# Hiyama Cross-Coupling of Arenediazonium Salts under Mild Reaction Conditions

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## Supporting Information

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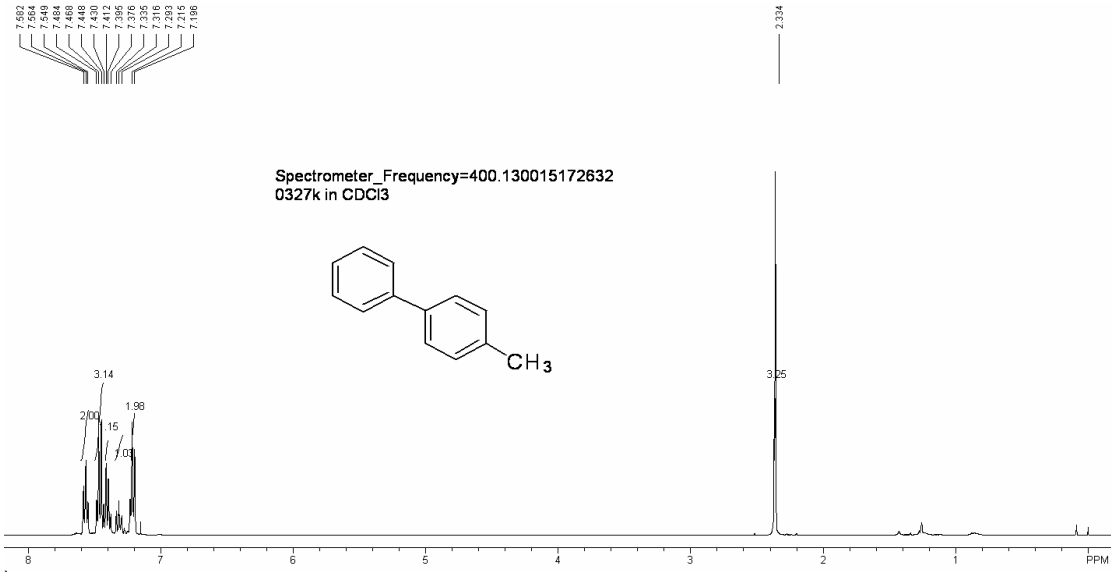
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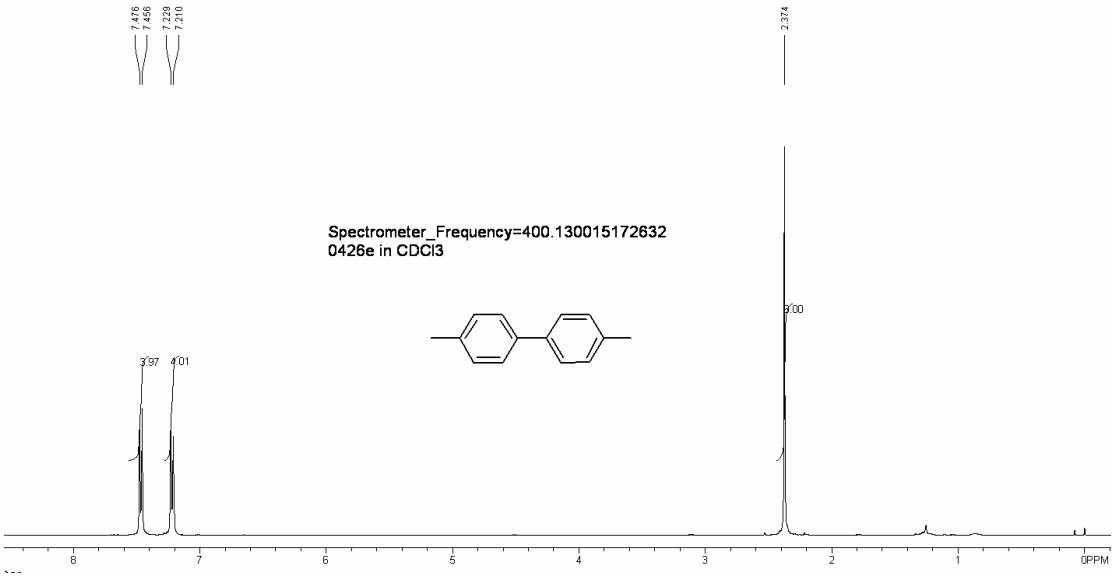
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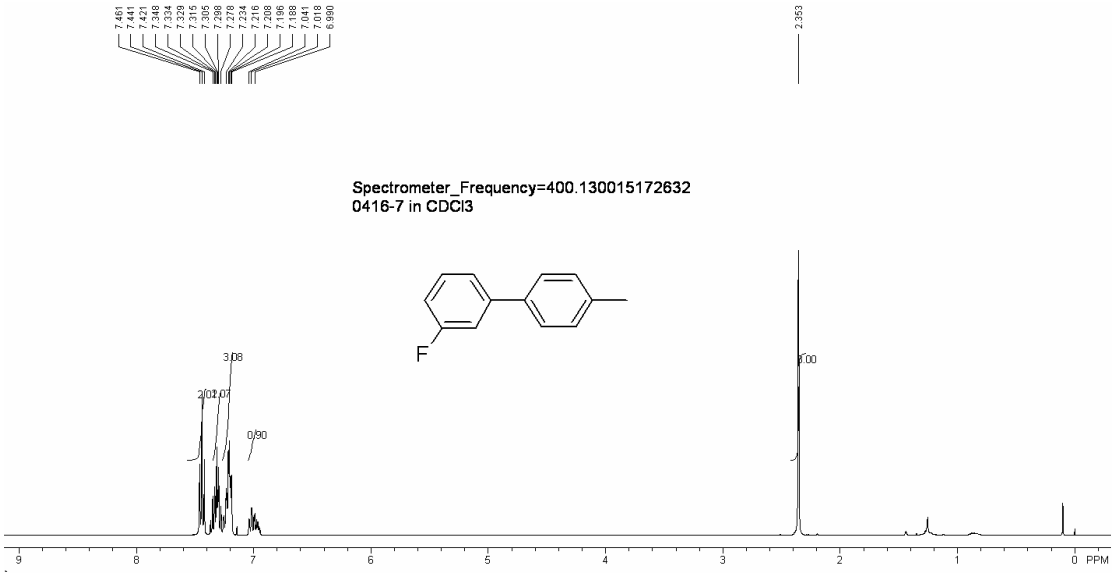
## 4-methyl-1,1'-biphenyl (T3-1, CAS#644-08-6)



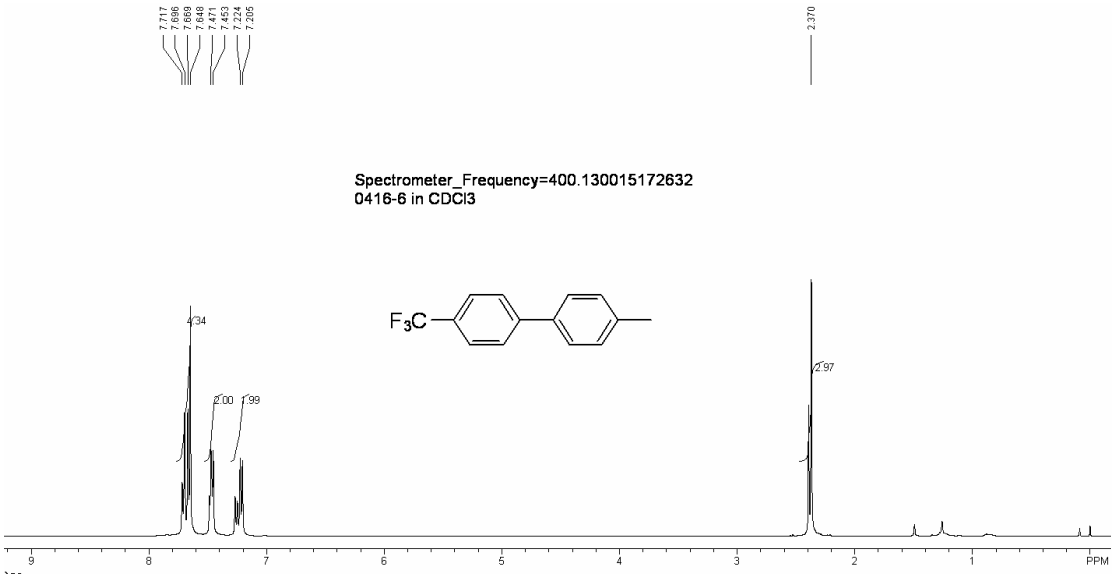

## 4,4'-dimethyl-1,1'-biphenyl (T3-4, CAS#613-33-2)



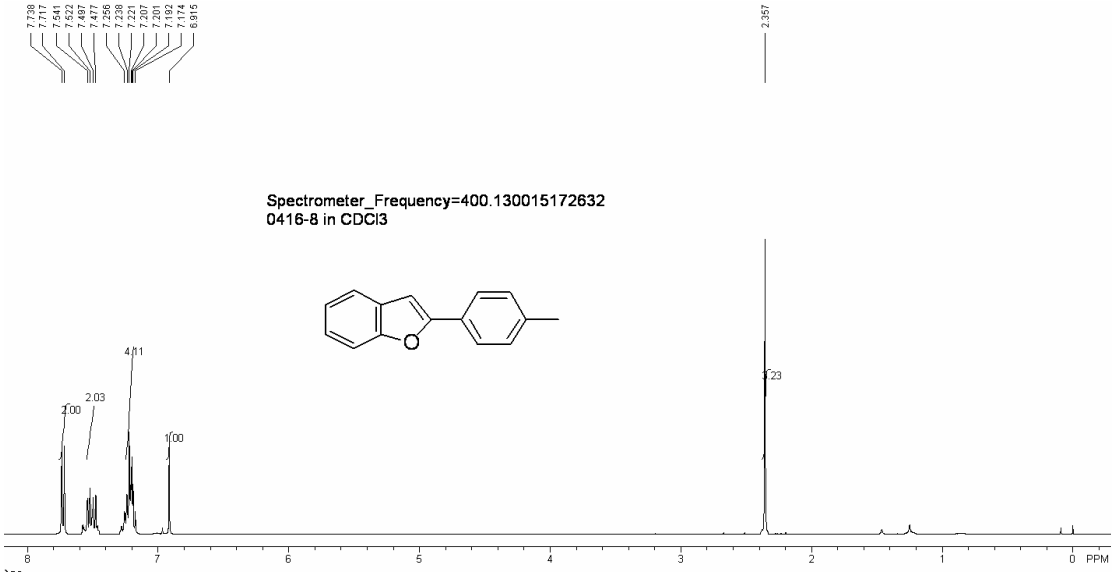
## 3-fluoro-4'-methyl-1,1'-biphenyl (T3-5, CAS#72093-42-6)



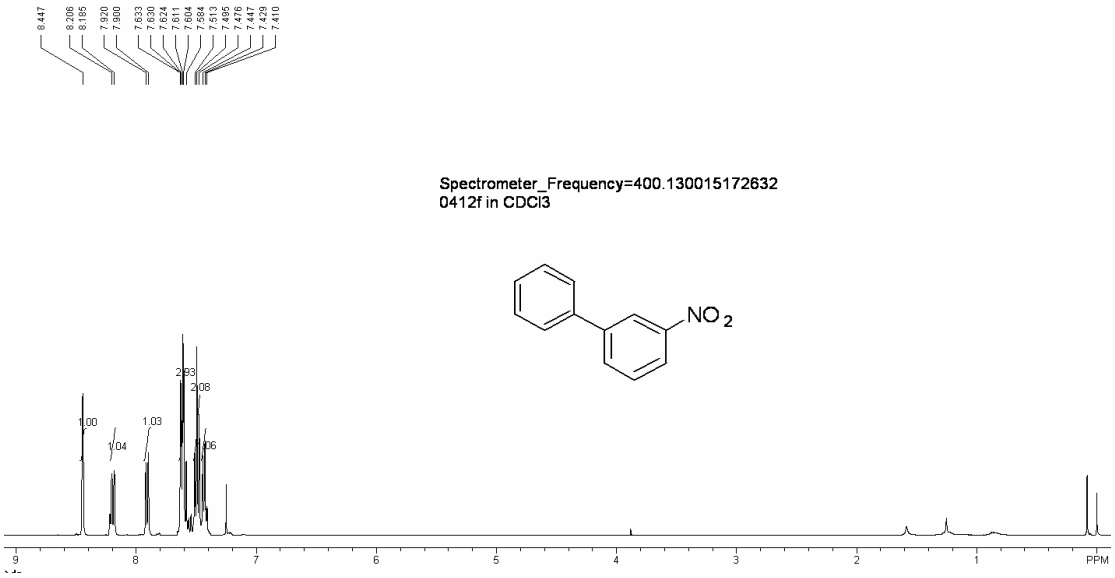

## 4-methyl-4'-(trifluoromethyl)-1,1'-biphenyl (T3-6, CAS#97067-18-0)



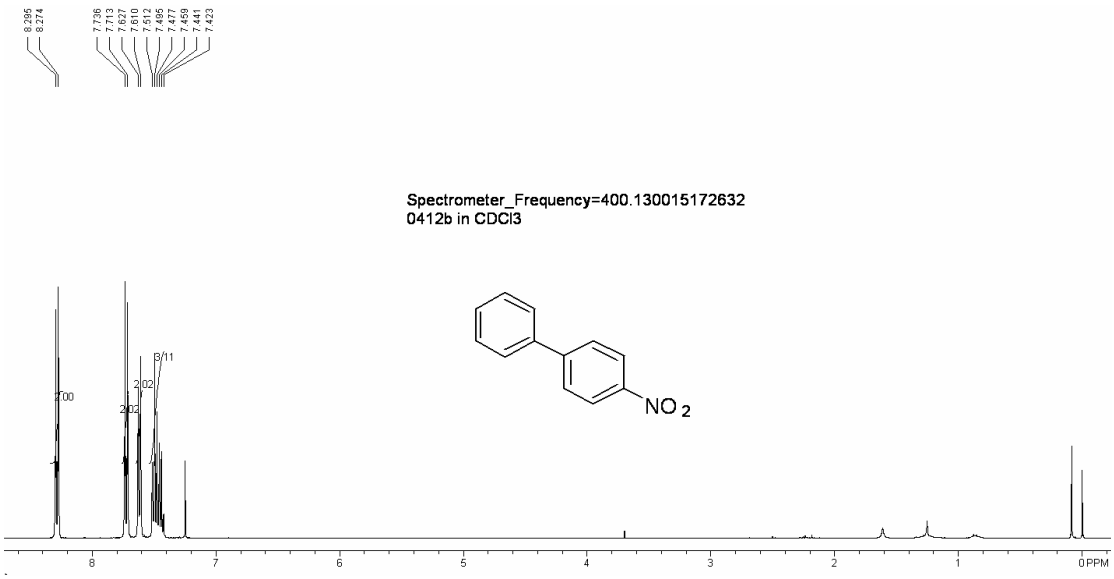
## 2-(p-tolyl)benzofuran (T3-7, CAS#25664-48-6)



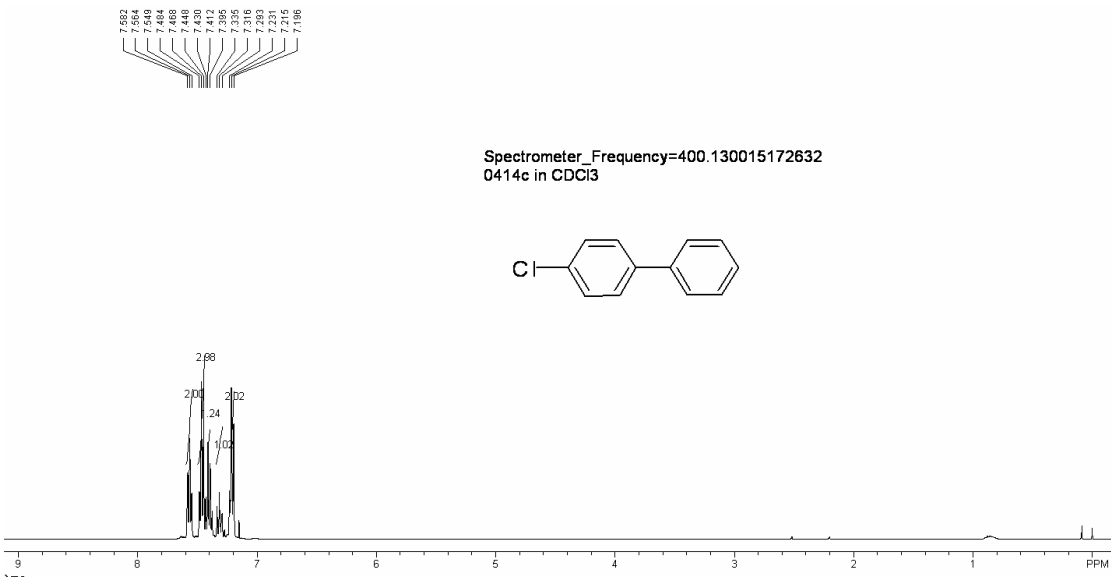

## 3-nitro-1,1'-biphenyl (T4-1, CAS#2113-58-8)



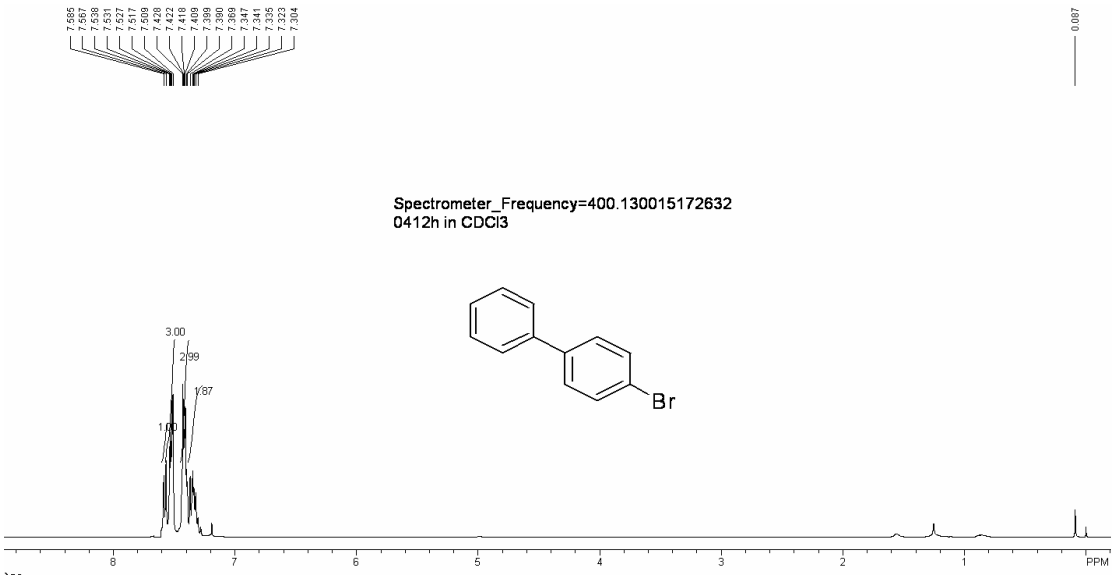
## 4-nitro-1,1'-biphenyl (T4-2, CAS#92-93-3)



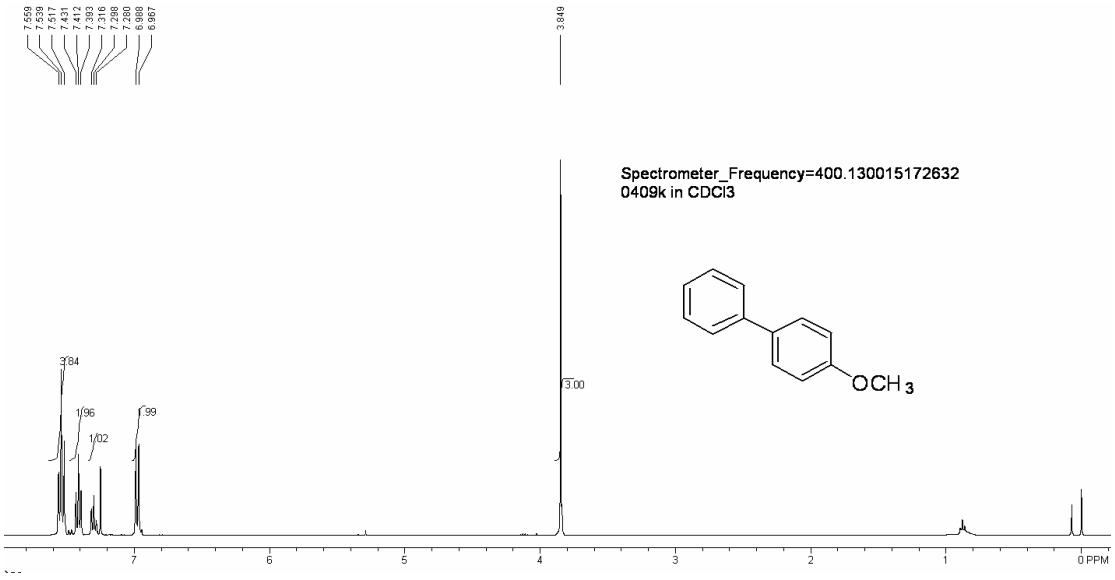

## 4-cholro-1,1'-biphenyl (T4-3, CAS#644-08-6)



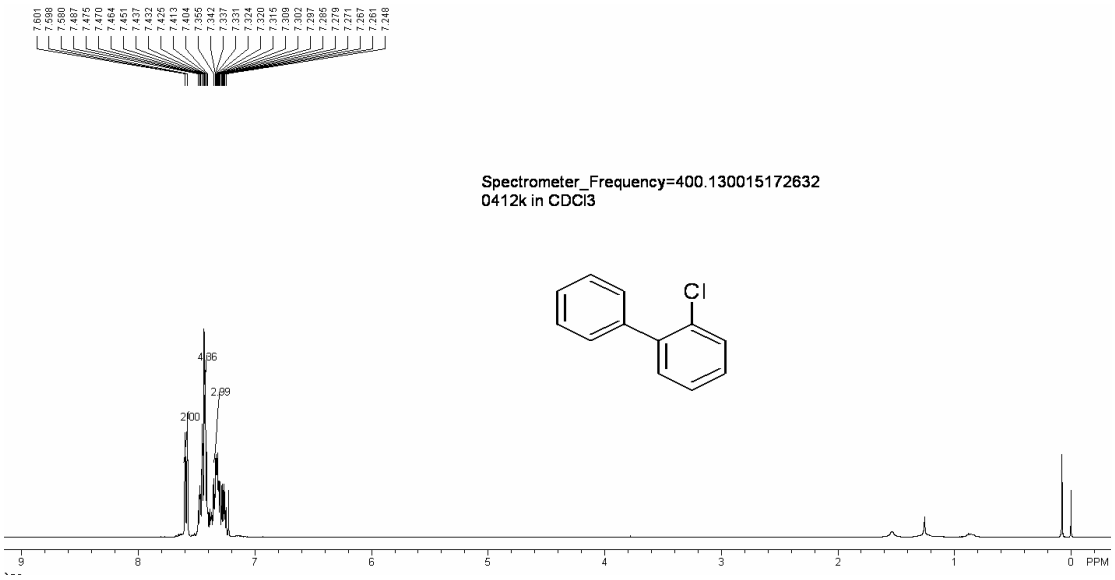
## 4-bromo-1,1'-biphenyl (T4-4, CAS#92-66-0)



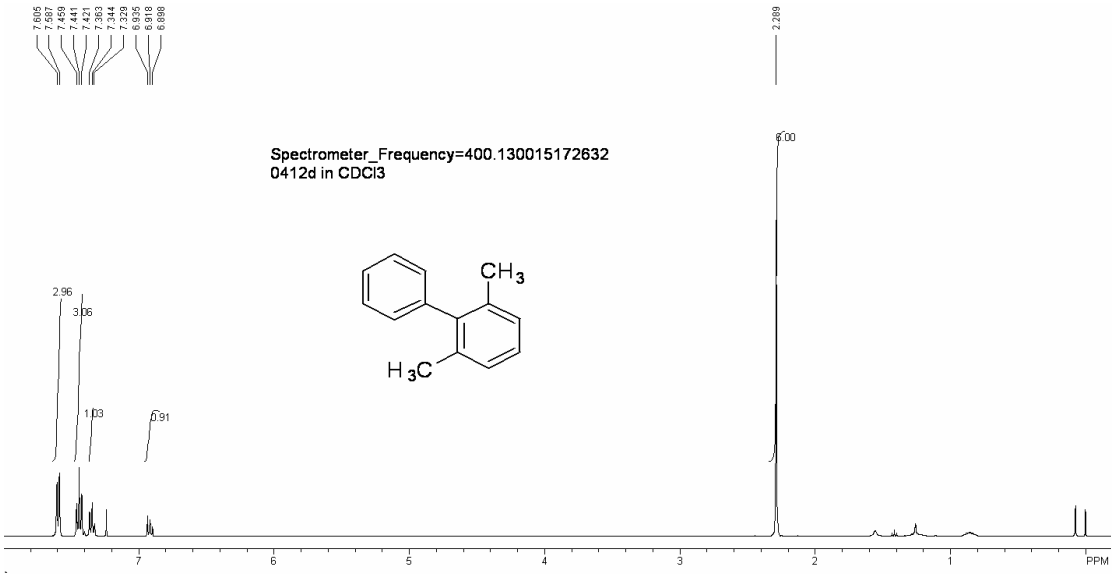

## 4-methoxy-1,1'-biphenyl (T4-6, CAS#613-37-6)



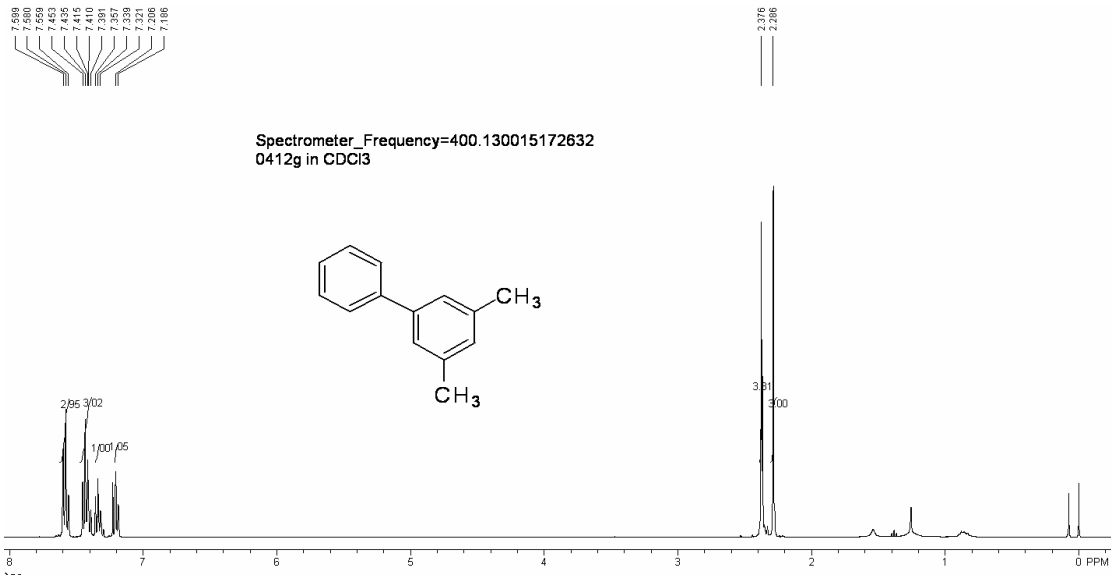
## 2-chloro-1,1'-biphenyl (T4-7, CAS#2051-60-7)



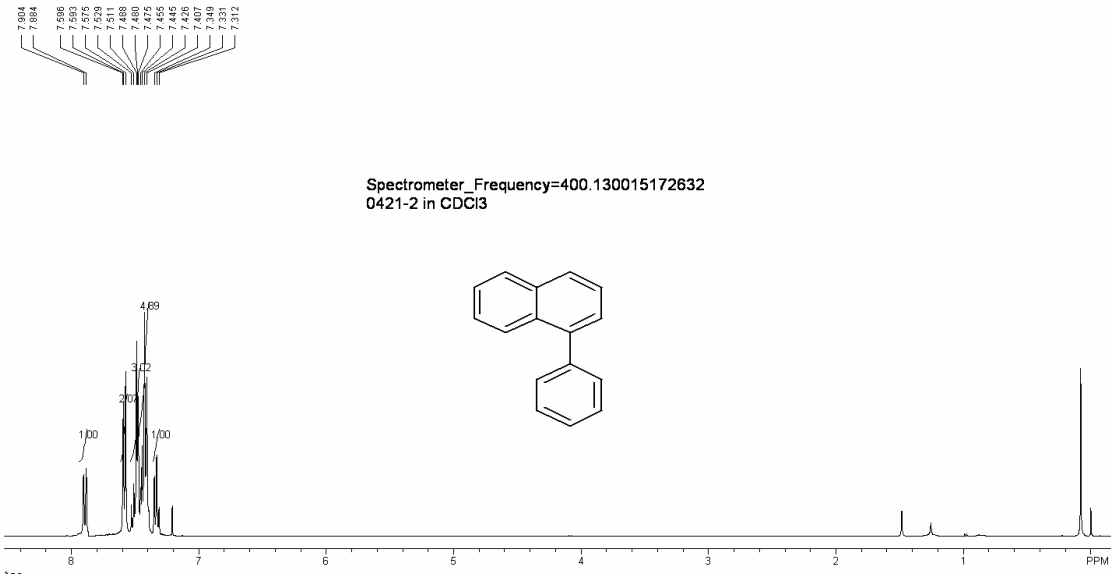

## 2,6-dimethyl-1,1'-biphenyl (T4-8, CAS#3976-34-9)



## 3,5-dimethyl-1,1'-biphenyl (T4-9, CAS#17057-88-4)




## 1-phenylnaphthalene (T4-10, CAS#605-02-7)



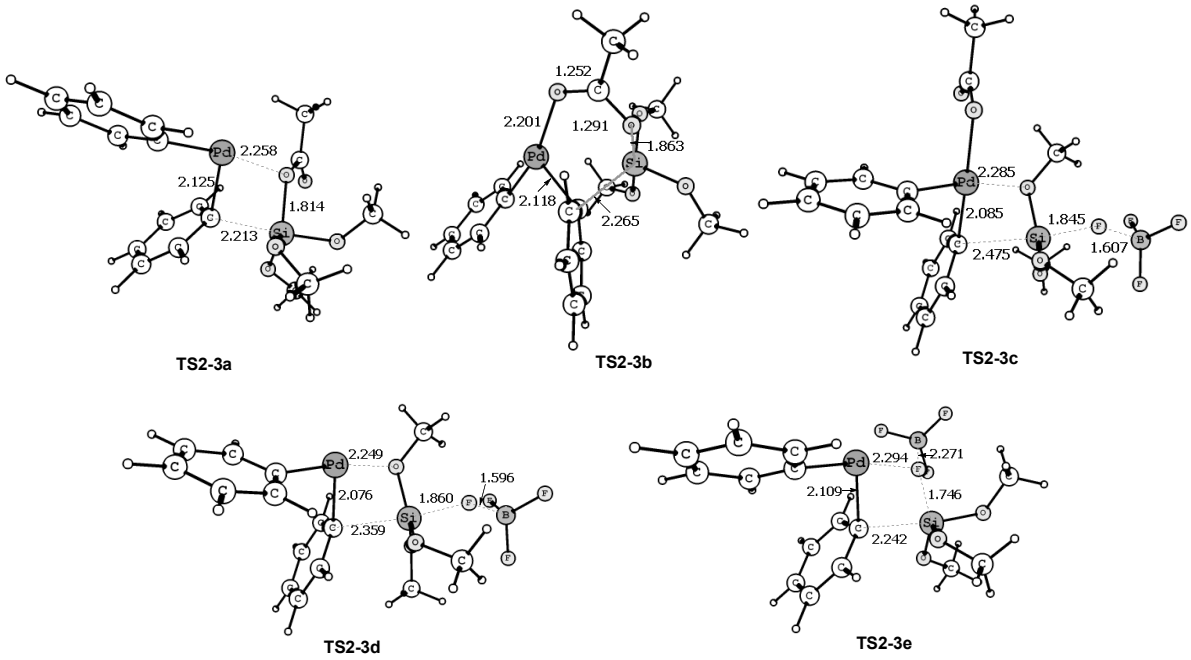



**Figure S1.** Optimized structures of the transition states as shown in Scheme 3.

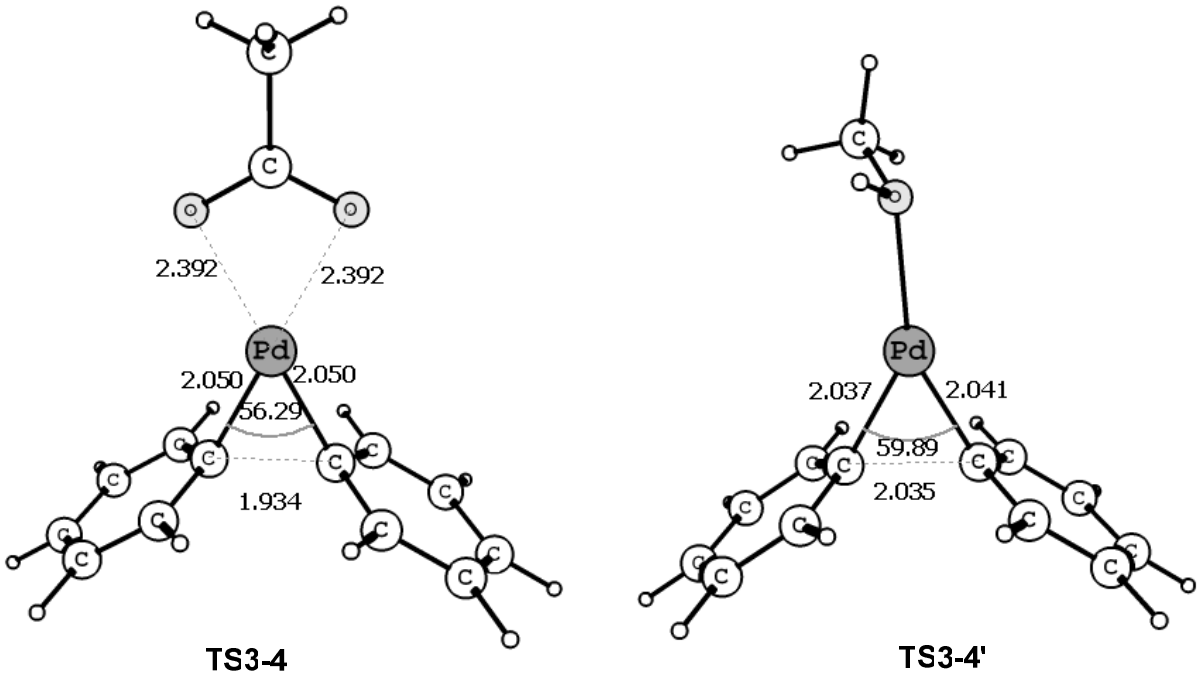



**Figure S2.** Optimized structures of relevant transition states involved in the reductive elimination step.

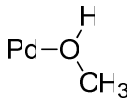
# Energy properties and Cartesian Coordinates of Reactants, Intermediates and Transition States

## $CH_3OH$

TCG(Thermal correction to Gibbs Free Energy) = 0.028492，

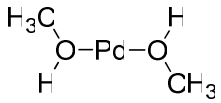
E(M06) = -115.7036056

| | | | |
|---|---|---|---|
| 6 | 0.667328000 | -0.018783000 | 0.000000000 |
| 1 | 1.089514000 | 0.990097000 | -0.000002000 |
| 1 | 1.030060000 | -0.547908000 | -0.892335000 |
| 1 | 1.030060000 | -0.547905000 | 0.892337000 |
| 8 | -0.753098000 | 0.123689000 | 0.000000000 |
| 1 | -1.128821000 | -0.771098000 | 0.000000000 |



TCG = 0.024175, E(M06) = -242.4292412

| | | | |
|---|---|---|---|
| 46 | -0.756300000 | -0.040345000 | 0.003592000 |
| 8 | 1.357581000 | 0.595254000 | -0.125933000 |
| 1 | 1.490113000 | 1.287619000 | 0.541814000 |
| 6 | 2.407062000 | -0.382740000 | 0.026130000 |
| 1 | 2.235001000 | -1.145062000 | -0.733792000 |
| 1 | 3.380850000 | 0.090807000 | -0.141080000 |
| 1 | 2.380815000 | -0.843089000 | 1.018527000 |



TCG = 0.072182, E(M06) = -358.1562238

| | | | |
|---|---|---|---|
| 46 | 0.001344000 | -0.206499000 | -0.009630000 |
| 8 | -2.108409000 | -0.195025000 | -0.423846000 |
| 1 | -2.437886000 | -1.092462000 | -0.249610000 |
| 8 | 2.119374000 | -0.269953000 | 0.359957000 |
| 1 | 2.236635000 | -0.200149000 | 1.322140000 |
| 6 | -2.969210000 | 0.742758000 | 0.261263000 |
| 1 | -2.600253000 | 1.738595000 | 0.017445000 |
| 1 | -3.994955000 | 0.626747000 | -0.103659000 |
| 1 | -2.935571000 | 0.592213000 | 1.344194000 |
| 6 | 2.974090000 | 0.711098000 | -0.270707000 |
| 1 | 4.014048000 | 0.524032000 | 0.015867000 |
| 1 | 2.857638000 | 0.579923000 | -1.346155000 |
| 1 | 2.681511000 | 1.726728000 | 0.010518000 |

HOAc

TCG = 0.028492，E(M06) = -115.7036056

| | | | |
|---|---|---|---|
| 6 | -0.090843000 | 0.120088000 | -0.000106000 |
| 8 | -0.641665000 | 1.205725000 | 0.000022000 |
| 8 | -0.780957000 | -1.040756000 | -0.000002000 |
| 1 | -1.732326000 | -0.816636000 | 0.000162000 |
| 6 | 1.395960000 | -0.112967000 | -0.000001000 |
| 1 | 1.681127000 | -0.693075000 | 0.883658000 |
| 1 | 1.681055000 | -0.695394000 | -0.882133000 |
| 1 | 1.920417000 | 0.842623000 | -0.001197000 |

$AcO^{\ominus}$

TCG = 0.021351, E(M06) = -228.5928353

| | | | |
|---|---|---|---|
| 6 | 0.192961000 | -0.000259000 | -0.007927000 |
| 8 | 0.796166000 | -1.110022000 | 0.001766000 |
| 8 | 0.727085000 | 1.145502000 | 0.001614000 |
| 6 | -1.353454000 | -0.033595000 | -0.002489000 |
| 1 | -1.723259000 | 0.272298000 | 0.985449000 |
| 1 | -1.758035000 | 0.680461000 | -0.729165000 |
| 1 | -1.741755000 | -1.033477000 | -0.220821000 |

$^{\ominus}$
PdOAc

TCG = , 0.016388 E(M06) = -355.3280048

| | | | |
|---|---|---|---|
| 46 | -1.267239000 | -0.020019000 | 0.009194000 |
| 8 | 1.647781000 | 1.376024000 | -0.012782000 |
| 6 | 1.721519000 | 0.132049000 | -0.032561000 |
| 8 | 0.733659000 | -0.694669000 | -0.076644000 |
| 6 | 3.098133000 | -0.537249000 | 0.041248000 |
| 1 | 3.861509000 | 0.104800000 | -0.406851000 |
| 1 | 3.363011000 | -0.688665000 | 1.095464000 |
| 1 | 3.099047000 | -1.514887000 | -0.448247000 |

$Pd(OAc)_2^{2-}$

TCG = 0.056713, E(M06) = -583.9509963

| | | | |
|---|---|---|---|
| 46 | 0.000331000 | -0.324873000 | -0.007074000 |
| 8 | -2.784702000 | 1.201637000 | -0.951415000 |
| 6 | -2.960597000 | 0.306430000 | -0.099922000 |
| 8 | -2.052177000 | -0.439713000 | 0.424322000 |
| 6 | -4.385633000 | -0.002313000 | 0.373479000 |

| | | | |
|---|---|---|---|
| 1 | -5.016093000 | 0.888665000 | 0.303280000 |
| 1 | -4.820955000 | -0.774001000 | -0.274439000 |
| 1 | -4.395339000 | -0.383323000 | 1.398726000 |
| 8 | 2.052239000 | -0.436458000 | -0.440357000 |
| 6 | 2.963537000 | 0.267481000 | 0.134286000 |
| 8 | 2.791475000 | 1.102404000 | 1.045950000 |
| 6 | 4.377808000 | 0.051600000 | -0.415934000 |
| 1 | 4.487061000 | -0.932342000 | -0.880013000 |
| 1 | 4.584614000 | 0.811630000 | -1.180455000 |
| 1 | 5.120118000 | 0.171366000 | 0.378860000 |

$BF_4^{\ominus}$

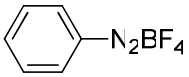
TCG = -0.010905, E(M06) = -424.6525076

| | | | |
|---|---|---|---|
| 9 | 0.811896000 | 0.811896000 | 0.811896000 |
| 9 | -0.811896000 | -0.811896000 | 0.811896000 |
| 9 | -0.811896000 | 0.811896000 | -0.811896000 |
| 9 | 0.811896000 | -0.811896000 | -0.811896000 |
| 5 | 0.000000000 | 0.000000000 | 0.000000000 |

$N_2$

TCG = -0.012842, E(M06) = -109.4971984

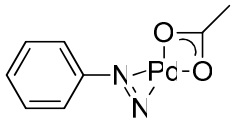
| | | | |
|---|---|---|---|
| 7 | 0.000000000 | 0.000000000 | 0.552521000 |
| 7 | 0.000000000 | 0.000000000 | -0.552521000 |




TCG = 0.070087, E(M06) = -765.4414159

| | | | |
|---|---|---|---|
| 6 | -0.844038000 | -1.383967000 | -0.021349000 |
| 6 | -0.970284000 | -0.001514000 | -0.020040000 |
| 6 | -2.277408000 | 0.517351000 | -0.001761000 |
| 6 | -3.443647000 | -0.270929000 | 0.015966000 |
| 6 | -3.273278000 | -1.646924000 | 0.014301000 |
| 6 | -1.983753000 | -2.197667000 | -0.004694000 |
| 1 | 0.151642000 | -1.811106000 | -0.035160000 |
| 1 | -0.102468000 | 0.648647000 | -0.031405000 |
| 1 | -4.422242000 | 0.193247000 | 0.030311000 |
| 1 | -4.144583000 | -2.292228000 | 0.027643000 |
| 1 | -1.867813000 | -3.276803000 | -0.005929000 |
| 7 | -2.428969000 | 1.883717000 | -0.002143000 |
| 7 | -2.551174000 | 2.988305000 | -0.002744000 |
| 5 | 2.984030000 | 0.056382000 | 0.004576000 |
| 9 | 2.342636000 | -1.197385000 | -0.088249000 |
| 9 | 2.005849000 | 1.078461000 | -0.018057000 |

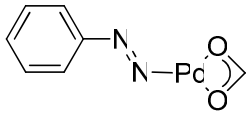
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|---|---|---|---|
| 9 | 3.700570000 | 0.127411000 | 1.206179000 |
| 9 | 3.848808000 | 0.219745000 | -1.085282000 |



**1a**

TCG = 0.108131, E(M06) = -696.1938569

| | | | |
|---|---|---|---|
| 6 | -4.694400000 | -0.646593000 | 0.014681000 |
| 6 | -3.373797000 | -1.081363000 | 0.011630000 |
| 6 | -2.355465000 | -0.115216000 | 0.001290000 |
| 6 | -2.628189000 | 1.256140000 | -0.005898000 |
| 6 | -3.958538000 | 1.672012000 | -0.002843000 |
| 6 | -4.986871000 | 0.724542000 | 0.007461000 |
| 1 | -5.498588000 | -1.375533000 | 0.022700000 |
| 1 | -3.123071000 | -2.136560000 | 0.017155000 |
| 1 | -1.809502000 | 1.968240000 | -0.013729000 |
| 1 | -4.191446000 | 2.731851000 | -0.008456000 |
| 1 | -6.021905000 | 1.052639000 | 0.009913000 |
| 7 | -0.994866000 | -0.506058000 | -0.001899000 |
| 7 | -0.449004000 | -1.575640000 | 0.000319000 |
| 46 | 1.064972000 | -0.254891000 | -0.007115000 |
| 8 | 3.183683000 | -0.835417000 | -0.009561000 |
| 6 | 3.531442000 | 0.393120000 | -0.008386000 |
| 8 | 2.634343000 | 1.298045000 | -0.014423000 |
| 6 | 4.991671000 | 0.763606000 | 0.034582000 |
| 1 | 5.325228000 | 0.773707000 | 1.079306000 |
| 1 | 5.589738000 | 0.025028000 | -0.504941000 |
| 1 | 5.148588000 | 1.758998000 | -0.386834000 |

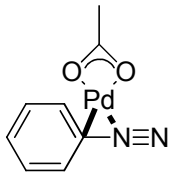


**1b**

TCG = 0.105863, E(M06) = -696.1828185

| | | | |
|---|---|---|---|
| 6 | 4.736638000 | -0.994266000 | 0.002069000 |
| 6 | 3.345541000 | -0.983592000 | -0.002908000 |
| 6 | 2.682207000 | 0.254126000 | -0.002769000 |
| 6 | 3.386353000 | 1.462866000 | 0.001759000 |
| 6 | 4.780644000 | 1.434688000 | 0.007591000 |
| 6 | 5.454095000 | 0.209957000 | 0.007571000 |
| 1 | 5.265175000 | -1.942739000 | 0.001571000 |

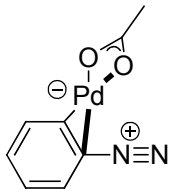
| | | | |
|---|---|---|---|
| 1 | 2.776578000 | -1.907336000 | -0.007495000 |
| 1 | 2.838653000 | 2.399453000 | 0.001310000 |
| 1 | 5.338242000 | 2.365942000 | 0.011846000 |
| 1 | 6.539773000 | 0.189685000 | 0.011608000 |
| 7 | 1.261403000 | 0.352586000 | -0.008129000 |
| 7 | 0.487182000 | -0.556201000 | -0.000251000 |
| 46 | -1.369273000 | -0.596066000 | 0.000109000 |
| 8 | -2.629966000 | 1.276334000 | -0.036373000 |
| 6 | -3.686430000 | 0.562598000 | -0.013876000 |
| 8 | -3.597282000 | -0.708037000 | 0.005956000 |
| 6 | -5.041232000 | 1.226881000 | 0.022685000 |
| 1 | -5.401428000 | 1.240097000 | 1.058380000 |
| 1 | -4.981146000 | 2.255701000 | -0.338296000 |
| 1 | -5.758289000 | 0.657586000 | -0.574657000 |




**1c**

TCG = 0.104439, E(M06) = -696.1750343

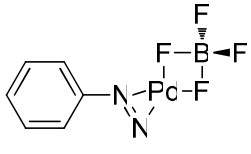
| | | | |
|---|---|---|---|
| 6 | -3.134026000 | -1.025133000 | -1.215281000 |
| 6 | -2.171364000 | -0.017531000 | -1.228958000 |
| 6 | -1.696744000 | 0.458721000 | 0.004483000 |
| 6 | -2.160753000 | -0.030936000 | 1.236745000 |
| 6 | -3.123581000 | -1.038397000 | 1.220427000 |
| 6 | -3.606505000 | -1.530450000 | 0.001926000 |
| 1 | -3.517733000 | -1.411980000 | -2.153902000 |
| 1 | -1.803992000 | 0.406772000 | -2.157112000 |
| 1 | -1.785637000 | 0.383482000 | 2.166265000 |
| 1 | -3.499230000 | -1.435441000 | 2.158045000 |
| 1 | -4.360432000 | -2.311630000 | 0.000903000 |
| 7 | -0.777519000 | 1.697643000 | 0.007828000 |
| 7 | -0.884299000 | 2.849915000 | 0.012104000 |
| 46 | 0.532472000 | 0.256023000 | -0.003717000 |
| 8 | 2.752502000 | 0.645257000 | -0.007199000 |
| 8 | 2.054704000 | -1.456853000 | -0.026656000 |
| 6 | 2.998940000 | -0.607615000 | -0.016488000 |
| 6 | 4.437627000 | -1.073707000 | 0.021013000 |
| 1 | 5.081572000 | -0.382426000 | -0.528580000 |
| 1 | 4.776850000 | -1.094111000 | 1.063859000 |
| 1 | 4.528379000 | -2.081554000 | -0.390376000 |



**1d**

TCG = 0.104994, E(M06) = -696.1779289

| | | | |
|---|---|---|---|
| 6 | 2.768051000 | -1.215940000 | 1.278630000 |
| 6 | 2.401278000 | 0.099128000 | 1.228871000 |
| 6 | 1.719279000 | 0.575999000 | 0.041387000 |
| 6 | 1.461673000 | -0.298926000 | -1.104409000 |
| 6 | 1.929547000 | -1.651755000 | -0.972849000 |
| 6 | 2.531425000 | -2.098737000 | 0.176978000 |
| 1 | 3.266737000 | -1.592366000 | 2.166399000 |
| 1 | 2.603530000 | 0.794479000 | 2.035843000 |
| 1 | 1.377622000 | 0.132012000 | -2.099775000 |
| 1 | 1.811413000 | -2.311691000 | -1.827328000 |
| 1 | 2.868596000 | -3.128275000 | 0.246728000 |
| 7 | 1.752039000 | 1.934988000 | -0.181858000 |
| 7 | 1.785742000 | 3.043536000 | -0.335733000 |
| 46 | -0.362416000 | 0.107039000 | -0.163209000 |
| 8 | -2.361902000 | -0.893879000 | -0.655922000 |
| 6 | -2.969982000 | -0.181623000 | 0.208001000 |
| 8 | -2.356952000 | 0.687772000 | 0.900901000 |
| 6 | -4.465909000 | -0.363441000 | 0.381115000 |
| 1 | -4.986925000 | 0.189716000 | -0.409836000 |
| 1 | -4.737994000 | -1.418156000 | 0.284440000 |
| 1 | -4.797643000 | 0.021434000 | 1.348126000 |

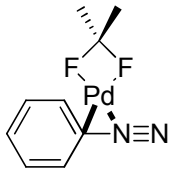


**1a'**

TCG = 0.071061, E(M06) = -892.2146666

| | | | |
|---|---|---|---|
| 6 | -5.025436000 | -0.675608000 | 0.000135000 |
| 6 | -3.701449000 | -1.096946000 | 0.000095000 |
| 6 | -2.695825000 | -0.115141000 | -0.000006000 |
| 6 | -2.980666000 | 1.254958000 | -0.000033000 |
| 6 | -4.315232000 | 1.653347000 | -0.000014000 |
| 6 | -5.331875000 | 0.692727000 | 0.000075000 |
| 1 | -5.821478000 | -1.413147000 | 0.000179000 |
| 1 | -3.437466000 | -2.148700000 | 0.000107000 |

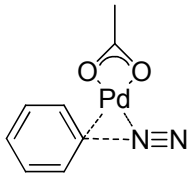
| | | | |
|---|---|---|---|
| 1 | -2.170090000 | 1.975751000 | -0.000133000 |
| 1 | -4.561228000 | 2.709985000 | -0.000075000 |
| 1 | -6.370456000 | 1.008952000 | 0.000098000 |
| 7 | -1.340357000 | -0.495303000 | -0.000075000 |
| 7 | -0.721629000 | -1.511075000 | -0.000009000 |
| 46 | 0.774122000 | -0.234979000 | -0.000093000 |
| 9 | 4.348887000 | 0.466063000 | -1.148890000 |
| 9 | 2.506187000 | 1.254506000 | -0.000017000 |
| 9 | 4.348468000 | 0.465796000 | 1.149371000 |
| 9 | 2.958872000 | -0.977963000 | -0.000172000 |
| 5 | 3.605236000 | 0.313041000 | 0.000109000 |




**1c'**

TCG = 0.067278, E(M06) = -892.20452

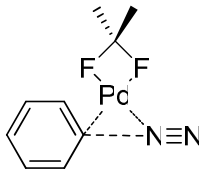
| | | | |
|---|---|---|---|
| 6 | -3.397971000 | -1.028784000 | -1.218386000 |
| 6 | -2.463614000 | 0.003293000 | -1.237396000 |
| 6 | -2.013157000 | 0.501540000 | -0.000110000 |
| 6 | -2.464904000 | 0.004835000 | 1.237296000 |
| 6 | -3.399273000 | -1.027210000 | 1.218523000 |
| 6 | -3.862871000 | -1.538123000 | 0.000139000 |
| 1 | -3.767690000 | -1.430103000 | -2.156138000 |
| 1 | -2.106151000 | 0.436884000 | -2.164557000 |
| 1 | -2.108359000 | 0.439505000 | 2.164303000 |
| 1 | -3.770043000 | -1.427353000 | 2.156364000 |
| 1 | -4.596716000 | -2.337866000 | 0.000286000 |
| 7 | -1.103740000 | 1.672137000 | -0.000512000 |
| 7 | -1.047198000 | 2.823580000 | -0.001144000 |
| 46 | 0.240985000 | 0.235583000 | 0.000097000 |
| 9 | 3.859474000 | -0.681781000 | 1.150187000 |
| 9 | 1.982889000 | -1.370039000 | -0.001239000 |
| 9 | 3.860833000 | -0.679894000 | -1.149250000 |
| 9 | 2.557539000 | 0.836872000 | 0.000924000 |
| 5 | 3.116871000 | -0.485532000 | 0.000173000 |




**TS1-2**

TCG = 0.106378, E(M06) = -696.1750444

| | | | |
|---|---|---|---|
| 6 | -3.130311000 | -1.032782000 | -1.215733000 |
| 6 | -2.163717000 | -0.028828000 | -1.228701000 |
| 6 | -1.685920000 | 0.442949000 | 0.004883000 |
| 6 | -2.153705000 | -0.043032000 | 1.236788000 |
| 6 | -3.120466000 | -1.046810000 | 1.220083000 |
| 6 | -3.604716000 | -1.536937000 | 0.001262000 |
| 1 | -3.515583000 | -1.417682000 | -2.154548000 |
| 1 | -1.794777000 | 0.394317000 | -2.156787000 |
| 1 | -1.777375000 | 0.369456000 | 2.166700000 |
| 1 | -3.498116000 | -1.442543000 | 2.157489000 |
| 1 | -4.361659000 | -2.315212000 | -0.000157000 |
| 7 | -0.776735000 | 1.705789000 | 0.008721000 |
| 7 | -0.905985000 | 2.854419000 | 0.014599000 |
| 46 | 0.535767000 | 0.269610000 | -0.004296000 |
| 8 | 2.039589000 | -1.456044000 | -0.024296000 |
| 8 | 2.757152000 | 0.639076000 | -0.009221000 |
| 6 | 2.992261000 | -0.615955000 | -0.016273000 |
| 6 | 4.426296000 | -1.095523000 | 0.021503000 |
| 1 | 5.078153000 | -0.406208000 | -0.521090000 |
| 1 | 4.762150000 | -1.127283000 | 1.065168000 |
| 1 | 4.508717000 | -2.101126000 | -0.397109000 |

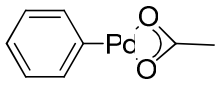



**TS1-2'**

TCG = 0.068533, E(M06) = -892.2022251

| | | | |
|---|---|---|---|
| 6 | -3.269708000 | -1.185665000 | -1.219051000 |
| 6 | -2.335573000 | -0.151783000 | -1.236811000 |
| 6 | -1.868746000 | 0.321559000 | 0.000041000 |
| 6 | -2.335466000 | -0.151975000 | 1.236861000 |
| 6 | -3.269598000 | -1.185856000 | 1.219028000 |
| 6 | -3.730899000 | -1.698300000 | -0.000031000 |
| 1 | -3.642632000 | -1.584727000 | -2.156829000 |
| 1 | -1.981945000 | 0.282798000 | -2.165098000 |
| 1 | -1.981772000 | 0.282476000 | 2.165185000 |
| 1 | -3.642446000 | -1.585055000 | 2.156778000 |
| 1 | -4.465461000 | -2.497550000 | -0.000060000 |
| 7 | -1.142939000 | 1.781973000 | 0.000086000 |
| 7 | -1.375562000 | 2.898601000 | 0.000158000 |
| 46 | 0.271210000 | 0.437674000 | -0.000042000 |

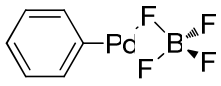
| | | | |
|---|---|---|---|
| 9 | 3.734163000 | -0.855945000 | 1.149625000 |
| 9 | 1.794517000 | -1.352214000 | -0.000247000 |
| 9 | 3.734582000 | -0.855856000 | -1.149369000 |
| 9 | 2.585857000 | 0.783782000 | -0.000011000 |
| 5 | 3.017196000 | -0.592148000 | 0.000004000 |




**2**

TCG = 0.100016, E(M06) = -586.7113716

| | | | |
|---|---|---|---|
| 6 | 3.650995000 | -0.630926000 | -0.069266000 |
| 6 | 2.299985000 | -1.004005000 | -0.066968000 |
| 6 | 1.321539000 | -0.009604000 | -0.002950000 |
| 6 | 1.654461000 | 1.343250000 | 0.050976000 |
| 6 | 3.008809000 | 1.703442000 | 0.048761000 |
| 6 | 4.002288000 | 0.721157000 | -0.011139000 |
| 1 | 4.419350000 | -1.397915000 | -0.118790000 |
| 1 | 2.027906000 | -2.059051000 | -0.116287000 |
| 1 | 0.882433000 | 2.106072000 | 0.095317000 |
| 1 | 3.282976000 | 2.754348000 | 0.094155000 |
| 1 | 5.050102000 | 1.008406000 | -0.013999000 |
| 46 | -0.489330000 | -0.717422000 | 0.029604000 |
| 8 | -1.600110000 | 1.046818000 | -0.078765000 |
| 6 | -2.760426000 | 0.472919000 | -0.039982000 |
| 8 | -2.838164000 | -0.781784000 | 0.024532000 |
| 6 | -3.979555000 | 1.358361000 | -0.041457000 |
| 1 | -4.162497000 | 1.711292000 | 0.980454000 |
| 1 | -3.820062000 | 2.232900000 | -0.677223000 |
| 1 | -4.853411000 | 0.797504000 | -0.379423000 |




**2'**

TCG = 0.062357, E(M06) = -782.7280898

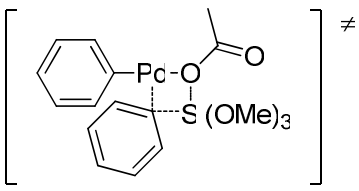
| | | | |
|---|---|---|---|
| 6 | -3.660243000 | -0.864527000 | 0.846031000 |
| 6 | -2.300059000 | -1.069376000 | 0.569626000 |
| 6 | -1.607837000 | -0.028161000 | -0.036976000 |
| 6 | -2.162980000 | 1.212278000 | -0.326873000 |
| 6 | -3.524510000 | 1.392184000 | -0.040706000 |
| 6 | -4.264568000 | 0.358760000 | 0.541544000 |
| 1 | -4.234141000 | -1.663471000 | 1.307023000 |
| 1 | -1.816175000 | -2.011351000 | 0.816387000 |
| 1 | -1.573203000 | 2.012991000 | -0.766478000 |
| 1 | -3.993510000 | 2.345050000 | -0.269207000 |

| | | | |
|---|---|---|---|
| 1 | -5.315184000 | 0.511770000 | 0.770565000 |
| 46 | 0.188452000 | -0.376679000 | -0.626828000 |
| 9 | 3.475628000 | 1.437059000 | 0.178351000 |
| 9 | 1.507281000 | 0.551878000 | 0.999254000 |
| 9 | 3.505760000 | -0.560564000 | 1.316209000 |
| 9 | 2.543854000 | -0.445608000 | -0.779006000 |
| 5 | 2.818380000 | 0.256076000 | 0.445332000 |

## $PhSi(OMe)_3$

TCG = 0.174655, E(M06) = -866.494976133

| | | | |
|---|---|---|---|
| 6 | 2.934598000 | -0.911733000 | 1.105706000 |
| 6 | 1.544448000 | -0.854918000 | 0.982749000 |
| 6 | 0.932988000 | -0.006531000 | 0.039849000 |
| 6 | 1.765018000 | 0.786492000 | -0.775050000 |
| 6 | 3.155275000 | 0.733128000 | -0.654672000 |
| 6 | 3.741819000 | -0.117662000 | 0.286332000 |
| 1 | 3.387162000 | -1.572431000 | 1.840420000 |
| 1 | 0.929947000 | -1.473524000 | 1.631448000 |
| 1 | 1.322460000 | 1.458073000 | -1.506919000 |
| 1 | 3.779342000 | 1.354977000 | -1.291020000 |
| 1 | 4.823560000 | -0.160252000 | 0.382229000 |
| 14 | -0.915603000 | 0.065443000 | -0.177062000 |
| 8 | -1.420915000 | 1.557798000 | -0.684498000 |
| 8 | -1.484589000 | -0.883541000 | -1.411231000 |
| 8 | -1.557904000 | -0.370757000 | 1.285265000 |
| 6 | -2.968668000 | -0.492514000 | 1.511578000 |
| 1 | -3.112809000 | -0.924519000 | 2.505204000 |
| 1 | -3.454219000 | 0.489112000 | 1.476284000 |
| 1 | -3.434137000 | -1.148050000 | 0.767451000 |
| 6 | -1.240163000 | -2.292218000 | -1.487515000 |
| 1 | -0.168977000 | -2.515242000 | -1.419796000 |
| 1 | -1.766816000 | -2.827020000 | -0.688785000 |
| 1 | -1.612826000 | -2.643420000 | -2.453299000 |
| 6 | -1.273129000 | 2.733904000 | 0.118552000 |
| 1 | -0.228301000 | 2.886270000 | 0.412670000 |
| 1 | -1.599095000 | 3.589177000 | -0.479102000 |
| 1 | -1.892710000 | 2.674962000 | 1.020622000 |

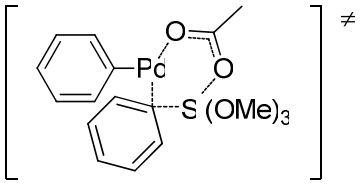



**TS2-3a**

TCG = 0.301901, E(M06) = -1453.193457

| | | | |
|---|---|---|---|
| 46 | 0.771365000 | -0.918508000 | -0.318735000 |
| 6 | 2.652404000 | -0.576785000 | 0.108841000 |
| 6 | 3.161886000 | -1.293620000 | 1.201817000 |
| 1 | 2.495331000 | -1.828403000 | 1.875235000 |
| 6 | 0.041545000 | 1.066396000 | -0.113344000 |
| 6 | 0.041135000 | 1.547299000 | -1.458647000 |
| 14 | -1.893882000 | 0.239475000 | 0.572010000 |
| 6 | 0.730964000 | 1.865123000 | 0.845595000 |
| 6 | 0.634298000 | 2.758712000 | -1.808231000 |
| 6 | 1.306987000 | 3.085623000 | 0.505575000 |
| 1 | 1.798783000 | 3.689665000 | 1.263245000 |
| 6 | 1.262069000 | 3.530129000 | -0.822539000 |
| 1 | 1.718226000 | 4.479831000 | -1.089583000 |
| 6 | 3.513984000 | 0.153774000 | -0.719602000 |
| 6 | 4.894073000 | 0.115744000 | -0.485934000 |
| 1 | 5.563699000 | 0.671281000 | -1.138011000 |
| 6 | 4.544656000 | -1.326776000 | 1.426303000 |
| 6 | 5.410073000 | -0.623931000 | 0.583125000 |
| 1 | 6.481100000 | -0.641836000 | 0.765907000 |
| 1 | 0.603625000 | 3.109236000 | -2.836240000 |
| 1 | -0.483091000 | 0.984446000 | -2.226554000 |
| 1 | 0.766508000 | 1.525402000 | 1.874993000 |
| 1 | 3.121804000 | 0.749114000 | -1.539285000 |
| 1 | 4.938240000 | -1.891836000 | 2.267599000 |
| 8 | -1.158465000 | -0.051493000 | 2.059732000 |
| 8 | -3.437880000 | -0.424971000 | 0.878546000 |
| 8 | -2.463127000 | 1.774442000 | 0.200083000 |
| 6 | -1.882518000 | -0.066765000 | 3.293571000 |
| 1 | -2.480965000 | -0.976792000 | 3.404514000 |
| 1 | -1.146889000 | -0.029936000 | 4.103143000 |
| 1 | -2.544570000 | 0.801630000 | 3.386084000 |
| 6 | -3.686030000 | -1.802407000 | 1.091827000 |
| 1 | -4.569068000 | -1.906310000 | 1.733967000 |
| 1 | -3.895284000 | -2.320594000 | 0.145121000 |
| 1 | -2.847481000 | -2.316025000 | 1.580944000 |
| 6 | -3.835572000 | 2.170550000 | 0.132687000 |
| 1 | -4.374754000 | 1.602930000 | -0.632122000 |
| 1 | -4.343832000 | 2.038430000 | 1.092847000 |
| 1 | -3.850228000 | 3.232044000 | -0.135507000 |
| 8 | -1.464592000 | -1.088887000 | -0.586410000 |
| 6 | -2.100429000 | -1.346504000 | -1.751935000 |
| 8 | -2.957641000 | -0.606079000 | -2.200073000 |
| 6 | -1.621141000 | -2.611624000 | -2.417795000 |

| | | | |
|---|---|---|---|
| 1 | -0.561346000 | -2.509797000 | -2.678408000 |
| 1 | -1.711385000 | -3.455853000 | -1.726889000 |
| 1 | -2.203524000 | -2.801629000 | -3.320271000 |

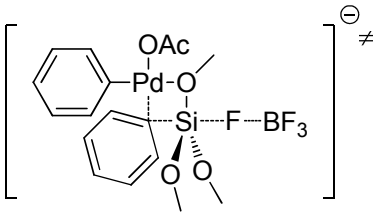



**TS2-3b**

TCG = 0.305149, E(M06) = -1453.199653

| | | | |
|---|---|---|---|
| 6 | -0.829451000 | 3.149716000 | 0.952194000 |
| 6 | -0.582395000 | 1.778377000 | 0.958341000 |
| 6 | 0.080206000 | 1.131325000 | -0.121953000 |
| 6 | 0.407317000 | 1.949850000 | -1.241485000 |
| 6 | 0.139895000 | 3.317142000 | -1.258579000 |
| 6 | -0.473518000 | 3.922805000 | -0.157068000 |
| 1 | -1.312596000 | 3.613524000 | 1.807717000 |
| 1 | -0.872143000 | 1.204713000 | 1.826622000 |
| 1 | 0.891760000 | 1.518303000 | -2.108666000 |
| 1 | 0.410931000 | 3.909322000 | -2.128056000 |
| 1 | -0.673903000 | 4.990771000 | -0.164452000 |
| 14 | 1.747792000 | -0.133504000 | 0.743199000 |
| 8 | 2.859111000 | 1.023378000 | 1.225678000 |
| 8 | 0.902268000 | -0.259465000 | 2.217429000 |
| 8 | 2.316462000 | -1.730505000 | 0.661882000 |
| 6 | 2.559503000 | -2.591707000 | 1.769052000 |
| 1 | 3.506320000 | -3.114117000 | 1.590203000 |
| 1 | 2.634459000 | -2.045908000 | 2.714675000 |
| 1 | 1.764339000 | -3.341167000 | 1.860924000 |
| 6 | -0.073287000 | -1.223073000 | 2.560391000 |
| 1 | -1.043952000 | -0.739816000 | 2.730034000 |
| 1 | -0.207046000 | -1.982722000 | 1.780988000 |
| 1 | 0.224964000 | -1.732480000 | 3.485159000 |
| 6 | 2.848730000 | 1.711967000 | 2.471486000 |
| 1 | 1.924955000 | 2.287203000 | 2.603842000 |
| 1 | 2.955584000 | 1.024317000 | 3.316977000 |
| 1 | 3.695716000 | 2.405897000 | 2.469221000 |
| 46 | -0.595220000 | -0.720529000 | -0.896834000 |
| 6 | -2.399915000 | -0.484311000 | -0.139617000 |
| 6 | -3.236091000 | 0.587645000 | -0.483538000 |
| 6 | -2.937954000 | -1.617782000 | 0.489978000 |
| 6 | -4.612275000 | 0.502142000 | -0.238521000 |

| | | | |
|---|---|---|---|
| 1 | -2.828636000 | 1.479846000 | -0.948781000 |
| 6 | -4.316282000 | -1.694938000 | 0.729451000 |
| 1 | -2.298181000 | -2.445468000 | 0.785948000 |
| 6 | -5.153214000 | -0.635303000 | 0.368368000 |
| 1 | -5.258893000 | 1.329495000 | -0.520664000 |
| 1 | -4.728374000 | -2.580262000 | 1.207394000 |
| 1 | -6.220408000 | -0.693184000 | 0.564800000 |
| 8 | 1.126399000 | -1.254507000 | -2.160508000 |
| 6 | 2.229251000 | -0.686508000 | -1.988730000 |
| 8 | 2.521206000 | 0.015301000 | -0.945256000 |
| 6 | 3.311112000 | -0.784085000 | -3.034147000 |
| 1 | 4.114079000 | -1.424118000 | -2.650642000 |
| 1 | 2.919543000 | -1.208753000 | -3.959343000 |
| 1 | 3.739135000 | 0.204830000 | -3.221852000 |

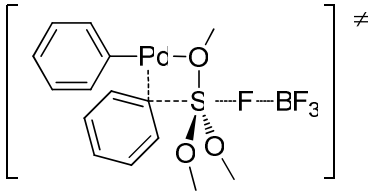



**TS2-3c**

TCG = 0.304973, E(M06) = -1877.850288

| | | | |
|---|---|---|---|
| 46 | -1.109026000 | 0.490511000 | -0.172746000 |
| 6 | -2.827256000 | -0.168373000 | 0.582266000 |
| 6 | -3.950539000 | -0.366787000 | -0.237441000 |
| 1 | -3.873712000 | -0.233853000 | -1.314025000 |
| 6 | -0.504530000 | -1.459340000 | -0.594515000 |
| 6 | -0.384520000 | -1.715263000 | -1.983551000 |
| 1 | -0.246424000 | -0.884811000 | -2.672153000 |
| 14 | 1.565471000 | -0.353302000 | 0.191120000 |
| 9 | 3.009698000 | 0.661201000 | 0.727944000 |
| 8 | -1.761572000 | 2.518873000 | 0.139666000 |
| 6 | -1.898239000 | 3.232266000 | -0.927795000 |
| 8 | -1.694196000 | 2.834901000 | -2.092518000 |
| 6 | -2.360616000 | 4.667244000 | -0.677399000 |
| 1 | -3.382739000 | 4.659565000 | -0.281136000 |
| 1 | -1.724633000 | 5.147703000 | 0.073579000 |
| 1 | -2.340852000 | 5.250206000 | -1.601154000 |
| 6 | -2.967080000 | -0.358537000 | 1.967050000 |
| 6 | -5.184267000 | -0.736032000 | 0.315357000 |
| 6 | -4.201329000 | -0.725830000 | 2.519135000 |
| 1 | -4.288811000 | -0.864623000 | 3.594688000 |
| 6 | -5.314668000 | -0.916449000 | 1.695447000 |

| | | | |
|---|---|---|---|
| 1 | -6.271660000 | -1.203680000 | 2.123698000 |
| 1 | -6.042127000 | -0.884459000 | -0.337141000 |
| 1 | -2.112373000 | -0.224720000 | 2.626496000 |
| 6 | -0.690998000 | -2.582649000 | 0.244615000 |
| 6 | -0.429673000 | -3.012859000 | -2.501526000 |
| 6 | -0.595498000 | -4.101351000 | -1.639833000 |
| 1 | -0.625803000 | -5.112802000 | -2.036955000 |
| 6 | -0.724368000 | -3.882509000 | -0.263648000 |
| 1 | -0.858360000 | -4.725683000 | 0.409947000 |
| 1 | -0.336175000 | -3.174715000 | -3.572691000 |
| 1 | -0.799624000 | -2.434814000 | 1.314631000 |
| 8 | 1.111568000 | -0.631770000 | 1.742313000 |
| 8 | 1.049768000 | 0.878746000 | -0.811966000 |
| 6 | 1.613500000 | 2.201831000 | -0.997993000 |
| 1 | 2.634334000 | 2.112754000 | -1.370822000 |
| 1 | 0.975670000 | 2.699416000 | -1.727560000 |
| 1 | 1.603875000 | 2.754862000 | -0.056652000 |
| 6 | 2.010927000 | -0.764543000 | 2.861389000 |
| 1 | 1.475714000 | -1.323024000 | 3.632212000 |
| 1 | 2.919798000 | -1.304964000 | 2.585689000 |
| 1 | 2.280447000 | 0.222647000 | 3.246330000 |
| 8 | 2.442438000 | -1.568991000 | -0.465542000 |
| 6 | 3.051080000 | -1.566966000 | -1.766010000 |
| 1 | 3.604566000 | -2.503734000 | -1.861434000 |
| 1 | 2.284670000 | -1.522901000 | -2.545363000 |
| 1 | 3.740439000 | -0.726136000 | -1.872150000 |
| 5 | 4.615456000 | 0.678787000 | 0.659118000 |
| 9 | 4.883227000 | 0.997498000 | -0.645536000 |
| 9 | 4.986622000 | -0.582501000 | 1.022309000 |
| 9 | 4.939286000 | 1.651508000 | 1.556183000 |

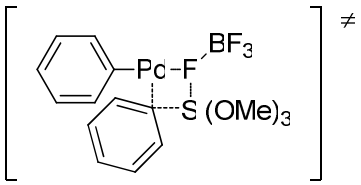



**TS2-3d**

TCG = 0.263235, E(M06) = -1649.218592

| | | | |
|---|---|---|---|
| 6 | 0.957168000 | 3.262676000 | -1.367048000 |
| 6 | 0.665936000 | 1.900543000 | -1.411583000 |
| 6 | 0.738525000 | 1.091678000 | -0.245363000 |
| 6 | 1.168844000 | 1.710948000 | 0.954527000 |
| 6 | 1.457532000 | 3.075782000 | 1.000022000 |

| | | | |
|---|---|---|---|
| 6 | 1.356363000 | 3.850396000 | -0.160450000 |
| 1 | 0.879752000 | 3.865585000 | -2.267644000 |
| 1 | 0.344401000 | 1.459176000 | -2.350433000 |
| 1 | 1.257180000 | 1.117960000 | 1.857781000 |
| 1 | 1.770491000 | 3.533304000 | 1.934590000 |
| 1 | 1.589117000 | 4.911287000 | -0.125584000 |
| 14 | -1.356472000 | 0.053583000 | 0.067495000 |
| 8 | -0.915006000 | -0.308565000 | 1.609522000 |
| 8 | -2.174627000 | 1.431015000 | -0.276133000 |
| 8 | -0.925836000 | -0.815180000 | -1.297823000 |
| 6 | -1.686784000 | -1.785535000 | -2.057048000 |
| 1 | -1.120452000 | -1.977484000 | -2.968926000 |
| 1 | -1.799298000 | -2.708361000 | -1.484375000 |
| 1 | -2.666054000 | -1.373462000 | -2.301384000 |
| 6 | -2.399355000 | 2.521299000 | 0.629870000 |
| 1 | -3.215840000 | 2.272938000 | 1.312656000 |
| 1 | -1.495858000 | 2.756812000 | 1.199829000 |
| 1 | -2.678785000 | 3.390219000 | 0.029786000 |
| 6 | -1.754745000 | -0.784850000 | 2.678370000 |
| 1 | -1.978886000 | -1.846139000 | 2.541983000 |
| 1 | -1.191597000 | -0.648573000 | 3.604151000 |
| 1 | -2.689354000 | -0.222235000 | 2.734761000 |
| 46 | 1.243330000 | -0.868639000 | -0.707278000 |
| 9 | -2.899934000 | -0.972774000 | 0.219666000 |
| 6 | 3.056443000 | -0.742823000 | 0.041085000 |
| 6 | 4.134054000 | -0.537156000 | -0.835296000 |
| 6 | 3.305328000 | -1.075391000 | 1.381753000 |
| 6 | 5.447892000 | -0.720171000 | -0.384264000 |
| 1 | 3.959248000 | -0.243380000 | -1.867469000 |
| 6 | 4.620828000 | -1.256338000 | 1.825740000 |
| 1 | 2.481704000 | -1.198368000 | 2.080786000 |
| 6 | 5.692176000 | -1.081160000 | 0.943983000 |
| 1 | 6.277538000 | -0.570971000 | -1.071096000 |
| 1 | 4.806201000 | -1.528846000 | 2.861938000 |
| 1 | 6.712588000 | -1.214248000 | 1.293422000 |
| 5 | -4.469559000 | -0.694731000 | 0.146111000 |
| 9 | -4.693977000 | 0.263682000 | 1.098327000 |
| 9 | -5.005663000 | -1.914165000 | 0.442680000 |
| 9 | -4.682018000 | -0.280285000 | -1.139097000 |

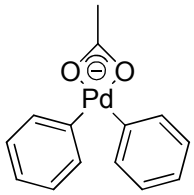



**TS2-3e**

TCG = 0.261341, E(M06) = -1649.196553

| | | | |
|---|---|---|---|
| 46 | 0.852827000 | -0.941404000 | 0.054461000 |
| 6 | 2.770957000 | -0.616919000 | 0.213878000 |
| 6 | 3.352058000 | -1.098024000 | 1.396027000 |
| 1 | 2.733079000 | -1.431529000 | 2.226226000 |
| 9 | -1.440683000 | -0.965616000 | 0.004028000 |
| 6 | 0.242761000 | 1.040593000 | -0.326867000 |
| 6 | 0.100030000 | 1.091090000 | -1.746719000 |
| 14 | -1.663927000 | 0.590395000 | 0.763770000 |
| 6 | 1.008737000 | 2.079581000 | 0.275803000 |
| 6 | 0.635016000 | 2.132570000 | -2.501185000 |
| 6 | 1.528244000 | 3.132203000 | -0.472109000 |
| 1 | 2.083113000 | 3.929128000 | 0.015518000 |
| 6 | 1.345488000 | 3.155755000 | -1.861033000 |
| 1 | 1.759446000 | 3.973009000 | -2.445894000 |
| 6 | 3.572376000 | -0.140275000 | -0.830423000 |
| 6 | 4.966012000 | -0.200320000 | -0.708627000 |
| 1 | 5.590228000 | 0.156404000 | -1.524164000 |
| 6 | 4.747942000 | -1.155965000 | 1.504959000 |
| 6 | 5.553770000 | -0.708473000 | 0.454256000 |
| 1 | 6.635887000 | -0.744515000 | 0.545976000 |
| 1 | 0.499471000 | 2.156086000 | -3.578984000 |
| 1 | -0.475453000 | 0.320815000 | -2.250888000 |
| 1 | 1.151288000 | 2.065041000 | 1.350695000 |
| 1 | 3.124799000 | 0.272523000 | -1.729680000 |
| 1 | 5.198726000 | -1.539251000 | 2.416902000 |
| 8 | -0.804627000 | 0.783889000 | 2.191785000 |
| 8 | -3.172768000 | 0.091015000 | 1.371302000 |
| 8 | -2.239572000 | 1.917741000 | -0.073146000 |
| 6 | -1.422176000 | 1.185601000 | 3.420448000 |
| 1 | -0.619106000 | 1.442123000 | 4.117780000 |
| 1 | -2.059380000 | 2.066381000 | 3.283088000 |
| 1 | -2.023016000 | 0.380658000 | 3.854727000 |
| 6 | -3.381576000 | -1.161534000 | 2.007244000 |
| 1 | -4.257569000 | -1.078637000 | 2.660833000 |
| 1 | -3.570878000 | -1.951243000 | 1.271008000 |
| 1 | -2.525385000 | -1.467265000 | 2.623997000 |

| | | | |
|---|---|---|---|
| 6 | -3.610701000 | 2.317694000 | -0.175162000 |
| 1 | -4.210711000 | 1.546879000 | -0.668086000 |
| 1 | -4.044945000 | 2.530754000 | 0.806314000 |
| 1 | -3.633032000 | 3.229090000 | -0.780804000 |
| 5 | -2.569926000 | -1.877062000 | -1.743026000 |
| 9 | -1.453450000 | -2.014766000 | -2.446751000 |
| 9 | -3.022273000 | -2.895352000 | -1.028678000 |
| 9 | -3.323581000 | -0.801459000 | -1.917477000 |




**3**

TCG = 0.18066, E(M06) = -818.673075

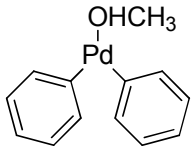
| | | | |
|---|---|---|---|
| 46 | 0.691617000 | -0.000162000 | -0.027019000 |
| 6 | -0.749773000 | -1.387972000 | 0.021544000 |
| 6 | -0.994167000 | -2.107334000 | 1.208693000 |
| 1 | -0.482485000 | -1.830454000 | 2.128376000 |
| 6 | -0.749181000 | 1.388208000 | 0.021866000 |
| 6 | -0.995095000 | 2.105925000 | 1.209690000 |
| 1 | -0.484870000 | 1.827526000 | 2.129723000 |
| 8 | 2.700568000 | -1.110360000 | -0.092827000 |
| 6 | 3.324090000 | -0.000507000 | -0.106679000 |
| 8 | 2.700751000 | 1.109485000 | -0.092431000 |
| 6 | 4.840318000 | -0.000268000 | -0.102548000 |
| 1 | 5.194112000 | 0.009714000 | 0.935872000 |
| 1 | 5.229679000 | -0.900369000 | -0.584974000 |
| 1 | 5.228937000 | 0.891436000 | -0.601067000 |
| 6 | -1.452763000 | -1.784981000 | -1.132374000 |
| 6 | -1.884571000 | -3.188691000 | 1.236259000 |
| 6 | -2.339446000 | -2.869097000 | -1.109988000 |
| 1 | -2.861155000 | -3.157162000 | -2.020624000 |
| 6 | -2.561196000 | -3.575852000 | 0.075766000 |
| 1 | -3.253272000 | -4.414149000 | 0.095735000 |
| 1 | -2.050234000 | -3.725982000 | 2.168037000 |
| 1 | -1.311276000 | -1.246983000 | -2.067460000 |
| 6 | -1.450349000 | 1.787077000 | -1.132516000 |
| 6 | -1.885239000 | 3.187486000 | 1.237510000 |
| 6 | -2.560083000 | 3.576488000 | 0.076589000 |
| 1 | -3.252009000 | 4.414903000 | 0.096767000 |
| 6 | -2.336786000 | 2.871392000 | -1.109859000 |
| 1 | -2.857115000 | 3.160886000 | -2.020831000 |

| | | | |
|---|---|---|---|
| 1 | -2.052131000 | 3.723469000 | 2.169821000 |
| 1 | -1.307667000 | 1.250373000 | -2.068167000 |

S $(OMe)_3OAc$

TCG = 0.134965, E(M06) = -863.4521293

| | | | |
|---|---|---|---|
| 14 | -0.522378000 | 0.046932000 | -0.040071000 |
| 8 | -0.647643000 | 1.628431000 | -0.429594000 |
| 8 | -1.492562000 | -0.801346000 | -1.053110000 |
| 8 | -0.851683000 | -0.159970000 | 1.548422000 |
| 6 | -2.087659000 | 0.247368000 | 2.158305000 |
| 1 | -2.050562000 | -0.053706000 | 3.207480000 |
| 1 | -2.207664000 | 1.333749000 | 2.099406000 |
| 1 | -2.941715000 | -0.239318000 | 1.675716000 |
| 6 | -1.582153000 | -2.234090000 | -1.067432000 |
| 1 | -0.619636000 | -2.679749000 | -1.338642000 |
| 1 | -1.895661000 | -2.616292000 | -0.090243000 |
| 1 | -2.328712000 | -2.511010000 | -1.815185000 |
| 6 | -0.483574000 | 2.156118000 | -1.755017000 |
| 1 | 0.547131000 | 2.019989000 | -2.099113000 |
| 1 | -1.168592000 | 1.671021000 | -2.457368000 |
| 1 | -0.708068000 | 3.224198000 | -1.713650000 |
| 8 | 2.145185000 | 0.850073000 | 1.042947000 |
| 6 | 2.154159000 | -0.106857000 | 0.293792000 |
| 8 | 1.025340000 | -0.589581000 | -0.285914000 |
| 6 | 3.375053000 | -0.888768000 | -0.105541000 |
| 1 | 3.490095000 | -0.862840000 | -1.194104000 |
| 1 | 4.260261000 | -0.469614000 | 0.373420000 |
| 1 | 3.252367000 | -1.936958000 | 0.186634000 |




**3'**

TCG = 0.186245, E(M06) = -705.752877

| | | | |
|---|---|---|---|
| 6 | 3.412327000 | 1.627590000 | -0.440962000 |
| 6 | 2.096215000 | 1.171960000 | -0.585458000 |
| 6 | 1.683710000 | -0.045663000 | -0.016428000 |
| 6 | 2.633367000 | -0.781626000 | 0.722677000 |
| 6 | 3.950286000 | -0.327063000 | 0.868629000 |
| 6 | 4.344170000 | 0.881020000 | 0.286528000 |
| 1 | 3.708777000 | 2.569531000 | -0.897645000 |
| 1 | 1.390568000 | 1.777157000 | -1.147660000 |
| 1 | 2.352253000 | -1.724730000 | 1.189515000 |

| | | | |
|---|---|---|---|
| 1 | 4.663395000 | -0.915330000 | 1.442069000 |
| 1 | 5.364302000 | 1.238385000 | 0.402029000 |
| 46 | -0.049246000 | -0.995561000 | -0.284233000 |
| 6 | -1.110493000 | 0.659516000 | 0.012850000 |
| 6 | -1.757945000 | 0.855013000 | 1.244204000 |
| 6 | -1.339994000 | 1.575307000 | -1.026247000 |
| 6 | -2.626753000 | 1.939652000 | 1.425457000 |
| 1 | -1.595178000 | 0.166236000 | 2.068779000 |
| 6 | -2.214023000 | 2.654830000 | -0.842373000 |
| 1 | -0.842986000 | 1.456634000 | -1.985508000 |
| 6 | -2.858529000 | 2.841893000 | 0.383672000 |
| 1 | -3.117897000 | 2.077235000 | 2.386091000 |
| 1 | -2.386659000 | 3.349592000 | -1.661200000 |
| 1 | -3.531763000 | 3.683118000 | 0.526301000 |
| 8 | -1.808306000 | -2.373753000 | -0.653734000 |
| 1 | -2.383091000 | -1.933646000 | -1.302578000 |
| 6 | -2.621821000 | -2.771679000 | 0.470905000 |
| 1 | -3.423639000 | -3.434226000 | 0.131810000 |
| 1 | -1.965528000 | -3.310481000 | 1.155065000 |
| 1 | -3.043905000 | -1.898141000 | 0.976814000 |

$BF_3$

TCG = , -0.012244 E(M06) = -324.5795188

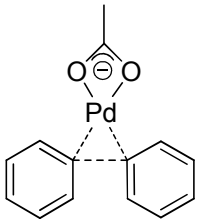
| | | | |
|---|---|---|---|
| 5 | 0.000000000 | 0.000000000 | 0.000000000 |
| 9 | 0.000000000 | 1.318995000 | 0.000000000 |
| 9 | -1.142283000 | -0.659498000 | 0.000000000 |
| 9 | 1.142283000 | -0.659498000 | 0.000000000 |

$FS(OMe)_3$

TCG = 0.096186, E(M06) = -1059.456219

| | | | |
|---|---|---|---|
| 14 | 0.000156000 | -0.299568000 | 0.130162000 |
| 8 | 1.288703000 | -0.633939000 | -0.817977000 |
| 8 | -1.286344000 | -0.624872000 | -0.823700000 |
| 8 | -0.002680000 | 1.205260000 | 0.779053000 |
| 6 | 0.001444000 | 2.393263000 | -0.030130000 |
| 1 | -0.112068000 | 3.248521000 | 0.639521000 |
| 1 | 0.946489000 | 2.487056000 | -0.575047000 |
| 1 | -0.828945000 | 2.384988000 | -0.743913000 |
| 6 | -2.643575000 | -0.386712000 | -0.415874000 |
| 1 | -2.958525000 | -1.131881000 | 0.322008000 |
| 1 | -2.757605000 | 0.615439000 | 0.009965000 |
| 1 | -3.274246000 | -0.473196000 | -1.303313000 |
| 6 | 2.645152000 | -0.384324000 | -0.414782000 |
| 1 | 2.915147000 | -1.004807000 | 0.446220000 |

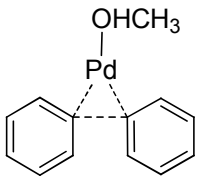
| | | | |
|---|---|---|---|
| 1 | 3.290445000 | -0.643400000 | -1.256857000 |
| 1 | 2.791043000 | 0.670832000 | -0.161645000 |
| 9 | -0.003275000 | -1.251618000 | 1.429611000 |




**TS3-4**

TCG = 0.180502, E(M06) = -818.4000606

| | | | |
|---|---|---|---|
| 6 | 2.144726000 | 2.787144000 | 1.213996000 |
| 6 | 1.421271000 | 1.592373000 | 1.210497000 |
| 6 | 1.033493000 | 0.967147000 | 0.001009000 |
| 6 | 1.437488000 | 1.591864000 | -1.203430000 |
| 6 | 2.161057000 | 2.786535000 | -1.197745000 |
| 6 | 2.520426000 | 3.394145000 | 0.010465000 |
| 1 | 2.417177000 | 3.245095000 | 2.162491000 |
| 1 | 1.159815000 | 1.135809000 | 2.161449000 |
| 1 | 1.188699000 | 1.134987000 | -2.157620000 |
| 1 | 2.446311000 | 3.244003000 | -2.142702000 |
| 1 | 3.089925000 | 4.319707000 | 0.014095000 |
| 46 | -0.774127000 | -0.000024000 | -0.010171000 |
| 6 | 1.033552000 | -0.967098000 | 0.000996000 |
| 6 | 1.437645000 | -1.591706000 | -1.203465000 |
| 6 | 1.421219000 | -1.592436000 | 1.210463000 |
| 6 | 2.161172000 | -2.786403000 | -1.197827000 |
| 1 | 1.188956000 | -1.134730000 | -2.157634000 |
| 6 | 2.144627000 | -2.787236000 | 1.213914000 |
| 1 | 1.159674000 | -1.135962000 | 2.161433000 |
| 6 | 2.520408000 | -3.394140000 | 0.010359000 |
| 1 | 2.446495000 | -3.243794000 | -2.142800000 |
| 1 | 2.416967000 | -3.245293000 | 2.162390000 |
| 1 | 3.089863000 | -4.319728000 | 0.013953000 |
| 8 | -2.891081000 | -1.112790000 | -0.019468000 |
| 6 | -3.501556000 | -0.000056000 | -0.016575000 |
| 8 | -2.891030000 | 1.112651000 | -0.019699000 |
| 6 | -5.023684000 | 0.000099000 | 0.032900000 |
| 1 | -5.346301000 | 0.002215000 | 1.081718000 |
| 1 | -5.430874000 | 0.894442000 | -0.446142000 |
| 1 | -5.431047000 | -0.895946000 | -0.442766000 |




**TS3-4'**

TCG = 0.186719, E(M06) = -705.73796

| | | | |
|---|---|---|---|
| 6 | 3.039614000 | -1.607178000 | -1.066901000 |
| 6 | 1.821086000 | -0.927562000 | -1.154149000 |
| 6 | 1.066373000 | -0.645445000 | 0.002609000 |
| 6 | 1.590061000 | -1.040781000 | 1.250591000 |
| 6 | 2.808725000 | -1.720713000 | 1.333504000 |
| 6 | 3.539786000 | -2.007510000 | 0.176270000 |
| 1 | 3.600191000 | -1.820060000 | -1.974124000 |
| 1 | 1.462864000 | -0.609147000 | -2.128968000 |
| 1 | 1.050487000 | -0.811438000 | 2.165167000 |
| 1 | 3.188239000 | -2.022859000 | 2.306805000 |
| 1 | 4.491366000 | -2.527881000 | 0.243329000 |
| 46 | -0.961213000 | -0.570178000 | -0.178573000 |
| 6 | 0.116126000 | 1.154428000 | -0.008992000 |
| 6 | 0.096047000 | 1.824318000 | 1.231210000 |
| 6 | 0.306324000 | 1.922588000 | -1.175792000 |
| 6 | 0.227273000 | 3.214661000 | 1.296758000 |
| 1 | -0.016585000 | 1.260780000 | 2.152931000 |
| 6 | 0.436604000 | 3.312726000 | -1.105592000 |
| 1 | 0.359017000 | 1.436000000 | -2.145533000 |
| 6 | 0.397744000 | 3.966606000 | 0.130022000 |
| 1 | 0.199724000 | 3.709383000 | 2.264815000 |
| 1 | 0.572982000 | 3.884055000 | -2.020813000 |
| 1 | 0.507598000 | 5.046322000 | 0.183746000 |
| 8 | -2.985502000 | -1.483074000 | -0.422545000 |