.644605000	0.512737000
C	2.666201000	0.277629000	1.036339000
N	2.082915000	-0.808357000	1.574424000
O	3.857592000	0.348850000	0.758143000
O	1.693814000	1.856223000	-1.491355000
H	1.353065000	-0.468697000	-1.046774000
C	2.460044000	2.922285000	-0.898352000
C	1.756349000	4.252993000	-1.123926000
H	0.730689000	4.205038000	-0.737148000
H	2.296105000	5.050457000	-0.596526000
H	1.729963000	4.491470000	-2.195032000
C	3.866349000	2.867720000	-1.458155000
H	4.313624000	1.898008000	-1.217510000
H	3.839874000	3.011467000	-2.546418000
H	4.471795000	3.668948000	-1.014934000
C	2.761525000	-2.094003000	1.744729000
C	-2.717107000	1.349895000	0.818123000
C	-4.384593000	-0.331706000	1.431123000
C	-5.406217000	0.452116000	0.906839000

C	-5.088748000	1.686593000	0.328596000
C	-3.043738000	0.092612000	1.383321000
C	-3.764029000	2.125905000	0.298208000
H	-4.602639000	-1.305923000	1.868660000
H	-5.875429000	2.313595000	-0.094526000
H	-3.533986000	3.098393000	-0.139688000
H	-1.476455000	3.015863000	0.597401000
H	-6.439268000	0.103990000	0.938321000
O	2.453803000	-1.684535000	-1.559942000
C	2.112767000	-4.009109000	-1.997602000
C	1.621663000	-2.608259000	-1.702664000
Pd	-0.210242000	-0.459265000	-1.040472000
O	0.356985000	-2.457789000	-1.575085000
H	-0.906997000	2.026347000	-1.444478000
H	-5.296514000	-0.717710000	-2.256667000
C	-3.358707000	-1.270733000	-1.705183000
C	-4.730955000	-1.625582000	-2.006953000
N	-2.271804000	-0.981645000	-1.445062000
H	-5.182357000	-2.103339000	-1.126957000
H	-4.754944000	-2.321118000	-2.857217000
C	-2.006476000	-0.849015000	1.860394000
O	-2.244495000	-1.926833000	2.382333000
H	-0.959249000	-0.539550000	1.697440000
H	1.084370000	-0.781832000	1.733282000
H	1.361392000	-4.583833000	-2.551703000
H	2.290282000	-4.511866000	-1.034660000
H	3.059829000	-3.981618000	-2.548846000
C	3.653111000	-2.089321000	2.988521000
H	4.385832000	-1.273864000	2.935838000
H	4.197244000	-3.041489000	3.068291000
H	3.046066000	-1.959039000	3.896927000
C	1.709376000	-3.199153000	1.791949000
H	3.390747000	-2.230742000	0.854450000
H	1.069144000	-3.083716000	2.680307000
H	2.195424000	-4.181472000	1.848209000
H	1.068134000	-3.174487000	0.901869000

TS8
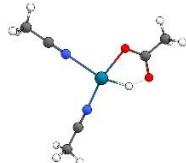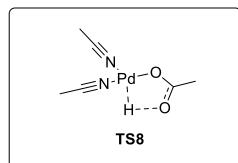
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Multiplicity: 1
$E_{B3LYP-D3}$: -622.8281241 a.u.
ΔG_{corr}: 0.099126 a.u.
One imaginary freq: -966.8673 cm^{-1}

H	3.978770000	-3.137780000	0.896089000
C	3.359389000	-3.287443000	-0.000002000
H	3.978766000	-3.137783000	-0.896096000
C	2.261756000	-2.338252000	-0.000001000
N	1.383613000	-1.583058000	0.000000000
H	2.964404000	-4.313439000	0.000001000
H	3.349628000	4.036536000	-0.896178000
Pd	-0.075541000	-0.220748000	0.000002000
H	-1.388623000	-1.291273000	-0.000004000

N	1.268138000	1.842171000	0.000009000
C	1.908980000	2.805728000	0.000002000
C	2.713479000	4.015082000	-0.000007000
O	-1.976779000	0.817397000	0.000003000
H	-4.415894000	1.509383000	0.000001000
H	2.056929000	4.896595000	0.000001000
H	3.349650000	4.036535000	0.896148000
C	-2.908592000	-0.026601000	-0.000002000
C	-4.343488000	0.416767000	-0.000001000
H	-4.849883000	0.007547000	0.885981000
O	-2.674518000	-1.290513000	-0.000006000
H	-4.849883000	0.007551000	-0.885986000

TS9
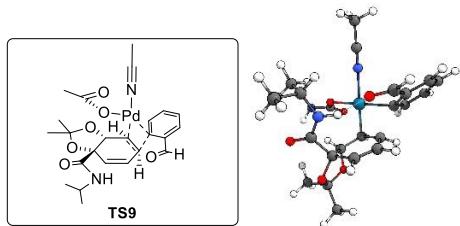
Charge: 0
Multiplicity: 1
$E_{B3LYP-D3}$: -1622.129966 a.u.
ΔG_{corr}: 0.432092 a.u.
One imaginary freq: -312.0805 -cm^{-1}

C	1.367679000	-1.127129000	-2.066771000
C	0.282569000	-1.859268000	-1.779036000
C	-0.172612000	-2.083956000	-0.395510000
C	0.570852000	-1.485797000	0.694700000
C	2.202566000	-0.410159000	-1.037568000
C	1.936042000	-0.899509000	0.414741000
H	1.705848000	-1.022971000	-3.098749000
H	-0.283194000	-2.344627000	-2.574431000
O	3.564616000	-0.764409000	-1.259837000
C	2.074363000	1.145077000	-1.108384000
N	0.877957000	1.588723000	-1.517565000
O	2.902889000	-1.946618000	0.557687000
H	2.160837000	-0.090219000	1.119939000
C	4.062192000	-1.555509000	-0.166508000
C	4.733233000	-2.799627000	-0.716435000
H	4.021064000	-3.361142000	-1.333180000
H	5.598557000	-2.516510000	-1.329295000
H	5.082182000	-3.435359000	0.107731000
C	4.990538000	-0.704885000	0.695593000
H	4.458090000	0.167568000	1.090655000
H	5.378997000	-1.305310000	1.528963000
H	5.835072000	-0.350756000	0.089989000
C	-2.096307000	-1.554647000	-0.167371000
C	-4.200556000	-1.775833000	-1.396063000
C	-4.747789000	-2.542572000	-0.370472000
C	-3.968716000	-2.832962000	0.755864000
C	-2.892931000	-1.256383000	-1.306987000
C	-2.652922000	-2.375562000	0.833623000
H	-4.797275000	-1.543948000	-2.280582000
H	-2.035722000	-2.674579000	1.681977000
H	-0.532289000	-3.096542000	-0.225506000

H	-5.768401000	-2.918441000	-0.450083000
Pd	-0.913295000	-0.086256000	0.777075000
H	0.554541000	-2.033392000	1.640247000
H	-4.376455000	-3.438730000	1.566665000
O	0.213188000	1.235307000	1.950071000
O	0.268193000	-0.143141000	3.725223000
C	0.595533000	0.894439000	3.132311000
C	1.555288000	1.887183000	3.773741000
H	2.540128000	1.776241000	3.294050000
H	1.219517000	2.918131000	3.599535000
H	1.658607000	1.697237000	4.848141000
H	-3.941692000	3.935845000	-0.393442000
C	-4.313237000	3.181920000	0.314723000
H	-5.223534000	2.717325000	-0.088996000
C	-3.297807000	2.166346000	0.509660000
N	-2.484353000	1.359646000	0.652114000
H	-4.542843000	3.664519000	1.274982000
C	-2.500995000	-0.351928000	-2.400105000
O	-1.532668000	0.388442000	-2.421531000
H	-3.201206000	-0.359921000	-3.263513000
O	3.016422000	1.859304000	-0.772665000
C	0.469972000	2.996427000	-1.611956000
H	0.155502000	0.910608000	-1.746780000
C	1.241935000	3.723860000	-2.716872000
H	2.310907000	3.772418000	-2.471231000
H	0.863416000	4.749909000	-2.827947000
H	1.125773000	3.205609000	-3.678979000
C	0.546880000	3.722385000	-0.266507000
H	-0.586361000	2.944450000	-1.908433000
H	0.082231000	4.714262000	-0.358623000
H	1.590516000	3.853266000	0.046229000
H	0.027775000	3.151696000	0.511327000

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